A modular structure for scientific articles in an electronic environment
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Chapter 1

Introduction

Sir Isaac Newton wrote: “If I have seen farther than others, it is because I have stood on the shoulders of giants”\(^1\) And if Newton stood on the shoulders of giants, it is because he had located helpful giants and found the means to climb on their shoulders. Without communication, he wouldn’t even have been aware of their existence. In the words of Francis Crick, who won a Nobel prize for the discovery of the molecular structure of DNA: “Communication is the essence of science”\(^2\).

The problem is that this communication is not always as effective and efficient as it could be. These days, two major trends can be identified: firstly, scientists are increasingly dissatisfied with the communication process; secondly, new, electronic communication channels are emerging. These two trends invite the question of how the new technology can contribute to a substantial improvement of scientific communication. Only part of the answer to this question can be found in further technical developments for it. It is also important to examine the organisation of the communication process, as well as the organisation of the scientific information that is communicated.

Against this background, we will propose in this thesis a new, modular structure for electronic scientific articles. In the introduction, we flesh out the context in more detail in section 1.1, before giving the outline of the thesis in section 1.2.

1.1 Communication in physics

1.1.1 The explosion of scientific journals

In general, two types of communication channels can be distinguished: informal channels such as discussions between colleagues, and formal or archival channels. To communicate science to a larger audience systematically, across both distance and time, formal channels are indispensable. The predominant formal means of communication in science is the scientific journal article. In our research we focus on communication via this channel.

The emergence and evolution of the scientific journal, and of the process of scientific communication by means of journals, have been prompted by the needs of scientists

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\(^1\)This famous quotation is derived from a letter from Newton to Hooke dated February the 5th 1676 [Turnbull et al., 1959].

\(^2\)Crick’s statement, made in a discussion on the BBC, is quoted in [Garvey, 1979, p.ix], a book titled *Communication: the essence of science.*
and by the possibilities offered by the publication media. A significant factor in the
shaping of scientific journals is the continuing endeavour to protect the scientists from
being ‘‘undated’’ by the information flow. The amount of information communicated
via journals has been growing considerably since the emergence of the scientific journal.
Roughly speaking, the number of titles doubles every 10-15 years and, at the same time,
more articles are published in each journal and the articles get longer. Scientists have
long been struggling to manage this increasing information flow and to find the relevant
drops of information without drowning. Nowadays, scientists believe they are only reading
40% of the relevant literature. Faraday reported the same problem already in 1826:

It is certainly impossible for any person who wishes to devote a portion of his time
to chemical experiment, to read all the books and papers that are published in
connection with his pursuit; their number is immense, and the labour of winnowing
out the few experimental and theoretical truths which in many of them are embar-
rassed by a very large proportion of uninteresting matter, of imagination, and error,
is such, that most persons who try the experiment are quickly induced to make their
selection in their reading, and thus inadvertently, at times, pass by what is really
good.

To manage the information flow, the scientific community has for centuries been adjusting
their communication channels.

The first scientific journals were established in the second half of the seventeenth century.
Until then small groups of scholars communicated with each other via private correspon-
dence. Taking Great Britain as an example, we see that the subsiding of social unrest
allowed for a more systematic organisation of the scientific effort. As a result the Royal
Society was formed in 1662. In the beginning, Henry Oldenburg, the secretary of the
society who corresponded extensively, read relevant letters aloud at the meetings of the
society. However, the correspondence soon started to overburden him. He tackled this
problem by printing and distributing the most important letters; thus, the journal Philos-
ophical Transactions: Giving Some Accompot of the Present Undertakings, Studies and
Labours of the Ingenious in Many Considerable Parts of the World was established. This
development was possible because of the ‘‘inventio sine qua non’’ of the printing press.

By 1789, the Neues medizinisches Wochenblatt für Aezzte complained: “This is truly
the decade of the journal, and one should seek to limit their number rather than to in-
crease them, since there can also be too many periodicals”. At that time, the sciences
started to differentiate and, in fact, the problem was that there were too many general
science journals but not enough specialised journals to allow the reader to filter the informa-
flow. Thus, in response to this problem, many specialised journals were founded in
the nineteenth century. The trend of specialisation, and the related trend of profes-
sionalisation, have restricted the number of journals that a scientist must consult in order

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3The history of the scientific journal is described in more detail in [Meadows, 1974], [Meadows, 1998],
4The growth of the scientific literature is shown, for example, in [Meadows, 1998, p.16]
5In [Meadows, 1998], this result of a recent user-survey is mentioned on page 211, and Faraday is
quoted on page 19.
6The Philosophical transactions were first published on 6th of March 1665, a few months after the
very first scientific journal appeared: Le Journal des Scavons, which was published in Paris on the 5th
of January of that year.
7This quotation is given in [Meadows, 1974, p.72].
to stay informed of the developments in his domain. These trends also have restricted
the readership of specialist journals: nowadays only scientists in a very specific branch of
a domain can understand the articles published in such journals.

In the beginning of the nineteenth century the information flow via specialised journals,
in particular journals published by specialised learned societies, was increasing. The
information flow, however, was far from smooth: there was an unacceptable publication
delay. One of the causes for the delay was the habit of reading submitted papers in the
annual society meeting before they could be published in the journal. Further delay was
caused, in particular in smaller learned societies, by the fact that it took a long time to
collect sufficient articles to warrant the publication of a journal issue. Distribution was
hampered by the high costs of postage and it was so limited that a large part of the
potential readership could not be reached. The situation improved when the publishing
efforts of the learned societies became as professional as the scientific effort of the members.
This professionalisation of the publishing effort was boosted after the Second World War
by the sudden growth of the number of journals published by commercial publishers.

In response to the growth of the number of journals, secondary literature was estab-
lished at an early stage: ‘abstract journals’ assisting the scientist in managing the primary
literature. At first, abstracts were only published separately in abstract journals, but later
abstracts were also included in the article itself. A present-day example of secondary lit-
erature is Current Contents, published by the Institute for Scientific Information (ISI),
which contains bibliographic information about primary journals in a particular domain.

With the professionalisation of science, the nature of the scientific experiments changed.
The content and format of scientific articles changed accordingly. In [Bazerman, 1988,
p.66,68], experimental reports published in the Philosophical transaction between 1665
and 1800 are compared:

In the first volume of the Transactions, a number of experiments reported are simply
cookbook recipes for creating marvellous effects or effects of practical use. [...] By
volume 90 authors talk about the necessity of establishing general knowledge and
the role of experiment in testing our beliefs as well as filling out our knowledge.

Thus, the article had started to play a role in the scientific debate. Consequently, method-
ological issues gained in importance, and the results of the experiments were reported with
increasing attention to precise and quantitative detail. At the same time this profession-
alisation was reflected in the formalisation of the discourse in the article. This led to the
prototypical sections in scientific articles: Introduction, Methods, Results, Discussion and
Conclusions.

These changes not only involved the content of the scientific discourse of the article,
but also the bibliographic aspects of the article. Since the first scientific articles simply
reported loosely connected experiments, they contained few references if any. In the sec-
ond half of the nineteenth century, however, most articles do refer to previous work, which
may be a sign of the increasing integration of scientific effort. However, many readers had
difficulties in locating the cited work using the incomplete references that were given at
that time. The situation improved with the standardisation of the references in particular
and of the bibliographic information in general.

Since the Second World War, the problem of the information overload has become acute.
The information flow has increased so dramatically that it is sometimes referred to as
an ‘information explosion’. For the individual scientist it has become difficult to keep up even with the secondary literature, let alone the primary literature. The scientist not only has to cope with the current journals, but also with the accumulated archives. As an indication of the scale, the Institution of Electrical Engineers scans over 4000 scientific and technical journals and some 2000 conference publications for the bibliographic INSPEC database. At the end of 1997, the Database contained nearly 6 million bibliographic records and is growing at the rate of 330,000 records a year [IEE, 1999].

The main cause of the information explosion is the rapid growth in the number of scientists since the Second World War. Another factor is the mechanism of funding research on the basis of the number of publications [Coles, 1993, p.12]:

The case study interviewees agreed that, although publications are necessary to establish the worth of a scientist, the importance placed on publications by assessment regimes fuels the volume of published science. The pressure to publish was seen to lead to ‘salami slicing’, multi-authored papers, repetitious publishing and the continuance of some journals of dubious quality.

The communication system has not been able to keep up with this information explosion. Consequently, “in some disciplines it is occasionally easier to repeat an experiment than it is to determine that the experiment has already been done.” [Garvey, 1979, p.8]. Thus, although a massive amount of information is available, it does not flow to the scientists who need the information.

The emergence of electronic media can help to tackle this problem, as the new technology can greatly facilitate the storage, retrieval, and dissemination of scientific information. However, simply increasing the amount of available information using this technology will only aggravate the information overload. It follows therefore, that the communication system and the information that is to be communicated must be well-organised, taking into account the possibilities offered by the technology.

1.1.2 The emergence of the electronic media

Nowadays, the computer has become pervasive in scientific communication. It has played an important supportive part in the communication process since scientific texts have been written using word processors, rather than typewriters, so that they are immediately available in digital form. In that form, they can be stored electronically and either consulted on the screen or printed on paper. With the advent of networking technology, the electronic media have started to play a leading part in communication processes: the electronic transmission of messages.

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8In physics, this cumulative effect is tempered by the fact that information is absorbed relatively quickly into the ‘common knowledge’, so that the original article in which it was published does not have to be referred to for a very long time. According to [Meadows, 1998, p.222], half the literature cited in an article has been published maximally 4.6 years before the publication of the article.

9Another consequence is the library crisis, which is described, for example, in [Butler, 1999]. Because of the number of journals and of the increasing subscription prices, the university libraries can no longer afford to subscribe to all relevant journals. And the more subscriptions are cancelled, the more prices will go up, so that publishers and libraries are caught in a downward spiral.

10A medical metaphor often used to describe this phenomenon is that of an ‘information infarct’: the circulation of information is obstructed, because the circulatory system is overloaded.
1.1. COMMUNICATION IN PHYSICS

Although electronic communication channels also include carriers like CD-ROMs, the most popular channel is the Internet and its various services.\textsuperscript{11} The Internet is a network of electronically linked computer networks. Its development started with the ARPAnet: a network established in 1969 by the US Department of Defence to connect the military with their contractors and with the universities doing military-related research. Using this network, files could be transferred and computers could be accessed remotely. Electronic mail quickly became the most popular application.\textsuperscript{12} Other networks were added. TCP/IP software (developed in the seventies and adopted in the early eighties) provided computers in different networks with a common language, so the loose collection of dozens of networks was welded into a real ‘internet’.

The World Wide Web (WWW) was initiated in 1990 at the Centre Européen de Recherches Nucléaires (CERN), as a new service on the emerging Internet. Tim Berners-Lee, the ‘inventor’ of the WWW, describes it as a “distributed heterogeneous collaborative multimedia information system” [Berners-Lee, 1991]: all information, from any source, can be accessed in a consistent and simple way. The main feature of the Web is that it is a hypertext system. It was after the introduction of the graphical interface Mosaic in 1993, that the Internet became a ‘household appliance’. To give an indication of the scale of the Internet, the online population in June 1999 is estimated to be about 200 million people and the number of hosts more than 43 million.\textsuperscript{13}

The Internet can assist scientists in the communication process at different levels. Electronic mail is used for informal discussions, instead of the telephone. Electronic mail services also take the place of traditional mail for a rapid exchange of data and manuscripts, for example between authors, between authors and editors and between editors and referees. The computer files can be distributed via the Internet and stored in on-line electronic databases, from which they can be retrieved again via the Internet. In this way, both scientific articles and practical messages can be made public. For example, The Internet Pilot To Physics [TIPTOP, 1999] is a unified physics resource, which includes an index of physics resources around the world, bulletin boards and notification services concerning practical issues, such as conference deadlines and job openings, and a forum for informal

\textsuperscript{11}The term ‘Internet’ has been officially defined in the following resolution [FNC, 1995]:

“The Federal Networking Council (FNC) agrees that the following language reflects our definition of the term ‘Internet’. ‘Internet’ refers to the global information system that -

(i) is logically linked together by a globally unique address space based on the Internet Protocol (IP) or its subsequent extensions/follow-ons;

(ii) is able to support communications using the Transmission Control Protocol/Internet Protocol (TCP/IP) suite or its subsequent extensions/follow-ons, and/or other IP-compatible protocols; and

(iii) provides, uses or makes accessible, either publicly or privately, high level services layered on the communications and related infrastructure described herein.”

A (rather technical) account of the history of the Internet is given in [Leiner et al., 1998] by a group of authors involved in the development of the Internet.

\textsuperscript{12}Basically, sending a message from one computer to the other entails the following steps. Software at the sending computer breaks down the message into little ‘packets’ of information and provides each with an address. The packets are delivered to that address via any suitable and available route. At the destination computer, software mirroring that at the sending computer reassembles the message.

\textsuperscript{13}Internet statistics about the online community are provided at the web site of an on-line marketing company [Global Reach, 1999]: in the version of June 15, 1999, the total online population was estimated to be 204 million. The Internet Software Consortium (ISC) identified in their domain survey of July 1999 56,218,000 hosts, i.e. computers that act as sources of information [ISC, 1999].
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communication.

In the recent years, we have seen an explosive growth of the use of the Internet for the publication of electronic scientific articles. In [Hitchcock, 1995], which is titled ‘A survey of STM on-line electronic journals 1990-1995: the calm before the storm’, 83 online journals in the domain of science, technology and medicine (STM) were examined. Since then, the storm has broken: the major science publishers have created electronic versions of all, or most of, their journals and made these available on the World Wide Web. According to [Butler, 1999, p.195] “A journal without a web version is now rare, and probably endangered.” To give an indication of the scale of the electronic endeavour, the distributor and agent Swets & Zeitlinger provided in June 1999 access to 9624 electronic journals in the domain of science technology and medicine.\textsuperscript{14}

The first electronic journals were close copies of their printed ancestors. Printed articles were scanned and made available as bitmap files after the publication of the original articles. In this approach to electronic publishing, the new technology was merely used for ‘long-distance photocopying’. Many publishers of electronic journals even stated explicitly that their electronic journal had to look as closely as possible like a printed journal. This seems characteristic of the application of a new technology: in a similar way, the first automobiles mimicked coaches to be horse-drawn. But the coach-like appearance of automobiles was gradually replaced by a form more appropriate to the new technology, when the advantages of an aerodynamic design were taken into account. So, the question now is: how to ‘streamline’ electronic journals to make them more suitable vehicles for the ‘information highway’?

Since the beginning of the nineties, various electronic publishing initiatives have been taken. Different possibilities offered by the new technology were used to improve particular aspects of scientific communication, such as the distribution of articles, the presentation of information in the articles, and the organisation of feedback.

One of the first important initiatives for electronic publishing in physics was concerned with ‘preprints’ (or ‘e-prints’, as the electronic versions are called) rather than regular articles. Preprints are part of the ‘grey literature’, i.e. in the grey area between informal and formal communication. The Los Alamos e-print archives provide a fully automated electronic archiving and distribution of preprints. For current awareness, the reader can browse a daily list of e-prints submitted in his area of interest (on the World Wide Web or sent by e-mail). In practice, the reader prints an e-print on paper in order to read it. Thus, the Internet is used for the dissemination of the same document that used to be disseminated via traditional preprint mailing lists.

This e-print service has proven so efficient that in certain domains it has supplanted traditional scientific journals as a channel for communication between scientists.\textsuperscript{15} Thus,

\textsuperscript{14}With respect to physics in particular: the Institute of Physics published in June 1999 33 electronic journals, the American Physical Society 8 and the American Institute of Physics 40, and Elsevier Science listed 169 electronic titles under the heading of physics, which include some journals in materials science and related domains. These numbers of electronic journals have been derived from the Web sites of the various distributors and publishers: [Swets & Zeilinger, 1999], [IOP, 1999], [APS, 1999], [AIP, 1999] and [Elsevier, 1999].

\textsuperscript{15}The archives started in 1991 as a documentbase for a small community of 200 researchers in theoretical high energy physics. In 1996, the archives were used by 35,000 scientists and contained over 75,000 e-prints [Ginsparg, 1996]. By July 1999, the archives have grown to over 100,000 e-prints and continue to grow by over 2000 e-prints a month. The user statistics are given at the Web site of the
this communication channel for grey literature is becoming more formal. The main difference is that the e-prints have not been certified by means of peer review. To fill that gap, a peer reviewed electronic journal has been established in collaboration with the e-print archives: *the Journal of High Energy Physics* [JHEP, 1999]. In the publication of this journal, as much as possible of the administrative work involved in the refereeing and editing process, in addition to the archiving and distribution, is automated or mediated by software robots.

Another initiative that bridges the gap between informal and formal literature using the Internet has been taken by Steven Harnad [Harnad, 1991]: *Psycoloquy* is a refereed electronic journal, in the domain of psychology and some related disciplines, established in 1989 on the basis of an electronic bulletin board [Psycoloquy, 1999]. In this journal, articles are published along with peer commentary, all contributions being refereed by an editor. The purpose of this journal is to provide scholars with an international forum of colleagues, to whom ideas in the formative stage of their research may be submitted and from whom rapid feedback obtained. Once the research has been completed the outcome can be published elsewhere.

With respect to purely formal communication, most electronic journals currently available on the World Wide Web were launched as electronic versions of existing printed journals. The electronic versions of articles published in such journals have some additional features, although often these are limited to the implementation of references in hyperlinks, at least within the article and preferably also to the publications cited in the article. However, in some electronic journals it is possible to include items that cannot be printed. For example, the publisher of the electronic journal (with an additional paper version) *New Astronomy* [New Astronomy, 1999] emphasises the possibility of including large data sets and multimedia files (e.g. animations). An important feature of this journal, and of other journals in the domains of astronomy and astrophysics, is its link with major scientific data centres (the cited data being too extensive for efficient publication in print).

In some electronic journals, particular aspects of electronic publishing technology are used to add features to the communication process, rather than just to the article itself. For example, it is possible to search the full text of all issues of the electronic version of *The Astrophysical Journal* [APJ, 1999]. The Institute of Physics offers personalised services, such as alerting services, to assist the reader in managing the information flow in its journals [IOP, 1999].

In short, some aspects of the communication process are facilitated by the new media. In addition, compared with print articles, electronic articles have some additional features. However, the organisation of the information in present-day electronic journals does not differ fundamentally from the way the information is organised in the print version.

### 1.1.3 The project ‘Communication in Physics’

In the physics community, different programmes have been initiated to deal with the issue of scientific communication in the context of the emerging technology. In 1989, archives [Los Alamos, 1999]. The archives consist of 38 sections for particular subjects in the area of physics, as well as 37 in the related areas of mathematics and non-linear sciences. For computer science, the Computing Research Repository was created in 1998, in connection with the Los Alamos archives.
the American Physical Society (APS) formed a ‘Task Force on Electronic Information Systems’ to review the state of affairs and develop a plan for the physics information system, because:

[it] is clear that the world of physics is on the verge of a revolution, a revolution that is driven by technology, but whose true nature will be determined by the response of the world scientific community. The revolution will change what and how physicists read, how they become aware of what they read, and even what ‘read’ means. [APS, 1991]

The task force has defined a long term goal: a world scientific information system. In this system, the world’s formal and less formal literature would be available on-line in an interactive environment. Individual documents, rather than entire journals, would be the fundamental entities. In 1993, the International Union of Pure and Applied Physics (IUPAP) also formed a task force to “investigate how the means presently available, and new means expected to become available soon, can be integrated into a first version of a system of communications, to provide fully electronic submission, publishing, large scale storage, fast retrieval and selection.” [IUPAP, 1993].

Here in The Netherlands, the research programme ‘Communication in Physics’ was launched in 1994 by the Foundation Physica, an organisation promoting the advancement of physics in The Netherlands. The foundation was moved to initiate this programme as a result of a meeting at which both the increasing dissatisfaction with the flow of scientific information was voiced and the emergence of the new technologies of computer networks and electronic publishing were signalled [De Waard, 1993]. This thesis reports on research performed in the context of this programme.

The starting point of the programme is the following: rather than being dragged along by the technological developments, the physics community should determine how it prefers the scientific communication process to function. Subsequently, the specific technology can be developed to implement this vision. Therefore, the first goal of the research programme is to gain insight into the nature of scientific information itself and of the management of this information. The second goal is to develop new models for the representation of scientific information and for scientific communication that can be implemented using the particular features of the new technology.

In order to increase our understanding of scientific information and the communication system, different aspects have to be considered: technical, social and financial aspects, as well as more ‘conceptual’ aspects. With respect to the technical aspects, for example, presentation, storage and automatic indexing techniques have to be developed. With respect to the social and financial aspects, issues like intellectual property and research policy and motives of scientists must be addressed. Many of these issues are the subject of current research and reported in journals like the Journal of Electronic Publishing, the Journal of Documentation and the Journal of the American Society for Information Science.

In the literature, however, the organisation of the scientific article itself is not considered systematically. Usually the authors aim to solve communication problems by developing sophisticated new techniques to deal with the article as it is. For instance, we agree with Liddy that there is a problem with the retrieval of information [Liddy, 1991, p.78]:

Current retrieval systems allow users to require only that the concepts they are interested in occur somewhere within the free-text representation. It is not possible
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for the user to specify what roles the concepts of interest should play in the retrieved documents or to specify the relationships that should hold between the concepts.

However, we approach this problem from a different angle. Liddy proposes

[a] system that can detect the structure of abstracts and is capable of providing this type of detailed representation [that] could improve the retrieval process by allowing the user to specify in advance the particular role they require each searched concept to play.

Contrary to Liddy, who aims to improve information retrieval by improving the retrieval system, we propose a fundamental restructuring of the article itself, so that the same retrieval system can work more effectively and efficiently. Thus, we take a step back and focus on a fundamental question concerning the scientific article: what is the basic ‘streamlined’ shape that allows for substantial improvement of scientific communication in the context of the new technology of electronic information transfer? Our basic idea is that, in an electronic environment, scientific information may be communicated more effectively and efficiently if it is presented as a network of articles with a modular structure, rather than as a set of linear, essay-type articles. An article with a modular structure consist of a coherent collection of explicitly linked modules, representing a coherent network of related conceptual information units within the larger network of published information. This structure allows the user to take into account the role that concepts of interest should play within a document, as well as the relations between specified concepts.

1.2 Outline

This thesis addresses the general problem of how to structure the presentation of scientific information in electronic articles. Given the idea of modularity, we focus on the following questions: (1) Is it possible to develop a systematic model for a modular structure for electronic scientific articles? (2) Does the modular structure indeed allow for more effective and efficient scientific communication?

The adequacy of the structure of such a presentation depends on the needs of the scientists involved in this type of communication. Therefore, we first analyse in chapter 2 the characteristics of scientific communication via articles in order to formulate an ‘interactants profile’. This profile summarises the characteristics and the needs of the prototypical readers and authors of scientific articles, and it yields communication criteria for the presentation of scientific information.

The definitions pertaining to the idea of a modular structure are given in chapter 3. In chapter 4, the idea of a modular structure is realised in a modular model for articles on experimental sciences: a model for the creation and evaluation of modular articles. In the modular model, the basic notions are complemented with a typology for the different types of modules and one for the different types of structured links that can be created using the model.

In order to make the modular model applicable to the creation and evaluation of concrete modular articles, the typologies have to be specified for the scientific domain at hand. In addition, specific rules for the composition are necessary, in order to determine which modules and links are required, and which are allowed, in a particular modular
article in this domain. In appendix A, we provide such a specification in terms of guidelines for authors of modular articles in the field of experimental molecular dynamics.

The general modular model for experimental science and its specification for experimental molecular dynamics are developed in conjunction with an empirical analysis of a corpus of published, linear articles. The bibliography of this corpus is given in appendix B. This analysis involved modularising articles from the corpus, i.e. reconstructing linear articles in modular form, rather than writing new modular articles, in order to ground our work in the existing scientific practice. We firstly aimed to determine whether it is indeed possible to write articles with a modular structure that satisfies both the abstract definitions and the concrete guidelines. Hypertext examples of modularised articles are given in the electronic version of this thesis, in appendix C. Secondly, we compared the modularised versions with the original articles in the light of the communication criteria, to see if the modular structure can indeed meet the requirements specified in the interactants profile, better than the structure of the original articles. Thus, we tested if the model allows for more effective and efficient scientific communication via electronic articles. This discussion takes place in chapter 5.

In chapter 6, we give an overview of our main findings. We also illustrate the applicability of the model to other types of publications by means of examples, which are discussed in more detail in appendix D. Furthermore, we briefly consider how the modular model can be implemented and tested, discussing in particular the demands on the technical realisation of modular articles in an electronic environment.
Chapter 2

Effective and efficient communication via electronic scientific articles

In this chapter, we determine the requirements that the structure of an article has to fulfil in order to satisfy the needs of the scientists. In section 2.1, we analyse the characteristics of scientific communication via articles. In section 2.2, we formulate the basic requirements for scientific communication via articles, specifying an ‘interactants profile’ of the scientists involved in it. The intrinsic characteristics of electronic publishing are discussed in section 2.3, in terms of the impact that the new medium may have on the fulfilment of the requirements. This leads to the formulation of ‘communication criteria’ for the structure of electronic scientific articles in section 2.4.

2.1 Scientific communication via articles

For a systematic discussion of the requirements and of the possible impact of electronic publishing on scientific communication via articles, we set out in section 2.1.1 the subsequent steps that we distinguish in the process of this type of communication. We examine in more detail the specific characteristics of communication in science in section 2.1.2, and the specific characteristics of communication via articles in section 2.1.3.

2.1.1 A model of the process of communication via scientific articles

In this thesis, we concentrate on the structure of scientific articles. For that purpose, we have to distinguish in our analysis between the organisation of the information and the actual phrasing used to present the information in the article. In addition, we have to separate the organisation of the article from the organisation of the communication process, which for instance involves the question of how peer review is organised. In this endeavour, we also have to separate between, on the one hand, conceptual issues pertaining to the organisation of the information and the communication process, and, on the other hand, the technical issues of the implementation of the article and the communication system. These different aspects are taken into account in the model of the process of scientific communication via articles that we give in this section.

Here, we first clarify how we use the terms ‘information’ and ‘communication’ in this
thesis, because in the literature these terms are used in different ways. By *communication* we mean the transfer of information from a human sender to a human receiver, for the purpose of increasing the receiver’s knowledge, enabling him to carry out tasks, or influencing his attitudes and behaviour. If the receiver also acts as a sender, the one-way transfer of information becomes a two-way exchange of information between human interactants. Depending on the type of communication, the senders and receivers are the speaker and listener in oral communication, or the writer and reader in the case of written communication.

By *information* we mean a conceptual representation of aspects of a ‘universe’¹ for the purpose of communication. Because information is a *conceptual representation*, it cannot be directly communicated to others; it first has to be represented in a message that can be encoded and transmitted.² Thus, communication entails at least three ‘representation levels’:

1. **Conceptual level:** *information*. Information is a *conceptual representation* of particular aspects of the universe.

2. **Symbolic level:** *message*. The message is a *symbolic representation* of the conceptual representation of an aspect of the universe. It can be formulated textually, in mathematical or chemical formulae, in pictures, or in any other ‘language’.³

3. **Technical level:** *signal*. The message is *encoded* (in different stages) in a physical or electronic signal that can be transmitted.

In a universe, separate entities can be distinguished, as well as relations between these entities. The same ‘granularity’ can be seen at the conceptual level: the information about these entities forms related *information units*. For example, information about the results of a particular type of measurement on different specimens can be divided into different information units. The complete set of rules for the performance of a particular task also form an information unit. We need such a notion of a ‘quantity of information’ to

¹That universe usually is the ‘real world’, but it can also be a simplified ‘ideal universe’ hypothesised for the sake of an argument, or a ‘fictional universe’ Aspects of that universe can be ‘static’ entities, such as physical objects and abstract entities, but also processes and lines of reasoning involving various relations between simple and complex concepts. These aspects of the universe are the most basic level we take into account. Loosely speaking, it could be seen as ‘that what the information is about’.

²Information also has the following characteristics. It is *wrong* if a particular aspect of the universe has not been represented properly at the conceptual level. It can ‘exist’ without being communicated *successfully*. It is *aimed at communication*. In this respect, information differs from knowledge, which we consider primary as an internal representation reflecting a true justified belief about some aspect of the universe. New information allows the receiver to add to, confirm or modify his beliefs and thereby to increase his knowledge. In this thesis on scientific communication, we deal with information, rather than knowledge. In addition, information can be complex. We do not use the term ‘information’ exclusively for simple, factual information; for that specific type of information we use the term ‘data’.

³The distinction between the conceptual level and the symbolic level in the communication process is also made in a cognitive model of the communication process described in [Conklin, 1987, p.24]:

[in writing, a] loosely structured network of internal ideas and external sources is first organised into an appropriate hierarchy [...], which is then ‘encoded’ into a linear stream of words, sentences, etc. [...] 

[reading is] taking the linear stream of text, comprehending it by structuring the concepts hierarchically and absorbing it into the long-term memory as a network.
2.1. **SCIENTIFIC COMMUNICATION VIA ARTICLES**

be able to develop an adequate structure for the representation of scientific information. If information can be considered as a network of units, we should structure a scientific article (in which the scientific information is represented) as a network of modules, each representing a unit. The question as to what can constitute an information unit, however, can only be answered in the context that determines what is similar information about similar subjects. We shall return to this question in sections 3.1.1 and 3.2.

The notion of information we use allows us to follow an information unit through the communication process, from the sender to different types of receivers. In this process, the amount and the nature of information conveyed is considered fixed, regardless of the question as to whether a particular receiver already is aware of the information or whether the signal is intact when it reaches him.\(^4\)

Our notion of communication is based on sending and receiving. In this respect, it fits with most models for communication, according to the *International Encyclopaedia of Communications* [Barnouw et al., 1989]:

Most communication models employ a small number of basic concepts: a sender; a process of encoding into signals or symbols; a message; a channel; a receiver; a relationship; a process of decoding; a range of things to which the messages refer (‘referents’); and an actual or probable effect, intended or not. Some models incorporate a feedback link from receiver to sender.

The communication models of this type are based on the mathematical theory of communication developed in [Shannon and Weaver, 1949]: a sender encodes a message in a signal that is transmitted through a channel and then decoded by a receiver.\(^5\) Shannon and Weaver developed their model to describe telephone conversation from an engineer’s point of view. They were not concerned with either the meaning of the message or the

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\(^4\) Whereas our notion of communication is compatible with the mathematical approach, our notion of information is not. In the *mathematical approach*, information is a property of a signal, providing a measure for the reduction of the uncertainty of the receiver. Thus, a transmitted signal does not carry any information if the receiver is already fully aware of it. In our approach, we connect the reduction of the uncertainty of a receiver to the adequacy of the different steps of the communication: if the goals of the interactants are not achieved, the communication has not been adequate. Thagard distinguishes two other basic approaches to the notion of information, which intuitively highlight its different aspects [Thagard, 1992]: the ‘ecological approach’ and the ‘information-processing approach’. In the *ecological approach*, information is a property of situations: it already exists in the environment and the role of ‘cognitive agents’ is to select and pick up the information that suits them. They must be able to pick up information about one situation from another situation, which leads to the question formulated in [Barwise and Seligman, 1997, p.25] as “how is it that information about some components of a system carries information about other components of the system?”. We do not consider this philosophical question, as we concentrate on practical communication between people. Furthermore, we concentrate on scientific information, which is not so easy to ‘pick up’ and can turn out to be incorrect. To emphasise that aspect, we consider information as a conceptual representation of an aspect of the universe, so that the sender has to play an active role representing a particular, complex situation. Thus, we follow the *information-processing approach*, rather than the ecological approach. In that approach, information is considered as an object, which can take the shape of a mental object that is operated on in cognitive activities, or a computational object in a computer algorithm.

\(^5\) These models can be visualised with the ‘conduit metaphor’ of sending information packages through a conduit. In [Gärdenfors, 1996], two metaphors are given for communication: the machine-oriented conduit metaphor and the more human-oriented ‘resonance metaphor’, in which information emerges only when the interactants can ‘resonate’ with the material. We shall use an (enhanced) conduit metaphor, because that metaphor allows us to visualise the different aspects and stages of communication.
reason for its transmission. Unlike Shannon and Weaver, we do take these aspects into account. For that purpose, we add steps to their model of the communication process. We describe the meaning of the message as the information represented in it. The reason for transmission is then taken into account in the goals of the sender and the receiver and thereby in their criteria for the adequacy of the communication.

We visualise communication between senders (authors in particular) and receivers (readers) as follows: packages containing information are transmitted to a receiver via a communication conduit (e.g. a telephone line, or a regular mail service). The communication, however, involves more than the transmission of packages through the conduit. Analytically, we distinguish four main stages. In the first stage, the sender creates the information package. Then, a connection has to be established with the receiver and the package has to be transmitted. This involves two stages: in the second stage, the dissemination, the package is made available to the receiver, and in the third main stage the receiver acquires it. The fourth stage is the assimilation, in which the receiver unwraps the package, consumes the information.

For the process of communication via scientific publications, these four main stages can be further refined into an idealised sequence of seventeen different activities. We emphasise that this is an analytical model of the communication process; in practice, the activities may be performed in a different order or simultaneously, or they may be repeated, guided by feedback, until the result is satisfactory. In the following, we examine the model in more detail.

Stage I: Creating

1. We start with the scientist generating and gathering raw scientific information in some research activity, by forming a conceptual representation of some aspects of the universe at issue. (2) This information is organised and characterised at the conceptual level, based on an evaluation of the raw material in the context of the research programme. In this step, the ‘raw output’ is both moulded and filtered. Some information is discarded as uncertain, irrelevant, superfluous or unimportant.

2. Then, the author actually writes the article, i.e. he creates a symbolic representation of the information. The author decides which ‘language’ or symbolic means he will use to communicate the different types of information: natural language (and which one), mathematical or chemical formulae, pictures, tables, animations, et cetera. Then, he chooses the structure of the document, the exact wording, the appearance of the non-verbal presentation, and the precise terms (e.g. key words) by which the information is characterised.

3. In order to allow for transmission, the document is encoded in an analog signal (e.g. by printing it on paper) or a digital signal (a computer file) that can be transmitted.\footnote{In Garvey, 1979, an influential model of the scientific communication system is given: a series of models incorporating information technology based on that model is given in Crawford et al., 1996.}

4. In Garvey et al., 1972, the information-exchange process associated with the creation of journal articles is described in detail, including feedback impacting on the research itself, on its representation at the conceptual level and on its representation at the symbolic level.
2.1. SCIENTIFIC COMMUNICATION VIA ARTICLES

Figure 2.1. A model for the process of scientific communication via articles is sketched. The main stages are: creating, disseminating, acquiring and assimilating. The arrows indicate the idealised sequence in which the steps are taken. There are several possible short-cuts in the process. Usually articles reach the receiver by way of an archive (a traditional or digital library), but they might also be delivered personally to a particular set of receivers, jumping from step (9) to (13). In communication by way of preprint archives, rather than publication in scientific journal, the document is not explicitly subjected to quality control: steps (6) and (8) are skipped in that case. The author can also give the preprint personally to particular receivers, cutting from (4) immediately to (13).
Stage II: Disseminating

(5) The first activity in this stage is the collection of encoded documents for publication. The editor of a particular journal can actively solicit them, or the author can submit them directly. The encoded document can be made public and archived immediately, in a ‘preprint’ archive [Ginsparg, 1996]. In communication via articles published in a journal, however, more value is added first.

(6) For scientific quality control, the correctness of the information and the clarity of the presentation are judged in some form of peer review. In principle, quality control does not have to take place before publication. Comments and ‘quality labels’ could be added to the article after publication. Different forms of peer review are proposed, for example, in [Harnad, 1991]. If this control takes place before publication, feedback can lead to an improvement of the article to be the published article. The editor of the journal may further enhance the quality. (7) Indexing also adds value to the document. The document can be characterised using controlled index terms chosen from a thesaurus, for example, or using free terms.

The next activities are not concerned with the scientific content of the article but with other added value. Usually, these mainly technical, administrative and financial tasks are performed by publishers and librarians. (8) Value can be added to the technical aspects of the presentation of the document and its encoding in a signal. The presentation can be professionalised and the document can be encoded (in different steps) in several types of signals. The technical aspects of editing and presentation involve, for example, visual design, typesetting, printing and format conversion. (9) The publication, in the literal sense of making the information public, then allows the audience to become aware of the existence of the information. At this stage, the (encoded) article can be distributed directly to the intended readership. However, it is usually transmitted to a (physical or digital) library, from which the receiver can retrieve it immediately after publication or later. (10) Thus, value is added by archiving the article for future reference.

Stage III: Acquiring

Supposing that the article created and disseminated in the previous stages contains information that is of interest to a prospective receiver, that receiver first has to acquire the signal in which the entire article, or the relevant part of it, is encoded.

(11) In this stage, the first activity involves locating relevant information, which implies a selection process. Relevant information can be found in two ways: by scanning or

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8 We shall get back to these different types of documents in section 2.1.3.
9 We do not consider these tasks in detail. A study of the roles of publishers and libraries in the scholarly information process and the types of value they can add, including legal support, financial management and marketing activities, is presented in [Sovill, 1995].
10 In [Belkin et al., 1993], this activity is considered in terms of Information Seeking Strategies, which have four dimensions or factors: 1) method of interaction (scanning–searching); 2) goal of interaction (learning–selecting); 3) mode of retrieval (recognition–specification); and 4) resource considered (information items–meta-information).

Scanning is mostly associated with retrieval by recognition and searching with retrieval by specification. Both seeking patterns are common in scientific communication. In a user-survey cited in [Meadows, 1998, p. 212], it was found that “some two-thirds of the information obtained via this usage of refereed articles, colleagues, books, on-line databases and abstracts” was deliberately sought. The remaining third of the information was gained unexpectedly.”
2.1. SCIENTIFIC COMMUNICATION VIA ARTICLES

browsing, and by searching. When browsing, the receiver navigates through (selected) sources, trying to encounter interesting information he was previously unaware of. Using this method, the browsing scientist locates information by recognising it as relevant.\(^\text{11}\) The searcher specifies in advance the characteristics of (potentially) relevant information. For both searching and browsing, both the contents of articles and the ‘meta-information’, i.e. the information about the articles, can be used.\(^\text{12}\)

(12) After locating the relevant information, the prospective receiver has to retrieve the ‘signal’ (e.g. the computer file).

Stage IV: Assimilating

(13) Once the receiver has retrieved the signal, he first decodes it, to obtain the document (i.e. the article, or the relevant part of an article) it contains. (14) Then he reads the document, reconstructing the information underlying it.\(^\text{13}\) Comprehensive reading involves following the discourse linearly from the beginning to the end. In their field of interest, however, scientists often read selectively: they usually neither study the article as a whole, nor in the prescribed order [Dillon et al., 1989].

(15) The receiver ‘absorbs’ the information (by fitting it into his own conceptual representation of the universe), and (16) evaluates it. (17) If it is satisfactory, he incorporates the information in his own research. This can involve increasing his personal knowledge, as well as a concrete utilisation of specific information. Generating new scientific information, the scientist now exchanges his role of receiver for that of sender, which brings us back to (1).

2.1.2 Communication in experimental science

In this section, we examine some characteristics of experimental science that influence its communication and hence lead to a specification of the requirements for adequate scientific communication.\(^\text{14}\)

\(^\text{11}\)In this thesis, we call ‘browsing’ all methods of locating relevant information by navigation through sources, and ‘searching’ all methods of locating relevant information by pin-pointing information by its characterisation. In [Ellis, 1989, p.178], six characteristics of the information seeking patterns of scientists are discussed: 1) Starting: activities characteristic of the initial search for information; 2) Chaining: following chains of citations or other forms of referential connection between material; 3) Browsing: semi-directed searching in an area of potential interest; 4) Differentiating: using differences in sources as filters on the nature and quality of the material examined; 5) Monitoring: maintaining awareness of developments in a field through the monitoring of particular sources; and 6) Extracting: systematically working through a particular source to locate material of interesting. Chaining, browsing, monitoring and extracting, as discussed by Ellis, involve locating relevant information by (more or less directed) navigation through selected sources. ‘Starting’ can involve searching for a starting point for browsing. Differentiating is important in both searching and browsing. The scientists whose behaviour is discussed in [Ellis, 1989] are social scientists, but in [Ellis et al., 1993] it is shown that there are no overriding differences between social scientists and physicists in this respect.

\(^\text{12}\)Searching in the contents of the article is free-text searching. The meta-information used in a search can consist of index terms associated to the document in activity (7).

\(^\text{13}\)Here, we use the term ‘reading’ as shorthand for ‘decoding a symbolic representation of the information (in terms of some natural, pictorial or other ‘language’).’

\(^\text{14}\)Of course, we do not pretend to give an exhaustive account of the precise nature of science. As Meadows puts it: “A picture, or more accurately a series of vignettes, of science built up from conjectures such as Kuhn’s and Popper’s provides a helpful framework for discussing research and communi-
CHAPTER 2. EFFECTIVE AND EFFICIENT COMMUNICATION

Communication is the essence of science, because science is a co-operative effort.\textsuperscript{15} Scientists can incorporate previous work in their own research, and they can use feedback to improve their work. This co-operative effort is usually organised in a research programme: a set of methodological rules, with a constellation of beliefs, values and techniques shared by a particular scientific community.\textsuperscript{16} In experimental science, this sharing is very important, because experimental science is supposed to refer to the ‘real world’, so that all scientists try to explain the same real world.\textsuperscript{17}

Another important characteristic of science is that it is always open to critical scrutiny. In empirical science, no scientific information is permanent and irrefutable.\textsuperscript{18} If a particular theory does not explain the observations, the theory may be invalid, or the empirical data may be unreliable. However, disagreement between theory and observation does not automatically entail that either has to be definitively discarded. Finding that the theory turns out not to be applicable to the observation, i.e. that it turns out not to be valid in the domain of the observations, leads to the specification of restrictions of the theory. The canonical example is the ‘overthrow’ of the Newtonian theory of gravity by Einstein’s theory of general relativity. Newtonian physics have not been discarded but restricted: in situations in which the gravity is sufficiently low it is still applied, but in the neighbourhood of a neutron star, for instance, the theory of general relativity explains the observations better. Thus, scientific information is not permanent, and it can be restricted to a particular range or domain.

In this thesis, we consider research as a problem-solving process. This problem-solving can involve the induction of general statements from specific observations, the deduction of specific predictions from general theories, and the testing of hypotheses. In practice, the research usually cannot be realistically described as pure induction, nor as deduction, and the scientists do not necessarily make any hypotheses explicit. This is the reason why we take the broader problem-solution pattern as a starting point.\textsuperscript{19}
2.1. **SCIENTIFIC COMMUNICATION VIA ARTICLES**

In a prototypical problem-solving process, the following subsequent steps can be distinguished. First, the initial situation is determined. Then, the problem that arises in this situation is identified and analysed. In response to this problem, a method is developed and executed to solve the problem. This leads to results, which, in the last stage, are evaluated to see if the problem has indeed been solved. The way this process manifests itself in ordinary discourse is described, for example, in [Hoey, 1983] and [Jordan, 1984]. In practice, the steps of the process do not have to be taken subsequently, and the discourse describing it does not have to be read sequentially either: the structure can be non-linear.

In this thesis, we focus on experimental research: empirical research in which data are obtained in scientific experiments. This type of research is a particular type of problem-solving process: solving concrete problems in the context of a research programme. The interplay between experiment and theory can be very complex, but basically the response to the problem involves experimental methods, which lead to experimental results, which then are discussed in the light of a theoretical framework. The prototypical structure of scientific articles follows this problem-solving process: experimental articles are usually made up of the sections Introduction, Methods, Results, Discussion and (less prototypically) Conclusions. This structure is frequently abbreviated as IMRDC or IMRaD.  

2.1.3 **Scientific articles**

In this section, we specify the means of communication: published documents, in particular scientific articles. By a *document* we mean a symbolic representation of a quantity of information that can be stored and retrieved separately (when it has been encoded in some medium). Communication via published documents has two distinguishing features that may compromise its effectiveness and efficiency: it is strongly indirect and heterogeneous.

In strongly indirect communication, there is no immediate feedback. In addition, the interactants are not connected to each other by a direct communication channel. This hypothesis can be falsified (e.g. Popper). In this thesis, we study the structure of actual scientific articles, and in experimental science this approach is not explicitly adhered to. On the other hand, we are more ‘strict’ than sociologists of science such as Gross, who argues that scientific research is neither an inductive process, nor a deductive process, but that formal communication, in which a systematic pattern is made explicit, is “an *a posteriori* rationalisation of the real process."

> [r]ead ing experimental or descriptive papers in science, we invariably experience an inductive process, a series of laboratory or field events leading to a general statement about natural kinds; in theoretical papers we experience the opposite movement, a series of deductions whose conclusions invoke or imply confirming observations. [Gross, 1990, p.85]

In this thesis, we indeed consider scientific research as an idealised process, rather than as the every-day work performed in a laboratory that is studied by sociologists of science, because we need a normative description in order to formulate requirements for adequate communication.

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20IMRaD means Introduction, Methods, Results, and Discussion.

21Thus, a document is not necessarily verbal. It is a message that can be encoded e.g. in printed form or in a computer file. For a general discussion as to what is a document, see for example [Buckland, 1997].

22By *direct* communication we mean real-time interaction driven communication. In direct communication, the sender has to take into account the background knowledge and beliefs of the receiver, but he doesn’t have to prepare his entire contribution in advance, because he can use feedback to adapt it in the course of the communication session. Examples of direct communication are a face-to-face conversation, a telephone conversation, and Internet ‘chatting’.

In *weakly indirect* communication, there is a time lag between the contributions of the interactants,
means that the transmission of a message from the sender to a receiver is nontrivial. The message is put into some ‘information pool’, from which the receiver has to retrieve it, and the sender cannot be sure that the prospective receivers have indeed done so.

Communication by means of published documents is not only strongly indirect, but also heterogeneous: the audience consists of (potential) receivers with different needs. The needs of a receiver depend on the goals that he pursues at that particular moment and on his background, which determines what the receiver understands, accepts and finds interesting.

Narrowing down the type of documents, we concentrate on scientific articles. In a broad sense of the word, a scientific article is any document in which information on a particular subject obtained from scientific research is presented. We focus on scientific articles in a more narrow sense of the word: by a *scientific article* we mean a refereed full, original account of a research activity published in a scientific journal, that constitutes a coherent unit for the purpose of communication to peers.\(^{23}\) In other words, the article forms a self-contained publication unit, in the sense that it provides what the target audience is supposed to consider a full account of a finished ‘piece of research’.

By a *scientific journal* we mean a documentbase in which certified documents of a particular type, on a specified subject in science, aimed at a specific target audience are published, and in which some form of peer review is implemented. A documentbase is a structured collection of documents of a particular genre, which can be accessed by more than one person and/or used for more than one purpose. Thus, a journal is defined by its functions of certification and registration of articles, of (allowing for) archiving and of making the audience aware of it.\(^{24}\) In our broad definition of the word ‘journal’, we do not specify the medium. The journal may be published by any suitable means. The most obvious media in this context are the electronic medium and the paper medium. We do not specify the journal’s schedule either. A journal traditionally is a periodical, but ‘continuous journals’ can also be envisaged: articles can be published as a continuous stream instead of being gathered into periodically appearing issues.\(^{25}\)

The kinds of documents that can be published in a journal include scientific articles so that the receiver cannot give immediate feedback. Therefore, the sender has to convey the complete message, anticipating the receiver’s understanding and acceptance. For example, weakly indirect communication can take place by means of personal letters and by means of lectures in which the discussion is entirely postponed until the end. In strongly indirect communication, the interaction is even more restricted.

\(^{23}\)We focus on this type of article, because it plays a predominant role in present day scientific communication. The narrow definition excludes preprints, reviews and monographs. The difference between a preprint and an article in the narrow sense of the word is that a preprint has not been subjected to peer review. This feature has no direct relation to the structure of the presentation of the information, which we aim to analyse. The role of reviews and monographs and scientific communication differs from the role played by short articles on original research. Therefore, reviews and monographs may have a different format. In chapter 4, we shall present a modular model for articles in the narrow sense of the word. We take reviews and monographs into account by allowing for modules representing information with a wide range, in addition to the modules that are part of scientific articles. Many remarks we make on articles in the narrow sense also apply, less stringently, to other types of scientific documents.

\(^{24}\)These functions are discussed in [Kirz and Roosendaal, 1996]. We shall discuss them in section 2.2.2 in relation to the requirements of the interactants in the process of communication via scientific articles.

\(^{25}\)In this respect, our notion of a journal is broader than that used in [Crawford et al., 1996], where a communication model based on the article as the unit of distribution is called the ‘no-journal model’. 
2.2. REQUIREMENTS FOR SCIENTIFIC ARTICLES

according to our narrow definition, rapid communications, comments and reviews. The requirements or guidelines for articles that are to be published in some particular journal are usually specified by the editorial board. The aims and scope of a journal are often explicitly stated. The subject may for example be chemical physics and the intended audience chemical physicists or all broadly interested physicists. The target audience of the journal, and more particularly of the article, is restricted to a specified range of fellow experts or at least fellow scientists. Nevertheless, it is still rather heterogeneous, as not every member of the target audience has exactly the same needs (as we shall see in section 2.2.2).

2.2 Requirements for scientific articles

In this section, we consider the specific requirements that the information, the representation of the information in scientific articles, and the ‘information system’ for the transmission of those articles have to meet in order to allow for effective and efficient communication. We first examine, in section 2.2.1, the characteristics of rational communication and the general requirements communication has to meet to be considered rational, and we specify these requirements for scientific communication via articles. In section 2.2.2, we formulate in more detail an ‘interactants profile’ of the interactants in scientific communication via articles.\(^{26}\)

2.2.1 Rational communication

Rational communication is a goal-oriented interactional activity, which has three aspects. Firstly, the messages of the interactants are means to achieve some end and responsive to the requirements of the situation. Secondly, rational interactants take into account the goals and plans of the other interactants. And thirdly, rational interactants actually take up the other’s purposes working towards an accepted common goal, so that their interaction truly is a joint activity [Van Eemeren et al., 1993, p.6].\(^{27}\) Scientific communication, in particular, is rational communication in which the interactants are scientists and the primary common goal of the interaction is the advancement of science.\(^{28}\)

An influential theory that articulates standards of rationality for the usage of ordinary language is ‘speech act theory’\(^{29}\). According to [Searle, 1969], speech acts are performed successfully if they satisfy specific ‘felicity conditions’ for rational communication.\(^{30}\) The

\(^{26}\)For an empirically grounded interactants profile, a comprehensive user-survey is required.

\(^{27}\)The notion of rationality, in the context of communication, is discussed in [Van Eemeren and Grootendorst, 1994 i]

\(^{28}\)In principle, this definition excludes teaching and the popularisation of science, which are primarily aimed at the advancement of individual knowledge. However, there is no clear borderline separating these genres. Considering communication via published documents, we find communication via reviews and monographs in the grey area between scientific communication (via scientific articles) and instructive communication (via tutorials). The grey area between scientific communication (between scientists) and popularisation (by scientists or journalists for the benefit of the general public) includes, for example, the journal Scientific American, which is, according to the instructions for authors, aimed at “intelligent members of the general public”.

\(^{29}\)Speech act theory describes the use of language as an action, namely the performance of ‘speech acts’. See [Austin, 1962]

\(^{30}\)The four felicity conditions were first introduced in [Searle, 1965] and they are summarised
felicity conditions imply an abstract model of presumptions and expectations, shared by all language users, of what rational communication involves. The best known example of such a model is Grice’s Co-operative Principle, to which the participants of a conversation are assumed to adhere [Grice, 1975, p.45]:

Make your conversational contribution such as is required, at the stage at which it occurs, by the accepted purpose or direction of the talk exchange in which you are engaged.

Although the Co-operative Principle is formulated for conversation, Grice explicitly states that this principle also applies to other types of rational interaction. The maxims\(^\text{31}\) that Grice derived from this Co-operative Principle have been reformulated by Van Eemeren and Grootendorst, in terms of five rules of communication based on Searle’s felicity conditions.\(^\text{32}\) These rules read as follows [Van Eemeren and Grootendorst, 1988, p.501]:

1. Perform no incomprehensible speech acts.
2. Perform no insincere speech acts.
3. Perform no unnecessary speech acts. \(^\text{33}\)
4. Perform no pointless speech acts.
5. Perform no new speech acts that are not an appropriate sequel or reaction to preceding speech acts.

Grice’s Co-operative Principle and the ensuing maxims and rules represent the basic expectations of participants in a conversation: speakers generally act according to them and listeners may base their interpretation of an utterance on the fact that they expect the speaker to adhere to them. In discourse analysis, adherence to the maxims is often taken as a starting point and the Co-operative Principle is used as a tool for the reconstruction of discourse. The maxims, and the rules for communication derived from them, can also be interpreted as norms for a rational, effective exchange of information. As such, they in [Van Eemeren et al., 1993] as follows:

(1) The propositional content condition. The utterance must express propositional content appropriate to its force. For example, promises must refer to future states, while reports of occurrences must not refer to future states. (2) The essential condition. Making the utterance ‘count’ as an expression of a certain objective, within some set of social understandings. (3) The sincerity condition. The sender must actually believe, want, and intend anything represented as believed, wanted, or intended. (4) The preparatory condition. The sender must have adequate justification for undertaking to achieve the underlying objective and must believe that performing the speech act itself will help lead to the achievement of the objective.

\(^\text{31}\)According to these maxims, the contributions have to be: 1) true (the Quality Maxim), 2) as informative as is required for the goals of the interaction (Quantity Maxim), 3) relevant to the goals of the interaction (the Relation Maxim), and 4) clear (the Manner Maxim).

\(^\text{32}\)Van Eemeren and Grootendorst have formulated these rules in the context of a normative theory for argumentation called ‘pragmatic-dialectics’ [Van Eemeren and Grootendorst, 1984], [Van Eemeren en Grootendorst, 1992]. The pragma-dialectical model describes argumentation as a methodical exchange of speech acts in a critical discussion aimed at the resolution of a difference of opinion. The pragma-dialectical model is an ideal model that specifies rules for the successive stages of a critical discussion. It can be used for heuristic-analytical, critical-evaluative and instructive purposes.

\(^\text{33}\)The information is unnecessary if, for example, the receiver is already aware of it. It is pointless if it is clear in advance that the receiver will not be able to understand or accept the information anyway, e.g. because he lacks specialised background knowledge.
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can be made explicit into the following – intertwined – basic requirements for rational communication and then used to provide senders with guidelines: quantity, clarity, quality and relevance.

In order to determine if a particular message satisfies these requirements, the requirements have to be further specified, by determining the goals of the sender and receivers, and thereby the ‘communicative purpose’ of the message. Therefore, the ‘genre’ and domain of the message have to be specified. A (rather general) working definition of the concept ‘genre’ is given in [Swales, 1990, p.58]:

A genre comprises a class of communicative events, the members of which share some set of communicative purposes. These purposes are recognised by the expert members of the parent discourse community, and thereby constitute the rationale for the genre. This rationale shapes the schematic structure of the discourse and influences and constrains choice of content and style. Communicative purpose is both a privileged criterion and one that operates to keep the score of a genre as here conceived narrowly focused on comparable rhetorical action. In addition to purpose, exemplars of a genre exhibit various patterns of similarity in terms of structure, style content and intended audience.

In this thesis, we focus on the genre of experimental scientific articles, and we concentrate on the domain of experimental molecular dynamics in particular.

As communication via articles is strongly indirect, the author has to pay particular attention in advance to the fulfilment of the receiver’s potential requirements. These requirements are particularly important in scientific communication, because scientific research is a co-operative effort. Incorporating existing scientific information into new work is constructive only if the information has a high quality and if it is relevant to the new situation. It is feasible only if it is presented sufficiently clearly to allow the scientist to understand and evaluate it, and it is practical only if the information is presented in an appropriate quantity.

1. **Quantity:** The message is required to represent all information that is necessary for the achievement of the sender’s and the receiver’s goals, and no unnecessary or pointless information. In other words, the sender has to provide precisely the appropriate amount of information. This requirement is derived from the communication rules to perform no unnecessary and no pointless speech acts.

The existence of a research programme (an accepted model or pattern) in science has a direct impact on the quantity requirement of scientific communication. The sender is required to provide the receiver with all necessary information. This implies that he not only has to give a full account of his latest findings, but that he also has to make all relevant background information available. In the context of a shared programme, that background has already been established. Once the background has been properly presented, it does not have to be repeated in each publication.

The consequence of the heterogeneity of communication via articles is that it is difficult to fulfil the quantity requirement for all potential receivers.

2. **Clarity:** The message has to be clear, orderly and brief, avoiding obscurity and ambiguity, so that the receiver can understand and critically test it. This requirement is based on the communication rule to perform no incomprehensible speech acts. This implies that the restrictions of the information and all relevant dependency
relations between information units must be made explicit. It also implies that
the problem-solution pattern of the research has to be taken into account in the
presentation.

As all scientists are in principle supposed to study the same ‘real universe’ system-
atically, regardless of place and time, they must be able to communicate with each
other, regardless of place and time. Furthermore, in experimental science, relevant
information is related to the ‘real world’, so that scientists require the possibility to
claim their priority:

[Scientists believe] that there is just one real world waiting to be explored.
Since several scientists may be working along similar lines at the same time,
this means that the first to give public notification of a discovery pre-empts the
work of the others. Consequently, the communication system must be able to
establish clearly who has priority for each step forward. [Meadows, 1998, p.49]

Therefore, the organisation, presentation and implementation of scientific informa-
tion has to be compatible with the practices of scientists in other places and
times. Consequently, there are handbooks about writing scientific publications (such
as [Day, 1979]), and there is a prototypical format of (some types of) scientific pub-
lications.

3. **Quality:** The message is required to be correct or to have adequate grounds for
belief. The sender is supposed to be honest and to be reasoned, and he can be held
accountable for the message. This requirement is based on the communication rule
against insincere speech acts.

Absolute correctness can be guaranteed only in cases where rigorous proofs are
possible. Therefore, the requirement of quality is specified to the requirement that
the information has to be correct given the current state of affairs in science, i.e. that
it has to be based on adequate grounds for belief. This implies that the information
has to be controllable.

Consequently, scientific communication has to meet particular clarity and complete-
ness requirements. To control a scientific claim, the receiver requires a full and clear
description of the procedures and methods that have been used. In particular,
the receiver has to be made aware of the restrictions of these methods, and the
consequent restrictions of the validity of the findings. Furthermore, if information
depends on other information, that dependency relation has to be explicit. In par-
ticular, it is necessary to specify the sources of previous results used in this work.
When the dependency relations are made explicit, it is possible to trace the con-
sequences of adjustments or refutations of particular information to the validity of
other information. If, for example, an assumption used in a method turns out to be
unwarranted, all findings based on that method are suspect.

4. **Relevance:** The message has to be relevant given the goals of the interactants at each
stage of the interaction.\(^{34}\) In other words, the sender has to provide the appropriate
*type* of information. The requirement for relevance follows from the rule to perform
no speech act that is not appropriate at that point in the sequence of speech acts.

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\(^{34}\)For a discussion of the notion of relevance in discourse and argumentation analysis,
see [Sperber and Wilson, 1986] and [Van Eemeren and Grootendorst, 1994 ii].
2.2. REQUIREMENTS FOR SCIENTIFIC ARTICLES

2.2.2 A profile of the interactants in scientific communication via articles

Scientific information via articles is a particular type of goal-oriented communication. Therefore, we have to specify who are the interactants, what are the goals that the interactants try to achieve, and what requirements the communication system and the article must fulfill in order to allow the interactants to achieve these goals.

The interactants are scientists who play various roles, as senders and receivers, in the communication process we described in section 2.1.1. In this discussion, the emphasis lies on the receiver’s requirements, because the authors also concentrate on the prospective receivers (they must tailor their article to the receivers’ needs) and the requirements of the senders concerned with the added value coincide with receiver requirements.35

Senders

Senders creating documents: authors

In pure science, researchers both publish and read articles, alternating the roles of sender and receiver.36 Authors are scientists who create scientific information and represent it in scientific articles, in the first main stage of the communication process. We assume that these scientists not only have research skills, but also have sufficient presentation skills, such as writing skills. They may be assisted by referees and editors.

We concentrate on what we assume to be the author’s primary goal: the advancement of science. 37 This goal has two aspects: firstly, the author aims to add to the body of scientific knowledge, offering present and future colleagues information that they can use in their own research. Secondly, the author wants to advance his own research by soliciting feedback from colleagues.

In order to achieve this primary goal, the author has to achieve three interactional goals in the article: he has to 1) inform the receiver of his work, 2) convince him of its reliability, and 3) convince him of its relevance

Now, let us consider the requirements that must be fulfilled to allow the author to achieve his goals. The author’s primary goal can be achieved only if the receiver’s requirements for effective and efficient communication are met. Therefore, the author has to present the information in a clear and acceptable way when creating the document in the first stage. For that purpose, the standard format for articles has to be clear, so that the author understands how and where he has to represent the information. Furthermore, he needs appropriate tools and guidelines allowing him to present and encode, in a convenient way,

35 See also [Line, 1992], in which the requirements of the authors, publishers, libraries, and consumers that the system of making scientific and technical articles available must meet are discussed. See also [Van Rooy, 1995], which is based on a study performed for a publisher and in which acquisition needs with respect to the information and the acquisition process, and dissemination needs are discussed.

36 We concentrate on academic research. The conditions of industrial and military research are different: information is not freely and universally available. Researchers at Research & Development departments in these sectors predominantly play the role of receiver.

37 In a user-survey [Coles, 1993], most respondents indicated that their first motivation for publication was the dissemination of information. Many indicated, as a secondary motive, improved funding and career prospects.
all the information he considers relevant. This implies that the author should not be limited to textual or ‘printable’ representations, or limited by restrictions with regard to the amount of information. It also implies that the author should not be obliged to do unnecessary work: if part of the information that the author wants to convey has already been presented, he has to be able to re-use that previous presentation. Since the representation of scientific information requires a profound understanding of the information itself, it is more efficient for the scientist to write the article himself then to explain everything to a non-scientist professional writer and delegate the representation of the information.

For his (secondary) goal of gaining recognition, the author needs to establish his claims of priority and intellectual ownership. For that purpose, the author requires the registration of his work (in activity (5) of the scientific process, the collection), and its authenticity to be guaranteed in the archives (10). The author also wants his work to get a ‘seal of approval’. For that purpose, he requires the certification provided by the quality control performed in (6).38

With respect to the technical added value, the author would like a high quality ‘physical product’ (created in activity (8)). More important to him is high visibility in the publication (9), in order to attract as large a part of the target audience as possible. The integrity of the information is also an important issue, especially in the archives (10): no one ought to be able to change the information.

Senders disseminating documents: editors, referees and indexers

In the second main stage of communication (disseminating the message), scientists can play the role of journal editor, referee and indexer. Editors who actively solicit articles for publication aim to elicit all relevant information available, steering the flow of the information. For that purpose, they have to be aware of existing knowledge and interesting developments in the field.

The referees responsible for the scientific quality control must be experts on the subject of the article. The goal of the referee is to ensure the scientific quality of the article, by either eliminating or ameliorating incorrect, incomplete or unclear articles.

The goal of indexing is to provide index terms that characterise the information represented in the document in such a way that the receivers are enabled to locate the document if it is relevant to their information needs. These index terms can be provided by the author, by a professional indexer, or by an automatic indexing computer programme. If the author is responsible for the characterisation of the article, it can be seen as part of the creation of the article. If a professional indexer has to find adequate index terms, he has to read and understand the article.

Thus, the requirements of the scientists adding value to an article that they have not written themselves correspond to requirements of the receivers. Therefore, we shall consider the requirements of these types of senders in conjunction with the requirements of the receivers.

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38 According to [Kürz and Roosendaal, 1996], scientific journals have four main functions: certification, registration, archiving and awareness.
2.2. REQUIREMENTS FOR SCIENTIFIC ARTICLES

Receivers

The intended receivers (or ‘target audience’) of scientific articles are peers, i.e. scientists who have approximately the same background as the author. Nevertheless, as we already stated in section 2.1.3, scientific communication via articles is heterogeneous: not all members of the target audience are equally familiar with the subject. The receivers’ ‘degree of familiarity’ ranges from the least-informed to the most-informed receiver.\(^{39}\) The most informed receiver is the expert. The question as to who is the least informed receiver, i.e. what is the minimum of knowledge on a specified subject that the receivers are presumed to have, depends on the domain and the level of specialism of the article. The ‘degree of familiarity’ with the subject affects the receivers’ goals and their requirements for effective and efficient communication.

Receivers acquiring documents: searchers and browsers

The receiver can have different specific goals in the stage of information acquisition: 1) to find specific information, 2) to look for new ideas, and 3) to keep informed.\(^{40}\) To achieve these goals, the scientist engages in different activities.

To locate the desired type of information in activity (11), the receiver needs the means to differentiate between information sources, with respect to their nature and quality. Therefore, articles are required to be certified, as an outcome of the quality control (6).

Also, the following technical requirements must be satisfied: the article representing the relevant information has to be encoded (by the author in (4), and in particular by the publisher in (8)) in such a way that it can be archived efficiently (in activity (10)). And the receiver needs adequate searching and browsing tools at his disposal.

Browsing:

To see what is available, the scientist browses. In other words, he performs a semi-directed or an undirected search, skimming articles or tables of contents of journals, or wandering through larger repositories of information (e.g. the shelves in the library or an electronic documentbase). The browser’s goal is to encounter interesting information.\(^{41}\) Informed browsers mostly monitor the information system to keep informed [Ellis et al., 1993]. Scientists who are less familiar with the subject rather look for new ideas, in what is called in [Chang, 1993] ‘serendipity browsing’.

Especially for the less-informed browser, both the article itself and the larger depository of documents (e.g. the library) are required to be structured clearly and relevantly. This implies that the structure needs to be compatible with what the receiver expect and that it has to be made explicit. Therefore, both the documents and the connections between them must be characterised properly, so that the browser can decide quickly whether a particular document is worth inspecting or not. Making the structure explicit in a ‘road map’ would greatly assist the browser.

In order to obtain a clear structure, it has to be properly conceived on the conceptual

\(^{39}\)In [Kircz, 1991], three discrete types of receive are distinguished: uninformed, partially-informed and informed receivers.

\(^{40}\)In a user-survey [Coles, 1993, p.110], it was found that the main reasons for the most recent use of the information sources/services were 1) writing a paper, 2) background reading for new projects, and 3) generally keeping up with the literature.

\(^{41}\)Note that by ‘browser’ we mean the browsing scientist, not the software assisting him in this activity.
level in (2) and properly realised in the writing activity (3). The archives have to be clearly structured in (10).

The informed browser mainly tries to keep abreast of the latest developments in his field. Therefore, he wants to be alerted when potentially relevant information is published (9). The time delay in the publication process has to be minimised, in order to ensure the actuality of the information. For the sake of efficiency, the informed browser wants to see immediately what is the novel information (as opposed to the background information) that warranted the publication of the article.

Searching:
In order to find specific information, the scientist performs a directed search. For example, he can search for a number or a definition, for advice to help him solve a problem, for a review on a specific subject, or for the precise address of an author. The more informed the searcher is about the subject, the better he is able to perform such a search, either with or without the support of an information specialist assisting in the technical aspects of the manipulation of the information system.

The basic requirements for searching information are completeness and findability: if the particular information unit the receiver needs exists, 1) it has to be available, and 2) the receiver has to be able to locate it.

For completeness, all potentially relevant information has to be taken into account in the author’s organisation of the information at the conceptual level (2). A fundamental problem concerning the completeness is that the author does not know what information could be relevant in other contexts, even if he strives for the completeness of what he thinks essential. Then, all potentially relevant information is required to be expressed in the article in (3) (the actual writing of the article) and subsequently encoded in (4). Relevant information can be lost for technical reasons in these activities.

Completeness also implies that all articles containing relevant information must be made available. They risk being lost altogether, when they are not included in some appropriate collection (in activity (5)). In the quality control (6), relevant information can get lost, if it is rejected along with incorrect information. Furthermore, the information should not stay in the ‘publication pipeline’ too long, but it has to be published (9) quickly. Once articles have been made available, the searcher requires that they remain available, i.e. that the articles are properly archived (10). Access to the archives and the security of the articles have to be guaranteed permanently.

Supposing that relevant information is available, the next step is to find it. For that purpose, a correct characterisation is indispensable. The information has to be adequately characterised, and that characterisation has to be represented at the symbolic level in a set of index terms, which then must be associated to the signal encoding the document.

The characterisation must be correct (i.e. the index terms must correspond to the information they describe), clear and relevant (i.e. they should describe the information in a way that fits the receivers’ expectations and needs). It is also required to be complete (i.e. all information must be characterised), to reduce the risk of the receiver missing the target altogether. In terms of Information Retrieval, this point is mostly concerned with the ‘recall’ of the search result. For the enhancement of the ‘precision’ of the search result, the characterisation must also be sufficiently precise: it should be narrow (i.e. the

\[\text{Recall} = \frac{\text{number of relevant documents retrieved}}{\text{number of all relevant documents}}\]

\[\text{Precision} = \frac{\text{number of relevant documents retrieved}}{\text{number of retrieved documents}}\]

(see [Van Rijsbergen, 1979, p.10]).
2.2. REQUIREMENTS FOR SCIENTIFIC ARTICLES

combined index terms should not be more general, for example, than the information) and fine-grained, in the sense that the representation of each different type of information that the receiver may be looking for should carry its own index terms. The information that the searcher is trying to locate is not necessarily what is represented in an entire article. Therefore, the precision of the search not only implies that no irrelevant documents should be retrieved, but also that the retrieved documents that contain relevant information do not contain any irrelevant information, or that the representation of the relevant information is highlighted within the document. Therefore, smaller publication units than the article have to be explicitly labelled in the case that an article is composed of parts representing different types of information. In the next chapter, we shall see that in a modular article, each module carries a unique characterisation.

Retrieving:
Then, the receiver wants to retrieve the article quickly, easily and cheaply in activity (12). Therefore, there should not be insurmountable technical or financial barriers blocking the archives.


text

Receivers assimilating the information contained in documents: comprehensive and selective readers, and users

Decoding:
For the transmission (and in particular storage) of the document, the symbolic representation of the information may have been translated into some computer language. In that case, the receiver has to decode the signal (13) in order to obtain the article itself. For example, if information represented in terms of a picture has been transmitted as a computer file in a picture format, it has to be translated back to the pictorial language that the (human) receiver can interpret. For this purpose, the receiver requires appropriate ‘tools’. In cases of exotic or obsolete encoding formats such tools may be unavailable.

Reading:
The receiver aims to learn from the article and to use the information represented in it in his own research. When consulting a scientific article, he therefore has the following specific goals, which reflect the author’s interactional goals: 1) to get informed, 2) to evaluate the reliability of the information, and 3) to evaluate the relevance of the information in the light of his own needs. For this purpose, the receiver can read the article comprehensively or selectively in activity (14) of the communication process.

In the case of comprehensive reading, the receiver consults the article as a whole, following the discourse linearly from the beginning to the end. Traditionally, articles are written to be read in this way. According to [Bazerman, 1985], most comprehensive reading is for self-instruction in areas beyond the intimate knowledge of the receiver. Thus, the receiver studies the article as a tutorial [Dillon et al., 1989]. He has to be sufficiently informed to be able to read an article written for peers comprehensively without additional background information. The most informed receivers may read an article comprehensively, in order to judge its quality. However, they are not always interested in reading the entire article, being already familiar with most of its contents.

In the case of selective reading, the scientists do not consult the article as a whole. Instead, they extract only the specific parts they need. Bazerman has interviewed informed
physicists, to analyse their reading strategies. He found that the majority of the interviewees read the larger part of the articles selectively [Bazerman, 1985, p.11]. Receivers do not consult the article sequentially either. Instead, they start with the interesting part and then jump to additional information. Rather than studying the article like a tutorial, the ‘selective receiver’ consults the article more like a reference book. A special type of ‘selective reader’ consults the meta-information of an article, rather than its scientific content. This role is played by non-scientists for administrative purposes, but also by scientists who want, for instance, to contact an author or to find a specific reference.

To allow the receiver to assimilate the information represented in an article, it has to be *structured and expressed in a clear and readable way*, so that the receiver can absorb (15) and evaluate (16) the information easily. In particular, the coherence of the information has to be expressed. In this context, the problem of incompleteness, already mentioned for the acquisition of information, also affects the receiver: explanations, extensive calculations and interesting proofs cannot be replaced by a statement like “you can easily show that”.

We assume that, for the sake of clarity, the distinction between old and new work has to be made explicit. We also assume that the receiver wants the main claim of the article to be highlighted and that the receiver wants to be able to assess the contents of the article and evaluate its potential interest quickly. Therefore, it also has to be clear how the article fits in its context.

For comprehensive reading, readability implies that the receiver is guided smoothly from the beginning of the article to the end, while in the structure the main issues are separated from side-issues. For the purpose of selective reading, the article has to be organised in small coherent units, so that the relevant specific information is not encumbered by the rest. For the selective consultation of the meta-information, these data in particular are required to be grouped and clearly structured. Thus, comprehensive readers and selective readers have conflicting requirements. If receivers must be able to read same article in two different ways, the article will have to be structured in a particularly clear and flexible way.

Furthermore, the article has to be produced (8), published (9) and stored (10) in such a way that its (physical or electronic) ‘technical presentation’ is either directly user-friendly, or easily re-formatted as such. The reader has to be able to transport and store the article for (re)use at a later time, to compare information and annotate the article.

**Incorporating:**

If the receiver judges the information to be sufficiently reliable and relevant, he can incorporate it in his own work. For instance, he can utilise it directly as input in a calculation, as a guideline for the fine-tuning of his own experimental set-up, or for comparison with his own results. This implies, from a technical point of view, that the information has to be presented and stored in a manipulable form.

The information can only be used wisely if it is complete, in particular with respect to its restrictions. The more familiar the scientist is with the subject, the more natural it is for him to use information from the article, without first reading the whole story. If the receiver does not accept the information, he can contribute to science by explicitly refuting that information.

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43 In [Kircz, 1991], this is called a ‘non-reader’.
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In the context of scientific articles, this implies that the information has to be controllable. Therefore, the source of cited information must be made explicit and the acquisition of the cited material has to be easy, so that the information can easily be checked. Furthermore, the receiver requires assistance in judging the article, in particular if he is not sufficiently well-informed to recognise unreliable information as such, or if he wants to use the information directly. Therefore, *certification* plays a crucial role in this stage, informing the receiver about the reliability of the information.

Related to the requirement of scientific quality is that of the *integrity* of the information. In the archives, the article has to remain ‘intact’. However, the archives must be flexible enough to allow for the addition of new versions, comments and explicit corrections, to keep the information up to date and ensure that obsolete information can be recognised as such. The original version of a published article must not be changed.

Summarising, we have discussed the following requirements of the interactants in the process of scientific communication.

As a prerequisite, the communication system in general has to fulfil the following requirements, including *dissemination requirements*. It should:

- provide practical tools and guidelines that facilitate authoring;
- register publications, establishing their existence and securing the authors’ intellectual ownership and priority;
- disseminate rapidly;
- durably store publications in such a way that receivers can easily locate and retrieve them;
- guarantee that the authenticity and integrity of publications are preserved;
- enable receivers to obtain publications in a (physical, digital) form that allows them to easily consult, annotate, transport and store the publications, and to manipulate their contents;
- provide practical tools and guidelines for navigation, and for searching, retrieving and consulting publications.

Concerning the article, the author has the following requirements

- ‘*Creation requirements*’: The prescribed format of the article has to
  - spare the author unnecessary work;
  - be clear.

The scientific article itself has to meet the following criteria to satisfy the receiver:

- ‘*Acquisition requirements*’: The representation of the information has to be characterised completely, sufficiently precisely, correctly, clearly and relevantly
• ‘Assimilation requirements’: The represented information has to be:
  – the appropriate quantity, i.e. sufficient and not excessive;
  – clear, i.e. clearly structured and clearly formulated (or, generally speaking, clearly expressed in any language, e.g. natural language, formulae, graphics);
  – high-quality, i.e. based on adequate grounds for belief, and therefore it has to be controllable and certified;
  – relevant to the central problem of the article.

2.3 Electronic publishing

In the previous section, we have specified the requirements for efficient and effective scientific communication independently of the publication medium. In this section, we discuss the intrinsic characteristics of the electronic publishing technology (compared with the paper based technology) in terms of the impact they may have on the fulfilment of the requirements on scientific communication.

Distribution

We speak of electronic publishing when the article is encoded in an electronic signal and made public in digital form in activity (9) of the process of scientific communication described in 2.1.1.\textsuperscript{44} The electronic distribution of scientific articles is more efficient than the distribution of printed articles by the traditional distribution channels, as it is distributed more quickly and more directly. Information can be made available more quickly, when it is published on-line. Firstly, the distribution itself causes no delays. Secondly, articles or other publication units can be published as soon as they are ready, without waiting for the next issue of the journal. Thus, an electronic journal can lose its periodical character and the flow of information can become continuous.

The issue of speed and ease with which an article can be obtained has two sides. On the one hand, navigating within an on-line article, once it has been found, may be relatively slow due to network congestion. On the other hand, on-line publications from different sources are accessible directly from the scientists desktop, whereas a paper or off-line publication in most cases has to be separately consulted in or fetched from the library or some other central service. Thus, electronic publications can be obtained quickly and easily, provided that the infrastructure is sufficient and the user interface is adequate.

The author’s requirement for high visibility is not fulfilled by most of the present day electronic journals. At this moment, paper journals have a more serious image, a much higher status and a far larger audience then electronic journals.\textsuperscript{45} This is not an intrinsic characteristic of the medium, but a description of the status quo. We assume that the prestige of the new media will increase when enough important scientists have published articles in scientifically adequate electronic journals.

\textsuperscript{44}This implies that an electronic publication does not have to be either originally generated or read in electronic form, and that the same article can be published both in electronic form and on paper. We concentrate on on-line publication, because communication via that channel exhibits more characteristics specific to electronic publication than publication by means of e.g. CD-ROM.

\textsuperscript{45}This is not the case for the electronic versions of prestigious paper journals [Speier et al., 1999].
2.3. ELECTRONIC PUBLISHING

Storage

As a storage medium, an electronic memory is much more efficient than paper. Therefore, it is possible to present in an electronic article large amounts of information that cannot reasonably be published in a printed article. In an electronic environment, it is also possible to store and present messages that cannot be printed at all. For example, in an electronic article, the symbolic representation of the information can be a sound or a movie, instead of a text or a picture. The choice of the medium does not have an impact on the requirements with respect to the writing itself, but the electronic media can enhance the clarity of the article, because the most appropriate type of representation can be chosen.

The impact of electronic storage on the requirement of completeness is mixed. On the one hand, an electronic article can present material that cannot be printed, including intrinsically unprintable animations and amounts of data that are too large to be printed in practice. On the other hand, information may be lost, because the electronic media are not as secure as the print medium (yet).\(^{46}\)

Complex search operations

An important advantage of electronic storage is that it allows for complex search operations, within a document as well as within an entire archive. The receiver can locate relevant articles by searching in bibliographic databases with abstracts (e.g. INSPEC), as well as in full text ‘document bases’. In order to allow the receiver to take advantage of this possibility, the representation of the information has to be characterised clearly and correctly.

Separating the storage from the presentation format

Another advantage of electronic storage is that information can be stored independently of the presentation. Upon each retrieval of the information, it can be decided how it is to be presented – on screen or on paper, and which font, format and appearance are most suitable for a particular task. This feature is explicitly used in descriptive languages as Standard Generalized Markup Language (SGML) or Extensible Markup Language (XML), where the structure of the presentation is marked up in a functional way (labelling headers and sections) instead of a typographical description (in terms of fonts and sizes) \(^{[ISO, 1986]}\).

In an electronic environment, the production of a truly physical product can be entirely eliminated, or replaced by a print job on a laser printer in the receivers office.\(^{47}\) In the user-survey reported in \(^{[Coles, 1993]}\), all respondents indicated that they wanted print-on-paper versions of articles of interest; they preferred to restrict reading from the screen to article scanning. It must therefore be possible to obtain an adequate printed version of electronic articles. This requirement, however, is far more stringent for the comprehensive receiver than for the selective receiver, who does not read the entire article. At least using

\(^{46}\)The medium-independent aspects of the requirement of completeness, concerning the choices of the scientist representing and then presenting the information, are unaffected by the transition from paper to electronic publication of course.

\(^{47}\)Thus, electronic publishing may lower the cost of the publication, but that is not necessarily the case. The financial aspects of electronic publication are discussed in, for example, \(^{[Scovill, 1995]}\), \(^{[Coles, 1993]}\).
the current technology, paper is easier to handle than the computer for the reader. It is more pleasant to read from paper than from a computer screen. Also, a paper article is more portable and it can more easily be annotated. And viewing different documents (or parts of documents) simultaneously is more practical if they are spread out over a desk than if they are presented on the screen.

**Flexibility**

An electronic journal is more flexible than its paper equivalent. Information represented in an electronic article can be presented in such a way that the receiver can manipulate it. For example, experimental data can be presented in a machine-readable format, integrated with tools for calculation and plotting graphs.

In an electronic article, not only the presentation is flexible, but the storage as well. Whereas a printed article is fixed, an electronic article can be changed. In printed articles, effective updating is impossible, because the only instruments are errata, addenda and follow-up articles pointing back. In an electronic environment, various additions can be attached to the original article, such as comments or links pointing forward to later work on the subject. Thus, the correctness and the clarity of articles can be enhanced in an efficient way.

This flexibility can also be used to adapt the system of peer review. The essence of the certification of the information as such does not depend on the technology but on the social and philosophical ideas about science. However, it can be implemented in different ways and at different times. Nowadays, selection takes place before publication and the acceptance in that particular journal forms the certification. On-line electronic publication allows for spontaneous peer review after the article has been published without previous selection. The comments, made by referees before and after publication, can be attached to the article, giving a specific certification with all necessary nuances, instead of a simple acceptance by some journal. The receiver himself can then filter the information flow, aided by the certification of the articles or the lack thereof. The higher the status of the referee, the more convinced the receiver will be of the scientific quality.

The flip side of flexibility is insecurity. So far, electronically stored documents are less secure than printed documents. Firstly, files can be changed without authorisation. It is important to protect the integrity of the original article, to avoid confusion, e.g. by ‘watermarking’ original copies. This problem does not occur if the information has been stored on a read-only carrier, such as a CD-ROM. Secondly, the electronic information stored on any carrier can become inaccessible if the carrier breaks down or becomes obsolete. Technical and organisational solutions must be found for these problems.

**Non-linearity**

The electronic media provide us with a distributed storage environment, which allows for a flexible consultation of publication units. On paper, a linear, essay-like one-dimensional presentation of the text is natural: the readers is supposed to begin at the top of the first page and follow the line of the article until the bottom of the final page. The electronic media allow for a non-linear, hypertext presentation.\(^\text{48}\) According to [Conklin, 1987, p.36]:

\(^{48}\)For an introduction to hypertext, see [Conklin, 1987]. The word hypertext was introduced in 1965 by Ted Nelson to describe a set of texts and images that are linked in a complex way. Conklin defined hypertext as a synonym of non-linear text. In his definition, a text with notes and references is also
2.4. COMMUNICATION CRITERIA FOR ELECTRONIC ARTICLES

People [...] think in terms of ideas, facts and evidence. Hypertext, via the notion of nodes as individual expressions of ideas, provides a vehicle which respects this way of thinking and working.

If the structure of an article and of a larger repository of knowledge is non-linear, it can be organised and presented in such a way that the clarity is enhanced and navigation is facilitated.\footnote{On the larger scale, hypertext only makes sense if a large part or all of the information is available in this electronic form.} However, hypertext has a double-edged impact on the clarity of the representation of information. On the one hand, the representation can reflect the structure of the information more closely, and thereby more clearly, if the information is non-linear. On the other hand, the non-linear representation can lead to disorientation, and an increase of the 'cognitive load', as the reader has to make an additional effort to know where he is and how to get to the desired location. Therefore, the requirement of clarity is even more crucial in a non-linear presentation than in a linear presentation.

Thus, hypertext can provide a tool for the presentation of information in scientific articles, provided that an adequate structure is devised for the organisation of the information. In this thesis, we develop a model for a systematic non-linear structure for scientific articles.

2.4 Communication criteria for electronic articles

In the previous sections, we have discussed the needs of the scientists engaged as senders and receivers in scientific communication, as well as the characteristics of the electronic medium. In this section, we summarise the 'communication criteria' that the electronic scientific article itself, and in particular its structure, must fulfil to satisfy the interactants' needs.

A Firstly, the representation of the information has to satisfy the following ‘retrieval requirement’: the representation has to be characterised completely, sufficiently precisely, correctly, clearly and relevantly in order to allow the receiver to locate, by means of complex search operations, the information that satisfies his information needs.

Communication criteria for the characterisation:

- Each publication unit has to be precisely and uniquely characterised so that it can be localised by (and so that the receivers are informed of) at least:
  * its domain-oriented content (allowing the receivers to search for units on the desired subject);
  * its genre (allowing them to search for and to filter units with the desired aims, e.g. tutorial, article) and publication status (allowing them to filter unpublished material from published material);
  * its standard bibliographic data.
– The structure of the publication has to be predictable. This allows 1) the searcher who has located a publication unit using its characterisation (during the retrieval process) to find in this publication unit indeed the information that the characterisation led him to expect. This also allows 2) the receiver (during the reading process) to recognise the role of the unit in the discourse.

– The metadata of every unit must be made explicit and grouped in such a way that they can be used to locate the publication and that they can easily be consulted by the receiver during the reading process.

B Secondly, once the receiver has obtained the message, that message has to fulfil the requirements of quantity, clarity, quality and relevance. Structuring the article adequately can contribute most to the fulfilment of the quantity and the clarity requirement. In particular, the representation of the information in an article has to satisfy the following ‘reading requirements’ in order to allow the receiver to assimilate it.

1. Quantity: The requirement of quantity implies sufficiency and no excessiveness: all information necessary to fulfil the receiver’s information need has to be provided, but all unnecessary information must be avoided.

Communication criteria for the quantity:
– Each issue that will presumably be considered a separate subject by part of the target audience has to be dealt with in a separate unit.
– Each unit has to be self-contained, so that it can be located, retrieved, consulted, cited and used repeatedly as a separate entity

2. Clarity: The representation of the information is required to be clearly structured.

Communication criteria for the clarity:
– The representation of research information should have a structure reflecting the process of the research itself (reconstructed as a problem-solving process, not as a depiction of the day-to-day proceedings).
– The representation has to contain explicit, precise connections between the related parts of the article and between (parts of) the article and related (parts of) articles, so that:
  * the accounts of subsequent steps in the problem-solving process are connected (for content-oriented coherence: what depends on what);
  * the steps in the line of reasoning are connected (for argumentative or rhetorical coherence);
– The structure of the article in particular, and of the collection of articles in general, must be made explicit in a clear overview.
– The representation of information in a publication unit (or in a coherent collection of units) has to form a ‘readable’ discourse.
  * Receivers must be able to follow the main line without being bogged down in details or background information.
2.4. COMMUNICATION CRITERIA FOR ELECTRONIC ARTICLES

* All details and background information that are necessary for the members of the target audience to understand the discourse have to be made explicitly available. There is tension between the need for full detail and the need for a clear line of discourse mentioned above.

* The discourse has to contain summarising remarks that facilitate the receivers’ understanding of large and complicated parts of the discourse.

* The same information should not be unnecessarily repeated in a coherent discourse.

The repetition can be necessary 1) in summaries (following the previous criterion) or 2) to meet the criteria of self-containedness in order to meet the quantity requirement of receivers who do not follow the entire discourse. In the last case, there is tension between the need for repetition by selective receivers and the need for a smooth discourse by comprehensive receivers.

– A distinction has to be made between main points and side issues, and between new information and background information.

3. Quality: The information is required to be based on adequate grounds for belief, i.e. to be correct given the current state of affairs in science. To guarantee this claim of quality, the information has to be:

– controllable by the receiver;

Communication criterion: Details about all methods used in the research and about its outcome (in particular about their restrictions) must be made available to the receiver, to justify the reliability of the work.

– certified by an accepted authority (e.g. a referee, a PhD committee). In addition, the authenticity and the integrity must be guaranteed.

Communication criterion: The certification and authenticity must be expressed in metadata that must be made explicit and grouped for every publication unit in such a way that they can easily be consulted by receivers of the publication.

4. Relevance: The information represented in the article is required to be relevant to the problem of the article.

Communication criterion: If the relevance of the information to the problem is not immediately clear, it has to be justified.

C Thirdly, the publication format has to fulfil the following authoring requirements.

1. From the authors’ perspective, the quantity requirement means that they do not have to do more work than necessary.

Communication criterion: Information has to be represented in a way that allows for multiple use of the presentation by means of reference to a previous publication.

2. The requirement of clarity implies that the prescribed format has to be clear, so that the author understands how and where he should represent the information.
CHAPTER 2. EFFECTIVE AND EFFICIENT COMMUNICATION

**Communication criterion:** The format has to be systematic, allowing the author to follow practical guidelines and to get used to it.
Chapter 3

A modular presentation of information: general definitions

In this chapter, we present the general definitions of the notions needed in our model for modular articles. We define what we mean by a modular structure in section 3.1. In order to allow for the creation and evaluation of modular articles, this general definition has to be made concrete in a modular model, by specifying what types of modules and links can be distinguished. The role and nature of the typologies are discussed in section 3.2 and the characteristics of the modular model are given in section 3.3.

3.1 A modular structure

We define a modular structure, by specifying the definition of modules in section 3.1.1, the definition of links between modules in section 3.1.2 and the mechanisms for the composition of modules in section 3.1.3.

3.1.1 The general definition of modules

According to the criteria for effective and efficient communication via scientific articles that we specified in section 2.4, information concerning each separate subject should be presented in a unit that readers can locate, retrieve, consult and manipulate separately. Hence, we define a module as follows:

**Definition 3.1.1** A module is a uniquely characterised, self-contained representation of a conceptual information unit, which is aimed at communicating that information.

This definition can be applied to any coherent body of information. In practice, the question as to what can be a conceptual information unit underlying a module can only be answered for a particular domain and genre. In chapter 4, we shall concentrate on electronic articles on experimental sciences, and in chapter 5 we shall focus even further on the domain of experimental molecular dynamics. Here, we clarify the general definition of a module.

The first distinguishing feature of a module is that it is a particular kind of *document*. Information is represented in modules for the purpose of communication, in the same way
it is represented in traditional scientific articles for that purpose.\textsuperscript{1}

The \textit{conceptual} nature of the information unit represented in a module is the second feature: modules are identified by their underlying concepts.\textsuperscript{2,3} The distinction between different modules is independent of the language in which the information is represented (such as a particular natural language, mathematical formulae or pictures) and thereby independent of the storage format as well. A module neither has to coincide with a ‘storage unit’, like a file, nor with a ‘presentation unit’, e.g. a hypertext node.\textsuperscript{4}

The lower boundary of what can constitute a module is determined by its \textit{self--containedness}, which is the third distinguishing trait. Our criterion for a representation of an information unit to be self-contained is its meaningfulness when consulted independently of other modules. An adequate module represents sufficient information to satisfy the needs of the target audience. More specifically, a module is self-contained if at least the most informed members of the target audience can extract the scientific information.\textsuperscript{5} For example, a complete figure with experimental results can form a self-contained representation and, hence, a module. Error bars in the figure make the reliability of the measurements explicit. However, these error bars have no meaning independently of the results themselves, so that not even an expert can use them separately. Therefore, the representation of information on the reliability of the results cannot constitute a complete module.

The upper boundary of the information content of a module is given by the fourth feature of a module: a module focuses on a \textit{single concept}. Other concepts may be addressed in the module, but these are auxiliary to the concept that the module focuses on. In other words, a module treats only one subject, allowing readers to concentrate on that subject. The nature and the degree of specificity of a relevant ‘single concept’ depend on the domain in science and on the level of detail required by the target audience. For instance, a module in a general science tutorial can focus on the general concept of ‘molecules’, whereas a module in an article on molecular physics could focus on the more specific concept of ‘sodium halide molecules’. In section 4.2, we shall introduce the modules we defined for articles on experimental science.

\textsuperscript{1}We have to emphasise that the modules we define represent units of information in the article and not units of functions in the communication process (such as the steps in the process we described in section 2.1.1). Therefore, our notion of modularity differs from the one developed in Fodor [Fodor, 1983]. Their ‘cognitive modules’ are functional modules, such as components of a perceptual system and a language production system.

\textsuperscript{2}Following Thagard, we mean by a ‘concept’ a largely learned open mental entity. [Thagard, 1992] gives an overview of what can be meant by the notion ‘concept’.

\textsuperscript{3}In our modular model, the distinction of modules is primarily based on their underlying concepts. In section 4.2.1, we shall see that modules are further distinguished by additional features, namely the ‘range’ of the information and a specified set of bibliographic data.

\textsuperscript{4}In present-day electronic articles, presentation units are usually distinguished by the type of the representation of the information: the main text of articles, the figures and the tables are presented in separate hypernodes. Such hypernodes do not fit in our definition of a module. An example of the distinction of information units by the storage format is given in [Murray-Rust, 1997]. These ‘machine-oriented’ scientific information components, such as files in a particular picture format or text-only files, are not modules according to our definition either.

\textsuperscript{5}In section 2.2.2, the profile of more informed and less informed readers has been sketched in general. The specific target audience of a particular journal has to be determined by its editorial board.
3.1. A MODULAR STRUCTURE

A module forms a part of a larger representation of information (e.g., an article or a
document-base) that has a modular structure:

**Definition 3.1.2** A **modular structure** is a pattern of modules and explicit links be-
tween modules.

A modular structure consists of two components that are put together following specified
basic rules. The first component of a modular structure is a set of modules that satisfy
the general definition as given above. The second one, consisting of the links between the
modules, is addressed in the next section. Modules and links can be combined to form a
coherent pattern following basic rules for the composition of modules, which are given in
section 3.1.3.⁶

3.1.2 The general definition of links

Our definition of modules as self-contained representations of information units does not
imply that they are independent of other modules: readers can only understand and
accept the information represented in the module, when they are sufficiently aware of the
scientific context. In this respect, modules do not differ from ‘traditional’, linear articles,
which also are self-contained and yet depend on their context. Articles are embedded in
the literature on the research programme as a whole (see section 2.1.2). This dependence
of articles on their contexts is expressed, for example, by the fact that they are published
in a journal dealing with a particular topic or programme, and also by references to
related articles. While the representation of information in an individual module can be
consulted separately, that information coheres in particular with information represented

⁶In computer science, modularity plays a role in the organisation of computer programmes. Its
purpose is to allow for modules, containing related data and operations, that can be designed and revised
independently. The replacement of such modules by improved versions does not necessitate a revision
of the rest of the programme. In the traditional paradigm of ‘structural programming’, modularisation
primarily entails a meaningful grouping of subprogrammes. In the object-oriented approach, modularity
is more pronounced. In the context of object-oriented design, [Booch, 1994, p.52] defines modularity as
follows: “Modularity is the property of a system that has been decomposed into a set of cohesive and
loosely coupled modules. Thus the principles of abstraction, encapsulation and modularity are synergetic.”
Abstraction implies the identification of essential characteristics. Deciding upon the right set of
abstractions for a given domain is the central problem in the object-oriented design. The abstractions
can be organised in a hierarchy, which allows for generalisation and aggregation. The details of modules
are hidden, or ‘encapsulated’; only the essential characteristics that are necessary for the interaction with
other modules are visible from the outside, so that the module can function as a ‘black box’.

In our work, we also have to decide what are the essential characteristics by which different types of
information should be distinguished. A hierarchy in these characteristics leads to the composition of
modules, which we shall discuss in section 3.1.3. Our modules carry visible labels that allow readers
to locate them, and contain details that remain hidden until the module is consulted. The modules
can also be created and used in different contexts. However, the interdependence of the information
represented in related modules in a scientific article can be quite strong, so that the modules are not
always ‘loosely coupled’. If the function of a module is, for example, to inform readers of the apparatus
used in a particular experiment, a new version of that module can describe that apparatus in a clearer
way. However, this new version cannot entirely replace the old module, because others may have cited
the old text. In addition, the new version has to describe exactly the same experiment, because the
module is connected to a module about the results generated in that particular experiment. Rules can
be formulated to specify how different types of modules, that are connected in different ways to other
modules, can be designed and revised.
CHAPTER 3. GENERAL DEFINITIONS

in other modules within the same article and in general with information represented in
the literature as a whole.

As we stated in section 2.2.2, effective and efficient communication requires that the
coherence of the information is made visible in its presentation. In a modular environment,
this coherence firstly finds its expression in links made explicit between the modules, which
we discuss here, and secondly in the composition of the modules. By a link we mean the
following:

Definition 3.1.3 A link is a uniquely characterised explicit, directed connection, between
entire modules or particular segments of modules, that represents one or more different
kinds of relevant relations.

A link can, in principle, be followed from the source to the target, as well as in the
opposite direction. The source and target of a link can be either a complete module or a
particular segment of a module, such as a phrase, a paragraph, a mathematical formula
or a figure. Unless explicitly stated otherwise, we shall in the following mean by a ‘link
between modules’, a ‘link between modules or segments of modules’.

Links connect modules to other modules within the same article, or within the same
collection of related articles, or in other collections of articles. Thus, the modular article
represents a network of information that is embedded in the network of all information
represented in modular scientific documents. Readers can choose a route through the
network that suits their particular information needs.

In these links, we express relations that are relevant in the communication between
the author and the reader of a module. The ‘relata’\(^7\) of the relations that are expressed
in such a link can be 1) the modules or segments of modules, or 2) the information units
represented in those modules or segments of these information units, or 3) the ‘real world’
entities they refer to.\(^8\)

Different kinds of relations can be distinguished; two particular relata can be related in
more than one way. Different relations between two particular relata can be represented
in one single, complex link connecting the modules. Consequently, links between modules
can vary in function and hence in structure. The function and structure of a link can
be made explicit in the modular structure, in the full characterisation of the link. The
specific types of links that are allowed in a modular presentation must be defined for the
domain and genre at hand, i.e. for the readership that is intended to use the links. In
section 4.3, the definitions are given for articles on experimental sciences.

3.1.3 The composition of modules

The inter-dependence of information units is expressed not only by means of links between
modules, but also in the ‘composition’ of modules.\(^9\) By composition we mean putting
together ‘elementary modules’ to form ‘complex modules’.

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\(^7\)The term ‘relata’ refers to the objects that are related.

\(^8\)The difference between these entities, information and the symbolic representation of information is
explained in section 2.1.1.

\(^9\)The importance of the composition has already been suggested for hypertext nodes by Halasz in
his influential paper on hypermedia systems [Halasz, 1988]. In [Smith and Smith, 1977], a similar notion
is discussed from the angle of database research, in terms of abstractions: “An abstraction of some
system is a model of that system in which certain details are deliberately omitted. [...] The objective
is to allow users to heed details of the system which are relevant to the application and to ignore other
3.1. A MODULAR STRUCTURE

![Diagram]

Figure 3.1. In a modular environment, an elementary module is part of a complex module is part of a modular article. Traditionally, a subsection is a part of a section is part of an article.

**Definition 3.1.4** An elementary module contains information that cannot be represented in more than one separate module.

Elementary modules are the smallest characterised building blocks of scientific publications, and thereby the prototypical modules. They cannot be further subdivided into smaller modules, because the resulting fragments would not be self-contained as required by definition 3.1.1. Nevertheless, they have an internal structure, which can be made visible in order to enhance the clarity, for instance by sectioning the text.

Elementary modules represent information units that readers should be able to locate, retrieve, consult and manipulate as separate entities. When the information units are related, the relations between them can be expressed in links between the modules. However, the coherence of the information represented in a particular set of separate modules can be so strong that links do not suffice to express it. In those cases, readers should be able to deal with the linked elementary modules as a single entity. Hence, the modular model allows for the composition of strongly related modules into a complex module, as is illustrated in figure 3.1. Unlike an elementary module, a complex module does contain constituent modules satisfying definition 3.1.1: elementary modules or lower-level complex modules that are self-contained in their own right. Being a module itself, a complex module carries a single characterisation and represents a single concept. This is a ‘complex concept’, however, that is related to lower-level ‘constituent concepts’.

**Definition 3.1.5** A complex module consists of a coherent collection of (elementary or complex) constituent modules and the links between them.

The purpose of the distinction of elementary modules and complex modules is to balance on the one hand the self-containedness of the individual elementary modules, and on the other hand the coherence of the information represented in a collection of strongly related modules.

Elementary modules can be seen as atoms: the smallest building blocks. Subdividing the atom, into its protons, neutrons and electrons, eliminates its chemical meaning. A complex module can then be seen as a molecule. A molecule contains atoms, but its chemical properties are uniquely defined and differ completely from the properties of its constituting atoms: the atomic bonds cannot be disregarded without losing the essence details. In some applications a system may have too many relevant details for a single abstraction to be intellectually manageable. Such manageability can be provided by decomposing the model into a hierarchy of abstractions.” [p.105].
of the molecule.

There may be various kinds of relations between the central concept of the complex module and the ‘constituent concepts’ in the constituent modules. In other words, different composition, or ‘synthesis’ mechanisms are possible. In our model, we shall restrict ourselves to two specific mechanisms: aggregation and generalisation.\(^\text{10}\)

Aggregation is grouping related (albeit possibly dissimilar) objects to form an aggregate object on a higher level. The classical example is that two legs, two arms, a trunk and a head aggregate into a body. An ‘aggregate complex module’ is a complex module consisting of constituent modules that each represent a component of the aggregate concept. The molecule is such an aggregate – in chemical terms: a compound. Therefore, we call this kind of complex module a ‘compound module’.\(^\text{11}\)

**Definition 3.1.6** A compound module is a complex module that is an aggregate of (elementary or complex) constituent modules.

An example of a compound module is the module representing an experimental set-up that consists of different components, such as a source and a detector, that are separately presented in constituent modules (see section 4.2.2). The compound module can also represent a procedure that consists of different steps.

A compound module has to consist of a necessary minimum of constituent modules to be adequate as an aggregate. That necessary minimum depends on the central concept of the module: which components are gathered into the aggregate of that particular type. In the chemical metaphor, a water molecule must consist of two hydrogen atoms and an oxygen atom. In the case of less rigorously defined concepts, the necessary minimum of an aggregate is less clear cut than the chemical metaphor would suggest. In the canonical example of aggregation, a prototypical body is an aggregate of six components (two arms, two legs, a trunk and a head). A less prototypical body, however, may lack some of these components: one would still call the aggregate a body, if one arm were missing, but one would be less likely to allow for a missing trunk.

The second way of forming a complex module is by putting together similar modules into a generic module by generalisation: “A generalisation is an abstraction which enables a class of individual objects to be thought of generically as a single named object.” [Smith and Smith, 1977, p.107]. All specific kinds of birds, for example, can be grouped under the general term ‘birds’. Accordingly, a ‘generalisation complex module’ focuses on a general concept, whereas the constituent modules it contains represent specific cases.

In the chemical metaphor, this kind of complex module can be considered a cluster. In chemistry, a cluster is a collection of similar atoms or molecules with the same chemical properties as the individual particles, but different physical properties. A cluster does not change in nature when a particular particle is added or removed. Unlike a compound module, a complex module created by generalisation does not have a particular minimum

\(^\text{10}\) Whereas Halasz focuses in [Halasz, 1988] on aggregation as a mechanism to create composites, in [Smith and Smith, 1977] two types of abstractions are defined: aggregation and generalisation.

\(^\text{11}\) In the earlier articles [Harmsz et al., 1996] and [Harmsz and Kircz, 1998], we did not distinguish between these different kinds of complex modules and we used the adjective ‘compound’ (in a non-chemical sense) for all kinds of complex modules.
or maximum set of components. The minimum for a ‘generalisation complex module’ to be useful is to contain at least two constituent modules.

**Definition 3.1.7** A **cluster module** is a complex module that focuses on a single concept which is a generalisation of specific concepts dealt with in the (elementary or complex) constituent modules.

An example of a cluster module is the module with results on reactions with alkali atoms in general that contains constituent modules dealing specifically with results with sodium, potassium and lithium atoms.

Complex modules can be created at different levels. A modular article is a particular type of complex module: it is a a uniquely characterised self-contained representation of an information unit and it is composed of a specified set of related modules. Higher-order complex modules can also be identified, e.g. in a collection of articles. The articles that we have analysed for the development of our modular model are, for instance, aggregated into units corresponding to the different parts of the corpus (see section 5.1.1) and, at a still higher level, aggregated into the corpus that covers the research project as a whole.

### 3.2 Typologies for a modular structure

We have defined a module as a representation of an information unit that concentrates on a single concept, to allow for a presentation of information that meet the readers’ requirement of a focused account of a specific subject. Furthermore, a module has a single unique characterisation, to allow for complete and precise retrieval. Therefore, the questions are 1) how to group the information into units that satisfy a precise information need, and 2) how to characterise the resulting modules. This raises the more fundamental question: What types of concepts are of interest to the intended readership? These questions have to be answered in the context of a particular domain and a particular genre or, in other words, for a particular intended readership. Hence, a domain and genre dependent classification is required for the creation and characterisation of modules.

Readers can consider information from different points of view, such as its subject and its function in the research process. In that case, it is useful to distinguish information units from those different points of view: an information unit of a certain type, which forms a single entity from one point of view, can be further subdivided into units of different types from another point of view. The resulting characterisation of the modules in explicit labels then has to enable readers to locate relevant modules through combined approaches in complex search operations.

Following Bailey’s terminology [Bailey, 1994], a classification is considered a general process of grouping entities by similarity. The term ‘typology’ is used for a special case of classification, namely a multidimensional classification, in which the categories (i.e. the types) are distinguished from a conceptual rather than an empirical perspective. Thus, the general definition of a module has to be complemented with a multidimensional typology of information.\(^\text{12}\)

\(^{12}\)The modules carry a single characterisation (as specified in definition 3.1.1) that is complex: the components of the characterisation reflect the different dimensions of the typology.
To allow for a systematic creation and characterisation of modules, the typology has to satisfy the following conditions.\textsuperscript{13} Firstly, the typology should be exhaustive, in the sense that it allows for the identification and categorisation of all types of information that are relevant to scientific communication in the specified domain and genre. Secondly, the different types of information must be clearly defined and, thirdly, homogeneous, so that all modules of the same type indeed represent similar information. Fourthly, the typology has to be economical, in other words, as simple as possible. And fifthly, the types should be mutually exclusive: the types of modules, and hence the central concepts of the modules, may not overlap. We do not apply this condition so stringently that the modules themselves cannot overlap. Information of the same type can be included in different modules, because that turns out to be necessary for their self-containment.

In order to visualise the complex characterisation of the information following a multidimensional typology, we consider what we call a ‘characterisation space’: a space spanned by the dimensions of the typology. Then, the information is characterised by its location or the region it occupies in the characterisation space. In social science, a similar notion is used: the dimensions of a multidimensional typology are said to form a ‘property space’ [Barton, 1955].

We model our characterisation spaces on Gärdenfors’s idea of a ‘conceptual space’, which we briefly summarise here. In [Gärdenfors, to be published], a framework is introduced for representing information at the conceptual level. Gärdenfors distinguishes three cognitive levels of representation: the most abstract level is the symbolic level, on which the information is represented in terms of symbols that can be manipulated without taking into account their meaning. The least abstract level is the biomechanical level of the subconceptual representation of the information in some configuration of connected neurons. Bridging these two levels is the level of the conceptual representation, in which the concepts are explicitly modelled. As we emphasised in chapter 2, we make a similar distinction between the conceptual and the symbolic level, as we use a conceptual notion of information units and of relations, defining modules and links as representations of these units and relations. Likewise, the characterisation of the information at the conceptual level can be represented in a label assigned to the modules at the symbolic level, in terms of key words, classification codes or other index terms.

In Gärdenfors’s framework of conceptual spaces, concepts are represented in conceptual spaces spanned by ‘quality dimensions’.\textsuperscript{14} The quality dimensions represent aspects or ‘qualities’ of the concept. The canonical example, which is illustrated by figure 3.2, is the representation of the concept ‘apple’ in terms of a conceptual space that is defined by the six main aspects of the apple: its colour, shape, texture, taste, pomological characterisation and nutritional value. The concept apple is then represented by the following values: “green-red-yellow”, “roundish”, “smooth”, “sweet-sour”, “[a particular seed structure]” and “[a particular sugar and vitamin content]”.

There exists a hierarchy in the aspects of a concept: the aspects themselves may in their turn have different subsaspects. For example, the colour of the apple, can in its turn be represented in a three-dimensional ‘colour space’ spanned by the hue, the brilliance and

\textsuperscript{13}These conditions are based on, albeit less stringent than, the conditions mentioned in [Bailey, 1994] for adequate typologies. Notably, our typology does not have to be closed: types and even dimensions can be added, as long as they are consistent with the basic typology.

\textsuperscript{14}Concepts are represented as regions and particular instances as points.
the saturation, as is illustrated in figure 3.2. Its taste can be represented in a ‘taste space’ spanned by the four basic tastes: sweet, sour, salt, bitter. In this way, the concept ‘apple’ is represented in full detail in a nested conceptual space that has far more dimensions than six. The concept can then be characterised by its co-ordinates, such as its precise hue and sweetness.

The conceptual spaces have a structure. For instance, the space of perceived colour can be modelled as a ‘spindle’, in which the dimension of the hue is given by a circle, the dimension of the saturation by a line starting at grey and ranging to full saturation, and the brightness by a line ranging from black to white. The structure of the space, and thereby the representation of concepts, depends on its purpose. The salience of the colour versus the taste for instance, depends on the usage of the apple in a decorative basket or in a fruit salad. Thus, the structure of conceptual spaces allows for a sense of similarity that depends on the purpose of the representation of the concepts.

In the present work, we recognise what we call ‘characterisation spaces’: multidimensional spaces spanned by ‘characterisation dimensions’ representing the characterisation of the various aspects of the information at issue. Such a ‘characterisation space’ is similar, but not exactly equal, to a ‘conceptual space’. The difference is that conceptual spaces are in principle used to represent elementary concepts and we use our characterisation spaces to characterise, from different points of view, information units that focus on a particular concept.

The structure of characterisation spaces also provides a sense of distance and thereby a notion of similarity between information units. The complete characterisation of a particular information unit is given by its location in the characterisation space. In other words, the information unit is represented by a set of n co-ordinates, or an n-dimensional vector, where n is the number of different aspects of the information that are used in the characterisation.\(^{15}\)

\(^{15}\)In the domain of Information Retrieval, n-dimensional vectors are typically used for the characterisation of documents. The multidimensional vector spaces in that domain are spanned by all key
CHAPTER 3. GENERAL DEFINITIONS

Figure 3.3. A complex search operation in a multidimensional characterisation space for a particular type of reaction, particular collision partners and a specified energy range: differential cross section AND iodine atoms AND (sodium atoms OR potassium atoms) AND 7-10 electronvolt.

As in the case of the domains and quality dimensions of conceptual spaces, we allow for a hierarchy in the level of detail. For instance, an information unit about atomic collisions can have a one-dimensional characterisation, which is expressed in an unstructured label, such as the general ‘atomic collisions’, or the specific ‘differential cross sections of chemi-ionisation in sodium atom-iodine atom collisions between 7 and 10 eV’. The information can also be characterised in a five-dimensional space spanned by the measured quantity, the type of reaction that takes place during the collision, the two particles involved and the energy range. In the latter case, the resulting complete characterisation is structured: it consists of five labels that form a particular pattern (measured quantity: ‘differential cross section’; reaction: ‘chemi-ionisation’; projectile: ‘sodium atom’; target: ‘iodine atom’; energy: ‘7-10 eV’). The prominence of each dimension in the complete characterisation can vary, as in the case of the conceptual space. For example, the type of reaction is a more salient characteristic than the energy range.

The representation in a characterisation space provides us with a complex characterisation of the information allowing for complex search operations, as is illustrated in figure 3.3. Information thus characterised can be located by specifying a conjunction of co-ordinates in separate characterisation dimensions (as in a Boolean AND in the symbolic representation), a disjunction of co-ordinate values in the same dimension or in different dimensions (as in a Boolean OR), or a combination of these. Depending on the geometry of the characterisation space, these values may be discrete (e.g. an author name) or continuous (a time interval).

The purpose of the characterisation determines what the characterisation space looks like: how many dimensions it has, which dimensions can be summarised, which are words or by all words in a document, such that n is the size of the vocabulary, which is a very large number [Van Rijsbergen, 1979]. These vector spaces are not designed to aid the intuition of the characterisation of documents, but the calculation in large document bases of e.g. the probability of their relevance. Our characterisation spaces are spanned only by the different types of characterisation, allowing for an intuitive picture of the characterisation.

It can even be characterised in an n-dimensional vector space spanned by all key words to reproduce the standard Information Retrieval characterisation.

When modules with a different characterisation, in different specific characterisation spaces are involved, the dimensions they have in common are taken into account. For this purpose, subspaces can be
3.3. MODULAR MODELS

salient, and what is the resulting sense of how similar particular concepts are. In the context of this study, the purpose of the characterisation is to allow members of a particular target audience to locate, in a collection of publications of a particular domain and genre, the information relevant to their needs at that time. Therefore, the specific characterisation space would be determined by the domain in science and the journal in which the articles are published. In section 4.2, we introduce a general typology for the domain of experimental science, with four main kinds of characterisation, and we briefly sketch the characteristics of these four ‘characterisation dimensions’: 1) a characterisation by the conceptual function of the information, 2) a domain-oriented characterisation, 3) a characterisation by the range of the information, and 4) a characterisation by a specified set of bibliographic data.¹⁸

In order to realise the second component of the modular structure, we require a systematic classification of the links that can be created. The questions now are how to connect the modules in such a way that the reader’s need for coherence is satisfied, and how to label the resulting links between the modules. The underlying problem is to determine what classes of relations are relevant in the context of scientific communication via publications in a specified domain and of a particular genre.

Each relation having only one aspect, the classification of the relevant relations does not have to be multidimensional. The type of a link, however, can determined by the different, complementary relations it expresses. In that case, the full characterisation of the link yields a complex label. In section 4.3, we present a typology for the links by the relations identified as relevant in communication by means of articles in the domain of experimental sciences.

3.3 Modular models

The idea of a modular structure is made concrete in a ‘modular model’: the general definition of a modular structure is complemented with a typology for the modules and a typology for the links. Since the readers’ requirements, and therefore the style of writing, differ for the different disciplines, these typologies depend on domain and genre. The modular model also determines how modules and links can be composed to form an adequate modular structure.

Definition 3.3.1 A modular model is a model for structuring the representation of information in a distributed storage environment in a particular domain and genre. The modular model gives the definitions of the types of 1) modules and 2) links that can constitute a modular structure, and 3) the rules for the composition of a modular structure.

Definition 3.3.2 A modular article is an article with a modular structure, i.e. an article which consists of modules and links between modules that constitute a coherent unit for the purpose of communication.

¹⁸Concrete examples of labels expressing the complex characterisation of particular modules on the subject of experimental molecular dynamics can be found in appendix C of the electronic version of this thesis.
Based on a modular model, rules can be specified for the creation and evaluation of actual modular publications. Thus, a modular model has two functions. The first function is an instructive one of helping an author to organise and present scientific information in a modular publication. The second function is a critical-evaluative one, enabling readers and referees to evaluate a modular presentation of information.

The domain and the genre for which a modular model has been designed constitute its scope. The model we present in chapter 4 has been designed for the domain of experimental sciences and for the genre of the scientific article, in particular the refereed account of original scientific research dealing with a particular topic that is addressed to peers and published in a scientific journal. As the idea of a modular presentation of information is intimately connected to the electronic media, the scope of modular models is in practice restricted to the electronic environment.

As specified in definition 3.3, a modular model consists of different components, including the typologies for the modules and the links. The multidimensional typologies in their turn consist of different components, corresponding to the different points of view from which the modules and links are characterised. The components of the model interact with each other: the definition of the types of links depends on the types of modules that are defined, and the composition of the modules is based on the relations between them. Nevertheless, there is some leeway in the consistent choice of components.¹⁹

A modular model in one domain can serve as a basis for establishing a similar model in an adjacent domain. Certain components of the model can be substituted by other components with a similar function; for instance, a scientific classification can be replaced by another one. It is also possible to obtain a new model by removing components, or adding components that turn out to be relevant for communication in a particular context. For instance, the typology for the modules can be expanded, in order to classify the dangerous substances that are used, labelling them as toxic, radioactive or explosive, and to what degree.

We have developed a general modular model for electronic scientific articles in the domain of experimental sciences, which is presented in chapter 4. Based on this model, we have specified rules for modular articles in the domain of experimental molecular dynamics, as a test case for the application of the model to actual articles. These rules are given in appendix A.

Summarising, a modular model has the following distinguishing characteristics:

1. The purpose of the model is to structure the representation of information in a distributed environment. Rules obtained by specifying the model fulfil two functions: to support the creation and evaluation of modular articles in practice.

2. The scope of the model is a specified subject domain and a specified genre in an electronic environment.

3. The model defines a modular structure that satisfies the following general criteria. These criteria can in practice only be used in conjunction with an interactants profile, such as formulated in section 2.2.2.

¹⁹The choice proves to be consistent if it leads to a modular model which can be used in practice to write articles with a modular structure that satisfies the general definitions.
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- The modular structure consists of modules and links.
- Each module focuses on a single concept.
- Each module represents an information unit identified by the underlying concept.
- Each module is self-contained, i.e., meaningful to at least the most informed members of the intended readership when it is consulted separately.
- Each module and each link is uniquely characterised.
- Links between the modules express the coherence of the information.
- Each complex module consists of strongly related constituent modules and explicit links.
- Each complex module as a whole represents an information unit formed by the synthesis of lower-level information units that are represented in its constituent modules.

4. The model contains typologies for modules and links with categories that are exhaustive, clearly defined, homogeneous, and economical. The types of modules and links are also mutually exclusive, although particular information can be represented in more than one type of module.

The general definition of a modular structure is adequate, in the sense that it can allow for effective and efficient communication, if an adequate modular model can be designed. A modular model is adequate, if it has the distinguishing features listed above and if it yields adequate modular articles, i.e., articles that are consistent with the model (and thereby adequately modular) and that satisfy the interactants’ demands, so that they are adequate as articles.

We assume that an article has to meet the communication criteria given in section 2.4 to satisfy the interactants’ requirements. The practical validity of the modular approach can only be verified in user tests. In this work, we develop and examine a modular structure, on the assumption of the authors’ and readers’ requirements given in section 2.2.2.
Chapter 4

A modular model for experimental sciences

In the previous chapter, the idea of a modular structure has been introduced and defined in abstract terms. To realise this idea, we have developed a modular model for the creation and evaluation of modular electronic articles in the domain of experimental sciences. In this chapter, we first explain how we have developed the modular model, and we then present it in detail. The definitions of the different kinds of modules are given in section 4.2 and the links are addressed in section 4.3.

4.1 Developing a modular model

We have anchored our modular model in scientific practice, by developing it in conjunction with a domain-specific analysis of a corpus of articles on experimental molecular dynamics. We have analysed printed articles and recast the information contained in these linear articles in modular form. This led to the formulation of our modular model for experimental science in general, and the formulation of domain-specific rules for writing modular articles on experimental molecular dynamics in particular. In this section, we describe how we have developed the modular model. First we explain why we have modularised existing articles from a particular corpus. Then we discuss the actual development of the model.

4.1.1 The modularisation of published articles

The modular model is meant for the creation and the evaluation of new modular scientific articles, not for the recreation of published articles. In this work, however, the modular model is used to create modular versions of (or in other words to ‘modularise’) published articles, because we do not aim to write a particular modular article, but to develop and evaluate of a modular model, and modularising linear articles allows for the comparison of a linear version with a modular version of the same article.

We chose to modularise published articles in order to check if our modular model is compatible with scientific practice. The original versions of the published articles can be used as a bench-mark, because their publication in refereed journals supplied them with
a mark of approval.\textsuperscript{1} The established format of present-day scientific articles is, as we mentioned in section 2.1.3, the product of a long evolution, in which it has been adapted to the needs of the scientific community. We have taken that established format as a starting point in the development of the modular model.\textsuperscript{2}

We have at our disposal a corpus of publications on a coherent and complete research project in the field of experimental molecular dynamics. That research has been carried out by prof.dr. J. Los and co-workers at the FOM-Institute for Atomic and Molecular Physics in Amsterdam (AMOLF) between 1968 and 1986. The corpus is described in section 5.1.1 and the bibliography of the publications it comprises is given in appendix B.

The choice of a coherent corpus on a single research project allows for the analysis of not only individual articles, but also of the connections between the different articles. In a coherent corpus, the network of information represented in one article can be explored, as well as its embedding within the larger network of all available information. The restriction to a single research project, conducted at a particular laboratory and during a particular period of time, may limit the validity of our findings. We assume, however, that the research reported in our corpus is typical of its domain.

This particular research project has been selected because of its internationally recognised quality and its variety: experimental, theoretical and numerical aspects of the subject are studied. It has led to publications, which are widely cited, in different international journals, conference proceedings and theses. The publications conform to the standard practice of scientific publication, following the style favoured in the established journals. The fact that the senior author and project leader has been willing and able to assist us with our analysis also played a role in the decision to analyse a corpus on this particular research project.

We have chosen a corpus on the subject of experimental molecular dynamics for the following reasons. Firstly, experimental molecular dynamics, which forms a bridge between physics and chemistry, is a rather prototypical domain in science. It is an established field of ‘normal’, problem-solving science (see section 2.1.2). Secondly, publications in this domain are relatively accessible; no specialised mathematical skills are required for a basic understanding of the subject. Thirdly, whereas on the one hand articles on experimental molecular dynamics are simple enough to allow for a comprehensive analysis, on the other hand, experimental, theoretical and numerical aspects are intertwined in the problem-solution pattern, so that the structure of the research in the domain, and thereby of the articles about it, is complex enough for the analysis to be non-trivial.

So, a corpus has been chosen that is coherent, accessible and typical of publications in scientific practice.

\textsuperscript{1}An artificial article cannot be used as a benchmark, and we could not simultaneously (co-)author linear and modular versions of new “real” articles in the domain of experimental molecular dynamics, because we are not researchers that field. Therefore we have recast existing “real” articles in modular form.

\textsuperscript{2}Of course, a model based solely on a standard, paper-based, format might be restricted to the characteristics of that format. Hence, we have taken into account the requirements for scientific articles in general, as well as the intrinsic new possibilities of the electronic medium, in the development of our modular model.
4.1. DEVELOPING A MODULAR MODEL

4.1.2 Analysis and construction

The modular model for experimental sciences has been based on an iterative empirical analysis of the corpus of publications on a research project in experimental molecular dynamics. We have analysed a set of ten articles, in which an account is given of a coherent part of the research. We have focused on the standard journal articles on original research.\(^3\) From the perspective of physics, we have examined the different types of information that are presented in physics articles and the different types of relations that can be identified in them. The analysis is focused on the information at the conceptual level, abstracted from the actual representation of the information in terms of a language.\(^4\) This implies that neither the choice of the language, nor the formulation is addressed in detail. We investigate how the information can be organised in a new way that allows for effective and efficient communication, given the requirements of the interactants in the process of scientific communication via articles, which have been described in section 2.2.2 and will be further specified for the domain of experimental molecular dynamics in section 5.1.2.

To enrich the analysis from the physics perspective, the point of view of ‘speech act theory’\(^5\) is adopted as well. The speech act analysis is focused on the textual representation of the physics content of articles. The purpose of the empirical analysis from this point of view is to identify the different communicative functions of an article and to reveal the text structures designed to fulfil those functions. We have taken as a starting point the fact that scientific articles have reports aspects and argumentative aspects: they are not only aimed at informing readers, but also at convincing them of standpoints about the research presented in the article, in accordance with the requirements for rational scientific communication by way of articles.

In the iterative process of the development of the modular model, firstly an initial model has been hypothesised as a starting point. The first ingredient of a modular model is the typology that determines what is considered to be a simple concept and thereby determines what information unit is to be represented in a module (satisfying definition 3.1.1). Following standard practice, characterisations of the information by its physics contents and by its bibliographic information were taken into account, although these classification types have not been elaborated in terms of specific classifications. We have also taken into account a characterisation of the information by its role in the problem-solving process. For that characterisation, the starting point was a classification directly reflecting the prototypical sections of scientific articles: Introduction, Methods, Results, Discussion, Conclusions (abbreviated as IMRDC).

Guided by the initial model, we did an exploratory analysis of corpus articles. The analysis pertained to the nature, the completeness and the coherence of the scientific information: we studied the structure of the article, identifying the different types of information contained in them, in terms of information units and relations between them. We also identified those types of information that could contribute to a more effective and efficient communication, but were left implicit or were entirely absent from the articles.

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\(^3\)We have defined the notion of an article as we use it in section 2.1.3

\(^4\)By a language we not only mean natural languages, but also mathematical formulae, figures, tables and other codes for the representation of scientific information.

\(^5\)In chapter 2, we already used insights from the field of speech communication to formulate the requirements of the interactants in scientific communication.
In this manner, we reconstructed the information underlying the article that we assumed to form the complete message to be communicated. Doing so, we played a role similar to that of the actual physicist reading the article.

In the next step, we confronted the initial modular model with the corpus. For that purpose, we used the model to ‘modularise’ the corpus articles we explored. This modularisation did not entail a direct translation of the original ‘linear’ ones. The information underlying each original article has been represented in a different way, by recasting it in an explicit modular structure, as is illustrated in figure 4.1. In order to facilitate comparison between the versions, the modularisation entailed mainly restructuring, but as little as possible actual rewriting of the text. Writing the modular version, we tried to put ourselves in the position of the author, in order to gain insight in the feasibility of a new modular structure and in its advantages and disadvantages for the author as compared with the existing linear structure. Of course, the difference is that a ‘real’ author aims to directly present his own work, and we endeavoured to recast the work of others in our own mould. On the one hand, this confronted us with problems familiar to translators. On the other hand, it is difficult for authors to organise novel work that is not entirely crystallised into its final shape, whereas we could organise the information in hindsight. Those differences had to be taken into account in the evaluation of the modularisation process.

The resulting modular articles and the modularisation process itself were subject of an evaluative analysis, to determine whether all information could be recast in modular form and whether the resulting article was adequate in the light of the communication criteria specified in section 2.4. At the level of the individual article, the original articles
were compared with the modularised versions. We also compared the modules of the same type from different, related articles.\textsuperscript{6}

On the basis of this evaluation, our initial modular model has been adjusted. The adjusted model has in its turn been used to analyse and modularise other corpus articles, further adapting the model to scientific practice. In this process, we tried to keep the modular model itself general. The aspects that are particular to the domain of experimental molecular dynamics were taken into account in the formulation of domain-specific rules. As we stated in section 3.3, domain-specific rules must be specified to allow for the adequate application of a general modular model to the writing and evaluating of actual modular articles. The better the modular structure is tailored to the domain and genre, the better the resulting domain-specific modular articles will satisfy the particular needs of the interactants in that domain.

The final modular model, in which the different types of modules and links are defined, is presented in this chapter.\textsuperscript{7} The final domain-specific rules for the application of these definitions is given in appendix A. In appendix C of the electronic version of this thesis, we give the modularised versions of two standard articles, as well as several connected modules providing the necessary background to the modules that are part of the modularised articles.

4.2 Modules

The general definition of a module (definition 3.1.1) allows for a modular representation of information that satisfies the users' demands. As we discussed in section 3.2, it has to be complemented with a typology for the characterisation of the information and thereby for the grouping of similar information into units. In this section, we introduce the typology included in the modular model for articles on experimental sciences, indicating the various points of view from which the information is characterised in section 4.2.1, before discussing each in greater detail in the subsequent sections.

4.2.1 The typology of the information

In order to develop the modular model, we assume a set of requirements, which have been formulated in the interactants profile discussed in section 2.2.2. According to these requirements, scientific information should be characterised and organised from different points of view that are relevant in the process of scientific communication.

As we mentioned in section 2.1.2, the traditional structure of articles roughly reflects the (idealised) structure of the research process reported in the article as a problem-solving process. We make this structure more explicit in articles, by introducing in the modular model a characterisation of the information by the role it plays in the research at hand, which we call its 'conceptual function'. Characterising information by its conceptual

\textsuperscript{6}This analysis is facilitated by the generous co-operation of the leader of the analysed research program and senior author of the articles, Prof. Los. He gave us direct access to more information than has been represented in the articles, by providing a physical and technical background, and information on the (scientific and other) considerations for the development of the research programme.

\textsuperscript{7}Earlier versions have been reported in [Harmsse et al., 1996], [Van der Tol and Harmsse, 1997] and [Harmsse and Kircz, 1998].
function thus leads to the creation of modules corresponding to the stages in the problem-solving process. For instance, information about the methods used to solve the problem is represented in a module dealing with those methods, whereas information obtained as the outcome of the problem-solving process is grouped into another module. The conceptual function of the information is the leading principle for the distinction of different modules. Hence, the resulting modular structure of an article is based on a problem-solution pattern, which is further refined using the other characterisations of the information.

The second perspective for the characterisation of information in scientific articles is the domain-oriented one: the information is characterised by its scientific content. Traditionally, this characterisation is expressed in index terms, such as key words or classification codes. Characterising and grouping information by its scientific content allows readers to get information on a specific subject.

These complementary characterisations of the information, by its conceptual function and by its scientific content, allow for the identification of the conceptual information units. In order to meet the requirements for effective and efficient scientific communication, the modular model includes two additional points of view from which modules can be distinguished.

We introduce in the modular model a characterisation of the information by its ‘range’, which expresses how widely applicable the information and its representation in a module are. Given the fact that a modular presentation yields a network of linked modules, the representation in a separate module of the information with a wide range, which is applicable to other research situations than the one at hand, facilitates multiple use. For instance, all relevant information about a particular apparatus can thus be grouped into a module and linked to all articles concerning experiments conducted using the same apparatus.

Finally, a specified set of bibliographic data is used to characterise the modules, similarly to the traditional bibliographic characterisation of articles. These bibliographic data include the names of the authors of the module and its publication date; many of these data will apply to all modules in a modular article. The bibliographic characterisation is necessary, to allow readers to locate modules from the bibliographic point of view. It also supports the general communication functions of the article, such as the registration and certification (see section 2.2.2). For instance, the characterisation of each module by its authors’ names not only allows the reader to directly pinpoint all modules written by a particular author, but it also indicates the intellectual ownership of each module.

In order to allow for effective and efficient communication via modular articles, the modular model thus includes a typology for the characterisation, and for the grouping into units, of the information from four different points of view:

1. the ‘conceptual function’ of the information;

2. the scientific content of the information;

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8 Remark that the conceptual function characterises the information by the role it plays in the article at hand. The same information can play a different role in another article. For example, the outcome of an article can be used in a subsequent article in the methods to solve a new problem.

9 Remark that these bibliographic data describe the modules at hand. The term ‘bibliographic data’ does not refer to the list of references of the modules.
3. the ‘range’ of the information;

4. a specified set of bibliographic data associated to the information and its representation.

The characterisation along these four lines will be discussed in detail in the next sections.

The characterisation of the information units following this typology can be represented at the conceptual level in a multidimensional ‘characterisation space’ (see section 3.2). The characterisation is then represented by the location of the information unit in the characterisation space, as is illustrated by figure 4.2, which allows for complex search operations along one or more of the dimensions of the characterisation space.

The characterisation space is the product of four subspaces. The ‘domain-oriented space’ is usually multidimensional, as the domain-oriented characterisation consists of related key words. When the information is characterised by a single key word, this characterisation space is only one-dimensional. The ‘conceptual function space’ and the ‘range space’ are both one-dimensional, i.e. we characterise information using a single term describing its conceptual function and a single term describing its range. The ‘bibliographic data space’ is multidimensional, because the information can be characterised complementarily, e.g. by its author name and its publication date.

In the above, we have stipulated that scientific information is characterised and grouped into units distinguished by its scientific content, its conceptual function and its range. The resulting modules representing these information units are further characterised by specified bibliographic data. This last kind of characterisation is not used to create separate modules.

Apart from the representation of the scientific information that plays a role in the research reported in the modular article, it is also important to provide information about the article. Readers need a clear picture of the structure and contents of the article, that 1) allows them to assess its relevance to their information needs, 2) allows them to locate and retrieve it, and that 3) facilitates reading the article or parts of it. This need is particularly imperative in an electronic environment where readers browsing through an
extended network risk getting ‘lost in hyperspace’, as well as in a modular environment where the readers’ insight into the coherence of articles is threatened by fragmentation.

Hence, in addition to the modules representing scientific information units, the modular model distinguishes a module that represents information about the modular article and its constituent modules: the module m1 Meta-information. The module Meta-information is a support module, which serves as a ‘linchpin’ holding together the other modules of the article. It contains, for example, the author names, the title and an abstract of the article. Its function is to display and clarify the structure of the article and its relations to other publications, and to make explicit and compile the complete bibliographic information. This module with information about the article will be presented in detail in section 4.2.7, after the presentation of the modules representing the scientific information that form the core of the article itself.

4.2.2 The characterisation by the conceptual function

In standard, linear scientific articles, the problem-solving process is expressed roughly in the prototypical section headings Introduction, Methods, Results, Discussion, and Conclusions, abbreviated as IMRDC.\(^\text{10}\) In our modular model we distinguish nine types of modules by the conceptual function of the information, which each reflect a stage of the problem-solving process. They are grouped into five types of complex modules: m2 Positioning, m3 Methods, m4 Results, m5 Interpretation and m6 Outcome. In this section, these modules are discussed in detail.\(^\text{11}\)

The complete set of modules distinguished by means of the conceptual function, complemented with the module Meta-information, form the basic components of a modular article. Figure 4.3 gives an overview of these modules. They are further structured by means of the domain-oriented characterisation and labelled with the bibliographic characterisation. Using the range-based characterisation, similar modules can be created at a higher level to complement the article.

m2 POSITIONING

A problem-solving process starts with the identification of the problem that is to be solved in a specified situation. This amounts to positioning the research in its context. The compound module Positioning consists of two constituent modules: the first stage in the problem-solving process as described in section 2.1.2, determining the situation in

\(^\text{10}\)In [Paice, 1991], the rhetorical structure of scientific articles is studied for the purpose of indexing and abstracting on the basis of indicators. Paice identified the following components: Problem (with the Background and a specification of the Problem), Response (including the approach or hypothesis the methodology, and analytical techniques), and Outcome (Results, Discussion, Conclusions, Practical implications, and Ideas for the future). Note that Paice aims to use the rhetorical structure to improve the retrieval of traditional articles, whereas we propose to make the structure more explicit in new, modular articles.

\(^\text{11}\)The sequence of the identification codes m2 to m6 follows the sequence of consecutive stages of the problem-solving process, which is also the preferred sequence to consult the article as a whole. The identification code m1 has been reserved for the module Meta-information introduced in the previous section. This module is included in the list of main modules, because the information it contains plays an important role in the article, although it does not really play a role in the research process. It is even heading the list, because a sequential consultation of the article as a whole begins with meta-information, such as the title, the author names and the abstract.
Figure 4.3. The module meta-information and the modules distinguished following the conceptual function of the information.
which the problem arises, is represented in the module *Situation* m2a. The second stage is represented in the module *Central problem* m2b.\textsuperscript{12}

In the compound module POSITIONING, the contextualised scientific question addressed in the article is set out. This compound module contains constituent modules *Situation* and *Central problem*.

The situation and the central problem are presented in different modules, to allow for separate consultation of a clearly defined central problem. They are also grouped into the same compound module, to emphasise the strong dependency of the problem on the situation.

**m2a Situation**

In most domains, the research is embedded in a research programme or some other long-term research endeavour. In particular in experimental science, research tends to be organised in projects, because the required experimental set-up is too elaborate and too expensive to allow for isolated experiments. This implies that the readers must be sufficiently aware of that context, if they are to understand the research and accept its reliability and the relevance. In some domains, such as pure mathematics, research is not necessarily explicitly embedded in a context and can stand alone. In that case, an article giving an account of such research can be truly self-contained.

The prototypical *Introduction* section of linear scientific articles contains a sketch of the situation in which the research is conducted. In a given situation, more than one problem may arise, so that the same sketch may be useable in more than one article dealing with its own central problem encountered in that situation. In addition, more informed readers are probably already aware of the situation, whereas readers who are relatively unacquainted with the subject of the article need such an introduction in order to understand the article.

In a modular article, the situation is therefore represented in a separate elementary module *Situation*. This allows for efficient reading, as the module can be consulted by novices and ignored by experts. It also allows for efficient authoring, because the same *Situation* module can be used in more than one article.

The *module SITUATION contains an account of the situation in which the central problem addressed in the article has arisen.*

The description embedding the article in its context can be a comprehensive introduction to the subject at hand, e.g. from a historical point of view, or emphasise possible future applications. If the article contributes to a larger research project, by addressing a problem that is subsidiary to the problem to be solved in the project as a whole, this module includes a report on the status of the project and a description how this article fits into it. This provides an embedding of the article in a specific scientific discipline and more particularly in the research project. The module can also contain explicit argumentation.

\textsuperscript{12}In the first version of the model in [Harmse et al., 1996], this module, then called ‘Goal’, was organised in a constituent module m2a called ‘Problem’ and a constituent module m2b called ‘Embedding’. The present terminology and organisation are closer to the problem-solution pattern. In [Harmse and Kirez, 1998], we used the term ‘Situated problem’ for the compound module, but the term ‘Positioning’ (which has been suggested by Prof. Los) expresses the meaning of the module in a more intuitive way.
on the relevance of the problem in this situation and on the relevance of this research to other domains in science, or even to non-academic applications.

**m2b Central problem**
As a scientific article is supposed to reflect a problem-solving process, the article has to contain an explicit statement of the problem to be solved. In a modular article, the central problem is stated clearly and concisely in the elementary module Central problem, so that the aim of the work can be pinpointed easily.

The module CENTRAL PROBLEM contains a concise description of the central problem addressed in the problem-solving process reported in the article.

In regular research articles, in which the problem and the author’s response to it are clear cut, the problem can be described in terms of a well-defined goal. The central problem can also be formulated as a question that the authors attempt to answer in the article.

More, and different, research can be necessary to solve the same general problem, so that the Central problem module can contain a link to a description of that problem elsewhere. Nevertheless, the precise goals of the individual article are specific to that article and have to be described in this module. Even if the authors repeated some experiment, the Central problem would explicitly state that the article deals with a repetition, and provide a link to a further description of the problem elsewhere.

**m3 METHODS**
In the Methods module, an account is given of the response of the authors to the problem described in the module Central problem: ‘tools’ have been selected or developed, and applied to that problem. The Methods section of linear articles in the domain of experimental sciences predominantly deals with the experimental methods, particularly with the set-up. The Methods module defined in the modular model provides an account of all methods that were used:

The module METHODS contains a description and discussion of the different (experimental, numerical and theoretical) methods used to solve the central problem in the article, including their restrictions.

Authors have at their disposal ‘toolboxes’, which contain the theoretical, experimental and numerical methods and tools available at the time they did the research. Consequently, they can apply existing methods, with or without adaptation, to the situation at hand. The information on these existing methods may have been published elsewhere. In that case, a Methods module can just provide a link to that published module, instead of repeating the description and discussion of the method represented in that existing module.

When a new method that is likely to be used in later research is presented in an article, the information should be represented in such a way that the module can easily be used in subsequent articles, by the same authors or by other authors. For example, a report on an experimental set-up is provided elsewhere, in a module designed for multiple use, and included in the article at hand by link. However, the article-specific measurement parameters are described in the individual article itself.
When more than one method is used in the article, which is generally the case, the Methods module is a complex module consisting of constituent modules focusing on those different methods. The typology by the conceptual function of the information distinguishes between experimental, numerical and theoretical methods. The different methods can be the components of an aggregate ‘complete method’, in which case the complex Methods module is a compound module. In the case that various specific types of methods are used in parallel, the Methods module is a cluster module.

In the Methods module, sufficient information is made available to allow in principle even the least informed members of the target audience to understand, accept and reproduce the methods. That implies that the restrictions of the methods must be included.

m3a Experimental methods

The module EXPERIMENTAL METHODS contains:

- a report on the experimental set-up (general scheme and specific instrumentation) used in this work;
- a report on the measurement procedure for generating experimental data using the set-up;
- a report on the restrictions of the experimental methods, e.g. with respect to the range and precision of the measurements;
- optional argumentation on the reliability and on the relevance of the experimental methods.

The general modular model allows for a further distinction, for specific domains, of this module into a constituent module focusing on the set-up and one focusing on the measurement procedure. In the domains of biochemistry and medicine, for instance, measurements are often carried out following highly standardised protocols, which are explicitly given in journals like Bioorganic & Medicinal Chemistry.

m3b Numerical methods

The module NUMERICAL METHODS contains:

- a report on the tools from the ‘numerical toolbox’ that were used in this work (i.e. the computer hardware and software and the algorithms);
- a report on the parameters and procedures used to generate the data using the numerical tools;
- a report on the restrictions of the numerical methods, e.g. pertaining to the precision and speed;
- optional argumentation on the reliability and on the relevance of the numerical methods.

Numerical methods can be used to do ‘experiments on the computer’, or to approximate other calculations, like integrations, that cannot be executed analytically.
4.2. MODULES

m3c Theoretical methods

The module THEORETICAL METHODS contains:

- a report on the tools (e.g. models and theories) from the standard ‘theoretical toolbox’ used in this work;
- a report on the calculations performed using these theoretical tools to generate theoretical data;
- a report on the restrictions of the theoretical methods, e.g. with respect to higher-order terms;
- optional argumentation on the reliability and on the relevance of the theoretical methods.

In response to the central problem at hand, theoretical methods can be used to provide a qualitative explanation of observed phenomena or to calculate quantitative theoretical results. The ‘theoretical toolbox’ contains the existing theories and models, theoretical assumptions and approximations. We consider data analysis techniques to be part of the theoretical toolbox.

The module Theoretical methods gives an account of the theoretical methods, including their restrictions, which pertain to the assumptions made in the model and the calculations, such as neglecting higher order terms. Apart from a report on the theoretical methods, the choices that were made can be justified in this module, in order to convince the reader of the reliability of the theoretical methods and their applicability in the situation at hand or in other situations.

m4 RESULTS

In our domain, the methods are used to generate results, which are then interpreted. This process is reflected in the prototypical sections IMRDC, in which the Methods are followed by the Results and then by the Discussion of those results. Analogously, we distinguish the modules Methods, Results and Interpretation.

The module RESULTS contains the results (the raw data and the treated results) generated with the different methods described and discussed in the Methods module.

The reason why the modular model strictly separates the presentation of the results from the presentation of their interpretation, is that this separation allows the reader to consult and use the results as such, independently of the author’s original interpretation, and interpret them in his own way.

Nevertheless, it will often be difficult to distinguish a separate Results module. Although the results, and in particular the raw data, are supposed to be ‘objective’ and uninterpreted, they do depend on the context in which they were obtained.\(^\text{13}\) Also, it is often difficult to make a sharp distinction between the raw data and the interpreted results, considering experimental results, they depend in the first place on the experimental methods used to generate them. For instance, for electron affinities different values may be obtained using different methods. Therefore, the methods employed to determine the electron affinities are indicated in the reference tables in e.g. the Handbook of Chemistry and Physics [Lide, 1992, p.10, 180].

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results; there may be a grey area of results in the various stages of interpretation (see also [Buxton and Meadows, 1978] and [Dillon, 1991]). When experimental data are generated in an attempt to test a theory, that theory determines, at least to some extent, how the experiment is set up and executed. The resulting raw data must be analysed, i.e. filtered, synthesised, and otherwise interpreted. For example, in an experiment where a lot of noise is generated, the theory is used to distinguish the “real” events from that noise. In order to be suitable for a clear presentation, the analysed data are then converted into other units, e.g. multiplied with functions or plotted on a logarithmic scale. These various presentation forms also depend on the expectations of the readers and thereby on the context of the discussion.14

The interdependency of experiments, theories and results is inherent to the nature of scientific research. Hence, the results always must be linked explicitly to the method and tools that were used to get them, and they must be presented with their restrictions.

As a rule, the Results module is a complex module. It can be a cluster of modules with similar, more specific results, which are distinguished by means of the domain-oriented characterisation. It can also be a compound module consisting of complementary components: in experimental research, there may be raw data, in addition to treated results that are presented tabularly or graphically. In that case, the Results module contains the constituent modules Raw data and Treated results. Each of these constituent modules may in its turn be a cluster module containing constituent modules distinguished using the domain-oriented characterisation of the information.

m4a Raw data

The module RAW DATA contains:

- the raw data, i.e. the output from the measurements or calculations;
- a report on the restrictions of the data, with respect to the errors and the range;
- optional argumentation on the reliability and on the relevance of the data;
- an optional report on intermediary data.

In order to allow the reader to manipulate the data himself, the raw data should be presented in a manipulable (in practice, machine-readable) format. Intermediary data can

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14 Data analysis plays an important role in experimental sciences. For example, in the textbook ‘Statistical and computational methods in data analysis’ [Brandt, 1970], it is stated: “As for laboratory work, we define an experiment to be a strict following of a prescribed procedure, as a consequence of which a quantity or a set of quantities is obtained which constitute the result. These quantities are continuous (temperature, length, current) or discrete (number of particles, birthday of a person, one of three possible colours) in nature. Now, no matter how accurately all conditions and prescriptions are maintained, the result of repetitions of an experiment will generally differ. This is caused either by the intrinsic statistical nature of the phenomenon under investigation or by the finite accuracy of measurement.”

Another example is Braddock’s textbook on the physics of experimental methods [Braddock, 1963], which also contains a chapter ‘Errors and the treatment of experimental results’, explaining how systematic errors can be taken into account and how random errors can be calculated. Braddock has also included a chapter about ‘The natural limits of measurement’, in which he discusses noise caused by thermal agitation, the particular nature of matter and electricity and the ‘uncertainty’ limitations of quantum mechanics, which limit the accuracy of physical measurements. Not only the accuracy of the results is thus restricted, but also the domain in which they are valid. This domain is also determined by both these natural causes and the limitations of the instrumentation.
be generated in the course of some measurements or calculation. These intermediary data then can be copied or extracted from their original module (Methods or Interpretation) and included in this module.

The restrictions of the data are based on the restrictions of the methods used to generate these data. For example, when the raw data represent the output of a detector for some scattering reaction, the reliability of the data depends on the resolution of the detector. In an error discussion, the accuracy of the data is therefore connected to the precision of the methods. Restrictions can also pertain to the range of the data, resulting from the range of the methods.

In some domains, the raw data are already nowadays published in a database (for a brief discussion, see [Reichhardt, 1999]). Examples are the data on genome [Cameron, 1998], astronomical data [Boyce, 1998] and crystallographic data [Kennard, 1998]. In those fields, the module Raw data could simply contain a link to the appropriate address in the database.

**m4b Treated results**

The module TREATED RESULTS contains:

- a report on the treated results, with respect to the validity and the range;
- a report on the data analysis and presentation techniques used to treat the data;
- a report on the restrictions of the results;
- optional argumentation on the reliability of the results, and on their relevance in the situation at hand and possibly in other situations;
- an optional report on intermediary results.

The treated results can be presented in a format facilitating reader's comprehension, such as in a figure or in a concise table. They can also be presented in a manipulable (in practice, machine-readable) format.

Intermediary results can be generated in the course of some measurements or calculation. If they are to be retrievable as results, they must be characterised as such. That can be achieved by copying them from their original module (Methods or Interpretation) to include them in this module.

This module contains a report on the restrictions of the results in terms of an error discussion pertaining to the range and the precision of the results. These restrictions are based on the restrictions on the raw data (represented in module m4a), and thereby on the restrictions on the methods used to generate the data, as well as on the restrictions on the methods to treat the data. The discussion can include comparison with results obtained in other work.

**m5 INTERPRETATION**

The results are generally interpreted in the light of a theory or model. As we mentioned in the presentation of the Results module, there does not have to be a distinction between results and their interpretation. In practice, domain-specific criteria can be given to determine what information can be represented in the Results module and what in
the Interpretation module.\(^\text{15}\) In appendix A, such criteria are given for the domain of experimental molecular dynamics.

In this domain, the Discussion section in the original article and the corresponding Interpretation module in the modular version will probably always be long and involved. The Interpretation module deals with the explanation of the results in terms of natural phenomena. Different interpretations, both qualitative and quantitative, may be suggested and discussed with respect to their plausibility. The proposed interpretations can also be discussed with respect to their relevance to the problem-solving: does the interpretation help us to solve the problem? By the term ‘interpretation’ both the process of interpreting and its product can be indicated. Indeed, this module contains both the process and the product:

The module INTERPRETATION contains the interpretation of the results:
- a report on the interpretation(s) as a process of interpreting the results;
- a report on the resulting interpretation(s);
- argumentation on the plausibility of the interpretation(s);
- optional argumentation on the relevance of the interpretation(s);

The plausibility of the interpretation, or in other words its reliability, depends firstly on the reliability of the results represented in the module Results (which in its turn depends on the reliability of the methods used to generate them represented in module Methods). Secondly, it depends on the reliability of the theory used for the interpretation. This dependency has to be taken into account in any argumentation on the plausibility of the interpretation. This can involve comparing the results and interpretations to other results and interpretations of the same authors and to results and interpretations obtained in other relevant work.

m6 OUTCOME

At the end of the account of a problem-solving process, a summary is needed of what has been achieved. Therefore, we define an Outcome module reflecting the final stage of the problem-solving process of the research reported in the article. In the prototypical linear article, this stage is addressed in a Conclusions section.

The module is an aggregate of two different components: the findings of the research effort at stake and the formulation of problems that are candidates for further problem-solving research.

The module OUTCOME is a compound module giving an account of the outcome of the problem-solving process, containing a constituent module Findings and a constituent module Leads for further research.

\(^{15}\)In a first version of the model given in [Harmsse et al., 1996], a module Discussion is defined, which included the information now part of the Interpretation, plus the discussion of the reliability of the results. This original module is closer to the Discussion section of linear articles. The discussion of the reliability of the results has now been transferred to the Results module in order to get more systematic definitions of the modules: the discussion of the reliability of an object is part of the same module as the report on that object (see section 4.2.6). In addition, the Interpretation module, which can be very complex as we shall see in chapter 5, has been somewhat streamlined by the transfer of the discussion of the reliability of the results.
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m6a Findings
The authors’ findings constitute their answer to the central question of the article formulated in the module Central problem. These findings are made explicit in this constituent module of the Outcome:

*The module FINDINGS is an elementary module containing*
- the findings that are obtained in this work;
- optional answers to related questions;
- optional argumentation on the reliability and on the relevance of the findings.

In principle, this module gives an account of the completion of the problem-solving process represented in the article. In practice, however, the Findings do not necessarily provide a clear answer to the central question. The conclusion can be that the results are inconclusive and that further research is needed, for example, because the theory did not apply to the situation at hand, or because a better resolution of the data is needed for an unambiguous interpretation. On the other hand, answers may have been found to related questions that are not specified in the module Central problem.

Also, an overall judgement of the reliability and the relevance of the research presented in the article can be briefly given and justified. A more extensive justification takes place in the other modules.

m6b Leads for further research
Regular research generally leads to new problems, whether the problem at hand has been solved or not. Signalling these new problems provides readers with leads for further research. Hence, we define this constituent module of the Outcome:

*The module LEADS FOR FURTHER RESEARCH may contain:*
- a report on new problems related to the subject at hand;
- a reformulation of unsolved problems, with a suggestion how to solve them;

When no satisfactory solution has been found for the central problem of the article, that problem is put up for further investigation. Based on their research, the authors are able to suggest how it could be approached, or at least to warn the reader how it cannot be solved. When the authors have encountered new problems related to the problem at hand, these can also be made explicit in this module.

The most obvious aspect by which information in scientific articles is characterised is from a domain-oriented point of view, by its contents. Using this characterisation complementarily to the characterisation by the conceptual function given in the previous section, we can distinguish, for instance, between different Treated results modules focusing on different reactions.

The domain-oriented characterisation is generally implemented in index terms, such as key words or classification codes. The index terms can be uncontrolled terms invented by the author, or controlled terms that are derived from a classification certified and maintained by some indexing authority. The characterisation space of this aspect of the
SCATTERING:

INSTRUMENTATION Molecular beam techniques [source; selection; interaction; analysis; detection; energy]

SOURCES: sputtering, charge-exchange, ...

[...]

DETECTORS: surface ionisation, ...

[...]

QUANTITIES Cross section [reaction; material; material; energy]

Total cross section [reaction; material; material; energy]

Differential cross section [reaction; material; material; energy]

[...]

MOLECULAR DYNAMICS:

REATIONS charge transfer

ion-pair formation

chemi-ionisation

[...]

MATERIALS:

electro-positive atoms molecules

alkali K, Na, Li

electro-negative halogen: I, Br, Cl I2, Br2, Cl2

O, N, ... O2, N2, NO2...

[...]

Table 4.1

An excerpt of the physics terms we used in the modularised articles. The terms are organised in a hierarchy of general and more specific terms. Terms like ‘cross section’ can have arguments, e.g. specifying particles involved in the collision; the different types of particles are given under the heading ‘materials’

information is spanned by at least one dimension, with a variable corresponding with the elementary scientific concepts. But for an adequate representation, the conceptual space should be spanned by more than one dimension, allowing for a complex domain-oriented characterisation using different key words. The number of dimensions spanning the space is not limited a priori, but dependent on the requirements for an adequate representation.

4.2.3 The domain-oriented characterisation

We do not include in the modular model a detailed characterisation space for the domain-oriented characterisation. The development of a suitable characterisation of information by its subject is the key issue in the field of Information Retrieval.16 With respect to the geometry of a domain-oriented characterisation space, in the area of Information Retrieval, ‘concept maps’ are developed with a geometry and a sensible notion of distance [Salton, 1983]. Therefore, we assume that there will be a suitable domain-oriented typology available to characterise the scientific content of the information. (As an illustration, some of the terms we used are given in table 4.1.)

4.2.4 The characterisation by the range of the information

The characterisation of the information by its ‘range’ indicates in how wide an area the authors suppose the information will play a role, in other words, how widely applicable the information and its representation in a module are.

16A standard overview of the efforts and achievements in Information Retrieval is given in [Salton, 1983]. The Condorret project [Van Bakel et al., 1998], for instance, is a domain-specific Information Retrieval project aiming firstly at the development of structured concept systems (ontologies) which can be used to define indexing terms, and secondly at the development of a method for semi-automatic assignment of such indexing concepts to machine-readable documents or document descriptions.
4.2. **MODULES**

The characterisation of the information by its range is a characterisation of the way in which a concept is used in publications; a concept remains the same regardless of the scope in which it is relevant. Concentrating information with a similar range in the same module can facilitate multiple use and thereby increase the efficiency of the communication process. Furthermore, characterising the information from this point of view informs the reader of the status of the information and its representation in a module.

Generally, the research that an individual article reports on is part of a larger, coherent research endeavour. Key information in such a research project and its representation in a module are applicable to more than one article issuing from that project. Some information units are even more widely applicable and play a role on the level of the field in general. Consequently, we distinguish three ranges following this type of characterisation.

1. **Microscopic** information plays a role in that part of the research which is presented in one article. For example, microscopic information pertains to the precise settings chosen to carry out particular measurements.

2. **Mesoscopic** information plays a role in a research project as a whole, i.e. in a collection of related articles. Authors can use mesoscopic modules to set apart information for multiple use. An example of mesoscopic information is the information about elaborate instrumentation, such as a molecular beam source that is installed and used for a prolonged period.

3. **Macroscopic** information plays a role on the level of the research domain, and therefore is explicitly used outside the project. Basic scattering theory is an example of macroscopic information. A macroscopic module has a status comparable to that of an ‘advanced text book’, as it has a larger, less informed target audience.

These three levels basically coincide with the difference between the genres of the research article, the review papers and the textbook. Microscopic modules are always part of an article. Mesoscopic and macroscopic modules are part of a larger network of information. A microscopic module can include mesoscopic or macroscopic information through a link to the mesoscopic or macroscopic module representing that information.

This characterisation is used complementarily to the characterisations by the scientific content and by the conceptual function of the information. The modular model allows for microscopic, mesoscopic and macroscopic variants of all modules defined in the previous sections. Some types defined by the conceptual function are more likely than others to give rise to modules with different ranges. For instance, methods can often be suitably presented in mesoscopic or even macroscopic Methods modules. Raw data are usually restricted to microscopic modules. Nevertheless, a mesoscopic module Raw data could be used to present the output of particular measurements made with e.g. the Hubble space telescope, the LEP collider at CERN, or in another large-scale experiment.

4.2.5 **The characterisation by a set of specified bibliographic data**

The fourth type of characterisation used in the modular model is a characterisation by a specified set of bibliographic data. The bibliographic data do not actually characterise the information contained within a document, but rather give information about that
document: they are metadata. The function of this type of characterisation, as well as the characterisation by the range, is not to delineate concepts, but to distinguish between different uses of the presentations of the concepts. By the range, a distinction can be made between information that has been presented for inclusion in a single article or in more than one article. By the bibliographic data, a distinction can be made between different articles about the same concepts.

Like the characterisation of the information by its scientific content, this type of characterisation is traditionally used for indexing. Bibliographic data are used to label each module, and in particular the article as a whole, because most of the bibliographic data apply to the article as a whole as well as to all of its constituent modules. The bibliographic characterisation of the article is made explicit in a meta-module m1a Bibliographic information that lists all bibliographic data. This module will be presented in section 4.2.7. We do not address in detail the question as to which types of bibliographic data are most suitable to characterise the modules. We assume that a suitable bibliographic component for the typologies will be available. Examples of existing categories of bibliographic data are given in the bibliographic components of e.g. the highly detailed SGML DTD used by the publisher Elsevier Science [Elsevier, 1999], and the more general resource description record known as the Dublin Core [Dempsey and Weibel, 1996].

In the modular model, a rudimentary bibliographic characterisation takes into account at least the following types of bibliographic data, which are also included in the original corpus articles:

1. Article title;
2. Author names;
3. Affiliations of the authors;
4. Name of the journal the article is published in;
5. Date of publication;
6. A unique identification.

A module can then be characterised by its location in the ‘bibliographic space’. This bibliographic space is at least a product space spanned by dimensions corresponding to a) titles, b) author names, c) affiliations, d) journal names, and e) dates. There can be more than one author, with more than one affiliation, the number of authors determining the number of dimensions. The geometry of the subspaces with journal names, author names and affiliations can be determined in terms of ‘maps’ by scientometrics, which provide a sense of distance between the work of scientists (for example, [Van Raan, 1988]).

The user can search along the axes of the bibliographic space for a conjunction of these bibliographic data. We do not treat the unique identification number that we assign to each module on the same footing as the other types of bibliographic data, because it is redundant to use this type of bibliographic data in a search in conjunction with any other characteristic. Hence, the identification number is not associated with a character dimension in the ‘bibliographic space’.

17 As we stated in section 3.1.3, an article is special case of a complex module.
18 In a modular environment, citation studies can be specified by module. Two authors who use each other’s work in their account of their experimental methods could, for example, be considered to be closer than people who only cite each other’s work in a mesoscopic Situation module.
4.2. MODULES

4.2.6 The internal structure of modules

Although modules are defined as units, they are not monolithic: as we already stated in section 3.1.3, both complex and elementary modules have an internal structure.

Complex modules

Complex modules have an internal structure that is made explicit in the characterisation of the information and in the characterised links between its constituent modules. On the level of the article (which is a special case of a complex module), an abstract is required, to provide the reader with a content-oriented overview of the constituents, as well as a ‘map of contents’, to provide an organisational overview. We treat each complex module similarly: at the level of the complex module, we introduce a ‘module summary’, and we also provide a map of contents, which can be included in or an excerpt from the map of contents of the entire article.

The module summary gives an overview of the contents of a complex module, in particular of the coherence of the information distributed over its constituent modules. Contrary to the abstract, a module summary is only included in a complex module if the reader is unlikely to gain sufficient insight in the content of the complex module without this summary. In that case, a complex module consists of its constituent modules, the links between them and a module summary.

Elementary modules

By definition, an elementary module does not contain explicitly characterised components forming meaningful self-contained modules. Nevertheless, it still can consist of different parts, although these parts cannot be retrieved separately. For the sake of clarity, the internal structure can be made explicit in the presentation of the information within the module. Standard lay-out techniques, such as paragraphs and headings, can be used for that purpose, as well as indicators in the text. The different ways to represent information, such as tables, figures and other non-textual representations, can also be used to make the internal structure explicit.

We determine the internal structure of elementary modules from two points of view from which we do not distinguish separate modules: 1) a secondary conceptual function of some aspects of part of the information represented in a module, and 2) the communicating function of the information.

Nested problem-solution pattern

Firstly, we distinguish the different parts of an elementary module by considering its internal problem-solution pattern. The problem-solution pattern of the presentation of the research in the article can be nested: a more detailed ‘sub-problem-solving process’ can be required to adequately take a certain step of the main problem-solving process represented in the article. The core of this step is formed by the outcome of the sub-problem-solving process. The sub-problem-solving process has to be represented in the article when it is expected that part of the target audience cannot understand or accept its outcome without further elucidation or argumentation. When it is relevant to represent

19The author himself first decides whether a module summary is required; the referees then check if they agree with that decision.
the sub-problem-solving process, our model stipulates that it is represented in the internal structure of the module at hand, rather than in the explicit modular structure of the article representing the problem-solving process as a whole.

The elementary module Treated results can, for instance, contain a graphical or tabular representation of some measurements. It may be necessary to explicitly address the following problem: how to treat the raw data obtained from the measurements and to present the results in an insightful manner? The problem-solving process described in the article as a whole constitutes the context of this problem: the question as to what is an insightful representation depends on the intended uses of the results. The response is to use data analysis and representation techniques that are appropriate in this situation. The graphical or tabular representation thus obtained forms the outcome of this small-scale problem-solving process. That process can be represented in the internal structure of the module Treated results.

Another example is the elementary module Experimental methods about a complicated apparatus. When the description of the apparatus itself is not sufficient, the author gives the module a sub-problem-solution-pattern, by including an account of how the apparatus is constructed and the reasons why it is constructed in this way. The problem in the sub-problem-solving process recounted in that module is how to make the appropriate measurements, and the result is the apparatus itself and the way it is used in actual measurements. The fact that these modules have a problem-solution pattern similar to that of an article, is illustrated by the fact that there are indeed articles published in technical journals devoted to this type of problem.\footnote{An example of such a journal is ‘Measurement Science & Technology’, previously called ‘Journal of Physics E: Scientific Instruments’.

The conceptual function of the information can express the role the information plays within the context of a particular module that plays in its turn another role within the context of the article as a whole. This yields, for example, Results modules with ‘methods aspects’ and Methods modules with ‘results aspects’. Although the secondary conceptual function of the information could be used to identify the internal structure of modules, only the conceptual function at the level of the main problem-solution pattern is used to explicitly label the information and to distinguish the different modules. Otherwise, the information turns out to be fragmented too much, so that the resulting modules do not satisfy the criterion of self-containedness.

The sub-problem-solution-pattern within a module does not necessarily have the same elements as the one at the level of the article. Especially the modular model’s detailed distinction of the outcome of the problem-solving process, in terms of results, interpretations and final findings, does not seem appropriate in all cases. Since we use the sub-problem-solution pattern for implicit structuring of modules only, the global elements of a situation, a problem, a response and an outcome suffice.

Communicative function
Secondly, we determine the internal structure of elementary modules from the point of view of speech act theory (see section 2.2.1). A particular reader considers a module to be successful, if he understands the representation of the information (i.e. if the communicative effect has been achieved) and if he accepts it (i.e. if the intended interactional effect has been achieved). Accordingly, the module can have three communicative functions, of two basic types [Van der Tol and Harmsze, 1997]:
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- The module has to provide the reader with information about the steps in the problem-solving process that is represented in the module. This communicative function always has to be fulfilled.

- The module has to justify the success of the step in the problem-solving process. If the reader is unlikely to be immediately convinced of the success of a particular step in the problem-solving process, the module needs to fulfill two specific communicative functions:
  - to justify the reliability of that particular step;
  - to justify the relevance of that step for the solution of the problem.

Let us consider, as an example, the module *Experimental methods* concerning a molecular beam apparatus. Firstly, the author should inform the reader of the features of the apparatus. For that purpose a - more or less detailed - report is given. Secondly, if the intended readership presumably does not accept the reliability of the apparatus without further argumentation, the author should justify it. To fulfill that communicative function, the author gives arguments supporting the standpoint that the reliability of the apparatus is adequate. In the example of a molecular beam apparatus, this argumentation is concerned with the restrictions, such as the energy range, the precision of the velocity selector and the detector, as well as the purity of the beam. Thirdly, the author should justify the relevance, in other words the applicability of the apparatus to the problem at hand, if it is likely that readers will not accept it without further argumentation.

There is a specific relation between these communicative functions. Convincing the reader of the relevance of a step in the problem-solving process is only possible when the reader is already convinced of its reliability (otherwise it would merely be hypothetical relevance). And argumentation on the reliability is meaningful only if the reader is sufficiently informed about the matter at hand. Therefore, the second communicative function (convincing the reader of the reliability) can be fulfilled only when the first communicative function (informing the reader) has been fulfilled.

In practice, the means to fulfill these communicative functions are often intertwined in the article, in the sense that the same text can be used subsequently as 1) a report on some aspect of the research, 2) argumentation for its reliability and 3) argumentation for its relevance. Hence, the model does not include the communicative function in the typology for the distinction of different modules. Even so, taking into account the different communicative functions allows for a more systematic creation and evaluation of modules leading to a clearer modular structure.\(^{21}\)

All communicative functions can be fulfilled in almost all modules. Exceptions are, firstly, the module *Central problem*, which does not contain argumentation. Any problem-related argumentation is given in the *Situation* module, for the sake of the conciseness of the *Central problem*. Secondly, the *Meta-information* does not contain argumentation for the simple reason that it does not contain scientific discourse. An exception is the *Abstract*, but that is a reflection of the discourse in the ‘scientific part’ article, rather than a new discourse. The other modules contain a report and explicit argumentation on the reliability and relevance of the represented step in the problem-solving process.

\(^{21}\)The communicative function will also be used explicitly to characterise links between modules, when the target module has a particular communicative function with respect to the source module.
provided that not all members of the target audience are expected to be sufficiently aware and convinced of the reliability and relevance of the issue at hand.

4.2.7 The module Meta-information

In the module Meta-information, we group and represent the meta-information about an article and its ‘scientific’ modules, which are defined and characterised as stipulated in the previous sections. Meta-information is not part of the reported scientific problem-solving process itself, but it plays an important supportive role in scientific communication. Therefore this module is linked to all other modules in the article.

m1 META-INFORMATION

The module META-INFORMATION is a compound module providing information about the article in six constituent modules with different types of meta-information.

The modular model distinguishes six different types of meta-information, which together form the complete meta-information. The module Meta-information and its constituent modules do not directly represent scientific information, and consequently they are not characterised using the domain-oriented characterisation.

m1a Bibliographic information

Bibliographic data are used to characterise each module in order to allow readers to locate it. Once readers have found and retrieved a module, or an entire article, they can use bibliographic data to put the module in context. The author names, their institutions, the name of the journal in which the module has been published and the date of that publication all help the reader to judge the relevance of the module to his needs. An informative title plays an important role as an ‘ultra-short abstract’ of the article.

Furthermore, stating the authors’ names in this module indicates their intellectual ownership, and mentioning their affiliations at the time when the research was conducted gives due credit to those institutions. Providing the current addresses of the authors allows readers to contact them. Therefore, this information about the article is grouped and made explicit in full detail in the elementary module Bibliographic information, which in our case is defined as follows:

The elementary module BIBLIOGRAPHIC INFORMATION contains the bibliographic information identifying the article, which consists of at least the following explicit parts:

- The title of the article;
- The names of the authors;
- The name of the journal in which the article is published and its publisher;
- Dates;
- The affiliations of the authors at the time the research was conducted;
- A unique identification of the article.
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The contents of the module Bibliographic information largely coincide with the bibliographic labels associated to each module, which are further discussed in section 4.2.5. The model does not require a one-to-one correspondence between the information specified in this module and the bibliographic labels attached to the modules: firstly this module pertains to the article as a whole. Therefore, it contains the general unique identification of the article as a whole, and not the more specific unique identification of the individual modules. Secondly, this module can contain additional bibliographic information that is not explicitly used in the bibliographic labels to characterise the modules.

**m1b Lists of domain-oriented index terms**

As we stipulated above, the second point of view for the characterisation of the information is a domain-oriented one. From that point of view, modules about specific scientific subjects are distinguished. These are labelled with domain-oriented index terms, so that readers can perform complex search operations and assess the relevance of the module to their needs. This domain-oriented characterisation of the information has been discussed in section 4.2.3.

In order to provide readers with an overview of the subjects addressed in an article, all domain-oriented labels, specified by module, are made explicit in the elementary module Lists of domain-oriented index terms.

*The elementary module LISTS OF DOMAIN-ORIENTED INDEX TERMS lists the domain-oriented characterisation of the modules in the article, by specifying the key words or classification codes characterising each module.*

**m1c Map of contents**

It is crucial to provide readers with an overview of the information that is presented in a modular environment in order to prevent disorientation. In the map of contents, a graphical representation of the entire modular structure of the article, including all modules and the characterised links between them, is made available to the reader.

*The elementary module MAP OF CONTENTS contains an overview of the modular structure of the article, in the form of a ‘road map’ of the whole article.*

From this map, all modules in the article can be accessed directly. Such a road map of the article allows the reader to quickly assess the subject of the components of the article, survey the global coherence of the information, and navigate efficiently within the article.

**m1d Abstract**

Abstracts play an important role in the present day scientific communication. In a modular article, the abstract will even be more important. The abstract, connected to all modules, serves as a linchpin, holding the distributed modules together.

*The elementary module ABSTRACT contains a textual summary of the main issues and lines of the article.*

Like the Map of contents, the Abstract gives an overview of the article as a whole. Each main module can be accessed directly from the abstract, through characterised links.
An adequate Abstract has three functions. Firstly, it allows browsers and searchers to quickly evaluate the relevance of the article to their information needs. This is a selection function. Secondly, it provides readers who are only concerned with the broad outline with sufficient information, which is a substitution function. Thirdly, it assists readers of separate modules, by clarifying the broader coherence of the article. This orientation function is particularly important in a modular environment.\textsuperscript{22}

\textbf{m1e Lists of references}

From the modules in a modular article, various information units can be referred to using explicit links. An individual elementary module can be cited in this manner, as well as an entire article.

In addition to the direct links between the citing module and the cited module, a complete list of references to information units outside the article is provided in the elementary module \textit{Lists of references}. Such a list provides the reader with additional context of the article and the ‘environment’ in which the authors operate: “References are browsed by some readers in order to further their impressions of the article” [Dillon et al., 1989, p.186]). The list also gives the reader an additional opportunity to locate a relevant article and it creates another route for the browsing expert.

\begin{quote}
\textit{The elementary module LISTS OF REFERENCES contains the full bibliography of other works that are referred to in the different modules of the article.}
\end{quote}

The references are provided in two formats. Firstly, all references in the article are listed, with the identification of the modules in which they are cited. Secondly, for each separate module, a separate list is given of the external references, with the link types through which they are connected.

\textbf{m1f Acknowledgements}

\begin{quote}
The elementary module ACKNOWLEDGEMENTS is an optional component of the compound module Meta-information. It contains the names and roles of non-author contributors and sponsors.
\end{quote}

\textsuperscript{22}The functions and components of an abstract of a modular article are discussed in detail in [Van der Tol, 1999].
4.3. **LINKS**

In the module *Acknowledgements*, institutional acknowledgements (e.g. of financial support by funding agencies) can be included, as well as personal acknowledgements of contributions by supervisors, technical staff and colleagues. Acknowledgements are a way of assigning due credit for contributions that do not warrant a full co-authorship. The informed reader can be interested in this information, because it embeds the article in its context [Cronin, 1995]. This module can also be of administrative interest.

4.3 **Links**

In the previous section, we have defined the first component of a modular structure: the modules. Now, we address the second component: the links between the modules. Definition 3.1.2 gives the definition of a link as a uniquely characterised explicit, directed connection between modules (or segments of modules\(^{23}\)) that represents one or more different kinds of relevant relations. In this section, we first explore the structuring of the links. Then we identify relations that are relevant for communication through scientific articles: in section 4.3.2 we define different types of organisational relations, and in section 4.3.3 various types of scientific discourse relations.

4.3.1 **Structuring links**

The hyperlinks that nowadays proliferate on the World Wide Web provide a conduit for easy navigation between hypernodes. However, they do not supply any information about the relation between the nodes. In the modular model, links not only establish a ‘physical’ connection between modules, but they also make explicit different types of relations between the information units represented in the modules.

The idea of characterising links has already been brought up in the early work of e.g. Trigg [Trigg, 1983], who proposed a concrete, fine-grained classification of hyperlinks for ‘normal links’ connecting the nodes of scientific articles and ‘commentary links’ connecting statements about a node to the node itself. His approach is rather phenomenological. In another early work, De Rose has given an abstract taxonomy of a wide range of explicit and implicit types of links, that “differ not only in purpose, but in structure, function and preferred means of implementation” [De Rose, 1989, p.250]. His taxonomy is rather coarse-grained.

In this work, we try to establish a systematic, fine-grained typology for links between the different types of modules defined in the previous, in which the classes of relation we identified the corpus articles are taken into account. An appropriate characterisation of the links enables readers to make a well-considered choice as to whether or not to follow the link, and also enables them to take the links into account in the process of locating and retrieving relevant information. Links are, firstly, characterised by the relations they express. According to the modular model, each link can simultaneously represent one or more different types of relations, and therefore each link can carry a full characterisation including of one or more different labels. Secondly, a link has a particular source and target. Thirdly, each link is also characterised by well-defined meta-information, such as the name of its author and the date it was created. Consequently, both modules and links

\(^{23}\) As mentioned in section 3.1.2, when we speak of a link between modules, we imply that the link can also connect segments of modules, unless explicitly stated differently.
are uniquely characterised ‘information objects’ that can be manipulated using database management and retrieval techniques. This ensures the authenticity and priority of each ‘information object’ when new links or modules are added to published work. In our analysis, we have only considered links created by the authors when they write the article, so that the bibliographic data about the link coincide with the data about the modules they connect. Therefore we have left the characterisation of the links by the meta-information implicit. In the following, we shall consider the sources and targets of links, and their characterisation by the relations they express.

A link is a directed connection leading from a source to a target, where the source and the target can consist of:

- an entire module;
- a segment of a module, such as a phrase, a paragraph, a formula, a table or a figure.

The source and target of a link do not have to be of the same type.

The link types we distinguish are reversible: the links can be followed in the opposite direction by way of the explicit reverse of the link. In the case of symmetric links, the type of the link itself coincides with the type of its reverse. For instance, a link expressing the fact that two connected modules are part of the same article has the same meaning when followed in both directions. Asymmetric link types have the opposite meaning when followed in the opposite direction. An example of an asymmetric link is a link expressing the fact that the source module is a constituent module part of a complex target module; the reverse link then expresses the fact that the target contains the source.\(^\text{24}\)

\(^{24}\)The modular model allows for the assignment of weight to the links. In general, some types of relations can be stronger than others and, within a type of relations, some instances can be stronger than others. Nevertheless, in our practical rules given in appendix A we have endowed the links in the
4.3. LINKS

A single link can represent more than one relation. In figure 4.5, we illustrate this with an example of a source (a particular figure in a microscopic Treated results module) and a target (a particular paragraph in a mesoscopic module Theoretical methods dealing with the techniques for data analysis and treatment) that are connected by means of a link, in which the following relations are expressed. In the first place, the link expresses the fact that in the target of the link an elucidation is given of the source. In the second place, the fact is expressed that the results presented in the figure depend on the methods described in that Theoretical methods module. And in the third place, the link expresses the fact that the mesoscopic module has a wider range than the microscopic module.25

A relation is identified between ‘relata’. Each relatum of such a relation can be:26

- an entity in the ‘universe’ (e.g. a ‘real world’ phenomenon or object, such as a chemical reaction or an apparatus):
  - the entity addressed in an entire module;
  - the entity addressed in a segment of a module;
- a conceptual representation of an entity (i.e. an information unit):
  - an information unit underlying an entire module;
  - an information unit underlying a segment of a module.
- a symbolic representation (in a modular publication) of an information unit:
  - an entire module;
  - a segment of a module.

The relata of a particular relation each are either ‘real world’ entities, conceptual representations, or symbolic representations. One of the relata can be (or be represented in) a module as a whole, whereas the other one is (or represents) only a segment of a module. The relata can also be different types of representation, e.g. a text and a figure.

Now, let us examine how the source and target of a particular link can be associated to the various relata of the relations represented in that link. For simplicity, we concentrate our discussion on one end of the link, namely the source of the link and the corresponding source relata of the particular relations represented in that link. The following situations can arise (an overview is given in figure 4.6).

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25 The various relations are defined in sections 4.3.2 and 4.3.3.

26 These different types of relata correspond to the different levels we distinguished in section 2.1.1: the basic level of the universe itself, and three representation levels: the conceptual level of the information, the symbolic level of, for example, the text and the technical level of e.g. the computer file. We do not identify ‘technical’ relations between signals; this type of relations could be added to the modular model.
Figure 4.6. How can the source of a link correspond to the ‘source relatum’ of a relation represented in that link: a) the source coincides with the relatum, b) the source is part of the relatum, c) the source represents the relatum, d) the source is a part of the representation of the relatum. However, e) the source cannot contain the relatum, and f) the source cannot contain a representation of the relatum either.
a) Both the source of the link and the source relatum are the same module (or the same segment of a module). In that case, the source coincides with a relatum, as is illustrated in figure 4.6a.

For example, as the information represented in a particular microscopic module differs in range from the information in a mesoscopic module, a range-based relation can be identified between the entire modules (as the relata). A link is created between the modules (as a whole) to express this relation. In this case, the source and the target of the link coincide with the relata of the expressed relation.

b) The source of the link is a particular segment of a module and the source relatum is the entire module. In that case the source is a part of the relatum (figure 4.6b).

Consider, for instance, a link created between a particular sentence in one module (source of the link) and a paragraph in another (target) to provide the required elucidation of that source sentence. Suppose that the module containing the source sentence is a microscopic module and the one containing the target paragraph a mesoscopic one. Then the link should also express the range-based relation between those modules. As the source relatum for the range-based relation is the entire module, the source of the link is part of the source relatum of the range-based relation.

c) The source of the link is an entire module (or a segment of a module), and the relatum is 1) the information unit underlying that module (or segment of a module; see figure 4.6c1), or 2) an entity addressed in that module (or segment of a module; see figure 4.6c2). In these cases, the source represents the relatum.

Suppose that the microscopic and mesoscopic module in our example represent respectively results and the experimental methods used to generate them. A link between the two modules expresses the problem-solving dependency relation between the results and the methods as ‘real world’ entities. In that case, the source of the link is a representation of the source relatum of the dependency relation.

d) The source is a particular segment of a module, and the relatum is 1) the information unit underlying that module as a whole (figure 4.6d1), or 2) an entity addressed in that module as a whole (figure 4.6d2). In these cases, the source is a part of a representation of the relatum.

An example of such a case is a link connecting at one end the error bars in a particular figure, and at the other end, the specific paragraph about the restrictions of the experimental results. This link expresses a problem-solving dependency relation between the entire results and the entire experimental methods. Thus the source of the link (the error bars in the particular figure) is a part of the representation of the source relatum (the results).

The source cannot contain the relatum (figure 4.6e) or a representation of the relatum (figure 4.6f), because then the anchor of the link would be underspecified. For instance, a link connecting two modules cannot express a relation between two particular sentences in those modules. If a relation is identified between more specific relata, that relation has to be expressed in a (new) link connecting a more specific source and target.
As we characterise the links from different angles, corresponding to the different relations that can be identified, the typology for the links is multidimensional, like the typology for the modules. Visualising the geometry of such a characterisation space, the relation can be associated with a ‘label’ along the positive axis, the reverse along the negative axis, and the origin would provide a default for ‘neutral’ type of relations, for example expressing the fact that neither one of two connected modules contains the other. A relation can be of only one type, but a link between modules can represent different, complementary relations and thus carry labels that correspond to different, complementary characterisation dimensions. As in the case of the characterisation of the information, a multidimensional characterisation space can be visualised, in which the complete type of a link is determined by its position in the characterisation space, or in other words, by the values of the co-ordinates corresponding to the characterisation dimensions. An example of the characterisation of a link is given in figure 4.7.

We restrict ourselves to links that are made explicit in the article, in particular, the links put in place by authors of modular articles. De Rose calls these links ‘extensional’, as opposed to ‘intensional’ links that only implicitly connect a source to a target, e.g. by invoking a search. A valuable asset of an electronic, modular publishing environment for instance, would be a ‘dictionary’ or ‘encyclopaedia’ with standard definitions, providing a background for less informed readers. The links to such a dictionary do not have to be hardwired in the modules: the reader can extract the term he is unfamiliar with and feed it into a dictionary search engine, by means of an (in De Rose’s terminology intensional vocative) implicit link or an (intensional) retrieval link. The intensional link types can play a role in actual modular articles. These links, however, are not part of the model for the writing of modular articles, because they are reader-driven and are generated on demand. Trigg’s ‘commentary links’ [Trigg, 1983], which are related to De Rose’s annotational links, are not taken into account either, because the model concentrates on articles and not on comments on articles. Taking into account such other categories of links can lead to additional components of the modular model.

Our modular model distinguishes two basic kinds of relations that are represented in links. Firstly, organisational relations refer to the organisation of the article. The relata of an organisational relation are (in all cases but one) entire modules, without reference to their content. A link representing such a relation can express, for example, the fact
that the connected modules are part of the same article. Different kinds of organisational relations are introduced in section 4.3.2. Secondly, links representing scientific discourse relations express how the elements of the scientific discourse in the modules, the information units underlying them, and the entities they refer to are related. Different kinds of these relations are presented in section 4.3.3.\footnote{An earlier version of this typology is introduced in [Harmse and Kürz, 1998].}

4.3.2 Organisational relations

By connecting modules by links that express organisational relations, we make explicit the organisation of the modules in the network of modular publications and, in particular, in the individual modular article.\footnote{Organisational links are also distinguished in the classical paper about hypertext [Conklin, 1987] and in [Baron et al., 1996]. The inclusive links distinguished in [De Rose, 1989] are organisational in nature as well.} This provides readers with basic ‘road signs’ in the modular structure and allows them to easily navigate between the modules. The relata of organisational relations are only entire modules, not segments of modules.\footnote{Except for ‘representational relations’, which will be defined in the following.} Organisational relations deal with modules as complete entities, without reference to their content; this is the same approach as in classical document retrieval by the author’s name, in which documents are manipulated regardless of their content.

The identification of an organisational relation between modules does not always entail the creation of a link. Some types of organisational relations, rather than providing a reason for the creation of a new link, are represented only in links that have been created for the purpose of expressing another type of relation. They increase the complexity of the structure of such a link, by adding functions to it, and they give rise to additional labels in the full characterisation of the link.

We distinguish six subcategories of organisational relations, which are summarised in figure 4.8: hierarchical, proximity-based, range-based, administrative, representational and sequential relations, as well as two particular types of sequential relations.
1. Hierarchical relations

In section 3.1.3, we introduced the composition of modules: elementary modules can be composed into complex modules, which in their turn can be composed into higher-level complex modules. This hierarchy of composed modules entails asymmetric ‘hierarchical relations’: a complex module contains its constituent modules and, vice versa, these components are part of a complex module.

Hierarchical relations can be defined in any model that allows for composites of modules, or generally, composites of units. Conklin [Conklin, 1987] encodes more elaborate hierarchical information, with next-siblings, for example, and first-children, first-grandchildren. We distinguish in the “family tree” only hierarchical relations between ancestors and descendants in general, i.e. constituent modules which are part of the complex modules that contain them. Sibling relations are not expressed in terms of a hierarchy, but in a ‘proximity-based relation’.

2. Proximity-based relations

Given the composition of modules into “families” of modules, two modules can be related as “siblings” or more distant “cousins”. “Sibling modules” are part of the same complex module, and therefore they both are hierarchically related to that complex module. The direct relation between the siblings we call a proximity-based relation. Expressing a, symmetric, ‘proximity-based relation’ gives the reader a clear indication how close the connected modules are, and we assume that modules published in the context of the same article or research project have more in common than modules from different projects, or
4.3. LINKS

even from different domains in science. The crucial question here is whether the connected modules are part of the same collection of modules, in particular the same article. There relations are made explicit only in links that are created for the representation of other relations.

At least two types of proximity-based relations can be distinguished, i.e. two different proximity-based labels can be assigned to links to indicate how close the linked modules are: internal relations are identified between information units that are part of the same article and external relations go beyond the article.

As we mentioned in section 4.2.4, research in the domain of experimental sciences is usually organised in projects that result in the publication of a set of articles. In that case, three types of proximity-based relations can be distinguished. Internal links connect modules in the same article. External links connect a source module and a target module that do not belong to the same article, nor to articles that have been published in the context of the same research project. And the intermediate type of links connects modules that are part of different articles, albeit of the same set of articles on a coherent research project.\(^{30}\) The connection between hierarchical relations and proximity-based relations is illustrated by figure 4.9.

3. Range-based relations

Because of the composition of articles into sets of articles about the same project, we have defined different types of modules by the range of the information, to facilitate multiple use of modules in such a set (see section 4.2.4. As a consequence of this definition, we can identify range-based relations between microscopic, mesoscopic and macroscopic modules. If a microscopic module (which is part of an individual article) is linked to a mesoscopic module (which has a range corresponding to a research project) or a macroscopic module (with an even wider range), that link express an asymmetric 'range-based relation', indicating which module has a wider range.

In this manner, transitions from microscopic to mesoscopic or macroscopic modules, and from mesoscopic to macroscopic modules are marked explicitly.\(^{31}\) Range-based relations are made explicit only in links that are created for the representation of other relations.

\(^{30}\) The modular model allows for a more or a less detailed labelling of links representing the proximity-based relation. For a particular domain, the distinction of internal and external relations may suffice, whereas for another domain more elaborate proximity-based relations could be defined. The proximity-based relation depends on the notion of the distance between modules, which can be provided by the geometry of the characterisation space, in particular the bibliographic component of that space: articles by collaborating or competing research groups, who refer to each other's work, can be considered to be closer than articles by unrelated groups, but not as close as articles issued from the same project.

\(^{31}\) In [Harmsen and Kircz, 1998] this notion of the difference between information with a larger and a narrower range is included in the content-oriented category. In the model in its present form, we have included this notion in the organisational category, because the range of the information leads to a practical distinction of modules, rather than a distinction of different central scientific concepts. Furthermore, the links representing organisational relations connect only complete modules, rather than segments of modules.
4. Administrative relations

The module *Meta-information* is defined as the repository of all metadata of the article, i.e. it provides the reader with information about the article (see section 4.2.7). In order to fulfill its pivotal function in the article, the module *Meta-information* and its constituent modules must be explicitly linked to all other modules in the article. The asymmetric relation between the module representing scientific information and the module providing the meta-information about it is called ‘administrative’.

5. Sequential relations

One of the main characteristics of a modular presentation of information is that it allows readers to choose and consult modules from different publications, in their own preferred sequence. But in order to suit the needs of readers who wish to consult the entire article, a standard ‘sequential route’ has to be set out between its modules. That route is given by means of links expressing asymmetric ‘sequential relations’, which indicate the next module and the previous module along that route.

We specify two types of sequential routes through the article. Figure 4.11 illustrates the difference between the two sequential routes.

5.1 A **complete sequential route** provides a complete tour passing all modules contained in the article.

This route is made explicit in order to meet the demands of readers who want a sequential report of all available information without missing a single module.

5.2 An **essay-type route** follows the traditional line of discourse, by linking (predominantly) the *elementary* modules sequentially.

This route suits the needs of those who wish to follow the line of the article as a whole, without being disturbed by undue overlap. Therefore, this route avoids the ‘module summaries’ of complex modules (unless they are necessary for the reader’s understanding), directly leading to the constituent modules instead. It also avoids modules like the *Raw data* in which information is represented in a way that is computer-manipulable rather than reader-friendly.

The modular model allows for other, specialised sequential routes through an article in particular, or through a collection of modules in general. It may, for example, be useful to specify an ‘module summary route’ linking ‘module summaries’ provided in complex modules. A collection of module summaries could then be used as an extended abstract of the article.
6. Representational relations

The same information can be represented in different formats. In the module Treated results, for instance, results can be represented in a tabular as well as a graphical format. This holds in particular for a presentation of information in a hypermedia environment. The relations between different representations of the same information are asymmetric 'representational relations':

A representational relation is an organisational type of relation, as it deals with the symbolic representation of the information rather than the scientific content itself. Contrary to the other organisational relation types, the relata are not necessarily modules as a whole, but they can also be segments of modules. For example, the relata of a particular representational relation can be a pictorial representation and a textual representation of the same information. A link expressing that relation then carries labels indicating, in one direction, that a pictorial version of the text is given, and, in the other direction, that a textual version of the picture is given.

In our analysis, we focus on the organisation of scientific information, and not on its particular representation. Therefore, we shall not take representational relations into account. Still, the model explicitly allows for them, because the availability of different (audio-visual) means to express information is an important feature of the electronic, multimedia publishing environment.

4.3.3 Scientific discourse relations

Whereas organisational relations are concerned with the organisational structure of the modular article, scientific discourse relations32 deal with the content of the modules. The relata of scientific discourse relations can be entire modules, but usually they are specific segments of modules (e.g. speech acts, figures, tables or formulae). The relata can also be the underlying information units, or the entities that are referred to.

32In [Harmsze and Kircz, 1998], we called the same category 'referential relations'. We have renamed them in order to distinguish our relations from the more general referential links used in [Conklin, 1987]. These relations correspond to the relational links in [De Rose, 1989], that also include annotational links. Our scientific discourse relations correspond to a subtype of these referential links. In De Rose's terminology, they are associative [De Rose, 1989], in Trigg's terms 'normal' [Trigg, 1983] and in the terminology of [Baron et al., 1996] these relations are content-based.
The different types of relations distinguished in this category are summarised in figure 4.12 and specified in the following. In appendix A, rules will be given for the representation of the different types of scientific discourse relations in links.

The modular model takes into account two basic kinds of scientific discourse relations. The first is directly concerned with the communication of the scientific information. These relations are based on the communicative function of one relatum with respect to the other. The second type of discourse relations consists of content relations between the relata.33

I Relations based on the communicative function

Scientific articles are aimed at a successful communication between authors and readers. For successful communication, the article and its constituent modules must fulfil certain communicative functions. In section 4.2.6, we used the communicative function of the representation of scientific information to determine the internal structure of modules. The communicative function can also be used to characterise links between modules.

The two basic aims of the author are to increase the reader’s understanding of the source, or to increase his acceptance of it. In order to understand and accept a module, readers may need additional information, for instance about the causes of a certain phenomenon. The author can make that information available to the readers by means of a link. The target of the link then consists of a representation (such as a statement, a figure or an entire module) which has a particular communicative function with respect to the source, for instance that of an explanation. This asymmetric relation based on the communicative function can be made explicit in the characterisation of the link. The relata of such a relation are representations of information units, which form modules or segments of modules. The different types of relations based on the communicative function are respectively elucidation, in particular clarification and explanation, and argumentation.

In practice, explanatory and argumentative discourse often cannot be easily distinguished.34 Both are concerned with the question “why is that the case”, as opposed to the question “what does that mean”, which requires clarification. The reasoning of an author can serve to increase both the readers’ understanding and their acceptance. Furthermore, scientific articles do not contain many explicit indicators of argumentation, as the preferred style is explanatory rather than argumentative, presenting the information

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33 When relata are speech acts, the term ‘communicative function’ refers to their ‘illocutionary’ level, and the term ‘content’ refers to their ‘propositional’ level [Austin, 1962] [Searle, 1969]. Here we use the terms ‘communicative function’ and ‘content’ not only for speech acts (i.e. for textual entities, such as a phrase or a more complex set of sentences), but also for non-textual relata, such as figures, tables and formulae. For example, a figure can serve as a clarification of the text, and the reader can ‘zoom in’ on a figure to obtain more details. An interesting set of relations between text elements is defined in the Rhetorical Structure Theory, in which the organisation of a text is described in terms of relations between its parts [Mann and Thompson, 1988]. In this set of relations, the distinction between these two levels is not taken into account systematically.

34 The difference between explanatory and argumentative discourse is discussed in [Houtlosser, 1995] and [Snoek Henkemans, 1999]. Explanation is aimed at increasing the reader’s understanding of how a particular state of affairs has come into being. The explained statements (explananda) must refer to a factual state of affairs and the explaining statements (explanantes) must state a cause of this state of affairs. Argumentation is aimed at increasing the reader’s acceptance of a standpoint. Unlike in the case of explanation, there are no restrictions on the propositional content of the statements serving as standpoint and argument.
4.3. **LINKS**

as objectively as possible. The reasoning is especially intertwined when the acceptability of a particular explanation also has to be justified, which usually is the case in scientific articles.\(^{35}\) Nevertheless, the modular model makes a systematic distinction between aiming at an increase in the readers’ understanding and aiming at an increase in their acceptance. This implies that a link aimed at both represents different kinds of relations based on the communicative function. In section 5.4 of the evaluation, we shall see how this distinction works in modularised articles.

I 1 **Elucidation relations**

An author can provide a link to a target for the purpose of increasing the reader’s understanding, i.e. to elucidate a particular representation of information. That link can be characterised by the asymmetric ‘elucidation relation’ between the ‘elucidandum’ (what is to be elucidated) in the source module, and the ‘elucidans’ (that what elucidates) in the target module. For example, in a Results module, the author states that the resonance energy of a particular reaction is \(H_{12} = 4.5 \times 10^{-2}\) eV. This statement may require an elucidation. In particular, it can require an explanation why the resonance energy has that particular value, supposing that the reader understands the statement itself. If that is not the case, the reader demands a clarification of what the author means by ‘resonance energy’, and in particular the formula defining \(H_{12}\).

I 1.1 **Clarification relations**

Suppose that the author anticipates that part of his intended readership will not understand what he means by a particular text or figure in a module. Then the author has to make a further clarification available to the reader, either within the module itself, or through a link to another module, which provides information that should increase the readers understanding. This link represents an asymmetric clarification relation between a “clarificandum” (what is to be clarified) represented in the source module, and a clarificans (what that clarifies) represented in the target module. The modular model allows for the distinction of different types of clarification relations. Van Eemeren and Grootendorst [Van Eemeren and Grootendorst, 1984] distinguish a particular type of speech acts, ‘usage declaratives’, that are aimed at facilitating or increasing the understanding of other speech acts. In the application of the model to the domain of experimental molecular dynamics in appendix A, we shall only use a ‘definition relation’ and a ‘specification relation’ as special cases of a clarification relation.

I 1.2 **Explanation relations**

When the authors anticipate that some of the readers will not understand how a state of affairs has been brought about, they can provide an explanation in which they inform the reader of the factors (such as the causes and circumstances) that determined how that state of affairs came about. The asymmetric ‘explanation relation’ between the explanandum (what is to be explained) and

\(^{35}\) A special case of reasoning is theorem-proving. We do not define this last case in greater detail, because the modular model concentrates on experimental sciences and formal proofs typically are not used in that domain.
Figure 4.12. The different types of scientific discourse relations distinguished in the modular model.
12 Argumentation relations

If the author can presume that not every reader in the intended readership will immediately accept a particular representation of information, it has to be justified. In the example of the value for the resonance energy presented in a Results module, the reader may not be convinced that the statement is reliable and relevant to the solution of the central problem of the article. In that case, arguments have to be put forward in favour of the standpoints that the statement indeed is reliable and relevant. Counterarguments aimed at refuting the standpoints can also be taken into account. The asymmetric ‘argumentation relation’ between the standpoint contained in the source module, and arguments supporting or attacking that standpoint represented in the target module can be made explicit in a link.

In a polemic domain, in which articles contain a lot of explicit argumentation, it is useful to take into account, in the characterisation of the links, whether a module provides arguments supporting the standpoint formulated in the connected module, or counterarguments aimed at refuting it. Therefore, the modular model allows for the explicit distinction of supportive argumentation and counterargumentation.

In the specification of rules for the domain of experimental molecular dynamics in appendix A, however, we shall not make this distinction.\(^{36}\)

II Content relations

In order to allow the presentation of scientific information to fulfil the communicative functions as specified in the above (i.e. to increase the reader’s understanding and acceptance of a particular module or segment of a module) the author can make available another module or segment that is related to it in one or more of the following ways: 1) one relatum depends on the other relatum, 2) one relatum gives an elaboration of the other, 3) one relatum is compared with the other, 4) one relatum is a synthesis of the other, or 5) the relata are causally related.

II 1 Dependency relations in the problem-solving process

As we stated in section 4.2.1, the modular structure has been defined to reflect the problem-solving process of scientific research. In the coherent problem-solving process, the different steps depend on the previous steps: the results, for example, depend on the methods used to generate them. A ‘dependency relation in the problem-solving process’ is an asymmetric relation indicating that the source depends on the target that is associated to a previous stage of the problem-solving

\(^{36}\)Depending on the perspective and the purpose of the classification, argumentation can be classified in different ways [Van Eemeren et al., 1996]. In a scientific context, it may, for instance, be useful to distinguish between rigorous proof and justification. In the justification, the author can argue that his methods were correct and appropriate, by stating the grounds for the choices he made. In the discussion of the internal structure of modules in section 4.2.6, we distinguished different types of argumentation by the type of standpoint, concerning reliability and concerning relevance. The modular model allows for the distinction of subtypes of the argumentation relation reflecting these different types of argumentation, although we shall not do so for the domain of experimental molecular dynamics.
process, or vice versa. The relata of this dependency relation are information units concerning a step in the problem-solving process, or entities.

In principle, the reader of a module representing information concerning a particular stage of the problem-solving process has to be sufficiently aware of the previous stages building up to the stage at hand, and to be sufficiently convinced that they have been completed successfully, in order to understand and accept the information in the module (see section 2.1.2).

II 1.1 Transfer relations
A special case of a dependency relation in the problem-solving process is the transfer relation. Specific items can be needed as input in a particular step of the problem-solving process. Such items are, for instance, numbers or formulae. These items are taken from another module and included in the module at hand. The cited target and source at hand are then connected by a link characterised by the asymmetric ‘transfer relation’, indicating the fact that a particular manipulable item from the target is used as input in the source, or vice versa.

II 2 Elaboration relations
An ‘elaboration relation’ is an asymmetric relation indicating that the target contains an elaboration of the representation of information provided in the source (meaning that it provides a more in-depth or “in-breadth” account of the subject), or vice versa. Its relata are representations, i.e. modules or segments of modules.

The mesoscopic sketch of the situation, for instance, provides both more details and a broader perspective than the microscopic Situation module. When one module provides more details, it does not necessarily provide more context as well. Therefore, we distinguish two subtypes, special cases of elaboration, that can be combined in a single link.

II 2.1 Resolution relations
A ‘resolution relation’ is an asymmetric relation expressing the fact that the target contains more in-depth details than the source, i.e. that it provides a finer-grained account of the subject, or vice versa.

An example of a resolution relation is a relation that is made explicit in a link between the module summary in the complex module Methods and a particular Theoretical methods module. The module Theoretical methods gives more details about the model than the module summary. The reverse link from the Theoretical methods expresses the fact that the information about the model is summarised in the module summary.

II 2.2 Context relations
A ‘context relation’ is an asymmetric relation expressing the fact that the target contains more “in-breadth” background than the source, i.e. that it provides a more broad sweeping account of the subject, or vice versa.

Although a particular module Theoretical methods gives more details about the theoretical model, the module summary in the complex module Methods gives more context and a wider perspective of the situation in which the method is used. Going from the module summary to the Theoretical methods module,
the reader focuses on a more narrowly defined subject, which is expressed in
the characterisation of the link from the module summary to the Theoretical
methods module.

There are two possible combinations of a resolution relation and a context relation.
The first one yields a general elaboration relation, in which one of the relata provides
both more details and more context. The second combination can be seen as a ‘zoom
lens’: zooming in reveals more details on a smaller area, as seen through a tele-lens;
zooming out provides a wide-angle lens that shows a wider area, but fewer details.

II 3 Similarity relations
To fulfil its communicative functions (of elucidating or justifying the content of the
source to the reader), the target can also provide information that is similar in
relevant aspects to the information represented in the source. For example, results
can be compared with the results on a similar system obtained by other authors.
This comparison can be used in an argumentation aimed at the justification of the
reliability of the results presented in the source. If a link expresses a (symmetric)
‘similarity relation’, the relata are similar enough for comparison. The comparison
can entail agreement or disagreement, or remain without unambiguous decision on
the agreement. The relata of a similarity relation are ‘real world’ entities.

II 4 Synthesis relations
In section 3.1.3, we introduced two ways to compose modules into higher-level com-
plex modules by synthesising the central concepts of the constituent modules: by
aggregation and by generalisation. The relation between synthesised concepts and
‘constituent concepts’ not only plays a role between complex modules and their
constituents, but also between other information units of different synthesis levels.

Expressing an asymmetric ‘synthesis relation’ in a link implies making explicit the
fact that the concept underlying the cited information represented in the target is
a synthesis (i.e. an aggregation or generalisation) of various concepts, including
a particular concept underlying the information in the source, or vice versa. The
category of synthesis relations has two subcategories:

II 4.1 Generalisation relation A ‘generalisation relation’ is an asymmetric rela-
tion between specific concepts and their generalisation. A link expressing a
generalisation relation makes explicit the fact that the concept underlying the
cited information (represented in the target) is a generalisation of a particular
concept underlying the information in the source, or vice versa.

Such a relation can, for example, be represented in the link between a micro-
scopic module Experimental methods about a specific molecular beam set-up
and a mesoscopic module representing more general information about that
type of set-up. The reverse of a link representing generalisation represents spe-
cialisation: following the reverse link the reader can navigate from the general
to the specific.

II 4.2 Aggregation relation An ‘aggregation relation’ is an asymmetric relation
between particular concepts and their aggregate. A link expressing an aggre-
gation relation makes explicit the fact that the concept underlying the cited
information in the target is an aggregate including a particular concept underlying the information in the source, or vice versa.

The reverse of a link representing aggregation indicates that the target represents a component of the concept underlying the source. In the example of the link between the microscopic Experimental methods and the mesoscopic module with more general information account, that mesoscopic module can focus on a component of the set-up. Then the link expresses the reverse of aggregation (from a complete set-up to a component of it, i.e. segregation), as well as generalisation (from a particular case to a more general one).  

II 5 Causal relations

In scientific reasoning, causal relations between cause and effect play an important role. However, the definition of what exactly are causal relations is a difficult one and we do not attempt to give it in general. As a rule of thumb, causal relations are concerned with the causes of a phenomenon, rather than with the reasons for choosing a particular course of action. The relata of this asymmetric relation are ‘real world’ entities, in particular, phenomena.

This concludes the presentation of our modular model for experimental sciences that allows for the creation of different types of modules (hierarchically organised in complex modules and constituent modules), and of different types of links connecting modules.

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37 The aggregation relation and the generalisation relation refer to different aspects of the same two complex, central concepts: the generalisation emphasises the fact that both concepts deal with an experimental set-up, one specific and one more general. The aggregation indicates that between the same two central concepts there is a difference in aggregation level: one is complete and the other one a component.
Chapter 5

Evaluation of the modular model

In this chapter, we evaluate the modular model that we presented in the previous chapter, investigating whether it is possible to write modular articles that satisfy the interactants’ requirements. We compare two particular modularised articles, which are given in appendix C of the electronic version, with the original, linear versions. We evaluate the feasibility of modular articles, by discussing the modularisation process, and the adequacy of the resulting modular articles: to what extent do the modular articles meet the communication criteria and thereby fulfil the readers’ requirements, in comparison with the linear articles?

We first introduce the domain-specific application of the modular model. Then we discuss, in section 5.2, the feasibility and the adequacy of modularised articles in general terms, before we specifically address the different types of modules in section 5.3, and the different types of links in section 5.4.

5.1 Applying the model to the domain of experimental molecular dynamics

Our modular model is a general model for the creation and evaluation of modular articles in experimental science. As we described in section 4.1, we have anchored our modular model in current scientific practice by analysing a corpus of printed articles on experimental molecular dynamics. On the basis of the model, we have specified explicit rules for writing modular articles in the domain of experimental molecular dynamics. These domain-specific rules are listed in appendix A. We have applied them to the modularisation of two sample articles from the corpus, which allows us to evaluate the modularised articles in comparison with their original versions.

We first describe the corpus. In section 5.1.2 we outline the domain-specific interactants profile. The two modularised articles are introduced in section 5.1.3.

5.1.1 The corpus of articles on experimental molecular dynamics

The full corpus contains a core of 28 full length articles on original research done at the FOM-Institute for Atomic and Molecular Physics in Amsterdam (AMOLF). It also contains seven articles published in Letter journals for the rapid publication of short
messages, five review articles that summarise the main stages in the research project and nine PhD theses issued from the project, as well as three additional articles and two theses on directly related work carried out by a collaborating group at the same laboratory. These publications have been selected and compiled by the senior author and leader of the research project we analyse. The complete list of all publications included in the corpus is given in appendix B.

The subject of the publications in the corpus can be summarised in hindsight as ‘vibronic coupling at intersections of covalent and ionic states’, in the domain of experimental molecular dynamics. Here, we briefly sketch the physics of the corpus, referring for a more detailed description to some modules created in the analysis of the corpus.

According to the tutorial survey of the field [Levine and Bernstein, 1974, p.1], “the subject of molecular dynamics deals with the study of elementary physical and chemical rate processes. It is concerned with both intramolecular motions and intermolecular motions, which together constitute the underlying ‘microscopic’ basis of all bulk rate phenomena.” Research in this domain addresses the forces acting between atoms or groups of atoms in such reactions, the intramolecular and intermolecular motions of the constituent particles, the energy flow between the different degrees of freedom during the interaction, and the mechanisms of bond-breaking and bond-making. In these mechanisms the interplay between valence electrons and nuclei is crucial. The systems that are studied cover uni-molecular systems, bi-molecular systems, clusters and molecule-surface systems.

The type of process addressed in the corpus1 is a one-electron transition in bi-molecular collisions that constitutes the first step of the chemical reaction

\[ M + XY \rightarrow M^+ + (X...Y)^- \rightarrow MX^+ + Y, \]  

(5.1)

where M is some electropositive atom (in practice an alkali atom, K, Na or Li) colliding with a vibrationally excited electronegative molecule XY\(^{\dagger}\) (a halogen molecule Br\(_2\), I\(_2\) or Cl\(_2\), for example, or O\(_2\) or NO).

This reaction has a relatively large cross section (meaning that the reaction takes place very efficiently), which can be explained by assuming the following reaction dynamics described in the ‘harpoon model’. Herschbach has given a comprehensive overview of this model in [Herschbach, 1966]. The valence electron of the electropositive atom jumps at a relatively large distance to the electronegative molecule. The resulting attractive Coulomb force creates an ionic bond. Since the ion molecule XY\(^{-\dagger}\) is vibrationally excited, it either immediately dissociates, or is easily dissociated by the Coulomb force, so that MX can be formed. The metaphor of the harpoon model is that of the small alkali atom catching a big halogen atom, by throwing its valence electron serving as a harpoon and hauling it in with the Coulomb force.

The focal point of the corpus is the first step of the harpoon reaction: the transfer of the valence electron of the alkali atom to the electronegative molecule. By isolating the charge transfer initiating the harpoon reaction, the ion-pair formation process

\[ M + XY \rightarrow M^+ + (X...Y)^- \]  

(5.2)

can be considered. The term used in the first part of the corpus for this charge transfer process is ‘chemi-ionisation’.

\(1\)The developments in the field of molecular dynamics leading to the research project at AMOLF are described in greater detail in the mesoscopic Situation module MESO-m2a included in Appendix C.
According to the atom-atom model for ion-pair formation in molecular collisions\(^2\) the charge transfer takes place via the crossing of the potential energy curves of the covalent state of the system \(M + XY\) and of the ionic state \(M^+ + XY^-\). At the crossing distance \(R_c\) both states have equal potential energy, so that the system can transform from the one state to the other through an electron jump between \(M\) and \(XY\). The electron can jump at two moments: when the particles arrive at the crossing distance of each other during their first approach and when they are again at that distance \(R_c\) when they move away from each other. The transition probability of the electron is given by the Landau-Zener formula [Herschbach, 1966].

The ion-pair formation is examined in the corpus by means of scattering: by measuring and calculating the total and differential cross sections of these reactions, using a molecular beam set-up. Scattering is well suited as a method for the study of molecular dynamics, and a molecular beam set-up in particular offers a way to specify the input parameters of the chemical reaction very precisely.

Collision physics is a major scientific discipline in its own right. The subject of atomic and molecular scattering deals with the behaviour of ions, atoms and molecules either in binary collisions or in a potential field. Experiments are designed in such a way that the initial and final state of the system are defined as accurately as possible, preferably in terms of a set of quantum numbers. A scattering event is described in terms of cross sections of different kinds: total, differential, double differential. These physical quantities contain all the information about momentum, energy (electronic, vibrational and rotational) and angular momentum transfer. Especially the earlier corpus articles are written in terms of scattering, rather than in the terminology of molecular dynamics.

For an explicit study of the ion-pair formation initiating the harpoon reaction, the relative velocity of the colliding particles has to correspond to a kinetic energy in the electronvolt range. At lower energies only an investigation of the reaction as a whole is possible. At AMOLF, methods and techniques were developed to generate well-defined electronvolt beams of neutral atoms and molecules and to detect the products of the chemical reaction. Later, other groups have studied these reactions using femtosecond lasers instead of scattering experiments.\(^3\)

At first, the aim of the research project at AMOLF was closely related to the molecular beam experiments on harpoon reactions of Herschbach and co-workers, whose experiments had inspired the AMOLF group to consider the initiation of the harpoon reaction. The research had a strong emphasis on scattering. In the course of the project, it evolved into a more general interest in molecular reaction dynamics between atoms and molecules. The main review paper, in which a thorough overview is given of the whole research project, is **Vibronic coupling at intersections of covalent an ionic states** (Kleyn, Los and Gislason, 1982; R4\(^4\)).

In retrospect, three sub-projects can be distinguished in the project. The program was initiated by the measurement of the total cross section in the electronvolt range of ion-pair

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\(^2\)See the *Theoretical methods* module MESO-m3c-mod in Appendix C for a detailed account of that model.

\(^3\)See, for example, [Manz and Wöste, 1993]

\(^4\)We have assigned codes of all publications in the corpus, indicating reviews with R and a number. Articles are referred to with A and thesis with T. The numbers are given in the bibliography provided in Appendix B. The identification codes are used and presented in greater detail in Appendix C. 1.
formation in collisions between halogen molecules and other electronegative molecules on the one hand, and alkali atoms K, Na and Li on the other hand. These measurements were interpreted qualitatively by reducing the atom-molecule problem to an atom-atom problem; for the electron transfer the Landau-Zener approximation is used. It was soon realised that this case was too complicated to be described as a simple binary collision.

The rest of this first part therefore consists of a detailed quantitative experimental study of the electron transfer in atom-atom collisions between a sodium atom Na and an iodine atom I

$$\text{Na} + \text{I} \rightarrow \text{Na}^+ + \text{I}^-,$$  \hspace{1cm} (5.3)

to test the Landau-Zener approximation in the domain in which it is supposed to be valid. In terms of scattering, both the total and the differential cross sections of this process were measured, and it was found that the Landau-Zener approximation for the transition probability indeed provides a very satisfactory explanation of the measurements of the total (Moutinho et al., 1971; A04) and the differential cross section (Delvigne & Los, 1973; A08). Thus, a solid foundation was created, on which further research and descriptions could be based.

The first part of this research project resulted in three Ph.D. theses: (Moutinho, 1971; T2) and (Baede, 1972; T3) with respect to the total cross sections, and (Delvigne, 1973; T4) with respect to the differential cross sections. It has been briefly summarised in (Los, 1976; R2) and more extensively in the conference contribution *Chemical ionisation by dynamic coupling* (Los, 1973; R1). Our analysis concentrates on this first subset of the corpus.

After the satisfactory conclusion of the first part, research proceeded at AMOLF to the much more complicated case of atom-molecule collision. The subject of the second part of the research project published in the corpus is the correlation between the transfer of the electron and the inter- and intramolecular motions of the nuclei in reaction (5.2).

The electron transfer itself can be considered instantaneous, compared to the other velocities involved. However, the time between the two passages of the crossing between the atom M and the molecule XY is long enough for the bond of the XY\(^-\) molecule which is formed at the first crossing to stretch. The influence of vibration on the electron transfer, i.e. the vibronic coupling at intersections of covalent and ionic states, was studied classically in the second part of the research project. In terms of scattering, the relation was studied between total and differential ion-pair cross sections on the one hand and the intramolecular motion of the halogen molecule during the collision on the other hand. This study of the reaction was executed systematically. The total cross section was measured, with variation in the initial energy and the internal energy of the XY molecule, along with the degree of dissociation of the (X...Y\(^-\)) anion. From these data the adiabatic and vertical electron affinity of the electronegative molecule were determined. The differential cross section was also measured.

The second part of the corpus is summarised in a conference progress report: *The dynamics of ion pair forming collisions* (Los, 1978; R3). The Ph.D. theses (Hubers, 1976; T5), (Aten, 1977; T6) and (Kleyn, 1980; T7) issued from this sub-project.

The same phenomena were studied from a theoretical point of view in a collaborating group at AMOLF. Evers worked on numerical studies, based upon the surface hopping trajectory model introduced by Tully [Tully and Preston, 1971], for collisions between alkali atoms and halogen molecules, especially K + Br\(_2\). This collaboration resulted among other things in the joined publications *Energy transfer and differential scattering for ion
5.1. APPLYING THE MODEL TO THE DOMAIN

pair formation in Na, K, Cs + I₂ collisions (Aten, Evers, de Vries and Los, 1977; A19) and Non reactive scattering of K by Br₂ in the energy range of 0-10 eV (Evers, de Vries and Los, 1978; A21).

The third and last part of the project consisted of the quantum mechanical treatment of the same problem of vibronic coupling at intersections. The subject of this part can be summarised as the study of the vibrational wave packets in one-electron transfer collisions. It has been set out in the theses (U.C. Klomp, 1982; T8) and (M.R. Spalburg, 1985; T9), and its outline is given in the conference progress report Non-Franck-Condon behaviour in inelastic atom-molecule collisions (Los and Spalburg, 1984; R5).

5.1.2 A domain-specific interactants profile

The characteristics and wishes that the interactants in the process of scientific communication are assumed to have are modelled in an “interactants profile”. We have introduced in section 2.2.2 a general profile of the interactants in the process of scientific communication via articles, in which we have made explicit their demands for effective and efficient communication. Here, we specify that profile for the domain of experimental molecular dynamics, in particular for the authors and readers of the articles in the corpus, and we formulate the domain-specific requirements.

The majority of the authors of the publications in the corpus were Ph.D. students at the FOM-Institute for Atomic and Molecular Physics in Amsterdam (AMOLF) and their supervisors, in particular the senior author and leader of the research project addressed in the corpus. They studied different aspects of the larger subject of the research project as a whole: the dynamics of ion pair formation, from the angle of molecular scattering. Because they collaborated, they were able to exchange results and share general information that plays a role in each author’s work. Because of the scale of the project, the general subject remained the focal point over a prolonged period of time, so that this general information also remained relevant to various publications.

In our modular model, we assume that the authors wish to take advantage of a common presentation of general information in their subsequent articles, once that has been created, rather than rewrite such a presentation for every single article. In this domain, we find multiple usage of information pertaining to the experimental methods and the theoretical model that is under scrutiny in the research project as a whole, and of a general introduction to the main subject and the background of the research project.

The set-up in a scattering experiment is rather elaborate. It consists typically of several components: a source of the primary beam, selection of the state of the particles in that beam, the interaction of the beam particles with their collision partners, the analysis distinguishing between the different reaction products and the detection of these products. Crucial parts of the set-up are custom-made at the laboratory workshop. Therefore, the experimental set-up takes an important place in the articles. The presentation of either the set-up as a whole, or elements of it are eligible for multiple use in various publications on different sub-projects.

A description of the salient points of the theory of scattering also plays a role in the interpretation of the experimental results in more than one publication. The ‘theoretical toolbox’ that the authors of the corpus-publications had at their disposal contained the harpoon model, the Landau-Zener model and the simplified surface hopping trajectory
model. Every author attempted to apply these theories and models, with or without modification, to a particular problem.

The target audience varied with the journal in which the article was published. The articles in the corpus have been published in the following journals: twenty in Chemical Physics, seven in Physica, which all belong to the first part of the corpus, and one in Journal of Chemical Physics. In these journals the following explicit ‘aim and scope’ are stated, indicating a target audience:

- **Physica**: “A journal specially devoted to theoretical physics, statistical physics, solid state physics, low temperature physics, atomic and molecular physics and ionisation phenomena in gases” (1971)

- **Chemical Physics**: “A journal devoted to experimental and theoretical research involving problems of both chemical and physical nature.” (1973)

And the editorial of the first issue in 1973 states: “[... ] It is felt essential that experimental papers published in this journal bear a relation to theory, and theoretical papers demonstrate their relation to present or future experiments. More specifically, subject matter in the field of spectroscopy and molecular structure, interacting systems, energy relaxation in molecules, fundamental problems in molecular quantum theory and statistical mechanics will constitute the main area of interest for which a good response is solicited [...].”

- **Journal of Chemical Physics**: “[... ] The purpose of The Journal of Chemical Physics is to bridge a gap between journals of physics and journals of chemistry. The artificial boundary between physics and chemistry has now been in actual fact been completely eliminated and a large and active group is engaged in research which is as much the one as the other. It is to this group that the Journal is rendering its principle service and makes its greatest appeal, both as a prompt and efficient medium of publication of research and as a convenient and carefully edited assemblage of pertinent information.” (1960)

The first set of articles was published in a journal that was supposed to cover a large part of physics. The main reason for choosing Physica was that it was considered one of the leading journals for the physics community in The Netherlands. Later articles were published in journals aimed explicitly at a more specialised audience engaged in experimental or theoretical research in chemical physics: the Journal of Chemical Physics and Chemical Physics have the same target audience, but the former is an American journal and the latter European.

In the domain-specific interactants profile, the reader is assumed to be a researcher working in the area of chemical physics. The domain of chemical physics is large enough to allow for a number of specialisms, so that not every member of the target audience is necessarily equally aware of the backgrounds of the subject of a particular publication. So, the target audience includes ‘less informed readers’ and ‘more informed readers’ as defined in section 2.2.2.

In the interactants profile, we assume, as did the authors of the corpus articles, that all readers are aware of the basics of the harpoon model, the Landau-Zener model and

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the simplified surface hopping trajectory model. These were available before the research project started. Nevertheless, the target audience is not assumed to be aware of all relevant details. Therefore, a description of the relevant theories and models, including their restrictions (i.e. their assumptions and approximations), has to be made available to the reader. This also applies to the theory of scattering. The basics are common knowledge, but only the more informed part of the target audience is assumed to be sufficiently aware of the more advanced aspects that are relevant to the subject.

The reader is also assumed to be aware of the general lay out and techniques of a molecular beam scattering experiment. The details of the construction of custom made components, however, are not common knowledge, nor are the specifications of the settings that differ for each experiment. An account of the restrictions of the apparatus (such as its energy range and precision) is also required in the article. The article must contain sufficient information, or refer to sufficient information, for the ‘averagely informed reader’, the prototypical member of the target audience, to perform the same or a similar experiment.6

Although some readers read the article as a whole, others are assumed to be interested in specific issues only. The authors of the corpus articles themselves regularly cite and use specific details from other articles. In particular, they refer to components of the set-up, expressions and parameters for the potential, and the results and interpretations of other measurements of cross sections. Both readers with a theoretical interest and those who are thoroughly familiar with the subject may find the full details of an experimental set-up of less interest. Experimentalists may on the contrary look for a description of the apparatus and a discussion of its applications and restrictions, for example, when they are involved in the construction of the same type of set-up themselves.

The research has an experimental and a theoretical component. Therefore, purely experimental articles, that report on measurements without interpreting them with respect to a theory, are rare. We assume that some readers are most interested in the interpretation of the results, whereas others want to consult the results of an article separately. The cross sections measured in a scattering experiment can for instance be used by the reader without the subsequent interpretation in terms of molecular dynamics. Parameters of a system, such as the potential parameters, are also useful as separate results. Firstly, the reader may wish to evaluate them directly, in which case the results must be represented in a comprehensive way, typically graphically for large amounts and tabular for small amounts of data. Secondly, he may wish to use them as input in his own research, to interpret the data using a different, updated theory or to compare them to his own results.

For the reader, it is important to know what methods have been used to generate the results. In order to enable the reader to understand how reliable the results are and to use them correctly, their error margins also have to be available; these error margins are related to the restrictions of the methods.

We assume that the reader wants to be able to locate information in a directed or semi-directed search, firstly by searching for the author names, journal names, periods in time, the group in which the author worked, or some unique identification for direct retrieval. Secondly, the reader also searches for physics terms. We assume that in this domain the reaction that is studied, the experimental method, including the sample and the energy range, and the theoretical model must be available for searching.

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6The experimental set-up for the molecular dynamics described in the corpus can be reconstructed and used in another laboratory, unlike, for example, the set-up for modern high energy physics.
5.1.3 Introduction to the examples

Applying our modular model for experimental sciences described in chapter 4 to the domain of experimental molecular dynamics, we have formulated domain-specific rules for writing and evaluating modular articles, which are given in appendix A. Following these rules, we have composed the modular versions of the two articles that are presented in appendix C. We assume that an appropriate hypermedia implementation of modular articles will be available to ‘real’ readers.\(^7\)

The first of these articles, (Delvigne and Los, 1972), is titled The differential cross section for chemi-ionization in alkali atom-halogen molecule collisions. Classical interpretation. In the bibliography of the corpus given in appendix B, it denoted as A05. The second article, (Delvigne and Los, 1973), is denoted as A08 and titled Rainbow, Stueckelberg oscillations and rotational coupling on the differential cross section of Na + I → Na\(^+\) + I\(^-\). The ‘tables of contents’ of the sections in the original articles and of the modules in the modularised versions are given in Table 5.1a.

These two articles are strongly related. The general problem addressed in the first part of the research project, and in particular in these articles, was the measurement of the cross sections of ion pair formation in molecular collisions and the explanation of the reaction as the first step of a harpoon reaction, using an atom-atom model. Previous to the publication of A05, sufficient insight was gained to conclude that the general explanation was viable and that is was possible to proceed with a more specific analysis. In A05, the authors reported that the experiment and the theory were in qualitative agreement for the differential cross section in reactions between sodium atoms and iodine molecules. This warranted an in-depth study of the reaction between sodium atoms and iodine atoms, which is reported in A08. In the latter case the theoretical model was more applicable than in the case of molecules, but the experiment was far more complicated, owing to the difficulties in creating a stable atomic iodine beam. The article A08 can therefore be seen as the follow-up of A05.

5.2 The feasibility and adequacy of modular articles

We discuss the modularised articles in the light of the interactants’ needs described in general in section 2.2.2 and specified for this domain in section 5.1.2. We compare the modular versions with the original versions, first from the author’s perspective and then from the reader’s perspective. In sections 5.3 and 5.4, the feasibility and adequacy of modular articles are discussed in detail for the various types of modules and links. In this section, we address them in general, for the entire article.

5.2.1 The feasibility of modular articles

Concentrating on a demand that is particular to the author, the modular article has to be feasible, we examine whether it is possible and practical to write modular articles. Since we have not written new modular articles, but recreated modular articles from linear ones, we evaluate the modularisation process, rather than the actual writing process. Therefore,

\(^7\)In the hypertext version of the appendix, the modularised articles are realised rudimentarily using the (insufficient) hypertext tools we have at our disposal, and in the printable version we provide them as a simulation of hypertext on paper.
<table>
<thead>
<tr>
<th>a) Sections of the original version</th>
<th>b) Modules of the modified version</th>
</tr>
</thead>
<tbody>
<tr>
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<td><strong>A05:</strong></td>
</tr>
<tr>
<td>1. Introduction</td>
<td>A05-m2 Positioning</td>
</tr>
<tr>
<td>2. Experimental</td>
<td>A05-m2a Situation</td>
</tr>
<tr>
<td>3. Results</td>
<td>A05-m2b Central prob</td>
</tr>
<tr>
<td>4. Discussion</td>
<td>A05-m3 Methods</td>
</tr>
<tr>
<td>4.1 $\Delta E$ determination</td>
<td>A05-m3a Experimental</td>
</tr>
<tr>
<td>4.2 $\alpha_{Br_2}$ determination</td>
<td>A05-m3c Theoretical</td>
</tr>
<tr>
<td>4.3 $R_c$ determination</td>
<td>A05-m4 Results</td>
</tr>
<tr>
<td>4.4 $\epsilon$ determination</td>
<td>A05-m4a Raw data (A05-m4aii)</td>
</tr>
<tr>
<td>4.5 $\rho$ determination</td>
<td>A05-m4b Treated results</td>
</tr>
<tr>
<td>4.6 $H_{12}$ determination</td>
<td>A05-m4bi Experimental</td>
</tr>
<tr>
<td>5. An appendix</td>
<td>A05-m4bii Theoretical</td>
</tr>
<tr>
<td></td>
<td>A05-m5 Interpretation</td>
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<td></td>
<td>A05-m5ai Classical</td>
</tr>
<tr>
<td></td>
<td>A05-m5a Quantum</td>
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<tr>
<td></td>
<td>A05-m5b Quantitative</td>
</tr>
<tr>
<td></td>
<td>A05-m5b Potential</td>
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<td></td>
<td>A05-m5bii Different</td>
</tr>
<tr>
<td></td>
<td>A05-m6 Outcome</td>
</tr>
<tr>
<td></td>
<td>A05-m6a Findings</td>
</tr>
<tr>
<td></td>
<td>A05-m6b Leads for further analysis</td>
</tr>
<tr>
<td><strong>A08:</strong></td>
<td><strong>A08:</strong></td>
</tr>
<tr>
<td>1. Introduction</td>
<td>A08-m2 Positioning</td>
</tr>
<tr>
<td>2. Experimental</td>
<td>A08-m2a Situation</td>
</tr>
<tr>
<td>2.1 Sodium beam</td>
<td>A08-m2b Central prob</td>
</tr>
<tr>
<td>2.2 Iodine beam</td>
<td>A08-m3 Methods</td>
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<tr>
<td>2.3 Detector</td>
<td>A08-m3a Experimental</td>
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<tr>
<td>2.4 Detection technique</td>
<td>A08-m3c Theoretical</td>
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<tr>
<td>3. Potential curves</td>
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<tr>
<td>4. Calculations</td>
<td>A08-m3ci2 Rotation</td>
</tr>
<tr>
<td>5. Measurements</td>
<td>A08-m3ciii Different</td>
</tr>
<tr>
<td>6. Comparison of the measurements</td>
<td>A08-m4 Results</td>
</tr>
</tbody>
</table>
the difficulties that we encountered are not necessarily inherent to the modular model, as they may be due to translation problems, or even to flaws in the original article.

For a modular article to be feasible, writing it has to be straightforward: it should be clear to the author how the information has to be organised. We discuss whether it was easy to identify in the original article the different types of information to be represented in the different modules. When this identification is easy, it will probably also be easy for an author to identify these types of information directly in the research process, and to group similar types of information in modules. In particular, we investigate to what extent the representation of the information could simply be copied from the sections in the original versions to the corresponding modules in the modular versions. Moreover, we discuss whether the relations that are to be expressed in hyperlinks could easily be identified.

For a modular article to be feasible, writing it should also be efficient: the author should not be forced to write more than is necessary for meeting the readers requirements. We examine this efficiency in a discussion on the size of the modular versions of the articles, as compared with the size of the original versions.

**Difficulty: from sections to modules**

Following the definitions of the modules given in section 4.2.1 and their specification in the guidelines given in appendix A, the information presented in the original, linear articles A05 and A08 has been recast in two modular articles (which consist of microscopic modules and links) and in a separate set of mesoscopic modules. The mesoscopic modules represent information that is used, and partly presented, in both articles. As an illustration, we have also provided two macroscopic *Theoretical methods* modules. The macroscopic modules are supposed to be parts of monographs or tutorials. One of them is based on a section of O’Malley’s book [O’Malley, 1971], rephrased to form a self-contained module.

At the microscopic and mesoscopic level, we have distinguished modules firstly by their conceptual function. As we saw in section 4.2.2, the definitions of such modules are based on the prototypical sections in scientific articles. As we see in table 5.1a, the original version of A05 indeed has a rather prototypical structure, which facilitates the comparison of the new modules with the original sections. The original version of A08 is less prototypical. It has more sections, as A08 is a long article of thirty pages. The theoretical component of the article is emphasised by the inclusion of the sections 3.*Potential curves* and 4.*Calculations*. However, these different sections still form an overall IMRDC structure. The collection of the sections 2.*Experimental*, 3.*Potential curves* and the first half of 4.*Calculations* could be grouped under the heading *Methods*, the collection of the second half of the section 4.*Calculations* and the 5.*Measurements* could be seen as *Results*, and the sections 6.*Comparison of the measurements and the calculations*, 7.*Discussion* and 8.*Rotational coupling* could be grouped under a higher-level heading *Discussion*.

To distinguish constituent modules within the modules created by means of the conceptual function, we have used a rudimentary physics classification sketched in table 4.1. This simple typology takes into account the INSPEC index terms associated to the original articles. The difference with the original terms is that we do not only use simple

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\[8\] Please note that this does not imply that all information in these sections is recast in the corresponding module.
5.2. THE FEASIBILITY AND ADEQUACY OF MODULAR ARTICLES

index terms, such as ‘rotational coupling’, but also complex ones, e.g. ‘differential cross section[chemi-ionisation; Na, I; 13-85 eV]’. We have used simple bibliographic data to characterise the modules thus created. The original articles are uniquely identified by the name of the journal, the volume and the page numbers of the published article. In the modularised versions of corpus articles we have characterised each module by the family names of the authors, the name of the institute, the name of the journal in which the article was originally published and the year of its original publication. We have also employed the corpus-specific unique identification code described in Appendix C.1.

The original versions of the articles are connected to other work by means of references, and occasionally different parts are connected by an internal reference, explicitly (e.g. “see appendix” in the section 3. Results of A05, p.67), or more implicitly (e.g. “[...] as will be derived later on in this paper” in the 1. Introduction of A05, p.62). In the modularisation process, we created characterised hyperlinks between modules and parts of modules, to express one or more different types of relations between those modules or parts of module, between information units underlying them, or between entities addressed in them. The different types of relations are defined in section 4.3, and in appendix A.3 guidelines are given for making these relations explicit in links.

In the modularisation process, the core of the various modules could easily be established. In many cases, information of a particular type was concentrated in a single section of the original article, so that a large part of that a section could be transferred directly to the corresponding main module. Other types of information were distributed over various sections, albeit in such a way that they could nevertheless be easily identified and coherently represented in a module, either by directly copying sentences or paragraphs, or after straightforward rephrasing. In A05, the sections 1. Introduction and 3. Results in particular contain a lot of information that did not fit in the corresponding modules Positioning and Results but that could easily be recast in other, more appropriate modules. In A08, the section 4. Calculations contains various kinds of information: information on the calculation methods, which we have recast in the module Theoretical methods, as well as a presentation and a discussion of the results of the calculations, which have been recast in respectively the Results and the Interpretation.9 In section 5.3, we shall compare the different modules and sections in greater detail.

Mesoscopic information concerning the situation, the central problem, the experimental methods and the theoretical methods could easily be identified. These are the types of information that, according to the domain-specific interactants profile we described in section 5.1.2, have to be represented in a form suitable for multiple usage. The contents of the mesoscopic modules could not solely be derived from the two original articles. In order to make the modules complete, as self-contained units that can be consulted by less informed readers, we derived information from other publications in the corpus (mainly review articles) as well. We also obtained information from the senior author of the research project in private communications.

9 In the modularised version of A05 in the electronic version of Appendix C, we have indicated typographically which parts of the modularised article have a one-to-one correspondence with parts of the original version, which parts correspond to rephrased parts of the original article and which parts have been added by us, as well as what information is represented in more than one module. We have suppressed these typographical indications in the modularised version of A08 in order to improve the readability.
Difficulties were caused by the borderlines between most modules. Creating the modular versions, we encountered the following kinds of problems.

Firstly, some information was inherently difficult to characterise unambiguously: it bore the characteristics of more than one type of information. In some cases, this problem could be solved by taking into account the internal structure of the modules, as described in section 4.2.6. For example, at the level of the entire article, we characterised the information about the way experimental results were presented in a figure as ‘results’. At the lower level of the Results module, we considered this particular information to play the role of a method in a sub-problem-solving process aimed at the final treated results. In the other cases when information could, from different perspectives, be considered to play different roles, we have presented it in more than one module in order to allow the reader to locate it using different labels. So, difficulties in the characterisation of information led to overlap between modules. Deciding on the exact type of particular information will always be difficult in some cases. However, it will be less difficult for the author of a new modular article, who has a thorough understanding of the information, than for the outsider who tries to modularise an existing article.

Secondly, even when the characterisation of the different ‘strands’ was unambiguous, some information of different types was interwoven so closely, that it was difficult to disentangle it. For example, the presentation of the results in the original version was intertwined with that of their (qualitative) interpretation. In practice, this intertwining led to some overlap between modules: the principle figures with the results were included in both the Results module and the Interpretation module. In the conversion of existing linear articles, this problem is unavoidable, as in the linear version the information has been interwoven intentionally, to form a single narrative. Directly writing a modular article will reduce the problem, although it probably cannot be avoided entirely when different types of information are strongly interdependent.

Thirdly, in order to obtain a complete module, it was necessary in some cases to add information to the information provided in the original version. This is merely a conversion problem. The author of a new modular article can follow the guidelines and directly include all required information.

With respect to the links between the modules, it was easy to identify and express the organisational relations. However, in many cases it was difficult to determine which scientific discourse relations have to be made explicit in links. In section 5.4 we shall discuss the different types of relations in detail.

Present-day authors are accustomed to writing experimental research articles with an ‘IMRDC’ structure. If an author is supposed to write an article with an entirely different structure, he will not find it feasible, as long as he has not become used to the new structure. This is one of the reasons why we have taken the prototypical section structure as a starting point in the development of the model; the basic structure of the modular article resembles the structure of the linear article. This similarity of the modular and the linear article is demonstrated by the fact that large parts of the modular articles could be copied from the original version, though the sequence of the paragraphs and sentences does not necessarily remain the same.

The modular structure is more fine-grained than the structure of the linear article. Therefore, the author of a modular article has to make more decisions concerning the
5.2. **THE FEASIBILITY AND ADEQUACY OF MODULAR ARTICLES**

Correct placement of the information, which could make it more difficult. However, the modular structure is more systematic and thereby provides the author with stronger guidance. Moreover, we have specified more elaborate guidelines for the author than is usual in traditional journals, which can be implemented in software assisting the author. The other side of the coin is that the modular structure is more rigid, which may frustrate authors who wish to elaborate in more essayistic prose.

We have found that the modular version differs distinctly from the original versions, so that articles written in linear form cannot easily be converted automatically into a linear form. As we have also found that it was difficult to reconstruct the information underlying an article written by someone else, we conclude that writing a modular article can be done most efficiently and effectively by the author himself, provided he has adequate tools at his disposal.

**Workload: the size of the article**

We examine the efficiency of writing modular articles, by comparing the size of the modular versions of A05 and A08 to the original versions. Table 5.2 gives an indication of the absolute and the relative size of the main sections in the original version and of the main modules in the modular version. The complete modular versions of the articles turn out to be longer than the original versions: the modular version of A05 is 113% of the original version and the modular version of A08 is 133%. If we restrict ourselves to the elementary modules, the modular versions are about as long as the original articles: the text in the modular version of A05 is about 100% and A08 108% of that in the original version. With respect to the size of the article, the definition of the modular structure has two opposing consequences: the modularised version can be smaller as well as longer than the original one.

On the one hand, information with a wider range can be represented in mesoscopic or macroscopic modules designed for multiple use and made available by means of links to the reader of a particular modular article. Consequently, the Positioning module in A05 is far smaller than the original section 1. Introduction, which includes a description of the model that in the modular version is given in a mesoscopic Theoretical methods module MESO-m3c-mod. This makes the efficiency of the process of writing the modular article higher than that of writing linear article.

On the other hand, the modularised article can be longer than the original version. In some modules, we had to provide additional information in order to make all required details available and to make the modules self-contained. These modules tend to be longer than the corresponding sections. Both in A05 and in A08, the modules Interpretation and Outcome are far longer than their counterparts in the original version. However, in cases where the same information had to be presented in more than one module for the sake of self-containedness, the workload was increased only when the different modules could not

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10 See for example the discussion of the module *Theoretical methods* in section 5.3.3

11 We aim to get qualitative idea of the size of the different versions, rather than a full statistical analysis. As an indication of the size, we count the number of words of the text in the sections and in the modules. We take into account neither graphical representations, which in particular form a large part of the results modules, nor the meta-information. We do take into account the text associated to the links, because the links are an integral part of the modular version and their creation is part of the author’s task.
## CHAPTER 5. EVALUATION OF THE MODULAR MODEL

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### c) Relative size

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### A08

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<td>7. Discussion</td>
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</table>

### Table 5.2

An indication of the sizes of the sections in the original versions and the modules in the modular versions of A05 and A08. a) For the main sections in the original versions, as well as for the complete collections of the sections (i.e., the entire articles excluding the meta-information), the absolute size is given in terms of the number of words. The relative size of the sections is given as the percentage of the total number of words in the complete set. In b) the absolute size and the relative size of the main modules, including the module summaries, are given, as well as the sizes of the complete set of all (complex) modules and of the subset of all elementary modules are given as well. In c) the relative size of the modules, compared with the corresponding sections, is given as the percentage of the number of words in the sections. In A08, the first 965 words of section 4, Calculations are considered part of the Methods, and the second 701 as part of the Results. In A05, the appendix corresponds to part of the Interpretation module, as does the first part of the section Discussion. The last 228 words in that section correspond to the module Outcome.
contain literal copies. In the two constituent modules of A05-m4bi, for example, a large part of the text about the experimental results could be recycled.

We have added ten module summaries in the complex modules in A05, and twelve in A08, in order to express the coherence of the information that is distributed over the different constituent modules. The module summaries could not be copied directly from the original version; the linear article generally contains only summaries of the complete text, in its abstract and in the Conclusions section. However, not all module summaries were difficult to write; for example, that of the complex modules Outcome are basically tables of contents of the constituent modules. In addition, writing these module summaries can form an intermediate step in the composition of an adequate abstract of the entire article, which the author should provide at any rate (see [Van der Tol, 1999]).

Creating a modular article, authors not only have to write the text and provide non-textual representations of scientific information in larger amounts than in a linear article. They also must make the structure explicit, more than in the case of a linear article: they must compose cohering elementary modules into different levels of complex modules, to make different types of relations explicit in links between modules and parts of modules, and to visualise the structure of the article in a map of contents.

In the modularisation process, all references in the original versions of the articles were recast in links in the modular versions. The linking in a modular structure is far more elaborate than the standard referencing in the original versions. Whereas the original version of A08 contains 34 references to 26 works, the modular version contains 386 explicit links between (parts of) 29 source modules and 58 targets, representing a total of 940 relations, characterised by 43 different types of labels. The main reason why there are so many links in the modular article is that the internal structure is made explicit systematically: about four fifths of the links express the internal coherence of the modularised articles. In addition, in the modularisation process we have isolated information in mesoscopic and macroscopic modules, which then had to be linked to the modules of the article.

We have found that the task of expressing by hand the structure in links, in the composition of modules and in navigation aids (such as the Map of contents) would increase the author’s workload to an unacceptable degree. However, in practice a large part of this additional task lends itself to automated procedures and tools. We shall discuss the requirements for such appropriate authoring tools in section 6.2.2.

Summarising, we conclude that modular articles are feasible. Although we have encountered some difficulties in delineating the boundaries of particular modules and in identifying the relevant scientific discourse relations, writing a modular article is sufficiently straightforward on the whole. Writing a modular article will probably require a greater effort than writing a linear article. However, if the modular article better fulfils the reader’s requirements, it will be worthwhile, as the author aims at communicating his work to the reader. In the next section, we therefore discuss the modularised articles from the reader’s point of view.
5.2.2 The adequacy of modular articles

The structure in general

Basically, the reader aims at locating, retrieving and consulting, in an effective and efficient manner, information that is relevant to his information needs. As we stated in section 2.4, the main requirements that we address in this context are clarity and efficiency. These requirements imply that readers should receive, by means of a clearly formulated and structured presentation, all information that they require in order to understand the message and to evaluate its reliability and its relevance to their information needs, and no unnecessary information. The appropriate presentation unit for that purpose is not necessarily the article as a whole: scientists often read articles selectively [Bazerman, 1985], [Dillon et al., 1989], [Line, 1988]. The basic feature of the modular structure therefore is that it explicitly allows for selective reading, as it consists of self-contained modules that can be consulted separately, and of links connecting them.

The modular versions of the articles are both more elaborately and more specifically structured and characterised than the original versions. To improve the readability, the original versions of A05 and A08 are organised in sections, some of which are in their turn subdivided into subsections (see table 5.1). However, a linear article is characterised only at the level of the article itself, and it can be retrieved only in its entirety. The modular articles are organised in modules, some of which are in their turn subdivided into three levels of ‘submodules’. All individual modules at the different levels (including the article, which is a special case of a complex module) are labelled, and designed to be retrieved and consulted both separately and in conjunction with related modules.

The modules are connected by explicitly characterised links. The links inform the reader of the relations between the module at hand and other modules, thus giving the reader insight in the organisational coherence of the article as well as in the coherence of the scientific discourse. The links also enable the reader to navigate to these other modules. In each module, all links associated to that module are listed in the navigation menu.

The structure of the modular article is not only more explicit and more fine-grained, it is also more systematic. This implies that, once readers have become accustomed to the modular structure, they have a clearer grasp of the structure of the article and they will be able to predict more accurately where the different types of information can be found. The basic modular structure (of the modules distinguished by the conceptual function) is not unfamiliar to the reader, as it reflects the problem-solving process of the research. In fact, the problem-solution pattern is more explicit in the modular version than in the original version. Hence the modular version is more adequate with respect to the communication criterion according to which the structure of the article reflects the ideal research process.

Each module is explicitly characterised by its physics content, the role that the information plays and its range (which is associated to ‘genre’), as well as by the traditional bibliographic data. In appendix C, this characterisation is visualised in ‘characterisation tables’, in which all labels associated to a particular representation of information are grouped. The complete bibliographic characterisation in the examples partly consist of a link to the module Bibliographic information, which supplements the concise bibliographic labels that are made explicit in the characterisation table. If modular articles are implemented in a publication environment with a retrieval system that takes into account
5.2. THE FEASIBILITY AND ADEQUACY OF MODULAR ARTICLES

this characterisation, the readers will be enabled to locate more effectively and efficiently relevant information, or vice versa, filter out irrelevant information.

The crux in matters of clarity and efficiency is that different readers, at different moments, have different information needs. Therefore, the relevance of the concepts differs, as well as the required degree of focus on these particular concepts, and the required level of detail of their presentation. We first examine these issues in general for all types of modules, before we discuss them for each specific module in section 5.3.

The level of focusing

For readers with a specific information need, the original versions of the articles A05 and A08 are not sufficiently focused. By meeting the communication criterion that separate subjects should be dealt with in separate units, the modular versions allow readers to consult specific modules representing the specific types of information they are interested in, and also to pass over the presentation of other types of information. For example, when the reader wants to understand the reasoning of the interpretation of the measurements, he can consult the module Interpretation, without consulting the full description of the theoretical methods in the module Theoretical methods.

Focusing on the representation of the required information in a separate module can cause problems, because the information may depend on the information presented in another module. For instance, the interpretation of experimental results depends on the theoretical methods used to interpret them. The reader has to be sufficiently aware of these methods in order to understand and assess the interpretation. Even if the reader thinks he understand it, he may be misled, if he is not aware of the restrictions of the methods and therefore of the validity of the interpretation. Hence, readers in particular less informed ones must be careful in consulting a separate module and using the information in their own work.

This problem is not restricted to modules. Readers of traditional articles must be sufficiently aware of information presented in other publications as well. It is impossible to include in a single publication all information that is relevant to a full understanding. It is the reader's own responsibility to familiarise himself with that information, as long as he has the opportunity to do so. A modular article explicitly provides the reader with this opportunity, as each module is connected to the modules on which it depends, by links explicitly expressing the dependency relations. Thus, readers are made aware of the existence of the related modules, informed about the relation between the module at hand and the other modules, as well as enabled to consult them. The main reason why we distinguish focused modules is that at least experts with a specific information need can consult the modules separately in a useful manner, as they already are sufficiently aware of the context of the module.

As the various parts of the modularised article are distributed over separate presentation units, it can be more difficult to follow the discourse of the entire article. The linear, essayistic article is, in the first instance, better suited for linear consultation of the entire article than the modularised version, because the modular structure has been designed to

\[\text{12}\] The relata of this dependency relation can also be the entities that the information is about.

\[\text{13}\] According to the definition of a module in section 3.1.1, an adequate module is self-contained, in the sense that an expert can consult it separately.
allow for selective reading. However, in the modularised articles, the essay-route guides the reader through the complete line of reasoning. Moreover, the structure of the modular article is visualised in a map of contents expressing the organisational coherence of the article. The structure is also made explicit in an abstract expressing the coherence of the scientific discourse in the entire article, as well as in various module summaries that express the coherence of the discourse in complex modules. This allows the modular article to meet the criterion for a complete and readable discourse.

The level of detail

Part of the target audience of A05 and A08 are less informed readers who aim for a full understanding of e.g. the experimental methods or the calculations performed using the theoretical methods to interpret the results. They require more details than the original versions of A05 and A08 provide. Writing a new modular article in an electronic environment, an author can include all required information, because there are no technical restrictions on the amount of details that can be provided. Recasting existing articles in modular form, we were unable to include the relevant details that were unavailable, but we have indicated where they could be provided.

From the perspective of readers who (at a particular moment) wish to grasp just the main lines of reasoning concerning a particular aspect of the research, the original versions provide, on the contrary, too many details to suit their needs. These details are not only redundant for these readers, but they also reduce the clarity. The main line of reasoning is often obscured by these details.

To solve this problem, the author of a printed article can make use of a paper-based form of hypertext: the main text refers to footnotes, endnotes and appendices. In physics articles, and in particular in the corpus articles, footnotes and endnotes are very unusual. The original A08 contains a few notes, but these are presented in the main text, at the end of section 6.Comparison of the measurements and the calculations and section 8.Rotational coupling. Appendices are used more often. For example, in A05 the mathematical details of the estimation of the wavelength are presented in an appendix. Likewise in the journal Bioorganic & Medicinal Chemistry the section with full description of the experimental methods is given at the end of the articles, after the conclusions. Another method of hiding such details is to use a smaller font size. As is pointed out in [Berkenkotter and Huckin, 1995, p.37], the Methods section of the Journal of Biological Chemistry is printed as a supplement in miniprint. The editors note that “miniprint is easily read with the aid of a magnifying glass”.

An electronic and modular environment is better suited for dealing with these contradictory needs for full detail and for a smooth, readable discourse. If the required details are part of a separate self-contained account (e.g. in a mesoscopic or macroscopic module), they can be made available to the reader of the discourse at hand by means of a link expressing that fact that the target provides details on the source. If the details do not form a self-contained account, they are presented within the module at hand, hidden from view.¹⁴ For example, in the Quantitative interpretation A08-m5bi the different steps

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¹⁴This presentation of the details can be compared to footnotes. However, we consider it to be part of the module itself, rather than a separate unit that has to be linked to the main text. Therefore, we have not defined an explicit type to express the relation between the main line and these details, contrary to, for example, [De Rose, 1989] and [Weber, 1995], who distinguish ‘annotational links’.
of the full calculation are outlined and the details of the calculations are hidden. In the electronic presentation of the modular versions of A05 and A08, the details are hidden in such a way that they can be unfolded and included in the discourse on the reader’s demand. In the presentation of the modules, we have indicated the parts of the module that are hidden typographically.

### Overlap

Some of the modules in the modular versions inevitably overlap. By ‘overlap’ we mean that the same information is represented in different modules. The overlap is necessary to achieve the efficiency required by readers who consult modules separately, which implies that the modules must be self-contained and complete. Further overlap results from the requirement of clarity, which demands the coherence of constituent modules to be expressed in module summaries. As a result of that, the overlap could reduce the efficiency for readers who consult the entire article or a large part of it linearly. However, we compensate by laying out an essay-route that avoids overlap and by hiding overlap from the reader’s view in the same way we mentioned in the previous section for hiding potentially redundant details.

![Table](image)

**Figure 5.1.** An indication of the overlap in the modules in A05: the percentage of the modules listed horizontally that overlaps with the modules listed vertically. Overlap between 0% and 9% is left white, overlap of 10%-49% is indicated in light grey, 50%-89% is dark grey, and 90%-100% is black. For example, 20% of the content of the module summary of the complex module Methods A05-m3 can also be found in the module Findings A05-m6a, and the modules Treated results A05-m5b1 and A05-m5b2 overlap at least 90%.

To get an indication of the overlap in the modular articles, we have examined the relative overlap between modules, i.e. the percentage of information contained in a module that is repeated elsewhere, versus the percentage of ‘new’ information that is contained only in the module at hand. Such an indication is given for article A05 in figure 5.1.15

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15We have estimated the overlap by counting the number of words in the textual representation of the information in one module and calculating the proportion of the text that is shared with the various other modules. We are interested in the information overlap between modules, rather than the overlap.
There are different types of overlap:

1. ‘**hierarchical overlap**’: overlap between summaries in complex modules (including the abstract of the article, which is a special type of module summary) and the texts of their constituent modules, as illustrated in figure 5.2a.

   The module summaries of complex modules summarise their constituent modules for the sake of clarity and completeness. They are not supposed to contain ‘new’ information that does not appear in the summarised document. Therefore, complex modules automatically overlap with their component modules. The module summaries of complex modules may also overlap somewhat with other modules, as a result of the coherence and completeness requirements.

   The module summaries make up about a fifth of our example-articles. Hierarchical overlap is not problematic, because the reader is aware of the ‘redundant’ status of the module summaries and can skip them. The essay-type route by-passes almost all modules summaries.

2. ‘**parallel overlap**’: overlap between modules that play similar roles in the problem-solving process, e.g. results for different but comparable systems obtained using the same methods (figure 5.2b).

   Parallel overlap is prompted solely by completeness considerations, catering for those who wish to consult only one module. This overlap can be quite massive and literal. For example, the two elementary Treated results modules with the experimental results in A05 contain almost the same text accompanying the different figures. Therefore, the overlapping part should be hidden from view in order to accommodate readers of more than one of the overlapping modules.

3. ‘**embedding overlap**’: overlap between the modules caused by the fact that they are embedded in the same article. (figure 5.2c).

   The modules can have an internal sub-problem-solution pattern. In order to make that pattern complete, the situation of the module has to be indicated. Therefore, in literal text. However, information as such is difficult to quantify. Therefore, we count the number of shared words, but we consider different representations, e.g. different phrasings, of similar information to be similar.
we include in each module an indication of the overall problem-solution pattern represented in the entire article, which embeds the module in its context.

Embedding overlap is prompted by efficiency considerations for readers who wish to consult only one module, as well as clarity considerations for those who may be interested in a larger part of the coherent reasoning presented in the article as a whole. To increase the readability for those who read more than one module, embedding overlap should not be too literal. The author can be instructed to avoid literal overlap of this type.

In the modular versions of A05 and A08, the ‘key concepts’ of the articles are repeated – in some form, in more or less detail and with different emphasis – in almost every module. An example of such a key concept is the fact that the chemisation of a certain kind of process is studied using a particular experimental technique and some particular theoretical model (see the table 5.3). This reference to the key concepts is kept very brief; a few words may be sufficient. Thus, embedding overlap forms a small part of the modularised articles. Massive embedding overlap would imply that the modules cannot be separated.

The situation in which the sub-problem-solving of a module takes place involves the entire problem-solving process of the article, but more particularly the previous step in the process. We specifically call the resulting overlap ‘serial overlap’.

4. ‘serial overlap’: overlap between modules that correspond to subsequent stages of the problem-solving process. (Figure 5.2d).

For example, the method is indicated in the module that describes the results obtained using that method. A special case of such overlap concerns the figures of results that are included both in a Results module, and in the Interpretation module about the interpretation of these results.

Massive serial overlap between particular modules would be a reason for merging the overlapping modules. In A05 and A08 serial overlap is quite small.

We conclude that, in general, it is possible to write modular articles that satisfy the reader’s and author’s requirements. The main drawbacks of a modular structure are that it entails a higher workload for the author, which can be alleviated by appropriate software, and that the modules tend to overlap. The most important assets of a modular structure in an electronic environment are its flexibility and explicitness. The flexibility allows readers to efficiently obtain information of interest, by allowing them to choose which module to consult, and in which sequence, and whether or not to ignore the details and overlap that is hidden from view. It also allows the author to repeatedly use published modules. Since the modular structure is more explicit than the structure of a linear article, modular publications can be clearer than linear publications.

5.3 A discussion of the modules

In this section, we evaluate the various modules distinguished by the conceptual function that form the basis of the modular structure of the modularised versions of the articles A05 and A08. We discuss how the information from the sections has been recast in modular
“Semiclassical differential cross sections have been calculated using the lowest-order stationary-phase approximation, JWKB phase shifts and the Landau-Zener transition probability.”

- In the modular version in: A08-m1d Abstract, A08-m2 Positioning [A08-m2a Situation, A08-m2b Central problem], A08-m3 Methods [A08-m3c Theoretical methods].

“For large impact parameters a serious discrepancy arises” [between the measured differential cross section and the one calculated based on the Landau-Zener coupling]

- In modules: A08-m1d Abstract, (summarised in A08-m5b Quantitative interpretation), A08-m5bii1 Quantitative interpretation, A08-m5bii2 Quantitative interpretation, A08-m6a Findings.

Table 5.3

Recurring issues in A08, original version and modular version. The phrasing is derived from the abstract.

form, and to what extent the resulting modules meet the communication criteria. In this discussion, we refer to the full presentation of the modularised articles in appendix C.

5.3.1 Meta-information (m1)

The meta-information given in the elementary module Bibliographic information (m1a) helps to satisfy the standard requirements for scientific publications. It makes the certification and the authenticity of the modules of the article explicit. In the modularised articles, we have presented the standard bibliographic data that are given in the original versions of the articles and that are easily collected, complemented with the corpus-specific unique identification code that is described in section C.1.

In the elementary module Lists of domain-oriented index terms, the content-oriented index terms of each module of the article are listed. This gives the reader an overview of the physics content of the modules. In the modularised articles, we have included physics labels as an illustration, rather than as a proposal for a systematic domain oriented typology. In assigning these physics index terms to the various modules, we encountered the standard indexing problems. However, these are put into a new light, because an adequate characterisation of the modules does not simply depend on the choice of physics index terms. An important factor is the way these terms interact in complex search operations with the other types of characterisation of the same module (in particular by the conceptual function), and with the characterisations of the related modules.

For example, the question is whether we include the terms describing the method in the characterisation of the module Central problem. If we do so, the characterisations of the Methods and the Central problem will overlap. Indeed, many different modules in the modularised articles carry the same physics terms. However, this overlapping physics characterisation is not necessarily a problem, because the characterisation of the modules
by their conceptual function expresses the different aspects of the same physics concepts.

In a modular environment it is not necessary to label each individual module with all relevant index terms. The module Central problem (and its characterisation) is linked to the method module (and its characterisation), so that the relation is also expressed indirectly. A user can search for a module Central problem characterised by a particular index term that is connected, by means of a link expressing a dependency relation, to a Methods module carrying another domain-oriented label.

Because the method used to solve the problem is an important aspect of the goal of the article, we have labelled the Central problem modules A05-m2b and A08-m2b with index terms indicating the type of theoretical model and the type of experimental set-up that are used. For a more detailed characterisation of the methods, the labels associated to the appropriate Methods modules has to be taken into account.

For navigational purposes, a Map of contents (m1c) is included in the modular article. It gives the reader an overview of the article, allowing for efficient navigation and for insight in the coherence of the article. The ongoing composition of the map also turned out to facilitate the creation of the modular structure. In the modularisation process, we filled in and refined the basic modules in the map in the course of the creation of the modules. In this manner, we had an overview of what had already been finished and what still had to be done.

The presentation of the contents in a map is more effective than a representation in a ‘table of contents’. A table of contents is a linear representation, which is typical for linear texts. In a map, non-linear texts can be visualised in more than one dimension. Such a map of contents can only fulfil its function when it is sufficiently clear itself. The implementation of the map as an interactive, graphical object therefore has to be carefully chosen.16 We immediately found that a complete presentation in a single picture of all modules in an article, as well as all links leading from and to these modules, is too complex to allow for insight in the structure of the entire article. The reader should be able to select the types of modules and links that are presented in the map, and to select how the modules are arranged.

In A08-m1c, we have given three kinds of maps. In the first one, the modules of the article are arranged by main module in order to provide a general overview of all modules (see figure A08-m1c-F1 in appendix C). In that map, we also present: the main physics terms characterising the modules, the sequential routes linking the modules, the directly related mesoscopic and macroscopic modules and the associated links expressing range-based relations, as well as the most important links representing ‘problem solving dependency’. In the second map, the modules are arranged following the essay-type route (figure A08-m1c-F2). That map presents all modules, highlighting only the modules that are visited by that route, and the links expressing the sequential routes. The third kind of map focuses on a particular module, namely the Theoretical methods module A08-m3ci (figure A08-m1c-F3). It presents A08-m3ci, with its full characterisation, the complex modules that include A08-m3ci, its constituent modules and all links leading to and from A08-m3ci, as well as the modules that are linked to A08-m3ci. Furthermore, the map shows the main modules of the article, but no details of any other unrelated module.

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16 Some possibilities and pitfalls are given in [Weber, 1995]. We discuss the implementation in more detail in section 6.2.2.
We have presented in the module Abstract the text provided in the original article, complemented with links. The abstracts of the modular articles can be improved. We do not address the issue of abstracting in detail in this work; it is the focus of another thesis prepared in our research project [Van der Tol, 1999].

The list of references of the original article is included in the module Lists of references (m1e). We have linked that list to the particular parts of the modules that cite the references, and added for each module a separate list specifying and characterising the references included in it. The management of the references is particularly tedious and has to be supported by appropriate authoring tools.

The Acknowledgements are copied directly from the original version of the article. We have added a link to the home page of the institutions that are acknowledged.

We conclude that the meta-information is easy to cast in modular form, once all information is gathered. However, collecting and presenting the full meta-information by hand is an inordinate amount of work. Therefore, the author has to be assisted with tools alleviating that task (see section 6.2.2). The resulting modules constituting the Meta-information allow the modular articles to meet the communication criteria: the metadata are made explicit and grouped.

5.3.2 Positioning (m2)

The contents of the module Positioning have mostly been derived from the Introduction section. In A05 and A08, however, this module does not precisely coincide with the original Introduction. On the one hand, we had to add new information to the modules in order to make them complete according to the rules specified in appendix A. On the other hand, some information presented in the Introduction section belonged to other modules than the microscopic Positioning or its constituents. Part of the information represented in the Introduction of the original version of A05 is represented in the modular version in a mesoscopic module Theoretical methods. Also, the Introduction of A08 already announces that a discrepancy has been found between the measurements of the differential and the calculations based on the Landau-Zener coupling and that this discrepancy could be removed by taking into account the rotational coupling as well. This agrees with the findings of [Swales and Najjar, 1987], where it was found that, in physics, authors tend to mention more often the main findings of their work in the Introduction. The Introduction has an orientation function, the reader is supposed to read the Introduction first. In the modular model, however, the module Positioning is not necessarily the first module that the reader consults, as he can enter the modular article at different points. In the modular article, the orientation function is fulfilled by the abstract, which may be more elaborate than in traditional article, and which is complemented with module summaries providing a more detailed summary of the complex modules.

Situation m2a

The modularisation process

Most of the text of the module Situation of article A08 could be copied from the In-
5.3. A DISCUSSION OF THE MODULES

Introduction section of the original article. Like the original Introduction, the Situation module extensively refers to article A05, which can be seen as the immediate predecessor of A08. Following the guidelines, we have included in the Situation modules a summary of the state of affairs in the research project. For that purpose we had to complement the information provided in the original version.

Information on the development of the domain and the relevance of this particular research project within the domain could easily be presented in a mesoscopic Situation module. The Situation module A05-m2a contains only a link to a mesoscopic module Situation, complemented with a brief summary of the state of affairs in the project. Part of the text in the mesoscopic module MESO-m2a has been copied from the first review article in the corpus, R1. We have added manually a short introduction, as well as a specification of the goal of the research project and the reason that particular goal was aimed for.

The resulting module

According to the communication criteria, an adequate article makes a distinction between new information and background information. The Situation module makes the modularised version better suited to meet this criterion than the original version. The microscopic module sketches the situation in which the central problem of the article arose, and the mesoscopic Situation module provides newcomers to the field with the necessary general background the research. In this way, the necessary details about the situation in which the research has been performed are made available, in such a way that they can be avoided by readers who are either already aware of, or not interested in, the embedding of the research in its context.

Central problem m2b

The modularisation process

Writing the modules Central problem required editing of the original text, because the relevant information was not isolated in the original version, but rather interwoven with the information that we have represented in the Situation. In the original texts, the central problem is implicit in the section Introduction and in the abstract. The central problem is hardly ever phrased as a problem, but rather formulated in terms of a programme, e.g.: “Here we report relative differential cross sections of some alkali atom-halogen molecule charge-transfer collisions” [A05, p.61] or a goal, e.g. “to test the semi-classical calculation method and the suitability of the Landau-Zener theory for this type of collision process” [A08, p.167]. In the microscopic modules Central problem, we have followed the original perspective and emphasised the goals of the measurement and calculation of particular variables in molecular collisions (in order to test a particular theory).

Following the ideal problem-solving process, we should have set out the central problem of the articles before addressing the methods used to solve it. However, in this domain of experimental research, the method is indicated in the module Central problem, because the method of scattering is interwoven so strongly with the problems of molecular dynamics that it more or less defines the research domain. Thus, the microscopic modules Central problem address the question as to what is to be done in each individual article. The higher level goals can be formulated in a related mesoscopic module: the general study of the reaction kinetics.
The resulting module
In the Central problem it is announced what is to be done, which then is executed in the other modules. Therefore, a lot of modules overlap with it, in particular the module summaries of complex modules. The Central problem resembles the abstract of the article: the main issues and lines of the article are set out. The difference is that the abstract includes a summary of the main results, their interpretation and the final outcome of the research, whereas the Central problem only states what results are aimed for, and what theoretical models and techniques the authors plan to use to interpret them. The Central problem is mirrored in the module Findings m6a, which summarises what has been done and what has been found.

The module Central problem helps the modular article to fulfil the communication criteria: the goal of the research is a subject that is of interest to readers who try to locate relevant articles, as well as to readers who have obtained the article and wish to be informed, in an efficient way, of its central problem. Also, the article should have an explicit problem-solution pattern, according to the communication criteria, and therefore it has to state explicitly what is the problem to be solved.

The general goal of the research project as a whole has been summarised (in a new text) in a mesoscopic module Central problem. This module allows less informed readers to locate a research project of interest, after which they can either consult further background information in the mesoscopic Situation and in a detailed account of the established methods in the mesoscopic Methods modules, or retrieve new state-of-the-art findings issued from the same project that are presented in microscopic modules.

5.3.3 Methods (m3)
In the modular version, all methods are gathered in the complex Methods module. This implies that all methods are labelled as such, allowing readers to locate them under that heading. The different methods are used in different stages of the problem-solving process; therefore the reader of the original version encounters them in different sections.

In a modular, hypertext environment, representing the different methods in a complex Methods module does not imply that readers have to consult those methods in conjunction: each particular Results and Interpretation module is connected to the appropriate constituent module of the Methods by means of a link expressing the fact that the result or the interpretation depends on that particular method. In addition, the essay-type route connects subsequent modules regardless of their covering complex module. In particular in the map of contents A08-m1c, it is shown clearly that the essay-type route visits the Methods modules at different stages (see figures A08-m1c-F1 and A08-m1c-F2).

The coherence of the complex module is made clear in the module summary, which briefly summarises the constituent modules and expresses the relations between them. The coherence can be made clear only when the methods are put into the perspective of the central problem of the article. Because the complex module Methods includes both the experimental and the theoretical (and in some articles numerical) methods, the module summary covers a large part of the article. In A08, for example, the module summary of A08-m3 describes the particular reaction that was studied (differential cross section of chemi-ionisation of sodium atoms-iodine atoms), the particular experimental method used to do so (beam techniques), and the particular theory (semi-classical atom-atom
model). These concepts are included in almost every module in the article, in different combination and in more or in less detail. Thus, the module summary overlaps a lot with its own constituent modules, with the Results module summary, with the Interpretation module summary and with the ‘summarising’ modules Positioning and Findings.

As stated in section 5.2.2, the requirement for efficiency causes tension, between the need for sufficient detail and the need to avoid redundancy. In science, the basics of most of the methods are available and it is generally accepted that they are useful. Scientists use these methods in their research, and in a particular article they describe how they have specified and applied the methods, also discussing the applicability of the methods to the problem at hand. In the original articles, The ‘standard’ methods themselves are not described in full detail. Therefore, the methods take up a relatively small part of scientific articles [Swales, 1990], [Buxton and Meadows, 1978]. However, the article is required to provide the readers with enough information to repeat the work, or at least to understand it and judge its reliability. Thus, the methods are obvious candidates for a representation in a mesoscopic or even a macroscopic module.

In the modularised articles the experimental set-up and the theoretical models and calculation techniques are represented in mesoscopic modules Experimental methods Meso-m3a and Theoretical methods Meso-m3c. The microscopic constituent modules of the Methods present the details that are specific to the article at hand and provide a brief summary of the method, for the sake of the self-containment of the microscopic module. Therefore, the constituent modules of the Methods overlap with the mesoscopic modules that they refer to, but that overlap is not literal. These modules do not overlap massively with other modules in the article.

**Experimental methods m3a**

**The modularisation process**

The Experimental methods module is certainly feasible, as it is easy to identify and group the information concerning the experimental set-up and the way it is used in measurements. In the linear versions of A05 and A08, the information concerning the experimental methods is predominantly presented in the sections Experimental, which also hardly contain any information of another type. Therefore, the modules Experimental methods A05-m3a and A08-m3a correspond rather closely to the original sections. In the modularisation process, we only had to decide what information to present in a microscopic module, and what to group in a mesoscopic module Experimental methods.

Both the general scheme of the experimental set-up and the individual components are presented at the mesoscopic level. The microscopic modules Experimental methods specify, for example, the size of the slit, the type of atom in the primary beam and the pressure in the collision chamber, which are parameters that vary in the course of the research project.

This module is also concerned with the measurement procedure used to generate experimental results with the set-up. In the domain of biochemistry, for example, measure-
ments are performed following highly standardised protocols, which are explicitly given in journals like Bioorganic & Medicinal Chemistry. In that case, the measurement protocol and the apparatus could be reported in two separate constituent modules. This is not the case in experimental molecular dynamics. In the examples, the accounts of the set-up itself and of the way to use it are intertwined. The information on the way how the set-up is used in measurements is mostly microscopic: what were the pressure and temperature during these particular measurements, how long did the measurements take and how many runs were made?

The resulting module

The sections Experimental in the original versions of A05 and A08 do not make all necessary details available, neither by including them directly, nor by referring explicitly to a publication in which they are given. For example, the original version of A08 mentions a surface-ionisation detector for the measurement of the relative intensity of the primary beam, without providing further details (A08, p.168). In A05 the same or a similar detector is mentioned, and it is specified that the detector consists of a 0.1 mm hot iridium wire and that its efficiency is expected to be energy dependent, which is supported by a reference to an article published in a journal devoted to instrumentation (A05, p.65). The previous articles A03 (A03, p.426) and A04 (A04, p.473) describe in greater detail how the iridium wire had to be treated in order to yield a stable detector, but the two articles give different, complementary details.

In the modular version, we have gathered all information concerning this type of surface ionisation detector in the mesoscopic Experimental methods module MESO-m3a-Ir and made them available to the readers of A05-m3a and A08-m3a by means of a link that expresses the following relations: MESO-m3a-Ir provides a detailed and focused clarification of a particular component of the general set-up of which a particular instance is used in A05-m3a and A08-m3a; furthermore, the mesoscopic module has a wider range than the microscopic modules, and the modules report on the same research project. These explicit links to a complete mesoscopic module make the modular versions of A05 and A08 clearer and more efficient than the linear versions: all details are made available to the readers of the articles, without bogging down the flow of the microscopic modules.

In this particular domain, the set-up consists of standardised components: a source, velocity selection, interaction, analysis and detection. Both in the original and in the modularised version, a schematic overview of the set-up is given. In some of the corpus articles, the structure of the set-up is reflected explicitly in the structure of the text by means of headings, although in A05 and A08 only a few components are thus set apart typographically. The microscopic modules Experimental methods do not contain constituent modules that represent these components of the molecular beam experiment. Since at the microscopic level the general set-up is only sketched, such constituent modules would not be self-contained. However, we have made the structure of the set-up explicit by means of paragraphs and by linking different components in the graphical representation to their description in the text. The mesoscopic module Experimental methods MESO-m3a, in which a full account is provided, does contain such constituent modules.
5.3. A DISCUSSION OF THE MODULES

Numerical methods m3b

Modules Numerical methods are quite rare in the core of our corpus. Some articles focus on numerical methods, but most numerical work has been done by a related group at the same laboratory. Evers, for example, gives in (Evers, 1977; E2) an account of the trajectory calculations that he performed, based on a trajectory surface hopping model, on a specified type of computer, using some specified numerical techniques. His goal was to select initial conditions and to integrate the equations of motion. The modularised articles that are given in the appendix do not contain Numerical methods modules.

Theoretical methods m3c

The modularisation process
The creation of the modules Theoretical methods was more difficult than the creation of the modules Experimental methods. In the original versions, the presentation of the theoretical methods is less localised than that of the experimental methods. The module A08-m3c1 is derived mainly from the section 3.Potential curves, A08-m3c2 from 8.Rotational coupling and A08-m3cii from 4.Calculations. The section 1.Introduction of the original A08 also contains some information on the theoretical methods, which is mostly repeated in the following sections, as does the section 7.Discussion. Most of the information represented in A05-m3c is derived from the section 1.Introduction in the original version of A05.

The boundaries of the module: entanglement
In the domain of experimental molecular dynamics, the theoretical methods are generally used to interpret the experimental results. The theoretical methods described in A05-m3c, for example, are used to explain the experimental cross sections (by comparing the experiment and the general theory in a qualitative interpretation) and, in particular, to calculate the theoretical cross sections based on the experimental results in a quantitative interpretation. The usage of the theoretical methods on the (experimental) results, and the fruits of that usage are presented in the Interpretation module. This makes it difficult to separate theoretical methods and the interpretation, which is reflected in the fact that the modules Theoretical methods and Interpretation overlap and are strongly linked.

We have represented the information on the theoretical model in the Methods module, rather than in the Interpretation module, to stress the fact that it is part of the ‘theoretical toolbox’ of models and theoretical assumptions and approximations available at that time. We have also considered the following alternatives:

1. To present in the Interpretation everything that happens later in the problem-solving process than the stage in which the experimental results are obtained. In this approach the experimental work is primary, and the theory is dedicated to the enhancement (namely the interpretation) of the experiment. This approach, however, leads to an intractable Interpretation module. In such an Interpretation module would be gathered a) the description of the model for the interpretation, b) the application of the model in terms of calculations, c) the outcome of these calculations, and d) the comparison of the results of the calculations with the results of the measurements. Therefore, we have decided not to accumulate everything associated with the interpretation of the experimental results in the Interpretation module.
2. To ignore the fact that the experimental results are used to generate the theoretical results (the calculated differential cross sections) and to reconstruct parallel experimental and theoretical problem-solving processes, where the experimental and theoretical results, obtained via the two methods, are finally compared at the point where the two parallel courses join again in an interpretation. This approach better fits the philosophical idea of science as a programme with predictions and testing. However, the two courses are not parallel logically speaking, as the experimental results are used as input in the calculations.

3. To present the model on the microscopic level in the Interpretation module, but to treat it on the mesoscopic level as part of the theoretical toolbox. In this manner, the fact that the theory is used to interpret the experimental results would be emphasised, hopefully without encumbering the Interpretation module too much, because this would take into account that the basic model is mesoscopic information anyway. Nevertheless, we prefer to stress the fact that the theoretical method are methods, so that readers can search for a particular theoretical method under that heading, regardless of the purpose for which it is used.

The criterion given in the guidelines for the presentation of a theoretical method in this module, is that the information should not depend on the experimental results (see appendix A). This implies that a model that is newly developed on the basis of experimental results, rather than used in the response to another problem, is presented in the Interpretation, rather than in the module Theoretical methods. This criterion works, in spite of the fact that in the original article the presentation of some theoretical methods often does depend on the experimental results, although the theoretical methods themselves don’t. In A05, for example, the atom-atom model for molecular collisions and the calculation methods for the differential cross section are clarified using figures of the potential curves and of the deflection function. These figures are based on experimental results. At this stage, however, the theoretical methods take into account only the general shapes and not the exact results. This is emphasised by the fact that in the original article A05 these theoretical methods are presented in the section 1.Introduction, rather than in the section 4.Discussion. Part of that account is also included in article A08, in the section 3.Potential curves. In the modular version, the model is presented in full in a mesoscopic module Theoretical methods.

Another example of a potential entanglement of the Theoretical methods and the Interpretation is the argument in the Theoretical methods A05-m3c supporting the standpoint that the model is not really applicable in the situation at hand, because vibration is neglected. That is not a conclusion of the article: the authors were already aware of it and stated it in the Introduction of the original article (The authors just tried to get a qualitative insight into the harpoon reaction using this, admittedly inadequate, theoretical model; in article A08, they addressed this problem by considering a more simple system for which the assumptions are valid.). In this discussion, the value of the electron affinity is used as an argument supporting the standpoint that the effect of vibration is large in this reaction and thereby that the model is not applicable. The electron affinity is calculated in the Interpretation, i.e. ‘later’ on in the problem-solution pattern (and later in the original article). For the sake of coherence, this argument has to be provided with the rest of the argumentation on the applicability of the model. We include the argument and the entire argumentation in the Theoretical methods module A05-m3c, thus group-
5.3. A DISCUSSION OF THE MODULES

ing all information concerning the model that was available to the authors before they started the experiment, including a discussion of its relevance to the problem at hand. The ‘forward reference’, firstly, is not very disturbing even in the original version, as it concerns only a simple value put into this module. Secondly, it is even less disturbing in the modular version, where the input value has been linked to the place it was obtained, thus sparing the reader some searching within the article. That link explicitly expresses the fact that the value of the electron affinity used in A05-m3c is input from the module Quantitative interpretation A05-mbi.

Within the module: internal structure
Once the information that is to be represented in the Theoretical methods is collected, the next question is how to structure that module using the physics characterisation. How do we deal with a conglomerate of theories, models, approximations that are all part of the ‘theoretical toolbox’? For example, in the Theoretical methods A08-m3c we discuss: the Landau-Zener with the potential curves, deflection functions, differential cross sections, the stationary phase approximation, the uniform approximation, JWKB phase shifts, and rotational coupling.

We have compromised between two following extremes:

1. To put everything in the same elementary module, because the information is inter-dependent; However, that module would be very complicated, addressing many different issues

2. To put each issue in a separate constituent module. This would lead to constituent modules that need to overlap quite seriously, if they are to be self-contained. In addition, the coherence of the constituents would be obscured.

We have created a complex module Theoretical methods that consists of two components. The constituent module A08-mci focuses on the transition probability. That module in its turn consists of two constituent modules, each focusing on a specific case of the transition probability: A08-m3ci1 on the probability associated to the Landau-Zener coupling and A08-m3ci2 on the one associated to the rotational coupling. The elementary module A08-m3cii presents the methods used for the following step: the calculation of the differential cross section based on the deflection function, with the stationary-phase approximation, the uniform approximation and JWKB shifts. The internal structure of this elementary module has been indicated typographically (using headings), to clarify the function of the different parts.

The resulting module
Because the module Theoretical methods presents the existing methods that are used in the article at hand, it is to be expected that those methods are already described elsewhere. In the original articles, the authors have also made that assumption. The information about the theoretical methods is not complete and the reader is assumed to know quite a lot about it. In the module version, A05-m3c and well as A08-m3c are complemented, by means of links, with mesoscopic modules and macroscopic which do cater for less informed readers. This allows the modular version to meet the communication criterion that the details of the background must be made available.

In fact, most of the theoretical methods can be given in a mesoscopic or macroscopic module. The Theoretical methods modules A05-m3c and A08-m3c refer to the same
mesoscopic accounts of the atom-atom model in MESO-m3c-mod and of the scattering theory for differential cross sections MESO-m3c-diff. However, the articles still contain non-trivial microscopic Theoretical methods modules, in which we summarise which theoretical tools have been used, how the different theoretical tools cohere, and in which we argued their applicability to the situation at hand.

5.3.4 Results (m4)

From a physics perspective, different types of results can be distinguished in A05 and A08: experimental and theoretical results. These results are firmly linked to the experimental and theoretical methods used to generate them. Some of these constituent modules in their turn contain constituent modules that are likely to be consulted separately.

The modular model allows for the distinction of separate modules that focus on the results for differential cross sections in collisions between particular types of alkali atoms and halogen molecules, at particular energies. That distinction turns out to be too fine-grained. We assume that usually readers would not wish to consult separately an elementary module focusing on the collision of atoms with a particular type of halogen molecule at a particular energy. The result of the experiment is the shape that all curves share, rather than the value for the cross section for a particular angle as given by the individual curves. In principle, only the difference between halogen molecules and other electronegative molecules, such as O₂ and CO, would justify the distinction of different modules. Accordingly, we have presented the experimental cross sections in collisions between Na and I at a wide range of energies in the one elementary A08-m4bi1, and the experimental cross sections for Li and Br₂ and for K and I₂ in the same module A05-m4bi2.

For a practical reason, however, the cross sections for collisions between K and Br₂ are presented in a separate elementary module A05-m4bi1. In the original version, the results are separated in a similar manner: the results for K + Br₂ are presented in Figure 4 and those for K + I₂ and Li + Br₂ in Figure 5. The reason is that the results K + Br₂ are explicitly referred to in the section Discussion in the original version and in the module Interpretation A05-m5 in the modular version. Isolating these specific results in a separate module allows readers to consult the Interpretation in conjunction with the specific module A08-m4bi1, without its ‘sibling’ A05-m4bi2. Nevertheless, the specific types of results cohere strongly and therefore they are grouped in a single covering cluster module A04-m4bi on alkali atom-halogen molecule collisions in general.

Also, different constituent modules are distinguished within the Results module, in particular in A08-m4, to represent results at different stages. First, the experimental differential cross sections are obtained and presented in A08-mlb1. In these curves, the rainbow structure is identified and presented in A08-mlb2. The compound module A08-m4bi is an aggregate of these two components. In the compound module A08-m4bi with the theoretical results, first the potential parameters are determined (A08-m4bi1). Using the potential as input, the theoretical differential cross sections are calculated (A08-m4bi2), in which then the rainbow structure is made explicit (A08-m4bi3).

Raw data m4a

The modularisation process

According to the guidelines, we should distinguish specific constituent modules Raw data
and Treated results in the module Results in the case that information is lost or substantially gained when the data generated in the measurements or calculations are further treated. However, the distinction between raw data and treated results is not clear cut. Firstly, opinions may differ as to how large a difference between the raw data and the treated results warrants the creation of separate modules. Secondly, the question as to what is the output of a measurement depends on the experimental set-up, or rather on the interpretation of what is the set-up and what are tools for the treatment of the raw data. Filtering and integrating data can be seen as an integral part of the measurement, or as a subsequent step.

In A05 and A08, differential cross sections are measured and plotted in figures as \( I(\theta) \sin \theta \) versus \( \tau \), as is usual for this type of measurements. A08 also provides figures of detector signals versus laboratory angles. Those latter figures present the 'raw detector signal' that has undergone a minimal treatment: for three of the four the curves, the measured points are substituted by interstitial points to reduce the statistical noise. The former figures, of the measured differential cross section, are the product of some more treatment. However, that treatment consists of straightforward mathematical manipulations that are performed by within the (computerised) set-up.

The results could have been treated significantly, by either deconvoluting the detector function and the measurements, or by convoluting that detector function with the calculations, so that the experimental and the theoretical results could be compared more precisely. But that was not necessary in this work, as the important features of the experimental and the theoretical results could be compared anyway.

We have presented the figures for the differential cross sections and the detector signals, as well as the figures of the rainbow structure and the general shape of the cross section, in the Treated results, rather than in a module Raw data. The reason is that in the guidelines we have stipulated that the primary results, i.e. the figures, are presented in the module Treated results, and that the 'rawier', underlying Raw data are only included when they differ non-trivially from the Treated results. It is also possible to stipulate, in another modular model, the primacy of the Raw data, so that a modular article always contains a module Raw data and only a module Treated results in cases where the data have been treated significantly.

In the modular versions of A05 and A08, we have not represented any raw data, because the 'really raw' data were not available in the original article. If the modular articles had been published directly in an electronic environment, raw data could have been represented in a module Raw data. Therefore, we have included Raw data modules in the example-articles, as an indication, but left them empty.

We could neither base precise guidelines for the raw data on the analysis of a corpus of articles, nor discuss the feasibility and adequacy of Raw data modules, as the articles do not contain any raw data. The editorial board of an electronic modular journal can specify further guidelines for this module.

The resulting module
For example, Raw data modules fulfil the information need of readers who try to interpret the same experimental results with a different theory: the raw data may contain features that the author has filtered out or obscured for his presentation in the Treated results. Most readers will not be interested in the 'really' raw data. The essay-type route, which the reader can follow when he is consulting the discourse of the article, accordingly avoids
the Raw data. Grouping these data in this module allows different readers to either focus on them or to skip them all, thus satisfying their respective requirements for efficiency.

**Treated results m4b**

The modularisation process

As we mentioned in section 4.2.2, there is no sharp distinction between the data and the conclusions, but a grey area, with the outcome of an experiment in the various stages of interpretation. In practice, it is possible to make the distinction between results and their interpretation, by focusing in the *Treated results* module on the graphical or tabular presentations and including in the *Interpretation* the discussion in terms of the theoretical model.

The idea of a *Results* module is based on the prototypical *Results* section. And indeed, the core of the *Treated results* module of the modularised version of A05 has been derived from that section. The original version of A08 does not include a section called *Results*; here the *Treated results* module with the theoretical results is derived mostly from the section 4. *Calculations* and the one with the experimental results from the section 5. *Measurements*.

The modules do not correspond exactly to the original sections. On the one hand, a lot of the information contained in the *Results* sections has been recast in the *Interpretation* modules. On the other hand, the *Treated results* modules represent a lot of information that has been derived from other sections as well. In the original version of A08, we have identified information concerning both the experimental and the theoretical results in the sections 6. *Comparison of measurements and calculations* and 8. *Rotational coupling*. The general shape of the differential cross section is presented and discussed in those sections, and the comparison of the experimental with the theoretical results includes a note discussing the reliability of the experimental results. In the modular version, the discussion pertaining to the interpretation of the experiment is given in the *Interpretation* module A08-m5bii, whereas the results themselves and the discussion on their reliability are also presented in the *Treated results* module A08-m4bii2.

In the original article A08, the data analysis techniques are described in the subsection 2.5. *Data* of the section 2. *Experimental*. In the modular version, this information has been represented in the constituent modules of the experimental *Treated results* module A08-m4bii, and in the mesoscopic module MESO-m3c-treat.

The problem how to analyse and present the raw data in an insightful way is addressed in an implicit ‘sub-problem-solving process’: in the context of molecular beam experiments, the results can be obtained from the data in the way described in this module. The outcome of this process are the results presented in a figure. Many details on the analysis and treatment of the raw data are applicable to the results on differential cross sections in general. This warrants the creation of a mesoscopic module MESO-m3c-treat, which is connected to the *Treated results* modules containing results on differential cross sections by means of a link expressing the fact that the mesoscopic module is more general and more detailed.

**The resulting module**

We assume that readers are interested in ‘objective results’ and try to interpret them using their own theories. For example, Bernstein and Levine have based an important
5.3. A DISCUSSION OF THE MODULES

theoretical article on Delvigne and Los's results of the differential cross section for sodium atom-iodine atom collisions that are presented in the Treated results module A08-m4b. Rather than taking into account the rotational coupling in the interpretation of the measurements, they have refined the application of the Landau-Zener coupling. Therefore, the different results are represented in different modules in order to allow the modular article to meet the communication criterion for efficiency.

The results in A05-m4bii and in A08-m4bii are copies from the interpretation module. These 'intermediate results' are included in the Results module in order to avoid for searching by the label 'results'. These are direct copies and as such overlap completely with the interpretation modules where they came from. This overlap inconveniences neither the reader, nor the author. The author does not have to do much extra work to create these modules, and the comprehensive reader can simply avoid them, as the essay-type routes pass over the modules A05-m4bii and A08-m4bii.

In A05-m4b, we see massive overlap between the 'parallel' Treated results modules, each with same type of results for different samples. These modules contain almost the same text. Information on the type of result, the methods used to obtain it and the reliability is repeated in each module dealing with a comparable results. However, the figures are very important here and those differ. The overlap between the parallels is a direct consequence of the criterion that the modules have to be self-contained: readers should be able to consult the modules separately. In order to allow the modular article to meet the communication criterion that there should be no unnecessary repetitions, those overlapping texts can be hidden from view, to accommodate those who consult more than one of the parallel modules. There is also some 'hierarchical' overlap with the module summaries of complex modules which provide a 'table of contents' of the constituent modules.

The core of the treated results are the differential cross sections of the scattering reaction, plotted against the scattering angle. These are represented graphically, once the raw data have been analysed and the variables have been multiplied with some function for the sake of clarity.

In the original version, comparable results are plotted in the same figure. For example, the experimental differential cross sections for K + I₂ and Li + Br₂ in Figure 5 of A05 (p.67). This not only saves space, but it also expresses the coherence and allows the reader to compare those results. This comparison is explicitly aimed at in Figure 11 of A08 (p.192), which presents both the experimental smoothed differential cross sections and the comparable theoretical ones.

In the modular version of A08, the comparison between the experimental result and the theoretical results is made in the Interpretation module A08-m5bii1. The experimental results themselves are also presented in A08-m4bi and the corresponding theoretical ones in A08-m4bii, in order to allow the reader to consult and manipulate these results separately. However, separating the results diminishes the cohesion. In order to restore the cohesion, we have connected the modules by means of a link that expresses the fact that these results can be compared. In addition, the reader has to be explicitly enabled to plot the results in the same figure, to facilitate that comparison. Therefore, the results should also be presented in a machine-readable format, allowing the reader to manipulate them. In the original articles, the results are not available in a machine-readable format, and therefore the modularised versions could not include such a presentation either.

Separating the raw data from the treated results and making the data-reduction meth-
ods explicit, allows the reader to obtain other results by using other data analysis techniques to treat the same data, or vice versa, by applying the same data analysis method to a different set of data. All dependency relations between the methods, the results and the interpretations are expressed by explicit links, so that the article can also meet the criteria for the clarity of the structure.

In order to be able to judge and then use the results, the reader has to be informed how reliable the results are, and to be convinced of that reliability. An account of the restrictions of the results includes an error discussion based on the restrictions of the raw data (m4a), and thereby on the restrictions of the methods, possibly on the reliability of the treatment techniques, and possibly on comparison to other people’s results. In the original section 3. Results of article A05 (p.66), it is stated that “The results for \( \theta < 2^\circ \) are less reliable due to apparatus effects”. According to the rules for writing a modular article, the notions of ‘apparatus effects’ in A05-mbi1 and A05-m4bi2 should be specified in greater detail, to allow the modular version to fulfil the reader’s requirements.

### 5.3.5 Interpretation (m5)

**The modularisation process**

In table 5.2, we have given an indication of the relative sizes of the modules and the sections. In the modularised articles, the Interpretation is by far the largest module: it takes up about half of the article A05. In the original version, the section Discussion (roughly speaking the counterpart of this module) also forms the largest section in the original version. The collection of the sections 6. Comparison of the measurements and the calculations, 7. Discussion and 8. Rotational coupling in A08, which can be grouped under a higher level heading of Discussion, is less dominant, but it still forms a large part of the article.

The main reason why Interpretation modules are comparatively large is because they play a central role in the article: in the Interpretation the experimental line of the article and the theoretical line are brought together. Moreover, the Results modules only seem to be very small, but that is artificial: firstly, only the text of the treated results is regarded in these size considerations, whereas the figures are the most important part of the treated results, as well as the most voluminous; secondly, as we saw, in the modularised version raw data could have been included, but they are unavailable in this case. Furthermore, the Interpretation modules are relatively large, because the Methods modules of the articles are kept relatively small, as a lot of information concerning the methods is represented at the mesoscopic level.

The Interpretation is not only an large module, but also a difficult one: it contains a lot of information that has to be dealt with in a clear manner within the module, and it is also rather entangled with the modules Theoretical methods and the Results.

*The boundaries of the module: entanglement*

The entanglement of the interpretation, the theoretical methods and the results is illustrated by the fact that part of the Interpretation is derived from sections that also contain information that is represented in the Theoretical methods or the Results. For example, a small part of the section 3. Potential curves is presented in A05-m5bi. The first part of the section 4. Calculations is given in A08-m3cii, whereas the second part was supposed to deal with the results of these calculations. However, most of that part is given in the
Interpretation, in particular in A08-m5a.

The theory or theories and technique(s) used for the interpretation are described and discussed (with respect to their reliability and applicability) in the Theoretical methods module m3c. The usage of these theoretical methods, however, in the process of interpreting the results, is included in the Interpretation, with the description and discussion of the resulting interpretation(s). This dependency of the Interpretation on the Theoretical methods is expressed by means of links. In the modularised versions of the analysed articles, most of these theoretical details are applicable to more than one article and therefore presented in the mesoscopic module MESO-m3c. For efficiency, most links in the Interpretation module are directly targeted at the mesoscopic modules. However, we have included at least one link to the module Theoretical methods of the article under consideration, in order to express the coherence of the article.

In the modularised articles, a Results module could be separated from an Interpretation module. In the domain of experimental molecular dynamics, interpreting the results obtained in terms of scattering implies explaining them in terms of reaction mechanisms specified in a molecular dynamics model. In the Qualitative interpretation module A05-m5a, for example, the main features of the curve of the experimental cross section are described in the light of a simple atom-atom model for molecular collisions. In the Quantitative interpretation, theoretical cross sections are calculated using that model and compared with the experimental ones.\(^{18}\)

Separating the results from their interpretation calls for overlap between the Results and the Interpretation module. In the first place, for the interpretation to make any sense, the core of the results has to be repeated in the Interpretation. In particular, the key figures representing the results that are to be interpreted are copied to the Interpretation module.

The description in words of the special features of the (graphically presented) results is included in the Interpretation module, rather than in the Treated results. For example, a description of the curves presented in A05-m4bi-ii is included in the Qualitative interpretation module A05-m5ai. The description of the curves leans towards the interpretation of the curve: the authors highlight features that they consider relevant for the solution of the central problem. A more practical reason is that the discussion of those features in the Interpretation can be performed more smoothly if the features are described in the same module.

The second reason for overlap between the Results module and the Interpretation is that intermediary results generated in the course of the interpretation are copied to the Results module in order to allow the reader to locate and retrieve them as results.

**Within the module: internal structure**

Once the author has decided what to represent in the Interpretation, the representation of that information in the module does not follow automatically: the module itself is rather complicated as well. It is a large module, which may contain different parts. It is

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\(^{18}\)On the level of a sub-problem-solution pattern, the results and the interpretation are not easily separable. For example, in the module Treated results the treatment and presentation techniques (as presented in MESO-m3c-treat) are used in response to the problem of the data analysis, and the outcome of that sub-problem-solving process are carefully analysed and clearly presented treated results. In that sub-problem-solving process, we cannot distinguish between results, interpretation and findings. However, that is not necessary, as the stages of this process are not explicitly labelled.
also argumentative in nature. The Interpretation module contains argumentation on the reliability of the interpretation(s), which is based firstly on the reliability of the results in the module Results (which in its turn depends on the reliability of the methods used to generate them in module Methods), and secondly on the reliability and applicability of the chosen interpretation theory.

Many of the external references to other work appear in the Interpretation modules. The function of the references is, for example, the comparison with the interpretations given by others for similar results, or input of factual information copied from another article into a calculation.

The resulting module

The Interpretation module is a very important one. In this domain, the interaction between theory and experiment is emphasised. The Interpretation can be seen as the ‘core’ of the argumentation in the article. The argumentation in the Interpretation is ‘supported’ by the arguments and detailed reports given in other modules. The Results module gives the details behind the salient features of the results that are explained in the Interpretation module, the Methods give the background of how those results were obtained and the details of the theoretical model taken from the theoretical toolbox to interpret the experimental results, the module Positioning announces what the author aims to do and why. The Outcome then summarises what has been achieved. Thus, the module Interpretation is strongly related to many other modules. For the sake of the coherence of the article, these relations, in particular the dependency relations, are expressed in explicit in hyperlinks.

Because the Interpretation is generally complicated, it is difficult to endow it with a clear structure. But it is also very important to do so in order to allow the reader to understand and accept the information. The importance of a careful explanation and a clear structure immediately becomes clear when the interpretation is consulted in the original articles: it is often difficult to keep track of the line of reasoning.

The act of interpretation may involve one or more sub-problem solution patterns in which different methods are used to interpret the results. The results can, for example, be explained qualitatively with respect to their general features. The results can also (additionally to the qualitative interpretation or not) be inserted as input into calculations based on chosen theories considered in parallel. These calculations can consist of a series of separate steps (each featuring a sub-problem-solution pattern), in which the output of each step is required as input in the next one. Or different types of results can be obtained independently, and then compared in the interpretation. Thus, there can be more than one complementary interpretation (qualitative and quantitative) that are merged into a complete interpretation. There can also be more than one explicit candidate interpretation before one is chosen. The guidelines for this domain allow for the distinction by the conceptual function of two constituent modules within the Interpretation: Qualitative interpretation and a Quantitative interpretation.

In A08-m5, two candidate interpretations are described and discussed. The measured differential cross sections are first interpreted qualitatively, using a simple semi-classical model that takes into account the Landau-Zener coupling (see A08-m5a). This qualitative interpretation is quite satisfactory. Then the authors proceed with a quantitative interpretation (in A08-m5b), in which they first determine the potential parameters (A08-m5bi). Subsequently, using those parameters as input, the differential cross sections are
5.3. A DISCUSSION OF THE MODULES

calculated in A08-m5bi1 based on the same semi-classical model. This quantitative interpretation, however, is not satisfactory. Therefore, the same experimental results are interpreted again in A08-m5bi2, this time taking rotational coupling into account as well. This last interpretation is singled out as the more successful one, because it provides an accurate, quantitative explanation of the reaction dynamics.

In these big and involved Interpretation modules the ‘module summaries’ in the complex modules, such as A05-m5, A05-m5a and A05-m5b, are particularly important. The module summaries of the ‘constituent complex modules’ A05-m5a and A05-m5b are almost literal copies of the highest level module summary. However, by making these aggregates explicit, and giving explicit ‘module summaries’ in each of them, the clarity of the module is clearly enhanced. The reader who consults a separate module needs the information to learn of the context and he does not encounter all copies. The reader who consults the article in its entirety or the Interpretation module as a whole following the complete sequential path does encounter multiple copies of the same text. The essay-type path avoids most module summaries, but in cases of large and complicated modules, the readers is more helped than hindered by a reminder of the overall structure of the module.

**Qualitative interpretation m5a**

**The modularisation process**

Within the Interpretation module A05-m5, firstly a qualitative interpretation is given in A05-m5a. This module Qualitative interpretation consists of two components. A classical explanation of the experimental results is obtained and discussed in a sub-problem-solving process presented in A05-m5ai. In A05-m5a(ii) a tentative quantum mechanical explanation is suggested for a particular angular range (namely, small angles). In the original article, this quantum mechanical interpretation was dealt with in an appendix. It consists of a calculated estimation of the quantum oscillation wavelength, which is then used in a rough argument for the explanation of an oscillatory feature of the experimental results.

The figure of the deflection function which is used for the basic explanation of the differential cross section in module A05-m5ai is part of the mesoscopic module MESO-m3c-defl. We have copied the figure to this module in order to make this module complete. In the original article, the figure referred to in the qualitative explanation is the *calculated* deflection function, which is determined in a later stage of the problem-solving process. Strictly speaking, this makes the original line of discourse inconsistent. However, only the general features of the figure are used. The qualitative explanation in A05m5ai still contains a ‘forward reference’: an assumption is made which is known to be satisfied only when the resonance energy for this system has been determined in m5bi. In a modular structure precisely targeted and explicitly characterised forward references can be taken into account more smoothly than a statement “(for the estimated value of $H_{12}$ given later)” [A05,p.67].

**The resulting module**

The use of isolating the qualitative from the quantitative interpretation, is that readers who wish to get the qualitative idea are not submerged in the elaborate quantitative calculations. On the other hand, this distinction causes some overlap, since some qualitative aspects are included in the module Quantitative interpretation as well in order to make that module self-contained.
Quantitative interpretation m5b

The modularisation process
A quantitative interpretation is given in A05-m5b, by calculating the theoretical differential cross sections. This interpretation consists of two serially connected sub-problem solution processes. Firstly, the potential for the reaction between potassium and bromide is determined in A05-m5bi, which implies a long and involved determination of a series of potential parameters. This determination of the potential parameters is almost entirely copied from the section Discussion in the original article.

The expression for the potential thus obtained (which can be consulted separately as a result, because it is also included in the module Treated results) is then used as input in A05-m5bii in order to calculate the deflection function and subsequently the theoretical differential cross section, which finally can be compared with the experimental values. In the original article, the deflection function was already presented in the Introduction, with forward pointers to the potential given in the section Discussion. In the introduction only the general shape of the deflection curve was referred to. That general shape has been presented in the modular version in the mesoscopic module Theoretical methods MESO-m3c-defl.

In both cases, a numerical evaluation of the deflection function is used to calculate the differential cross section, for which the method has been described in A06. In the original article A05 this was implemented via a forward reference to an article that was “to be published”. This untargeted forward reference is resolved in the modular version, where an explicit link has been added in module A05-m5bii.

The resulting module
In the modular version, the details of the calculation are hidden from view. Therefore, the main lines of reasoning can be followed more easily than in the original version. This satisfies the needs of readers who are only interested in these main lines, and of reader who need to an overview of the reasoning as a whole before they can understand the fully detailed account. The details can be unfolded to fulfil the requirements of readers who do not understand or accept the outcome. In principle, these details can be more elaborate than in the original version, because thus hidden they do not obstruct the main lines and in an electronic environment there do not have to be ‘page limits’. However, in the Interpretation modules of the examples, no additional details have been presented.

The mathematical elaboration does not form an information unit that can be consulted separately and therefore does not form a separate module.

5.3.6 Outcome (m6)
The components of the module Outcome provide the conclusions of the article. In long corpus articles, e.g. in A04, A08 and A14, which each have more than twenty pages, the conclusions were given in a specific section Conclusions. In the other (smaller) articles no Conclusions section was included. In A05, for example, the information that we included in the Outcome module was found at the end of the article, where such a section could have been made explicit. In other articles, such as A02, the outcome of the research is not summarised at the end of the article.
5.3. A DISCUSSION OF THE MODULES

The Outcome modules of A05 and A08 are a complex module, as each contains two elementary modules. They are not very complicated, so that they do not require an elaborate module summary. In particular the one in A05-m6 is hardly more than a table of contents.

Findings m6a

The modularisation process
The findings of the research are not always as explicit in linear articles as we might wish for. After reconstruction, this module is not too difficult to create, also because massive overlap is no problem here.

The Findings provide an explicit (at least tentative) answer to the central question of m2b. This answer in module m6a is linked to the question in the Central problem m2b by means of a characterised link indicating that the answer is dependent on the question. Examples of findings are conclusions about the validity or applicability of a theoretical model in the light of the obtained results. From a different view point, these amount to the equivalent conclusion that the results can be interpreted as the reflection of behaviour of the physical system as it is modelled by that theory. The usefulness and applicability of experimental techniques is also a subject for conclusions.

We think it is quite possible that in some articles the main conclusion is simply a particular value for, for instance, the adiabatic electron affinity of the molecule under consideration. Such a conclusion can be drawn after some discussion about the applicability of a theory, in which also a comparison is made with the values obtained by others. It is always possible to mention numbers in the conclusions, with a pointer to the results.

The resulting module
In this module a brief recapitulation is included of what has been achieved in this article. This recapitulation is linked to the modules that it recapitulates, using ‘problem-solving dependency’ links expressing the fact that the findings depend on these modules, which provide a more focused and detailed account of the concepts. Thus, Findings is a ‘summarising module’ and therefore it overlaps with a lot of (module summaries of complex) modules. In particular the Findings risk coinciding with the Abstract m1d given in the Meta- information. The difference is that the abstract has to provide an overview over the entire problem- solution pattern of all (main) modules in an article, whereas the Findings emphasise the resolution of the problem-solving process.

In spite of its overlap with other modules, we have included a module Findings in each modular article. The Findings can be seen as the final stage of the problem-solving process, in which its outcome is made explicit. In a linear article, the conclusions are often presented rather implicitly at the end of the Discussion section. Making the findings explicit can, firstly, clarify a complex discussion. Secondly, it caters for the needs of readers who are interested in the outcome, without being willing or able to follow the entire discussion. According to [Dillon, 1989], readers often browse the conclusions of an article to judge its relevance. Indeed, in the original version of the longer article A08, in which it may be more difficult to determine what is the outcome of the problem-solving process, an explicit section Conclusion is included. Thus, the module Findings allows the

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19 In the articles we have analysed, the determination of the electron affinity was considered a secondary goal of the research.
browsing reader to get news in an efficient way, and it clarifies the reasoning of articles in which there are many candidate interpretations cluttering up the Interpretations module.

**Leads for further research m6b**

**The modularisation process**

When present, the information that belongs in the module *Leads for further research* is relatively easy to isolate in the original article, but some additional information is generally necessary to form a complete module according to the guidelines formulated in appendix A.

In the explicit summary of the Findings A05-m6a, as well as in the section 4. *Discussion* of the original article, it is concluded that the theory gives only a qualitative explanation of the experimental results. An important reason for the failure of the quantitative interpretation is given by the fact that the theoretical model is not applicable to the reaction under consideration, which is explicitly stated in the *Theoretical methods* A05-m3c. In order to get an accurate quantitative explanation the resolution of the experimental set-up, as described in A05-m3a, should be increased. At the end of the original version of A05, and in the module A05-m6b of the modularised version, a suggestion is made to increase that resolution by replacing the source, one of the ‘standard’ components’ of the set-up, by another type of source.

**The resulting module**

The module *Leads for further research* is optional for solved problems (articles with finished proofs, for example). However, most ‘regular research’ is a continuing effort and therefore likely to given rise to new problems, even if the problem at hand is solved. In most of the articles we analysed, no adequate solution to the problem could be found. The ‘new problems’ that arise from the problem-solving procedures presented in the articles therefore mostly concern reformulations of the old problem. The *Leads for further research* module containing such a reformulation depends on the (inconclusive) Findings, which is expressed in the characterised link between the modules m6a and m6b.

The bottom-line of article A05, as is stated in the module Findings A05-m6a, was that the problem addressed in the module *Central problem* was solved only roughly and qualitatively: the simple classical model does not give a good explanation of the reaction. For a more accurate quantitative solution, a new approach is suggested in the module *Leads for further research* A05-m6b, and carried out subsequently in article A08 in which this problem is addressed by experimenting on a more simple system and by using a more complex model and a more complicated experimental set-up.

### 5.4 A discussion of the links

In this section, we discuss the second component of the modular structure: the links. We first focus on the representation of organisational relations and subsequently on the representation of scientific discourse relations.
Table 5.4

For each module in A08, except the module Meta-information and its constituents, the number of identified relations and the number of links used to express them, with the module at hand or a segment of it as the source, are listed: a) The number of relations of each type identified and expressed either only in the navigation menu or in the text as well. The columns add up to the total number of relations of any type made explicit in a particular module and the rows add up to the total number of times a particular type of relation was made explicit in any module. In the entire set of scientific modules in the article, 940 relations have been made explicit in a link. b) The number of links with the module at hand as the source created to express the relations identified in the module. In the entire set of scientific modules in the article, 386 links have been created to express the relations.
5.4.1 Representing organisational relations

In order to prevent the reader from getting lost in the network of modules that is formed by a modular article or a larger collection of modules, the organisational coherence has to be made explicit.

As an indication, we list in table 5.4 how many relations of the different types we have identified for each content module in the modular version of A08, and how many links we have created to express these relations. In A08, we identified, and expressed in explicitly labelled links, 377 organisational relations. The links provide the reader with roads to the various modules, the labels serve as signposts, and the module Map of contents as a road map.

The identification of an organisational relation usually did not lead to the creation of an explicit link in the text of the content modules. However, when we created a link to connect objects that were related by a scientific discourse relation, we also expressed the organisational relations between those objects in that same link. Thus, the reader is informed of the relation between connected objects, so that he can make a well-considered choice as to whether to follow the link or not. In the modular version of A08, organisational relations make up 40% of the complete set of relations that are expressed in the links: 18% are included in the text and 22% are only made explicit in the navigation menu.

Creating links expressing hierarchical relations, we aimed to give them access to the constituent modules of a complex module, and vice versa, to the covering complex module. Hierarchical relations automatically appear when complex modules are formed from constituent modules. The only links that can express a hierarchical relation, and thereby the fact that the complex module contains the constituent modules, are ones which connect modules that are also close according to the proximity-based relations. If one of the modules is microscopic, and thereby part of an article, they both have to be part of that article, so that the link is also characterised as ‘internal’. Mesoscopic and macroscopic modules that are connected by means of a link carrying a hierarchical label, are also part of the same (higher-level) entity.

In the examples, all elementary modules are part of a larger complex module, and in all complex modules the constituents are summarised (even if only in terms of a table of contents). Therefore we identified hierarchical relations for each module. Every hierarchical relation is expressed, at least in a link in the navigation menu.

Proximity-based relations can easily be established between any two modules: the author merely has to determine whether the modules are part of the same article, or both report on the same research project, or neither. In the original version of A08, about a third of the references are to other works written by the authors of A05 and A08 or by others in the same group; the rest refer to works by authors outside the project. In the modular version, only 6% of the links express an external relation and 11% a project relation; the rest represent internal relations.

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20 In this table, we have not taken into account the links starting from the module Meta-information, or any of its constituents, as the source.

21 Organisational relations do play a predominant role in the text of the module Meta-information or any of its constituents, in particular in the Abstract.
5.4. A DISCUSSION OF THE LINKS

Range-based relations always occur when a module with a wider range is referred to from a module with a narrower range, notably, when a mesoscopic modules is cited from a microscopic module. In A08, we have provided 39 links to higher-level modules, thus informing the reader of this difference in range. Most of these links appear in the Situation and the constituents of the Methods module.

Administrative relations are always expressed between each module containing scientific information and the modules providing the meta-information associated to the scientific information in order to allow the reader to navigate between the scientific content of the article and the meta-information. In A08, almost in almost every\textsuperscript{22} content module, three standard administrative relations are made explicit in the navigation menu, in links to the complex module Meta-information, the map of contents and the Abstract. The administrative labels can only be assigned to internal links, which connect modules within the same article.

Readers of a modular article are forced to take an active part, as they must decide in which sequence they want to consult which modules. This implies that for each link they must decide whether to follow it or not. The reader is less likely to get lost if he has at his disposal a sequential path. Creating these routes is certainly feasible. A default complete sequential route can be generated automatically. However, the author can optimise the route by choosing the most suitable sequence of similar constituent modules of, for example, the Treated results. We have provided the reader with easy-to-use connections to the next module and the previous one by expressing the sequential relations associated with two sequential routes.

All modules are part of the complete sequential route. Thus, the complete sequential route can guarantee the readers that they haven’t missed a single module. However, on this route the readability has been sacrificed for completeness. In the first place, the overlap between different modules (in particular with the module summaries in the complex modules) causes unnecessary repetition for the readers who consult the article via the complete sequential route. In the second place, the bothersome modules like the raw data obstruct the flow of the scientific discourse.

The essay-type sequential route is most suitable for consulting the article as a whole. The creation of the essay-type route requires a bit more attention than the creation of the complete sequential route: the resulting route is supposed to provide the sequential reader with a comprehensive account of the research that is represented in the article. In A08, the essay-type route connects all elementary modules, except the Raw data and the theoretical Treated results. It passes over all complex modules, with the exception of the covering Theoretical methods module A08-m3c and the Quantitative interpretation A08-m5b. These are included in order to facilitate the reader’s understanding of the discourse. This is necessary, because both the Theoretical methods and the Quantitative interpretation are very complex modules, which the essay-route visits more than once.

If the theoretical methods are used to interpret experimental results, the problem-solving process can be seen as serial: in order to solve the central problem of the article, an experimental sub-problem (of the measurement of, for example, the differential cross sections in chemi-ionisation in collisions between Na and I), and a theoretical problem (of

\textsuperscript{22}The exception is the module Positioning, in which the link to the Acknowledgements, created for the step back along the complete route, also expresses an administrative relation.
the interpretation of those cross sections in terms of an atom-atom model) are addressed sequentially. This sequence is expressed in the essay-type route, which allows readers to consult the article as a single discourse. In article A08, this route first passes through the Experimental methods and the two constituent modules of the Treated results that deal with the experimental results, before passing through any Theoretical methods modules. The last Theoretical methods module

Both the complete and the essay-type sequential route are part of an article and therefore connect microscopic modules. Therefore, the links are also ‘internal’. The essay-type route avoids most of the complex modules and therefore the links expressing that route are usually neutral with respect to the hierarchy.

Making explicit the organisational relations gives the reader insight in the organisational coherence of the collection of modules and allows him to navigate efficiently. The organisational types of relations can be identified and expressed in links rather easily. In fact, most of these relations can be made explicit automatically once the modules and the links expressing the relevant scientific content relations are created.

### 5.4.2 Representing scientific discourse relations

Contrary to the organisational relations, the scientific discourse relations did cause problems in the modularisation process. These problems were not unexpected: it is already pointed out in [Trigg, 1983] that it is difficult to characterise links in an informative and yet consistent way. In some cases, a particular link type can be assigned unambiguously, but in other cases no link type seems applicable, or a mix of most types. Because these types of relations are more difficult to identify in the empirical analysis, their definition in the modular model, which has been developed using that empirical analysis, is also rather tentative.

**Relations based on the communicative function**

In the modular version of A08, we have not expressed many relations based on the communicative function. Often, the target of a link implicitly provides, at the same time, a clarification, an explanation and a justification of the source. We have considered that to be the default. The reason is that in the text the communicative function of different parts is often not straightforward either. The usual writing style in science is to formulate the presentation as a report: the authors inform the reader of their research, its reliability and its relevance. The reports on the reliability and relevance can also be reconstructed as argumentation aimed at justifying standpoints with respect to that reliability and relevance. We assume that the author intended both to inform and to convince the readers. Therefore the target of a link can have different communicative functions with respect to the source, depending on the question whether the reader does not understand the source or is not convinced of its reliability or relevance. And therefore the link can express different relations based on the communicative function. We have only expressed a relation based on the communicative function when that function was explicit enough. For example, in A08-m32ii we created a link that explicitly expresses the fact that the cited article both elucidates the uniform approximation, and justifies its applicability.

In any case, we have only expressed relations based on the communicative function in
5.4. A DISCUSSION OF THE LINKS

links leading from a source that was something that had to be elucidated or argued, to a target providing the elucidation or argumentation. We have not made explicit a single instance of the opposite, a relation in which the target was something that had to be elucidated or argued.

We have made explicit some clarification relations, mostly in the Experimental methods and the Findings, in cases where the target relatum predominantly addresses the question ‘what’ rather than ‘why’. For example, the module Experimental methods A09-m3a refers to the mesoscopic modules that are part of MESO-m3a for a detailed and focused account of the components of the set-up. The communicative function of that account with respect to the text in A08-m3a is that of a clarification of what these components look like and how they work, rather than an explanation of why they do so, or a justification of their reliability.

We have identified only sporadically the more specific relations of definition and specification. In A08-m3cii, the term deflection function is linked to its definition in a mesoscopic module. In the examples, not many explicit definitions are given. In the implementation of modular publications, the reader could be enabled to look up definitions in a ‘scientific dictionary’ by means of implicit links, which are called intensional in [De Rose, 1989]. However, the modular model is restricted to explicit links, and such a dictionary is not available in the example.

In the Theoretical methods, we have used the more general elucidation relations, which imply both clarification and explanation. By making explicit an elucidation relation, we emphasise the fact that the target is aimed at informing the reader of what is meant and why the described state of affairs has arisen, rather than at justifying it.

In a few cases, we have made explicit an argumentation relation. For example, in the Findings A08-m6a it is concluded that “the Landau-Zener theory can be applied by the simple use of the transition probability”. We have added a link which expresses a clarification to a mesoscopic module about the theory. We have also added a link expressing argumentation to the Interpretation A08-m5bii1, where the applicability of the theory is justified. Argumentation relations form only one percent of all relations in A08.

The articles we have modularised are not very polemic. Therefore, a particular reader does not require the explicit possibility to search for advocates or adversaries of a particular standpoint. Hence we do not distinguish between supportive argumentation and counterargumentation.

Content relations

The relations pertaining to the dependency in the problem-solving process could be identified quite easily. In appendix A we have given clear rules for the identification of these relations between particular modules. In A08, we identified 47 of these relations, for example between the measured experimental cross sections represented in A08-m4bii1 and the molecular beam method given in A08-m3a.

The subtype of dependency relations, transfer relations, was also identified easily and frequently. Often, a particular value obtained in another module, in the same article or elsewhere, is used as input. For example, the value for the vertical electron affinity that is obtained in A05-m5bii is used as input in the discussion of the Theoretical methods in
A05-m3c. Figures are imported as well. For instance, the figure of the potential curves is generated in the Interpretation module A08-m5bi. It is copied to A08-m4biil, which is expressed in that Treated results module by a link carrying the label ‘input’.

About half the links in A08 express either a general elaboration relation, or a more specific resolution relation or context relation, or a combination of these. The general elaboration relation, where the one relatum provides more details as well as a wider context of the other relatum, is not very common in A08. Only 17 links are labelled as ‘is elaborated in’, and no link carries the opposite label. The other combination of the resolution relation and the context relation, where the details are more focused, is identified 75 times. More than a quarter of the links lead to a target that provides more details about a particular issue addressed in the source. For example, resolution relations can be identified between, at one end, most mesoscopic and macroscopic modules, and at the other end, the microscopic modules connected to them. Usually the authors of a microscopic module refer to these higher level modules, because they don’t want to provide all relevant details in the microscopic module. Therefore links to other articles are also often labelled as ‘is detailed in’.

The opposite, where the target relatum of the relation summarises the source, is expressed explicitly in about a eighth of the cases. Between module summaries in complex modules and constituent modules, both ends of this combination of resolution and context relations are made explicit. A link is made explicit in the constituent modules, leading to the module summary, which provides more context and less details. The opposite of these relations results in an explicit link from the module summary, to a more detailed and focused account in the constituent modules.

We have identified very few similarity relations in A08. Most of them are associated to the Treated results. The experimental and theoretical results that are compared in the interpretation, and that in the original version were presented in a single figure, are connected by a link expressing that comparison. In addition, the results are compared with the results of others, in the context of the discussion of the reliability of the results, by means of ‘external’ links. We have not labelled any links with the more explicit labels ‘agrees with’ or ‘disagrees with’.

Of all relation we have made explicit, 16% were synthesis relations. Most of them were identified between complex modules and constituent modules. For example, the specific experimental results for collisions between KBr₂, LiBr₂ and KI₂, represented in the elementary module A05-m4bi1 and A05-m4bi2, are grouped into a cluster module A05-m4bi, which deals with alkali atom-halogen molecule in general.

We have also expressed synthesis relations in links between microscopic and mesoscopic modules (which therefore also express range-based relations). For instance, the microscopic modules Experimental methods, in which the set-up used in a particular experiment is presented, refer to various constituent modules of the mesoscopic Experimental methods, in which the components of molecular beam experiments in general are presented.

A link expressing a segregation often also represent an elaboration relation: the target module provides a more focused and detailed account of a particular component of the central concept of the source module. These types do not necessarily coincide, as the
target can focus on a concept that is not a component of the aggregate central concept of the source module.

In the modular versions of A05 and A08, causality is expressed in the reasoning in the text within the modules. However, we have hardly expressed any *causality* relations in links. Causality relations can be identified between relata of an explanation, because explanation by definition involves causality. However, we have not labelled links expressing an explanation as causal by default, but we have only made causality explicit between relata that have a clear causal relation. This does not happen very often, as generally causality is intermingled with less strict reasoning, e.g. a justification of the choices that were made.

Summarising, we see that the methods *Positioning* and *Experimental methods* are quite easy to write. They also fulfil the needs of readers who either want to avoid unnecessary details (by avoiding these modules) or to get a fully detailed account (by consulting the modules in full detail). The module *Results* provides a focused account of specific results, that fulfils the readers’ requirements, and it is also feasible, if the guidelines are followed. The module *Theoretical methods* was somewhat complicated in the case where the theoretical aspects were emphasised, but in fact the account of the theoretical methods in the original version even more complicated, because the modular version is more explicitly structured and it contains module summaries that clarify the line of reasoning. The *Interpretation* module is also a difficult one to write, because it is a very complex module, just like the corresponding *Discussion* section.

Organisational relations, as well as dependency relations based on the problem-solving process and similarity relations, are easy to provide and quite useful. Other scientific discourse relations were more difficult to identify in the modularisation process, but may be easier to deal with by authors writing a new modular article.
Chapter 6

Conclusions

In this chapter, we give an overview of our main findings in section 6.1, and in section 6.2 we indicate how our work can be further developed. In section 6.2.1, we briefly discuss the applicability of our modular model to selected examples of publications in other domains, and in section 6.2.2 we provide suggestions for the implementation of modular articles.

6.1 Findings

In this thesis, we have shown that electronic scientific articles can be organised in a ‘modular structure’ that consists of modules representing different kinds of information units and links expressing various relations. Because the modules are uniquely characterised and self-contained, they can be located, retrieved and consulted separately. They can also be located, retrieved and consulted in conjunction with related modules, because the coherence of the information distributed over different modules is made explicit. In the first place, the coherence is expressed in the composition of elementary modules into complex modules. Secondly, it is expressed in the explicitly characterised links that connect related modules (or parts of modules). A single link connecting particular modules can express various relations between these modules, between the information units underlying the modules and between the entities that information is about. Since the links connect both modules within an article and modules that are part of different publications, the modular article forms a network within the network of all scientific publications. A modular presentation of information allows readers to navigate freely through the network of information, compiling their own reading-matter to suit their particular information needs.

We have developed a modular model for the structure of electronic articles on experimental science; we have also specified rules for the creation and evaluation of modular articles on experimental molecular dynamics in particular. The modular model has two main components. The first component is a multidimensional typology for the various kinds of information that are represented in scientific articles and thereby for the modules. In addition to the traditional bibliographic and domain-oriented characterisations, we have introduced a characterisation of the information by its conceptual function and a characterisation by its range. The second component is a multidimensional typology for the links by the relations they represent. These relations fall into two main classes: organisational relations and scientific discourse relations. The typologies that we have developed can be used for the creation and explicit labelling of modules and links in ar-
articles on experimental science. From our model, modular models for other domains and genres can be derived by deleting or adjusting the elements of the typologies that do not suit and adding suitable ones.

Starting from an ‘interactants profile’ with the needs of authors and readers, we conclude that the flexible and explicit modular structure allows for more effective and efficient communication in an electronic environment:

1. **Multiple usage**
   The modular structure allows authors to re-use modules that they have written themselves or that have been written by others. Particularly suitable for multiple use are modules with a wide range, i.e. mesoscopic and macroscopic modules. Therefore, writing a modular article is more efficient than writing a linear article.

2. **Locating relevant information**
   The modular structure allows for better information retrieval than the traditional structure, since the multidimensional characterisations of the modules and links allow for a complex search, as well as for a well-considered selection of a browsing path:
   - The *module labels* allow readers to locate particular modules from different, complementary perspectives;
   - The *link labels* allow readers to locate clusters of related modules and modules in a particular context, rather than simple objects only.

3. **Selective reading**
   The modular structure allows readers to selectively locate, retrieve and consult precisely those parts of the published works that interest them most: a single module, an entire article, or another set of related modules. Since selective reading is a common reading strategy, a modular article is more efficient than a traditional, linear article.

4. **Clarity**
   In an article with a standardised modular structure, scientific information is presented in a systematic way. The structure of a modular article is made explicit in the composition of modules and in the characterised links, and it is clearly represented in the *Map of contents* and in the *Abstract* and the module summaries. Thus, a modular article is more transparent for the reader than a linear article.

In order to allow for a substantial improvement of scientific communication in practice, the modular model must be implemented in such a way that the authors and readers can indeed take advantage of the benefits of the modular structure. Authors must be provided with tools that enable them to write modular articles in a straightforward, efficient and standardised way. For locating, retrieving and consulting modular articles, the reader needs appropriate reading aids. From our study, clear requirements emerge for tools supporting the process of writing modular publications, as well as for tools that enhance the product.
6.2 Leads for further research

We have shown that a modular structure for scientific articles is feasible and adequate. This suggests further research would be useful into the technical issues, concerning the implementation and testing of the modular model, and into the conceptual issues of extending, refining and adapting the modular model. Research should cover models both for electronic articles on experimental science and for publications in other domains and genres.

6.2.1 The applicability of our modular model

The components of our model

Our modular model for experimental science consists of a multidimensional typology of the information that can be used to distinguish different types of modules, and a multidimensional typology for structured links by the various relations they express. Each of the typologies consists of different components, corresponding to the various dimensions of the typology. Based on our modular model, new models can be formulated for other domains, by specifying, adapting or deleting these components, and by adding new ones.

In the typology of the information, it is straightforward to incorporate an appropriate domain-oriented characterisation in the model. For example, INSPEC terms can be used in physics; for chemistry they can be replaced by the terms defined for Chemical Abstracts. An appropriate bibliographic component can also be chosen for any domain. The set of bibliographic data we have used to characterise the information can be extended and refined in a straightforward way. We have not addressed the question as to what would be the most appropriate way of labelling modules by their domain-oriented and bibliographic characteristics; further research may be required.

The range component can be useful in any domain in which research is organised in projects and programmes with a shared background. Our characterisation by range can be refined, but it is also possible to replace our range component with a binary characterisation that distinguishes only between regular articles and ‘background modules’.

The component of the conceptual function is the main component of the typology of the information. The set of six main modules that we distinguish by the conceptual function can be used in areas of research with a problem-solving structure in which, using a particular method, results are generated and then interpreted. In other words, the basic modular structure with respect to the conceptual function may be applied to experimental and empirical research. In the physical sciences, experimental results are explained in terms of natural phenomena; in other fields the interpretation may be in terms of sociological, economical or other phenomena. Within these main modules, more and other constituent modules can be defined, to tailor the modular structure to a particular domain.

The typology for the links is less domain-specific than the typology for the modules. It has two main components: one for expressing organisational relations and the other for scientific discourse relations. Each of these components is subdivided into a hierarchy of smaller components. The organisational relations we have defined can easily be identified and expressed in any modular publication created using a modular model that has a range-component.
CHAPTER 6. CONCLUSIONS

The component of the scientific discourse relations has two main subcomponents: content relations and relations based on the communication function. Concerning the content relations, characterised links expressing dependency relations in the problem-solving process and those expressing elaboration relations can play an important role in publications of many genres in many domains. It is useful only to include our rather elaborate component for the communicative function in a modular model for a domain and genre in which different communicative functions (such as argumentation, explanation, clarification) are aimed for explicitly. The scientific discourse relations are also the most difficult to make explicit in links and the link typology remains open for further research. In particular, current research in discourse analysis and argumentation theory warrants a more elaborate analysis of the scientific discourse relations.

Our modular model is intended for the creation and evaluation of modular articles. It can be extended with a component dealing with comments on modular articles. Such an extension could be based on Trigg’s typology for ‘comment links’ [Trigg, 1983].

Based on the typologies for the identification of information units and relations, specific instructions must be formulated for the creation and evaluation of the different types of modules and links in which respectively the information and the relations are represented. A module that requires particular attention is the module Abstract, which fulfils an important role in the orientation of the reader. In this thesis, we have not addressed the question of how the abstract of a modular article should be structured and linked to the body of the article in order to fulfil this role. The abstract is the subject of a separate thesis within our project (see [Van der Tol, 1999]).

Examples of publications in other domains

As an illustration of how our modular model can be adapted to other domains, we consider four examples of publications on: 1) a predominantly experimental study of high temperature superconductors; 2) the development of a process for the synthesis of a particular compound in bioorganic and medicinal chemistry; 3) an empirical study in the domain of argumentation theory; and 4) abstract research on logic for artificial intelligence.

1) Generating experimental results: high temperature superconductors

In the domain of experimental molecular dynamics, both experiment and theory play an important role: experimental methods are used to perform measurements, and the results of these measurements interpreted are using the theory. In some domains of science, research is concentrated on experiments in which, for example, different samples are studied using the same experimental method, or where different types of measurements are performed on the same sample.

In appendix D.1, an example is given of a predominantly experimental publication: [Ihara et al., 1997], a short contribution to a major conference on materials and mechanisms of superconductivity. In this publication, a sample of a potentially good superconductor is prepared and studied using standard methods.

In a modular environment, a publication of this type does not have to include an Interpretation module. The core of the publication is a Results module. It is supplemented with a module Experimental methods about the sample preparation and further details about the experimental methods can be made available by links to mesoscopic or macroscopic modules. Modules Central problem and Situation can be included to explain what
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the authors tried to do and why. A module Findings can be included to allow reader to search for the main result under that heading. Of course, a module Meta-information has to be included as well.

2) The development of new methods: bioorganic and medicinal chemistry
In some publications in experimental science, the result reported is a newly developed method: a particular apparatus, technique or procedure, which can be used in subsequent research. A straightforward example of such a publication is described in appendix D.2: the result of the work presented in [Hutchison and Brouillette, 1998] is a procedure for the synthesis of a particular bioorganic compound. In a modular environment, the new procedure can be presented in a Results module, so that the reader can locate the original module in which the method was reported when it was first developed. When the new method is used in later work, it can be made available by means of a link in a module Experimental methods.

3) Empirical research in the humanities: argumentation theory
The main modules we distinguished for experimental science may be directly applicable to publications about empirical studies in the humanities and social sciences that traditionally have an IMRDC structure.

In appendix D.3 we consider [Van Eemeren et al., 1995], an article in the domain of argumentation theory. In this example, hypotheses are explicitly formulated and tested. In a modular environment, these hypotheses can be presented in a module Central problem, which is more extensive than the modules Central problem we have encountered in our analysis in the domain of experimental science. The methods pertain to the test design (experimental methods), statistical methods (numerical methods) and a theoretical framework (theoretical methods). The interpretation of the empirical results amounts to a discussion as to what extent the hypothesis has been confirmed.¹

4) Abstract research: logic for artificial intelligence
Our model must be more thoroughly adapted in order to be of service in more abstract domains, like mathematics. As an example, we discuss in appendix D.4 a contribution to a book published as a consequence of a conference on game theory and epistemic logic, in the domain of logic for artificial intelligence.

   Whereas the research reported in our corpus was concentrated on measurements and the interpretation of the experimental results in terms of a theory, the main activity in

¹According to [Buxton and Meadows, 1978, p.177], the proportion that the Discussion section takes up in in printed articles in social sciences (as opposed to the sections Introduction and Methods) differs from the proportion that its counterpart takes up in natural sciences. Buxton and Meadows explain this difference as follows. In natural sciences, the theoretical model used to interpret experimental results is usually part of the generally accepted paradigm. Therefore, it is clearer what measurements are relevant. However, once the measurements have been made, the authors have to clarify in the Discussion how the specific, new experimental results relate to the general, existing model. In hypothesis-testing research in social sciences, authors must formulate in the beginning a new model and an explicit hypothesis. Once they have formulated the hypothesis and performed the empirical work to test this hypothesis, they only have to point out in the Discussion whether the hypothesis was confirmed by the experimental results, so that this section can be short. Similarly, in a modular environment, the module Interpretation for this hypothesis-testing research may be shorter and less complex than the Interpretation modules that we have created in our work. This need not be the case for explorative research in the social sciences and humanities.
[Van der Hoek and Meyer, 1997] is proving theorems about a logic, consisting of a deductive system, a model and a language. Since the logic (with its three components) plays a central role in publications in this domain, it can be presented in a module Description of the logic (containing three constituent modules) that lends itself to multiple use. The counterpart of our module Methods may be a module Proving consisting of the constituents Proof techniques (which is suitable for multiple use) and Proofs. The result, a proven theorem, may then be presented in a module Theorems that the reader can directly locate, retrieve and consult.

In short, we see that the modular structure developed for experimental science can be adapted to other domains. The bibliographic component of the typologies may be standardised for all scholarly articles. The range-based component of the typology for modules and the typology for the links might be standardised for all domains in which articles are published in the context of research programmes. The domain-oriented component of the typology for modules must be customised for the domain in question. Concerning the component of the conceptual function, the modules Meta-information, Positioning (with a Central problem and a Situation) and Findings can probably be used in all domains. The distinction of the modules Methods, Results and Interpretation, or their specific equivalents, is less clear cut. For instance, in abstract domains there are no experimental results to be interpreted, and for research in which a new method is developed, that method is the result.

6.2.2 Technical requirements for implementation and testing

We have concentrated on the development of a modular model that is adequate given a theoretical interactants profile. As a test case, we have specified this model in terms of rules for writing modular articles on experimental molecular dynamics. Now that our modular model is available, the following two questions should be addressed in a representative user survey: how does the modular structure of articles affect the effectiveness and efficiency of scientific communication in practice, and do modular articles indeed meet the requirements of actual users?

The subjects of such a survey should be authors of real, new, modular articles and readers that are part of the target audience. Since the scientific community is under heavy pressure to publish in established journals, tests in mature fields with a high visibility might not be easy. Perhaps the best environment for testing a modular model is in a new area of research in which the pressure to 'publish or perish' is weaker. Another possibility is the patent literature: this literature is highly structured and compliant with various official rules. In this genre, efficiency is very important and, in addition, patents are assumed to be devoid of essayistic digressions.

For the user survey to be adequate, the users must have adequate tools and instructions at their disposal. The instructions we have given in appendix A (or similar instructions for another domain) must be further specified to guide the author in the actual presentation of the information. The implementation must satisfy the requirements formulated in the following description.

2For the textual representation of information, many standards exist. In an electronic environment, non-textual representations will play a more important role. Therefore standards must be developed for such representations as well.
The authors’ tools

Module templates

Storage and presentation of modules has to be sufficiently standardised to allow the reader to locate, retrieve and consult modules written by different authors in a similar fashion.\(^3\) Therefore, the authors must be provided with a template: a mould for their article.

The development of such templates is closely linked to the editorial policy and Instructions to authors of a particular type of publication. Given the necessity that storage of modular articles in a database must be a simple and automated process, the templates must, in their turn, be standardised by being compliant with the international standard for the definition of device-independent, system-independent methods of representing texts in electronic form: the Standard Generalized Markup Language (SGML) [ISO, 1986].

Starting from the modular model, creating a Document Type Definition (DTD) for modular articles is straightforward. The DTD defines the structure of this type of document and the tags that can be used to encode the structure of actual modular articles according to the SGML rules.\(^4\) A style sheet then determines how the tagged article is presented on screen or on paper.

The authoring tools must include the following templates:

- a template that: 1) prompts the author to create all modules required in a publication of a particular domain and genre; and that 2) allows the author to create all modules that are admissible in that domain and genre;
- a template for the internal structure of the modules. In particular, it must be possible, during the writing process, to tag details or overlap that can be hidden from sight in the reading process;
- a fine-grained template for the module Meta-information;
- ‘label templates’ for the characterisation of the modules and the links.

Furthermore, the authoring tools must connect the module Meta-information to the meta-information specified in each module in such a way that the consistency of the meta-information is ensured, and that the author needs to provide the meta-information only once. The tools must:

- connect the module Bibliographic information (m1a) to the bibliographic characterisation of each modules;
- connect the module Lists of domain-oriented index terms (m1b) to the index terms specified in the label of each module;

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\(^3\) Usually, modules will coincide with storage and presentation units, i.e. with files and with hypertext nodes. However, we emphasise that this is not necessarily the case. If a particular module is too large and cumbersome to be rapidly downloaded in its entirety, it can be stored in more than one file.

\(^4\) The DTD defines the elements that the article can consist of (e.g. different kinds of complex modules and elementary modules, module labels, overlapping text, figures, link labels) and rules for the relations between elements (e.g. the fact that a complex module has to be connected –directly or indirectly– to at least one elementary module, by means of a link expressing a hierarchical relation).
• connect both the Map of contents (m1d) and the module Lists of references (m1e) to the links in the navigation menus and in the text of the modules.

Map-making kit
The basic problem-solution pattern of scientific articles can be laid out in a map that provides an overview of the components the author has to create. The author can use that general map as a starting point for the Map of contents of the article he is creating. For that purpose, he requires a ‘map-making kit’ consisting of graphics software complemented with basic templates for the creation of a particular type of publication in a particular journal. The domain and genre specific templates must allow the author to customise his presentation within the limits established by the journal. The map-making kit must:

• enable the author to draw a map of a modular structure from scratch;
• represent finished modules automatically in the map;
• indicate automatically, or allow the author to indicate, the stage of completion of the different parts of the structure, distinguishing at least between:
  – components that are required by the basic guidelines;
  – components planned by the author;
  – finished components.

Link aids
As we concluded in chapter 5, identifying and expressing the different relevant relations is a complicated task. However, that task can be alleviated by ‘link tools’ for the generation, characterisation and presentation of the links.

• The link aids must enable the author to define the source and the target of the link (by hand, by browsing or by searching).

The author must be able to refer to a specific part of any new or published module, not just to the module as a whole. In the current version of the Hypertext Mark-up Language, HTML 4.0 [Ragget et al., 1998], a hyperlink to a particular point in a node is possible, but not practical. The first drawback is that it requires an anchor at the appropriate location in the target, and that anchor can only be inserted there by the author of the cited article, not by the author of the citing article. The second drawback is that there is no indication where the relevant part stops (i.e. where the reader can stop reading according to the author of the citing article). These problems may be solved by the development of the Extensible Markup Language (XML). Draft specifications are available of an XML Linking Language (XLink) and an XML Pointer Language (XPointer) [Maler and DeRose, in progress]. Using these languages it is possible to specify a new link annotating an existing document. It is also possible to specify links to multiple destinations, which can be targeted at specific places inside a document or specific portions of a document, even when the author had not specified an anchor at that particular place.

• The link aids must enable the author to select, in a pull-down menu, the different relations that he wants to express in the link;
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- The link aids must generate automatically the links expressing:
  - the administrative relations between the Meta-information (and its constituent modules) and any module representing scientific information that is created in the article;
  - the hierarchical relations that occur as soon as complex modules are created.

- The link aids have to characterise automatically any link that is created, by the author or by the system, with:
  - range-based labels;
  - proximity-based labels.

- Based on a standard set of links and the links specified in the text, the link aids must generate at least semi-automatically:
  - the table of navigation;
  - the representation of the links in the Map of contents;
  - the references in the module Lists of references.

The author should be enabled to adjust the automatically generated, characterised and presented links. When the author adjusts a link in the table of navigation, the Map of contents or the Lists of references, the other presentations of the links must be updated (semi-)automatically. In this case, the author also must be prompted to adjust the text of the source module: for example, the link aids can generate a list of the links that have been recently added or modified.

The system must keep track of both ends of a link (the source and the target). The navigation menu shows not only the links leading from the module at hand to other modules, but also the links from other modules to the module at hand as a target. A link to the module at hand may be created after the publication of this module; therefore, the navigation menu and the map of contents should not be stored hardwired into the modules, but be generated on the spot when the module is consulted, based on the collection of characterised links leading to and from the module.\(^5\)

- The link aids must provide a template for an explicit bibliographic label, in the event that a new link is created between published modules.

For the reader, it is not only important to know that particular modules are connected by a link of a certain type, but also to know who created that link and within what context. In other words, in order to meet the authenticity and integrity requirements of a scientific article, the links must be as fully characterised as the modules and all other ‘published items’.

When a link is created by the original author at the same time as its source module, its bibliographic characteristics are implicitly determined by the bibliographic characteristics of the link.

\(^5\)Using the XML Linking Language [Maler and D’Rose, in progress], it will be possible to specify bidirectional links, and to create link databases that allow for filtering, sorting, analysing, and processing link collections.
characterisation of the source module. This is the case for the links that we have created and discussed in this thesis, because we have concentrated on the creation of entire modular articles rather than on the addition of individual modules or links to published work. However, in a modular environment new links can be created by new authors between existing modules. These ‘added’ links should not only be characterised by the relations they express, they should also be endowed with explicit bibliographic labels.

The readers’ aids

A modular article in an electronic environment may have many complicated features. The reader therefore has to be able to customise the presentation, which implies that the most important goal of the readers’ aids is flexibility.

Locating, retrieving and printing

Readers require a search engine that allows for complex searches of entire articles, complex modules and elementary modules. It must be possible to search by:

- module labels;
- phrases from the full text in any particular module;
- link labels;

or combinations thereof. For instance, the reader must be able to locate a microscopic Results module, dealing with the differential cross section of collisions between sodium and iodine atoms, that is connected to a module Experimental methods, about a molecular beam set-up, by means of a problem-solving dependency link. Another example is the search for a mesoscopic Experimental methods module on surface ionisation, that is the target of at least ten links carrying proximity-based labels indicating that the source is not part of the same article and resolutions-labels indicating that the target provides details.

Once the reader has located the modules of interest, he should be able to print individual modules (automatically including the images and other non-textual but printable parts) as well as any selected collection of modules.

Modules

Just as for the traditional scientific article, the modular article, as well as each individual module, is a self-contained representation of scientific information. Therefore, we must keep in mind that many of the same presentation issues that have to be taken into account when writing a traditional article remain valid in the modular case. The internal structure of modules has to be made visible by means of typography, paragraphs and sections. If the reader prefers to print the module on paper, the presentation of the printed version may be adapted to the paper medium.

In addition to the traditional presentation requirements, the modular structure leads to requirements concerning the composition of modules and links. Complex modules, which consist of linked constituent modules and a ‘module summary’ summarising them, should be implemented in a ‘recognisable’ way. For example, the module summary may
be presented in a different font or colour than the elementary modules. The exact presentation should not be hardwired into the module, but rather stored in SGML type tags. The presentation then can be managed through the style sheet.

The reader’s main requirement concerning the implementation is that the presentation should be flexible. In particular, the reader must be able to unfold or hide:

- mathematical digressions and other details;
- parts of modules that overlap with other modules that the reader may already have consulted;
- the characterisation of the module and the navigation menu;
- full figures (which can be replaced by thumbnail figures);
- unprintable representations of information (e.g. java applets).

**Links**

The distributed presentation obscures the coherence of the information: if the reader does not understand the target and the nature of the links connecting the modules, he cannot make a well-considered choice as to whether to follow the links or not. Therefore, the type of the link must be made explicit as well as its target. Rather than identifying the target with an uninformative identification code, the author name and publication date of the cited module may be made explicit. In addition to the type and the target of the link, a short phrase can provide further clarification. This characterisation should be hidden from view, and only be made visible on demand. For example, the link may be represented in the text by a small icon (different icons may be used to indicate the main function of the link) and the characterisation may be shown in a ‘pop-up’ box when the reader moves his mouse onto the icon.

If a particular point in a module serves as a starting point for more than one link, the various links may be routed via a menu. For example, at a particular feature in the graphical of the results a link may be provided for zooming in on that feature, another for comparison of that feature to a similar feature in another Results module, and a third to its interpretation.

Many explicit links could also make a modular article unreadable. The reader must therefore be able to choose how the links are presented: as elaborate informative icons, as unobtrusive icons, as words, or completely hidden from view. The different types of links should in principle be distinguishable at first glance. Links that have been created to express an organisational relation may be presented using a different colour, font or icon than links created for the different kinds of scientific discourse relations.

Furthermore, the reader requires tools that enable him to:

- customise the organisation of his screen. For example, if he activates a link, he can view the target:
  - in the same window that the source of the link occupied previously;
  - in a separate window overlapping the window presenting the source;
  - in the other half of a ‘split-window’ that allows for simultaneous viewing.
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The organisation of the windows may depend on the type of the link. An external link may, for instance, be considered a detour and lead to a separate window, whereas a link expressing a similarity relation calls for direct comparison and thereby for two neighbouring windows; a sequential link would stay within the same window, and the Map of contents may be permanently kept in a corner of the screen.

• define a personal sequential path.

In the modular model, we have defined sequential relations that allow the reader to consult the complete article (via the complete sequential path) and to consult the modular article as if it were a traditional, linear article (via the essay-type sequential path). The reader must also be able to define a personal route through the article, which he then can follow by way of ‘next’ buttons. Navigation links for those paths should be provided at the bottom of a module, allowing the reader to simply ‘turn the page’ after reading the module, but also at the top to avoid forcing the reader to scroll through the entire module.

Overview
At all times, the reader of a modular article should have at his disposal the navigation menu of the module at hand, as well as the Map of contents and the Abstract of the article.

In an electronic environment, the map of contents must be interactive: the representations of the modules in the map must be linked to the modules themselves by hyperlinks. The map should also indicate (on demand) which ‘content module’ the reader is currently consulting and which modules he has accessed before (if any). The map of contents must be flexible, because it is too complex to be presented in full detail to the reader. The reader must be able to:

• choose which types of relations are visible and to what degree of detail he wants to view the map;

• zoom in on the details of modules and links. The default presentation includes each module in the article without links, except the complete sequential path. The reader may also hide all constituent modules and concentrate on the main modules, or add more details such as (all or some specified types of) links between (all or some specified) modules, the mesoscopic modules linked to the modules of the article, or the full physics characterisation of modules.

• generate a Map of contents representing the structure of a larger network of modular publications based on the information stored in the ‘journal database’ about the modules and the links connecting the various modules.

Publishing & archiving
Although our study suggests a novel way of publishing, we do not challenge the societal role and place of the scientific article. Our model may be directly applied in an electronic journal environment provided that the necessary software is in place. The editors of ‘modular journals’ can specify the modular model in terms of instructions to authors and templates. If the model is not immediately valid for the domain and genre at hand, it may be adapted.
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We assume that there is some form of peer review or editing process for checking the resulting modules and the labels in which their characterisation is made explicit, as well as the links and their labels. The refereeing of mesoscopic modules should be more rigorous with respect to completeness, comprehensiveness, and correctness than in the case of a microscopic module. A macroscopic module has a status comparable to that of an ‘advanced text book’, since it has a larger, less well-informed target audience. It has to be written explicitly as a macroscopic module and be evaluated more rigorously by the referee to ensure its quality.

The system must allow for updates and additions of modules and links. For example, in the module Bibliographic information the current addresses of the authors has to be kept up to date. Intermediary results may be identified and made explicit by the author at the time of publication, or at a later stage by the author or an editor, for example, in an update of the characterisation of the information. Links may be added between comparable Results and, if the Results turn out to be wrong, the reader must be warned and referred to the new insights.

Rules will have to be specified for the management of the database. For example, modules and links should not ‘disappear’ when they become obsolete, because that would compromise the integrity of the system. Rather than replacing the entire module or link, a new version may be created and explicitly linked to the old version, as well as to the related modules.
Summary

In this thesis we have developed a modular model for scientific articles. We propose to group the different kinds of information into different modules and to express the coherence of this information in the composition of the modules into complex modules themselves in explicitly characterised links that describe various relations between them.

In chapter 1, we have sketched the context of this thesis. Emerging electronic publication technology could make the overloaded process of scientific communication via articles more effective and efficient. The linear format of the traditional article is tailored to the paper medium but it is not necessarily equally suited to new media. We have aimed to define a structure for electronic scientific articles that fulfils the authors’ and readers’ needs and that takes full advantage of the specific characteristics of electronic media.

In chapter 2, we have set out the main features of scientific communication by the use of articles and the requirements of the scientists involved in that process. Readers require a clear presentation of precisely that information that is relevant to their information needs and sufficiently reliable, without being encumbered by redundant information. The authors require the capability to present all their work in a convenient way and, since they wish to communicate their work to the readers, they also require the readers to be able to locate, retrieve and consult it.

The main feature of new electronic media concerning the structure of articles is the possibility of hypertext – storing and presenting information in a well-defined distributed way, enhanced by a linking system. The scientific discourse in a printed article is presented and stored as a linear essay, and can only be retrieved in its entirety. In practice, however, readers often consult only particular parts of the article. In an electronic environment, this reading strategy can be anticipated: an electronic article can represent a network of information units within the network of all scientific information available in published work.

This chapter culminates in a set of ‘communication criteria’ that the structure of scientific electronic articles must meet in order to allow for effective and efficient communication.

In chapter 3, we have introduced the notion of a modular structure as a pattern of modules and links between them. A module is defined as a uniquely characterised and self-contained representation of a conceptual information unit, aimed at communicating that information. The most basic component of the scientific article is the elementary module. From this elementary level, we allow syntheses into complex modules.

In the modular structure, the coherence of the information is not only expressed by the
composition of modules but also by means of links. A link is defined as a uniquely characterised, explicit, directed connection, between entire modules or particular segments of modules, that represents one or more different kinds of relevant relations. In practice, a link is an explicitly labelled hyperlink.

In chapter 4, we have presented our modular model for experimental science. To determine what can be considered as similar information that is to be represented in a single module and to determine how the resulting module is to be characterised, the general definition of a module has been complemented with a domain-specific typology for grouping the information. Likewise the definition of a link has been complemented with a typology specifying the types of relations that can be expressed in a link.

The first main component of the model is the typology of the information. In the characterisation of the information we have chosen to take into account four different aspects: the conceptual function of the information, its domain-oriented content, its range, and its bibliographic characteristics.

Firstly, we have developed a characterisation of the information by its conceptual function, i.e. by the role that the information plays in the problem-solving process of the research. This forms the core of the model. The main modules of scientific articles represent information units distinguished by this characterisation. Following the conceptual function, we have defined the modules: Positioning (composed of Situation and Central problem), Methods (that can consist of Theoretical Methods, Numerical Methods and Experimental Methods), Results (that can be composed of Raw Data and Treated results), Interpretation and Outcome (to be made up of Findings and Leads for Further Research).

Secondly, the modules distinguished by the conceptual function are further refined from the domain-oriented point of view. For example, different kinds of results for different types of chemical reactions are represented in different modules. In this case, the Treated results is a complex module containing constituent modules with the specific results. The characterisation of the information by its domain-oriented content, in terms of key words or other index terms, is standard practice; we have not developed new terms.

Thirdly, we introduce in our model a characterisation of the information by its range. On the basis of the range, we can distinguish between information that is unique to the article itself (microscopic), information that plays a role in the research project from which the article is issued (mesoscopic), and information that plays a role in the field in general (macroscopic).

Finally, the modules that represent information units distinguished by these three aspects are labelled by specified bibliographic data, such as the authors’ names and the publication date. Since in the characterisation of the information by its domain-oriented content, the bibliographic data are already used in standard practice; we have not developed a new bibliographic approach.

In order to express all relevant bibliographic information we have also defined a module Meta-information in addition to the modules representing scientific information. This module serves as a linchpin holding the article together. Important components of this module are the Map of contents, which is an extension of the linear table of contents, and the Abstract.
The second main component of our modular model is a systematic typology for the links. The type of a link is determined by the different kinds of relations it expresses. We have found it both feasible and useful to distinguish two main classes of relations: *organisational relations* and *scientific discourse relations*.

Links representing organisational relations, which can be identified between entire modules, organise the modules into an explicit network. A useful type of organisation relation yields an ‘essay-type sequential path’, which guides the reader along the important modules in a way that mimics a linear essay. Links expressing ‘administrative relations’ allow the reader to switch between the modules representing scientific information and modules with meta-information about the article, such as the Map of contents. We also define ‘hierarchical relations’, ‘range-based relations’, ‘proximity-based relations’ and ‘representational relations’.

The class of scientific discourse relations is very broad. We distinguish two main subclasses of scientific discourse relations. The first is the subclass of ‘relations based on the communicative function’ that can be identified between entire modules or parts of modules: ‘elucidation relations’ and ‘argumentation relations’. The second is the subclass of ‘content relations’, which can not only be identified between modules or parts of modules, but also between the information units underlying the modules and between the entities that these information units are about. For instance, specific content relations express the dependency of particular results on the methods used to generate them, while others express the agreement between particular results or the fact that an elaboration is given of a particular part of a module. We furthermore distinguish ‘synthesis relations’ and ‘causality relations’.

To ensure that the model is grounded in scientific practice, we have developed the model in conjunction with an analysis of published articles. These articles concern experimental molecular dynamics, which can be considered as a prototypical experimental science. Our sample was a coherent corpus of high quality articles in this field. We have analysed original articles and recast them into modular form; in other words, we have ‘modularised’ linear articles.

Modularising linear articles has enabled us to compare the modular versions to their original versions in the light of the authors’ and readers’ requirements. We have used our experiences in the modularisation process iteratively, as feedback, to improve the modular structure. Thus, the evaluation of modularised articles has allowed us to determine useful specific rules for the creation of adequate modular articles on experimental molecular dynamics. These are given in appendix A. The instructions are in principle intended for authors writing modular articles from scratch, although we have applied them in practice as guidelines for the modularisation of existing articles. Two modularised articles are given as examples in appendix C in the electronic version of this thesis. Guided by the specific analysis, we have been able to formulate a more general modular module for experimental science. Other modular models for other domains and types of publications can be derived from this particular model.

In chapter 5, we have evaluated the feasibility and the usefulness of our modular model by discussing the modularisation process and the resulting modularised articles presented in appendix C in the electronic version.

Modular articles are not completely different from linear articles. The modules dis-
tinguished by the conceptual function of the information have been defined analogously to the sections in traditional linear scientific articles published on paper. Therefore, the basic structure of a modular article resembles the basic structure of a traditional article. Also, in modular electronic articles the same systems of domain-oriented index terms and bibliographic labels can be used as for linear, printed articles. However, the modules turn out to differ too much from their corresponding sections to make it practical or even possible to automatically transform linear articles into modular articles. The most efficient way of creating a modular article is to do so directly, instead of recasting a linear article in modular form. In order to be able to write a modular article in practice the author will need appropriate authoring tools.

The key difference between the modular structure and the traditional section structure is that the modular structure is more explicit, systematic and fine-grained. It is thus clearer and more flexible, allowing the reader to follow different paths through the information network and facilitating multiple usage by the author. Furthermore, the multidimensional characterisation of the modules and of the links allows for more complex searches. The index terms associated with a particular module can be far more precise than the index terms associated to an entire article, and the traditional labels are complemented with range-based labels and labels associated with the conceptual function. In addition, the characterisation of the modules is complemented with an explicit characterisation of the links that can be taken into account in complex searches.

Modular articles are designed for selective reading rather than for reading an entire article linearly. The first consequence is that when a reader wants to consult all components of the article he has to navigate. However, the creation of the sequential path has made this navigation as easy as turning pages. The second consequence is that in order to make each module self-contained we had to introduce different kinds of overlap between the modules. The overlap could be disturbing for readers who consult more than one module, but this problem can be solved in the implementation by using the possibilities of electronic media.

Mesoscopic and macroscopic modules increase the efficiency for the author, since published modules can be integrated into new modular publications by means of explicitly characterised links. In this way, the description of an apparatus or of a theoretical model, the presentation of important results, and other representations of information that are suitable for multiple usage can be re-used in a convenient way that gives full credit to the original authors. These modules increase the efficiency for the reader as well: firstly, they are more complete than the individual original articles were and secondly, the reader can easily avoid them.

We have found that mesoscopic information can easily be represented in the mesoscopic modules Situation, Central problem (about the context and the central problem of the research project as a whole), Experimental methods and Theoretical methods. The most obvious candidates for macroscopic modules are Experimental methods and Theoretical methods (with established experimental set-ups and theoretical models and theories).

The part of the article that lends itself best to modularisation is the account of the experimental methods, since in the original articles the set-up was restricted to a particular section. In a modular environment, modules Experimental methods may be easily created by the author. The reader can consult or avoid them in an efficient way, depending on the question whether he needs experimental details.

The modules Positioning and Outcome, and their constituent modules, were less easy
to recast. However, defining and determining rules for these modules was quite straightforward. It is probably easier to write these modules directly in a modular form. They are quite useful to the reader, the Situation being particularly useful for less informed readers. In particular if the interpretation of the results is complex, the module Findings plays an important role in the clarification of what has been achieved in the article, or in directly informing readers who only wish to consult the findings of the work. Defining and determining concrete rules for the module Results and its constituents was more difficult. Applying the rules to form modules, however, was not difficult and the resulting modules are likely to be consulted by many readers.

The part of the article that is most difficult to modularise concerns the interpretation of the results. This is probably the most difficult part to write in any representation of scientific research, since the interpretation involves a complex scientific discourse. Making explicit the structure of the discourse in the modular structure does clarify it, so that the modular version of the article turns out to be more readable than the original version.

The coherence of the information is adequately expressed by the composition of the modules and by the characterised links. In the modularised articles, several layers of complex modules were required to make the structure of the information explicit. The ‘module summaries’ of their constituents and the relations between these constituents turn out to play an important role in clarifying the article. In the original version, it is only the abstract that provides an overview of the content of the article. In the modular version the module summaries give the reader additional assistance.

Representing organisational relations in characterised links turns out to be quite simple. With respect to scientific discourse relations, we found that most content relations can also be easily and usefully expressed in links. However, it is often quite difficult to decide precisely which relations based on the communicative function, which synthesis relations and which causal relations should be expressed. Expressing such relations directly in new modular article will probably be easier than making them explicit during the modularisation process.

In chapter 6, we conclude that it is indeed possible to formulate a modular model for the structure of scientific articles that can allow for effective and efficient communication. The modular structure enhances the clarity of scientific articles and facilitates multiple use of modules. It also allows the reader to selectively locate and consult individual modules, as well as sets of related modules. Since we have developed multi-dimensional typologies for both the modules and the links, readers can locate a module representing relevant information by means of a well-considered browsing path or by means of a complex search in which they can take into account not only the different aspects by which the information is characterised, but also the module’s embedding in its context.

We have developed our modular model for articles in experimental science. By adapting and replacing components of the typologies for modules and link, modular models can be derived from our model for other domains. We illustrate the applicability of our model by considering examples of other types of publication in the light of the modular structure.

In order to determine whether modular articles can improve scientific communication in practice, the model must be implemented and subjected to a user-survey. We have formulated a set of requirements for this implementation to satisfy: the authors and readers need appropriate tools to take advantage of the benefits of the modular structure.
Our modular model has been developed for articles on experimental sciences. This thesis is a different type of publication. However, we can consider it roughly in terms of the modules that we have defined. The Situation pertains to electronic scientific publishing, and the authors’ and readers’ requirements, as described in chapter 2. Our Central problem is to determine the optimal structure for articles, given the requirements of the interactants and the characteristics of the electronic media. With respect to the Methods, we have developed a modular model by means of the analysis and modularisation of a sample of published articles on experimental molecular dynamics. The modular model given in chapter 4, with the associated specific rules for writing modular articles on experimental molecular dynamics that are specified in appendix A, form the Results. The modularised articles given in appendix C may be seen as intermediate results. We could not interpret our result in terms of some theory. In this thesis, the counterpart of the Interpretation is the evaluation of the model, by way of the evaluation of the modularised articles, in chapter 5. Our main Findings are listed in section 6.1, and in the section 6.2 we have suggested some Leads for further research.
Appendix A

Guidelines for writing modular articles

The modular model for experimental sciences presented in chapter 4 defines the types of modules and links that are allowed in a modular scientific article. In order to apply the model to the creation of actual modular articles in a specific domain, we have to specify which particular modules and links are required in a modular article, which ones are allowed, and how these modules and links can be put together to form an adequate modular article.

In this appendix, the modular structure for the field of experimental molecular dynamics is specified in terms of generic guidelines for writing modular articles. These guidelines do not include instructions to authors on technical details, for instance, with respect to the style of the bibliography. Instead, we indicate, in the form of side-remarks, what kind of specifications the publisher of a particular modular journal should provide its prospective authors with. A procedure for the creation of modular articles in this domain is given in section A.1. Then, more specific guidelines are given for modules in section A.2 and for links in section A.3.

Formulating the guidelines, we assume that authoring tools facilitating the creation of a modular article are available. For example, the author should have at his disposal a template for the basic modular structure and in particular for the module Meta-information, as well as user-friendly software to generate certain links automatically\(^1\). In an electronic environment, the guidelines for a particular type of module can be presented in an entirely self-contained unit, to assist the author in his work. We also assume that the information given in chapter 4 is available to the prospective author of a modular article, so that we can concentrate on the domain-specific guidelines without repeating the general definitions.

Two electronic modular articles created following these guidelines are given in appendix C of the electronic version of this thesis, and in chapter 5 the resulting modular articles are evaluated in the light of the interactants profile specified in section 5.1.2.

\(^1\)In section 6.2.2 requirements are given for such authoring tools.
A.1 Guidelines for a modular structure

A.1.1 Composition

The smallest building blocks of a modular structure are elementary modules, which can be composed into complex modules. There are two kinds of complex modules: 1) A compound module contains a set of constituent modules, each giving an account of a component, that are aggregated into a higher-level entity; and 2) A cluster module contains a set of similar constituent modules focusing on specific concepts that are generalised in the higher-level cluster module. A complex module contains:

1. its constituent modules (which can be elementary modules or lower-level complex modules);
2. the links between the constituents;
3. a Map of Contents of the complex module, as a separate map or as part of a larger map;
4. a module summary, if necessary for the reader's understanding.

In order to obtain a modular structure expressing the problem-solving process of the research, you have to represent the information in the ‘main’ scientific modules reflecting the steps of that process: Positioning, Methods, Results, Interpretation and Outcome (for which guidelines are given in the next section). A modular article in this domain is composed of at least:

1. one of each of the following ‘main’ scientific modules:
   (a) Positioning, containing a constituent module Central problem and a constituent module Situation providing at least a link (labelled as ‘More context in’) to a module published elsewhere providing an embedding of the research in its context;
   (b) Methods, containing at least a link (labelled as ‘Is detailed in’) to a module published elsewhere with an account of the methods used in the research;
   (c) Results, containing at least the treated results that have been obtained in the research reported in the article;
   (d) Interpretation, containing at least an (attempted) explanation of the results;
   (e) Outcome, containing at least a brief recapitulation of what has been achieved in a constituent module Findings;
2. a module Meta-information, with standardised meta-information;
3. a complete sequential path through the article expressing sequential relations;
4. links expressing administrative relations between the module Meta-information and each scientific module in the article.
A.1.2 Physics content

Characterise the physics content of the information by means of index terms.

The editorial board of a particular journal can specify what kind of index terms are allowed. If there exists a standard, certified and maintained classification for the domain at hand, it should be taken into account. In the domain of experimental molecular dynamics, the INSPEC Physics Abstracts classification scheme and the similar Physics and Astronomy Classification Scheme (PACS) are standard.

The editorial board of a journal can stipulate that only index terms derived from the standard classifications may be used. They can also stipulate that the controlled classification codes and keywords can be complemented by uncontrolled terms, which the author considers to be relevant but which are not included in the official classification. In that case, the uncontrolled terms must be explicitly indicated as such. The board can also allow for any scientific or technical term to be used in the characterisation of the information. Readers can also use free text searching to locate the information by its content, instead of using the index terms, or in addition to the index terms. The advantage of using standardised index terms is that the recall is not lowered by variations in the formulation of the label.

*Example:* Let us consider a reactive scattering process in which K atoms collides with Br₂ molecules, forming KBr and Br. The information can be characterised by a single compound label such as ‘scattering K + Br₂ → KBr + Br’. It can also be characterised by a set of five equivalent, unstructured simple labels, such as ‘reactive scattering’, ‘K’, ‘Br₂’, ‘KBr’ and ‘Br’. Information about scattering processes can also be represented in a structured multidimensional space. It is at least spanned by the following dimensions: a dimension representing the type of scattering (elastic, inelastic, reactive), two incoming interactants, one with the products, and also a dimension with the energy range. Just as every colour has a hue, a saturation and a brightness, every scattering process has its interactants, product and energy. In terms of keywords, the information on the scattering process can then be represented in a complex characterisation with arguments, such as ‘scattering[K,Br₂;KBr,Br;1eV]’.

A.1.3 Procedure

In order to cast the information in a modular structure, take the following steps:

1. **Problem-solution pattern:**
   First, organise the scientific information by its conceptual function, into a problem-solution pattern, dividing it into information units following the guidelines specified in section A.2.

   In a single article, report on a single problem-solving process. This process can be complex. If you have addressed in your research different problems, report on them in the same article only if they are related ‘sub-problems’ of a higher-level general or aggregate problem. In that case, indicate in the module *Positioning* how the central problem is structured.
Include in the article one and only one of each of the main modules summarised above, and group the modules of the same type, even if associated to the different lines of inquiry, within a single, complex module. For example, when different methods were used for the solution of the central problem, give an account of these methods in different constituent modules and include these modules in a complex Methods module.

- In a parallel problem-solving process, different sub-problems are addressed simultaneously, in parallel lines of research. These lines are brought together in the module Outcome, which addresses the solution of the central problem. For instance, in case you have tried different methods parallelly in order to solve the general problem, provide a report in separate, specific modules that are generalised in a compound Methods module.

- In a serial problem-solving process, different sub-problems are solved sequentially: the outcome of each sub-problem-solving process is needed for the solution of the next sub-problem. The final step then leads to the Outcome. For each step, give an account of the methods, results and interpretations in a constituent module that is a component of the main modules Methods, Results and Interpretation respectively. Use a sequential path connecting the constituent modules to indicate the sequence of the serial problem-solving process.

- If a step in the problem-solving process involved the solution of a subsidiary problem, i.e. if the problem-solving process was nested, express the subsidiary problem-solution pattern in the internal structure of the module representing that step.

II Physics-oriented structure:
Then, organise the information within those units by its physics content, dividing it into smaller information units that focus on one topic, following the physics classification.

III Range-based structure:
If your work is part of a research project, group the information with a mesoscopic range and the information with a macroscopic range.

- Check whether the mesoscopic and macroscopic information has already been represented adequately in a published mesoscopic or macroscopic module.

- If such a module does not exist yet, represent the mesoscopic information in a mesoscopic module designed for multiple use in various articles issued from the same project. Include in these modules a full report of the issue at hand and all argumentation that is necessary to inform and convince even the least informed part of the target audience.

If part of the information plays a role in the research domain as a whole, if you want to represent that information in a module, and if the information is not adequately represented in another macroscopic module, you can represent that information in a macroscopic module designed for multiple use in works by any author in the domain. However, it is not
recommended to created macroscopic modules as a simple side product of an article.

Because these higher level modules are designed for a wider and less informed audience, elaborate and strict guidelines are necessary for mesoscopic modules, and even more so for macroscopic modules. The guidelines we present here focus on the article. Mesoscopic and macroscopic are not really a part of the article itself, although they are part of the larger network of modular publications.

- If (or as soon as) such a module exists, link it to the microscopic module it corresponds to and represent in the microscopic module only the information that is specific to the current article.

In the resulting modules:
Represent the information units with a microscopic range (i.e. the information that you want to communicate to the reader in this particular article) in microscopic modules, by expressing the information in a 'language' (text, formulae, pictures, tables, or other audio-visual language).

| Make these modules self-contained, i.e. make sure that the modules contain sufficient information, that is represented sufficiently clearly, to allow at least experienced researchers in the domain of experimental molecular dynamics to satisfy a specific information need. Provide in each module a report of a specific stage or component of the research, in sufficient detail to allow the members of the target audience to understand it. In principle they must be able to repeat the work, and in practice they must be able to use the information in their own research. The details can either be included directly into the module, or made available by means of a link to a previously published module, in particular to a mesoscopic or macroscopic one.

- If the target audience is unlikely to be convinced beforehand of the reliability of the information, justify it by argumentation. If the target audience is unlikely to be convinced beforehand of the relevance (the applicability), justify that. You can also point out and justify the relevance of the research to other issues.

V Composition:
Following the guidelines given in section A.3, identify the relevant relations between the information units represented in the modules.

- Represent the collection of information units in a complex module, rather than in unconnected modules, if the complete collection can be considered a larger, single unit, so that separating them obscures the coherence of the information.

- Represent a coherent collection of information units in a complex module, rather than in a large but monolithic elementary module, if the constituent units can be represented in self-contained modules that members of the target audience are likely to locate, retrieve and consult.
• Represent information in an elementary module, if representing only parts of it would lead to a unit that is meaningless when consulted separately.

Compose into complex modules all elementary modules that represent:
• microscopic information units that resulted from a division of a unit with a particular conceptual function into smaller units by their physics content.
• in particular, any information units about the components of an aggregate, when you presume that members of the target audience will want to locate, retrieve, and consult the module representing the aggregate information unit as a whole (a compound module)
• in particular, any information units focusing on specific concepts that can be generalised, when you presume that members of the target audience will want to locate, retrieve, and consult the module focusing on the generalised concept (a cluster module)

1. Provide a map of the complex module for an organisational overview.

2. If readers are unlikely to grasp the coherence of the information distributed over the constituent modules, provide at the level of the complex module a content-oriented overview, similar to an abstract: a ‘module summary’ in which the coherence both of the information and of the constituent modules are expressed.

Given appropriate authoring tools, the map of a module could be generated from the complete ‘map of contents’ of the article, and included in a module by means of a link. Guidelines for the module summaries and the relation of the module summaries to the abstract of the article as a whole are discussed in [Van der Tol, 1999].

VI Meta-information:
Group the meta-information about the modules and the links, and represent it in a module Meta-information, following the guidelines given in section A.2.

• Make the characterisation of each module explicit in a unique label expressing the conceptual function, the physics content, the range of the information and a set of bibliographic data: the title of the article, your names and the names of the institutes where you conducted the research. When the article is accepted for publication, the name of the journal, the name of the publisher, the publication date and a unique identification have to be added (see the guidelines for the module Bibliographic information).

VII Links:
Represent the relations that have been identified in a –potentially complex– link connecting the source module to the target module, and characterise that link explicitly by assigning a label to it expressing 1) each relation represented in the link, and 2) the bibliographic information about the link

• At least represent in each module the following relations: administrative relations between the content module and the meta-modules Meta-information, Bibliographic information, Map of contents, and Abstract,
between the module at hand and the previous step and the next step on
the complete sequential path and the essay-type sequential path. Repre-
sent the hierarchical relations between every complex module and each
of its constituent modules. Represent the proximity-based relation and
the range relation in each link that is provided in the module.

- Create in each module a 'navigation table' listing all links, with their
characterisations, connected to that module as a whole or to a segment
of that module, either as a source and as a target of the link.

A.2 Modules

A.2.1 Meta-information (m1)

- In order to present the meta-information about the article, compose a
compound module Meta-information consisting of five compulsory constituent
modules (Bibliographic information, Lists of physics index terms, Map of
contents, Abstract and Lists of references) and one optional constituent
module (Acknowledgements).

The editorial board or the publisher will have to specify what meta-information is precisely
required, in what format, and who is responsible for it - the author or the publisher. The
different types of metadata and their manipulation are discussed from the angle of SGML.

- At the level of the compound module Meta-information, provide a table of
contents of the constituent modules.

- If you have created mesoscopic and/or macroscopic modules in conjunc-
tion with the article, also provide the meta-information about those mod-
ules. Connect each mesoscopic and macroscopic module to a module Meta-
information that consists of at least a constituent module Bibliographic in-
formation and a Map of contents that provides a graphical representation of
these modules and the modules connected to them. The other constituent
modules of the Meta-information are optional.

- Either compose a module Meta-information for individual mesoscopic or
macroscopic modules, or, if you have created (an addition to) a coherent
set of mesoscopic or macroscopic modules, link each module to a Meta-
information that is valid for all of these module.

Bibliographic information (m1a) Give in this module:

- the full title of the article; The title should be informative, so that readers
can select articles that are relevant to their needs by browsing titles.
In the domain at hand, scattering plays such an important role that the type
of scattering reaction under consideration usually should be mentioned in the
title.
Figure A.1. The module meta-information and the modules distinguished following the conceptual function of the information, and the sequential paths leading through the article. The dashed line indicates the complete sequential path, and the dotted line the essay-type sequential path.
A.2. MODULES

- the name of the journal in which the article is published, the name of the
  publisher of the journal, and the unique identification of the article as
  assigned to it by the publisher, which encodes the journal in which the article
  is published.

The unique identification has to be standardised for all publications in a wide area. It
would be handy if that unique identification could tell the expert something about the
article, for example, by encoding the journal name, the date and the type of module. Currently, there are various initiatives to assign a unique identification to publications
[Paskin, 1999].

- the family name and either the initials or the first name of each author. If
  applicable, specify which author is responsible for which module. In addition,
  provide the names and addresses of the institutions each author was
  associated to at the time the research was performed. If available, include
  the current address where each author can be reached. These addresses can
  include an e-mail address, the address of a home page and an address for
  postal mail.

The editorial board or publisher of a particular modular journal should provide specific
rules for these bibliographic data in order to standardise them. Author names, for ex-
ample, may cause many problems in practice. In general, each author’s family name and
first names should be provided in a particular format: first names first or first names last,
in full or in terms of initials.

Things get complicated when authors have non-standard western names, for instance,
without a specific first name. Even if the structure of the author names has been deter-
mined, the spelling and in particular in transcription of non-western alphabets, can vary.
In for instance [Borgman and Siegfried, 1992], these problems are discussed in detail.

The format of the addresses should also be specified: how to present the address
for surface mail, for example, and whether the address for ‘traditional’ mail, the e-mail
address and the URL of a home page are compulsory or optional.

The current addresses must be updated when authors move and they must be removed
when authors can no longer be contacted. This kind of update can be organised by way
of databases of universities, learned societies or publishers.

The publisher has to provide the date of the publication of the article. If modules are
modified after publication, the date of the modification has to be included, specified by
module.

The date when the publisher first received the manuscript may be included, as well
as the date the publisher received a revised version and the date of acceptance, if these
dates are made explicit by the publisher. These metadata can be standardised over a
wide range of journals.

Lists of physics index terms (m1b)

- List for each module in the article the keywords, classification codes, or
  other terms derived from controlled lists that characterise that module (e.g.
  materials index terms).
If the index terms are derived from a standard classification system (e.g. PACS codes), indicate which system is used and provide a link to the full thesaurus.

- Make sure that any overlap between the physics labels is not caused by the fact that each module carries the characterisation of the entire article.

'Map of contents' (m1c)

- Provide a graphical representation of:
  - all main modules in the article;
  - all constituent modules contained in these main modules;
  - all links between the modules, in particular the links expressing the sequential paths.

- Present the graphical representation in such a way that at least all main modules are visible at first view, with only the essay-type sequential path connecting the visible modules, and in such a way that the reader can make the other modules and links visible on demand. (see figure A.1)

- Provide a link (carrying at least the label 'To contents') from the graphical presentation of each module to the contents of the presented module. In each module of the article, a link (carrying at least the label 'To meta-information') has to be provided to this map.

Abstract: (m1d)

- Give a textual summary of the main issues and the main lines of the article, in which information represented in each main module (or its constituent modules) is summarised.

Specific guidelines can be given for the process of composing and evaluating an abstract. See [Van der Tol, 1999].

- Provide a link from the abstract (carrying at least the label 'To contents') to each main module (or directly to the relevant constituent module). In each module of the article, a link (carrying at least the label to 'To meta-information') has to be provided to this module.

Lists of References (m1e)

- List for the article as a whole, all modules and other representations of information units outside the article that are referred to from any module in the article. When a segment of a module is referred to, that module as a whole is included in the reference list. Specify the module in which the reference was made.

- Also list for each individual module in the article all modules and other representations of information units outside the article that are referred to from that particular module. Specify the characterisation of the referring links.
• Add to each reference in the lists an administrative link to each (segment of the) module in the article where the reference was made.

The editorial board or publisher of the particular journal normally prescribe a specific style for standardising the references in these lists, as well as the way the references are denoted in the discourse in the modules. An example of an existing style is given in the Chicago Manual of Style [Grossman, 1993].

Acknowledgements (m1f)

• If there are non-author contributors to the article, give their names and roles (e.g. acknowledge the contributions of technicians in the construction of the experimental set-up and the useful discussions with other scientists).
• If the work has been financially supported by an institution, other than the affiliations of the author(s), give its name and address (for surface mail and where available for e-mail and home page). If that financial support is channelled through a project with a number, specify that number.

A.2.2 Positioning (m2)

Situation (m2a)

• Provide an embedding for the central problem, by describing the situation in which the problem described in module m2b has arisen. When applicable, mention the techniques (e.g. molecular beam techniques), the materials involved (e.g. alkali atoms and halogen molecules), and the global energy range (e.g. the eV range). If this article is issued from a research project, embed it in that project in particular.
• If the situation has already been described in another (mesoscopic) module, make that module available by means of a link (carrying a label 'is elaborated in') to that module. The core of this module then contains merely pointer. Complement that pointer if necessary with, in particular, an update on the status of the research project.
• If members of the target audience are not likely to accept the relevance of the central problem in this situation, provide argumentation supporting that relevance in this module.

Central problem (m2b)

• State concisely the central problem addressed in the article. The problem can be stated in terms of a well-defined goal, or formulated as a question that you attempt to answer in the article.
• If this article is issued from a research project aimed at solving a global central problem, link this microscopic module (with a link characterised as 'wider range/is elaborated in/synthesis') to the mesoscopic module describing it. This module cannot consist of a mere pointer to another module, because the central problem addressed in the article is specific to that article.
• Include in the statement of the central problem an indication of the general
type of the method used in the response to the problem (e.g. scattering),
of the physical qualities to be determined, measured or calculated (e.g. dif-
erential cross sections), and of the system under examination (e.g. alkali
atoms, halogen molecules and their ions at relative energies in the eV range).
When new or unusual methods are used, name them and add a link (labelled
'Is detailed in/Is focused in'); to the relevant Methods module.

• If the article presents a complex problem-solving process, make explicit which
'subproblems' must be solved subsequently or conjunctionally in order to solve
the overall problem.

• Provide a link labelled as 'Is used for' to the module Findings representing
the dependency relation in the problem-solving process.

A.2.3 Methods (m3)

• Compose a complex module Methods consisting of one or more constituent
modules giving an account of the methods used in the research: Experimental
methods and/or Numerical methods and/or Theoretical methods and, if
necessary, provide a module summary of those constituent modules.

• If more than one of these types of tools (e.g. more than one experimental
method was used) is used and if more than one of these tools is described in
sufficient detail to warrant the distinction of a module that can be consulted
separately, create a complex module Experimental methods containing con-
stituent modules distinguished by their physics contents. The constituents
can be components aggregating into the complete experimental tool, or focus
on specific tools that are generalised in the complex module. If the differ-
ent experimental methods are only summarised and further made available
by means of links to other modules, present all of them in an elementary
Experimental methods module.

• Provide a link representing the dependency relation in the problem-solving
process labelled as 'Is used for' to the module Raw data and/or Treated
results and/or Interpretation giving results or interpretations based on these
methods

Experimental methods (m3a)

If experimental methods are used:

• Describe the experimental set-up (general scheme and specific instrumenta-
tion) used in this work, and give its restrictions with respect to the range,
the precision and the stability. The specifications of a commercial apparatus
for instance, can be included by a link (labelled 'Specifications given in') to
the manufacturer's documentation. In addition, describe the measurement
procedure to generate experimental data using the set-up.

Make sure that the module contains all information necessary to guarantee
the reproducibility of the experiment.
A.2. **MODULES**

- If more than a link to other modules (plus a short summary) is given, distinguish constituent modules that represent the components of the molecular beam experiment:
  1. Source; the source of the atom, molecule or ion beam(s).
  2. Selection; selection of the state of the beam particles, specifying the input parameters of the beam(s). Give the type of mechanical velocity selector or other velocity selection procedure. In addition, describe the beam collimators.
  3. Interaction; the interaction region between the particles in the two beams or between the beam particles and particles in a static gas, including a description of that static gas.
  4. Analysis; the analysis distinguishing between the different end products of the reaction, (e.g. fast ions and slows atoms).
  5. Detection; the detection of the beam before interaction and detection of the reaction products. Indicate the type of each detector in the set-up (e.g. hot wire, particle multiplier) and provide its characteristics (e.g. threshold values, slit function), preferably by means of a link to a module dedicated to that detector (labelled 'Specifications given in/Is detailed in/Is focused in'). If applicable, also name the amplifier characteristics.

If it is not possible to form self-contained constituent modules about these components, distinguish the components explicitly in the internal structure of the module **Experimental methods**.

**Numerical methods (m3b)**

Although in the domain of **experimental** molecular simulations dynamics (e.g. Monte Carlo) are not customary, they can be used in the research and reported in the article. Numerical methods can also support the experiment (electronic data acquisition) and support calculations that cannot be performed entirely analytically (e.g. integrations). If numerical methods are used:

- Describe the computer hardware and software and the algorithms used in this work, and give their restrictions. In addition, describe the parameters and procedure that are used to generate the data using the numerical 'tools'.

**Theoretical methods (m3c)**

If theoretical methods are used:

- Summarise the models and theories from the 'theoretical toolbox' used in this work, and their restrictions.

- Link this module to a mesoscopic or macroscopic module containing a full account. If no adequate higher level module is available, link to a microscopic module with a full account. If no other module provides an adequate account of the theoretical methods, describe them in this module.

This 'toolbox' includes: scattering theory, the atom-atom model for molecular collisions, the Landau-Zener approximation;
The editorial board of a journal can make a 'catalogue of the theoretical toolbox' available, by providing an index of the existing theories, models and approximations that are often used in the domain at hand, and specifying the modules in which they are properly described and discussed.

- A criterion for including information in the *Theoretical methods* module (rather than in the *Interpretation* module m5) is that the information in this module is independent of the results generated in this article. Calculations using the results of this article as input are considered to interpret the results and as such are made part of the *Interpretation* module. An existing model that you use for the interpretation of the results is part of the theoretical toolbox; include it in this module. On the other hand, if you have developed in the current article a new model for the purpose of explaining the results, present that in the *Interpretation* module.

- Report on the calculations performed with these theoretical tools to generate theoretical data, providing sufficient details for the reader to follow the calculations;

- If input parameters are used in the calculations, link them to their source by means of a linked typed as 'Input from'.

### A.2.4 Results (m4)

- Link all results (and their restrictions) to the method used to generate them (and their restrictions) by a link labelled as 'Depends on'.

- If available, describe intermediary results copied or extracted from their original module (*Methods* or *Interpretation*) into this module.

- Mention for all results, whenever applicable, the physical qualities to be determined, measured or calculated (e.g. differential cross sections), the system, (e.g. alkali atoms, halogen molecules and their ions) and the energy range (e.g. 13-85 eV), the type of reaction that is studied (e.g. chemionisation) and the units or dimensions (e.g. $I(\theta) \sin \theta$ in arbitrary units vs. $\tau$ in eV x degree).

**Raw data (m4a)**

If information is lost in the treatment of the raw data:

- List the raw data, the output from the measurements or calculations, and give their restrictions.

The editorial board can specify further guidelines for what can constitute the raw data, depending on the field and on the equipment normally used in that field.

- If the module *Treated results* is a complex module, create a complex module *Raw data* representing the raw data in constituent modules corresponding to the constituent modules with the treated results based on these raw data.
A.2. MODULES

Treated results (m4b)

- Report the treated results in clear units and dimensions, preferably SI units. For large amounts of results, complement a clear graphical or audio-visual presentation with a manipulable storage format.
  In this domain, the treated results generally include cross sections of the scattering reaction under investigation, plotted against the angle. These are represented graphically and the variables are multiplied with some function for the sake of clarity.

The editorial board can give specific instructions with regard to figures (in particular images and drawings), tables, and other non-textual representations).

- If 1) more than one type of results is obtained and if 2) more than one of these types of results is reported in sufficient detail to warrant the distinction of a module that can be consulted separately, create a complex module Treated results containing constituent modules distinguished by their physics contents. The constituents can be components aggregating into the complete results, or focus on specific results that are generalised in the complex module.

- Describe the data analysis and presentation techniques used to treat the data, if the target audience would otherwise not be sufficiently informed to understand and assess the results.

- Give the restrictions of the results, with respect to the range and the precision: the error discussion.

- Link the treated results (and their restrictions) to the raw data they are based on (and their restrictions), and where necessary to data analysis techniques used to treat the data (and their restrictions) by links labelled 'Depends on'.

A.2.5 Interpretation (m5)

- Report on the interpretation (as a process) of the results that are not described in the Methods or the Results. If this involves calculations, provide sufficient details for the reader to be able to follow the calculations.

- If input parameters are used in the calculations, link them to their source by a linked typed as 'Input from'.

- Describe the resulting interpretation(s) in terms of chemical or physical phenomena. For example, results obtained in terms of scattering can be explained 1) in terms of reaction mechanisms specified in a molecular dynamics model, or 2) in terms of intermolecular potential parameters. Different interpretations can be given, such as a qualitative and a quantitative explanation of the results, or interpretations in which different factors are taken into account (e.g. translational coupling only, or rotational coupling as well).

- Link the interpretation (and its restrictions) to the results that are interpreted (and their restrictions) and to the theoretical method used to interpret them (and their restrictions) by a 'Depends on' link.
• If the target audience is unlikely to be convinced beforehand of the reliability and the applicability of this interpretation to the solution of the central problem, provide explicit argumentation supporting the standpoints that the interpretation is reliable and helps to solve the problem. This discussion can include a comparison to the results and interpretations published in other work.

• If more than one interpretation is considered and if more than one of these interpretations is reported in sufficient detail to warrant the distinction of a module that can be consulted separately, create a complex module *Interpretation* containing constituent modules distinguished by their physics contents. The constituents can be components aggregating into the complete interpretation, or they can focus on specific interpretations that are generalised in the complex module. If the different interpretations are only summarised and further made available by means of links, present the entire interpretation in an elementary *Interpretation* module.

• If the interpretation is complicated and elaborate without warranting the distinction of separate constituent modules, start the elementary *Interpretation* module with a brief outline of its contents.

• If a separate qualitative and quantitative interpretation are described and discussed, distinguish two constituent modules, that can otherwise simply be made explicit as parts of an elementary module:

  1. Qualitative interpretation m5a The qualitative interpretation of experimental results can involve a discussion of special features of the results as given in a figure (such as oscillations, bumps or spikes) in terms of physical phenomena (such as interference).

  2. Quantitative interpretation m5b The quantitative interpretation of experimental results can involve a comparison of these results with theoretical results calculated on the basis of the experimental results, (e.g. by fitting or averaging). For a quantitative interpretation the dimensions of the quantities must be well-defined.

### A.2.6 Outcome (m6)

**Findings (m6a)**

• Summarise the main findings that are obtained in this work, which form:

  1. an answer to the central question formulated in the module *Central problem*

  2. a brief recapitulation of what has been achieved in the research reported in this article.

If the central question reads like "can the measurements of this particular reaction be interpreted by that particular model?", answered it by a conclusion such as "yes, even quantitatively", "only qualitatively", or "we still don’t know if that model can explain the experimental results".
If the question is a more experimentally oriented, e.g. “what are the cross section of these reactions?”, briefly summarise what has been measured and provide a link (carrying labels ‘Depends on/is detailed in’) to the Results module where the results are given. Furthermore, comment on the results: do they fall in the expected range, are the surprising in some sense?

If there is no clear answer to the central question, the conclusion can be that the results are inconclusive and that further research is needed, for example, because the theory did not apply to the situation at hand and the measurements need a better resolution.

- If any problems related to the central one have been solved in the course of the research, the solutions can be summarised in this module.

- If the target audience is unlikely to be convinced beforehand of the reliability or the relevance of the findings, justify them by summarising the ‘final judgement’ on the reliability and applicability of the research presented in this article in the given situation, and by linking to the appropriate modules for the arguments supporting that final judgement.

- If the central problem is considered through different specific problems addressed in parallel lines of problem-solving, or through the solution of a series of component-problems that form the subsequent steps of the process as a whole, explicitly state the structure how the different lines or components are brought together in this module.

- Link the module Findings to the findings of the problem-solving process that are represented in the Interpretation, where they have been obtained. In addition, link this module to the Methods and Results modules it recapitulates and to the Central problem that is supposed to be solved here, by means of a ‘depends on/is detailed in’ link.

**Leads for further research (m6b)**

- If any leads for further research related to the research reported in this article have been encountered, suggest the new problems that are to be solved.

- If no definitive solution can be reported in module m6a, then m6b is compulsory: reformulate the problem at hand. If you reformulate the problem, try to suggest as concretely as possible how the problem might be solved, and/or explicitly state what potential solution has been found to be inadequate.

- If the central problem is not solved, link this module to the inconclusive findings, by a ‘depends on’ link.

### A.3 Links

#### A.3.1 General guidelines for links

A module is a document representing a conceptual information unit. Likewise a link is a physical connection that represents different types of relations identified at the conceptual level.
Figure A.2. The source and the target of a link are 1) an entire module or 2) a segment of a module. The relata of the relation expressed in such a link are 1) an entire module or 2) a segment of a module, or 3) an information unit underlying an entire module or 4) an information unit underlying a segment of a module, or 5) an entity addressed in an entire module or 6) in one addressed in a segment of a module.
Relations can be identified between so-called 'relata', where each relatum can be
1) the 'real world' entity addressed in an entire module, 3) an entity addressed
in part of a module, 2) an information unit underlying an entire module, 3) an
information unit underlying a segment of a module, 4) an entire module itself, or
5) a segment of a module. A link expressing a relation can be created between
a source and a target, which can be 1) an entire module or 2) a segment of a
module. Accordingly, the source (and the target) of a link can 1) coincide with
the corresponding relatum, or 2) represent the relatum. The source can also 3)
be a part of the relatum, or 4) represent a part of the relatum. The source cannot
contain (a representation of) the relatum.

- Identify the organisational relations and scientific discourse relations that are
  relevant for the readers' insight in the domain in general and their under-
  standing of the module at hand in particular.

- Express these relations in the modular structure in terms of labelled hyper-
  links, provided that the relata correspond to different modules, or that they
correspond to widely different parts of the same module (in the case that this
module is large and complex, and that the relata are far apart). If a relation
can be identified between adjacent items in the same module, only make it
explicit in the text, not in a link.

- For each relation of a particular type that is made explicit in a link, use the
  appropriate label to characterise the link. The links are directed and the
  labels express how the citing source is related to the cited target. To an
  asymmetric relation, two labels can be associated, expressing the relation in
  the two directions. For example, to the hierarchical relations the label 'is
  part of' can be associated, as well as the label 'Contains' for the opposite
direction of the same relation. The labels for symmetric relations are the
  same in both directions.

A link between a source $S$ and a target $T$ is denoted schematically as

$$\text{S link type } \rightarrow \leftarrow \text{reverse link type } T,$$

where the 'link type' can be a complex characterisation consisting of more
than one label.

- If you create the link at the same time as the source module, check if the link
  is automatically endowed with bibliographic data associated with the source.
  If you create a new link, anchoring it in a published module as the source,
  provide the bibliographic data to make the characterisation of the new link
  complete.

- Characterise each link completely with the set of all labels associated to it
  and make the links thus characterised explicit in:

  1 the *Map of contents*. Present the links to modules outside the article also
     in the module *Lists of references*. Specific guidelines for these modules,
     that are part of the *Meta-information*, have been given in the previous
     section

  2 the 'navigation menu' of each module. List in the navigation menu,
     specifying the characterisation,
* each link from the module at hand to a target specified by its unique identification;
* each link to the module at hand from a source specified by its unique identification.

The format of this navigation menu will be specified for the journal in which the article is to be published. The author should have at his disposal software allowing him to automatically generate the navigation menu in the correct format, as well as the map of contents and the lists of references in the Meta-information. We suggest requirements for such authoring tools in section 6.2.2.

3 the text of the source module, if the link plays a role in the scientific discourse (rather than just in the organisation of the modules).
* Create in the text a hyperlink.
* Endow the link explicitly with the complete set of labels associated to the relations expressed in that link. Indicate which relations were the raison d'être for the creation of the link.
* Make explicit the unique identification of the target. A reference to an article as a whole is expressed in a link to its module Meta-information.
* If the readers are unlikely to understand immediately what are the source of the link, its target and its function (i.e. what relations between which objects warranted the creation of the link), also include in the presentation of the link a short phrase summarising these characteristics.

In the text of source module $S$, the target $T$ is referred to as: [link type: (link type); target: $T$] and explicit backtracking of that link from the module $T$ is then expressed as [link type: (reverse link type); target: $S$].

In the following, specific guidelines will be given for the identification of such relations and their representation in links.

### A.3.2 Organisational relations

Identify the organisational relations between modules, of which at least one is part of the article at hand. Express these organisational relations in links and present these links in the Map of contents and in the navigation menu of each of the modules. The different labels that can be associated to organisational relations are summarised in figure A.3.

The purpose of organisational relations is to identify the module's organisational context in the article and in larger collections of modules. The modules can be consulted separately, without their context in the article. Hence, organisational relations do not have to be made explicit in the text of the module itself. If, however, a link is given in the text to represent a scientific discourse relation between particular relata, that link should also express any organisational relations that can be identified between the corresponding relata, which implies that the link is
characterised by the labels associated to these organisational relations as well (see above for the correspondence of the source and target of the link, and the relata of the relations it can express).

1. Hierarchical relations (Is part of, Contains)

- Make explicit all hierarchical relations between the complex modules that you have created and their constituent modules.
- Check if between the relata a synthesis relation (aggregation or generalisation) can be identified as well, i.e. if the complex module is a clear-cut compound module or cluster module. If that is the case, express that relation in the same link. If no synthesis relation is made explicit, a link labelled ‘Is part of’ by default expresses implicit aggregation and generalisation.
- If the complex module contains a module summary, make explicit in the same link a resolution relation and a context relation, to indicate that the complex module provides fewer details and more context than the constituent modules.

**Notation:** The link ‘S Contains $\rightarrow$ Is part of T’ is denoted in the text of S as [link type: (Contains); target: T], meaning “the current module S contains module T”, and in the text of T as [link type: (Is part of); target: S], meaning “the current module T is part of the module S”.

**Example:** ‘A05-m2 contains $\rightarrow$ part of A05-m2b’: The compound module Positioning A05-m2 contains the module Central problem and reversely, the elementary module Central Problem is part of the Positioning.

2. Proximity-based relations (Article, Project, External)

A proximity-based relation indicates whether the connected modules are close to each other: are they part of different works or of the same work? Make this type of relation explicit between modules that are connected by a link created for the purpose of expressing another type of relation.

- **Article:**
  The label associated to a proximity-based relation between modules in the same article is ‘Article’. This is the default proximity-based relation: do not make that label explicit in the characterisation of a link.

**Example:** The Treated results module A08-m4bi and the module Experimental methods A08-m3c are part of the same article A08. The proximity-based relation between these modules could be made explicit in the link between them as ‘A08-m4bi Article $\rightarrow$ Article A08-m3c’, but these labels are not made explicit.

- **Project:**
  - Use the label ‘Project’ to express the proximity-based relation between modules that are part of different publications issued from the same research project.
  - Present all links that are labelled ‘Project’ in the Lists of references.
Notation The link ‘S Project →←Project T’ is denoted in the text of S as [link type: (project); target: T] and in the text of T as [link type: (Project); target: S], meaning that both modules are issued from the same project.

Example: The Situation module A08-m2a and the module Findings A05-m6a are both part of the corpus, i.e. issued from the same project, so that the link between them is labelled as follows: ‘A08-m2a Project →←Project A05-m6a’.

- External:
  - Use the label ‘External’ to express the proximity-based relation between modules that do not belong to the same article, nor to articles that have been published in the context of the same research project.
  - Present all links that are labelled ‘External’ in the Lists of references.

Notation The link ‘S External →←External T’ is denoted in the text of S as [link type: (external); target: T] and in the text of T as [link type: (external); target: S], meaning the connected modules are issued from the different research projects.

Example: The Situation module A05-m2a, links are given to articles by authors that do not collaborate within the same research project: ‘A05-m2a External →←External RfA05-7-m1’.

3. Range-based relations (To wider range, To narrower range)

- A range-based relation indicates the difference in range between the information represented in linked modules. Make this type of relation explicit between modules that are connected by a link created to express another type of relation. In this manner, characterise all links connecting the microscopic modules of the article to mesoscopic and macroscopic modules, as well as links connecting mesoscopic modules to macroscopic modules, with the label ‘To wider range’. Use the label ‘To narrower range’ to characterise links from mesoscopic and macroscopic modules to microscopic modules, and links from macroscopic to mesoscopic modules.

- Check if a link labelled as ‘To wider range’ should also be labelled as ‘Is generalised in’.

Notation: The link ‘S To wider range →←To narrower range T’ is denoted in the text of S as [link type: (to wider range); target: T], meaning “the information in module T has a wider range than the information in the module S”, and in the text of T [link type: (To narrower range); target: S] means “the module S has a narrower range than the information in the module T”.

Example: Mesoscopic modules have a wider range than microscopic modules, so that ‘A05-m3a To wider →←To narrower MESO-m3a’, where A05-m3a provides the article-specific information on the actual measurements performed at this time and MESO-m3a the information about the set-up, which plays a role in the research project as a whole.

4. Administrative relations (To contents, To meta-information)

Make explicit the administrative relations between, on the one hand, the module
Meta-information and its constituents, and, on the other hand, the 'scientific' content modules:

- Link each microscopic module (through the navigation menu) to the Meta-information, the Abstract and the Map of content and characterise those links with the label 'To meta-information'. In addition, link each mesoscopic and macroscopic module you have created (through the navigation menu) to their Meta-information and Map of contents.

- Provide in the modules Abstract, Lists of index terms and Map of content links labelled as 'to contents' to each module of the article, and as well as in the Lists of references to each module that contains 'Project' or 'External' links. In addition, provide links labelled 'To contents' from the meta-information about the mesoscopic and macroscopic module to the content of those modules.

Notation: The link 'S To meta-information $\rightarrow$ $\leftarrow$ To contents T' is denoted in the text of S as [link type: (to meta-information); target: T], meaning "the meta-information of the current module S is provided in module T", and in the text of T [link type: (to contents); target: S] means "the information associated to the current meta-information module T is provided in the module S".

5. Sequential relations

- Determine the sequence in which the modules can be consulted by readers who wish to read the entire article. Set out paths through the article that facilitate sequential consultation, by making explicit the asymmetric relations associated to the sequential path between the modules that the path passes through.

The standard sequence of microscopic modules in an article is: m1 META-INFORMATION, m1a Bibliographic information, m1b Lists of physics index
terms, m1c Map of contents, m1d Abstract, m1e Lists of references, m1f Acknowledgements, m2 POSITIONING, m2a Situation, m2b Central problem, m3 METHODS, m3a Experimental methods, m3b Numerical methods, m3c Theoretical methods, m4 RESULTS, m4a Raw data, m4b Treated results, m5 INTERPRETATION, m5a Qualitative interpretation, m5b Quantitative interpretation, m6 OUTCOME, m6a Findings, m6b Leads for further research.

- If these modules contain constituent modules distinguished by their physics content, choose the sequence that best corresponds to the steps in the problem-solving process, or start the path with the easy cases, before leading the reader to the more complicated cases. In the case of the components of the experimental set-up of a collision experiment, follow the course of a projectile particle from its source to the detection of the collision products.

5.1 Complete sequential path (Sq-next, Sq-back)
- Set out a complete sequential path that passes through each module in the article, which allows the reader to be certain that he has not missed any modules.
- Specify in each module a sequential link indicating the next step and the previous step, except for the module Meta-information, which is the starting point of the path and the module Leads for further research, which is the end.

**Notation:** A link ‘S Sq-next →←Sq-back T’ is denoted in the text of S as [link type: (Sq-next); target: T], meaning “following the complete sequential path, the next step from the current module S leads to module T”, and in the text of T as [link type: (Sq-back); target: S], meaning “retracing steps from the current module T by way of the complete sequential path leads back to module S”.

**Example:** ‘A05-m2b Sq-next →←Sq-back A05-m3’: Following the sequential path that we have established in the article, the next step along the complete sequential path after the module Central problem, leads to the Methods module.

5.2 Essay-type path (Es-next, Es-back)
- Set out an essay-type sequential path that passes through the elementary modules in the article, that allows the reader to follow the line of discourse of the article.
- Start the path in the module Situation for short or simple articles. For more complex articles, start the path in the Abstract. In addition, provide a starting point for the essay-type path in the module summary of the Meta-information.
- Only include a complex module explicitly in this path if its ‘module summary’ is absolutely necessary for the sequential reader’s understanding of a (particularly complicated) collection of elementary modules. Avoid the Raw data. In addition, avoid most of constituents of the module Meta-information, in particular the Lists of physics index terms and the Lists of references.
**A.3. LINKS**

**Notation:** A link 'S Es-next $\rightarrow$ Es-back T' is denoted in the text of S as [link type: (Essay-next); target: T], meaning "following the essay-type sequential path, the next step from the current module S leads to module T", and in the text of T as [link type: (essay-back); target: S], meaning "retracing steps from the current module T by way of the essay-type sequential path leads back to module S".

**Example:** 'A08-mb3c Es-next $\rightarrow$ Es-back A08-m4bi': Following the essay-type sequential path, the next step along the complete sequential path after the module *Experimental methods*, leads to the *Treated results* module focusing on the experimental differential cross sections.

An editorial board can specify stringent rules for the essay-type path. They may require the author to either include or to exclude the Bibliographic information and the Map of contents. These decisions may also be left to the author’s discretion.

6. **Representational relations [to be defined]**

If you have represented the same information in different formats, make explicit the representational relations between these different representations (for instance, in links connecting a textual representation, a figure and an animation).

In the modularisation of the corpus articles, we have not identified representational relations, because neither we, nor the authors of the original articles, have represented the same information in different formats. The editorial board of a multimedia journal can specify rules for this ‘technical’ type of relations.

### A.3.3 Scientific discourse relations

- Identify the scientific discourse relations that warrant the creation of an explicit link.

- Express the relevant discourse relations in links and present these links in the text of the modules involved, as well as in the navigation menu of each of the modules and in the *Map of contents*. The different labels that can be associated to scientific discourse relations are summarised in figure A.4.

<table>
<thead>
<tr>
<th>Relations based on the communicative function</th>
</tr>
</thead>
<tbody>
<tr>
<td>- Determine for each module if particular readers are unlikely to understand and/or accept all segments of the module. <em>(Remark: if all readers will probably have problems understanding and accepting the module, the module is not self-contained and you have to add information.)</em></td>
</tr>
<tr>
<td>In that case, include in the text of the module a link to a target that is aimed at increasing those readers' understanding and/or acceptance. In that link, express an elucidation relation, and/or an argumentation relation. Elucidation implies informative questions, whereas argumentation implies critical questions. The relata of such a relation can be, for example, particular statements made in the module, figures or formulae.</td>
</tr>
</tbody>
</table>
• The expression in links of relations based on the communicative function is aimed at answering the readers’ questions. To identify those relations, use prototypical questions that readers may have about the relatum corresponding to the source of the link, which are to be answered by the relatum corresponding to the target of the link.

• When you make a relation based on the communicative function explicit, check if the same link should also express one or more content relations: how are the link and target supposed to increase the readers understanding and acceptance of the source?

1 Elucidation relations (Is elucidated in, Elucidates)

- Determine which modules or segments of modules must be referred to in order to allow readers (that are less informed and/or more interested in the full details of the scientific discourse) to understand each part of the modules.

- Prototypical question: “What is that and why is that the case? I don’t understand this statement.”, as opposed to “I don’t accept this statement”.

- Connect by a link expressing an elucidation relation the segment of the module that some readers are likely to find unclear to the target that should elucidate it.

- If the relation is a general elucidation relation, rather than one of the specific types of elucidation given below, characterise the link expressing it with the labels ‘Is elucidated in’ and ‘Elucidates’.

Notation: ‘S Is elucidated in $\rightarrow$ Elucidates T’ is denoted in the text of S as [link type: (is elucidated in); target: T], meaning “(a segment of) the current module S is elucidated in or using the module T”, and in the text of T as [link type: (Elucidates); target: S], meaning that “S contains a statement or other part that the current module T elucidates”.

Example: In the Situation module A08-m2a Stueckelberg oscillations are mentioned. Bernstein elucidates the phenomenon, i.e. he clarifies what are Stueckelberg oscillations and explains what causes them. The elucidation is made available by a link ‘A08-m2a Elucidans $\leftrightarrow$ Elucidandum [Bernstein]’.

1.1 Clarification relations (Is Clarified in, Clarifies)

* If it is unlikely that all readers will understand what some statement or other representation in the source means, i.e. if some readers will find it unclear, provide a link labelled as ‘Is clarified in’ to a target that provides a clarification that is supposed to increase the readers understanding.

* A clarification relation is a specific kind of elucidation relation. Prototypical questions: “What is that? How does that work?”’, as opposed to “How did that come about”, which requires an explanation.

* When making an clarification relation explicit, check in particular whether the link should also express an elaboration (or in particular carry the label ‘Is detailed in’ or ‘More context in’) or a similarity.
A.3. LINKS

Notation: The link 'S is clarified in → ↔ Clarifies T' is denoted in the text of S as [link type: (Is clarified in); target: T], meaning "the (some piece of) module S is clarified in or using the module T", and in the text of T [link type: (Clarifies); target: S] means that "S contains an unclear statement or other representation that can be clarified by T".

Example: In the Theoretical methods module A08-m3cii, the Airy description is used. The reader who does not know what that description amounts to is referred to Airy's article for further clarification: 'A08-m3cii is clarified in → ↔ clarifies $R_{A08}^{f}$'.

1.1.1 Definition relations (Is defined in, Defines)

- If it is unlikely that all readers will understand what a particular notion or term in the source means, i.e., if some readers are probably unfamiliar with that term, provide a link labelled as 'Is defined in' to a target that provides a definition.

- Prototypical questions: "What does that term mean?" or "What is that object?". A definition relation is a specific kind of clarification relation. You can define an existing term (lexically) by describing its meaning, define new term (stipulatively) by establishing its meaning, and you can provide a (so-called 'real') definition of something (e.g., physical quantity, mathematical function), which is a description that allows the reader to identify its particular characteristics.

Notation: The link 'S is defined in → ↔ Defines T' is denoted in the text of S as [link type: (Is defined in); target: T], meaning "the definition of some particular term given in module S can be found in module T", and in the text of T as [link type: (Defines); target: S], meaning "that S contains something that requires a definition that is provided in T".

Example: In the Theoretical methods module A08-m3cii the deflection function is used. The definition of a deflection function is given in the mesoscopic module MESO-m3c-defl: 'A08-m3cii is defined in → ↔ Defines MESO-m3c-defl'.

1.1.2 Specification relations (Specifications given in, Gives specifications of)

- If it is unlikely that all readers will know what are the specific features of a particular object described in the source, provide a link labelled as 'Specifications given in' to a target that provides a specification. In particular, connect the mention of an apparatus to its full technical specification by a link expressing a specification relation.

- Prototypical questions: "What is the specification of that object?". In particular, the reader may ask "What are the technical specifications of that apparatus?" or "What are the particular features of that model?". A specification relation is a particular type of clarification relation.

- When making a specification relation explicit, check in particular whether the link should also express a resolution relation, i.e.
whether it should also be labelled as 'Is detailed in'.

**Notation:** The link 'S Specifications given in $\rightarrow \leftarrow$ Gives specifications of T' is denoted in the text of S as [link type: (specifications given in); target: T], meaning "the specification of some particular object described in module S can be found in module T", and in the text of T as [link type: (gives specifications of); target: S], meaning that "S contains the description of an object for which the full specification is given in the current module T".

**Example:** The multiplier used in the detection system described in the *Experimental methods* module A07-m3a is a Bendix M306. For the full technical specification of that apparatus, a link is provided to the manufacturers:

'\text{A07-m3a Specifications given in } \rightarrow \leftarrow \text{Gives specifications of (Bendix)}'.

1.2 **Explanation relations (Is explained in, Explains)**

* If the reader is unlikely to understand how the state of affairs given in the source came about, or what caused the phenomenon described in the source, provide a link labelled as 'Is explained in' to a target that provides an explanation that is supposed to increase the readers understanding.

* Prototypical question: “How did the state of affairs referred to in that statement come about?”'. For example, the reader may ask: “What caused this physico-chemical phenomenon, e.g. why is the harpoon reaction so efficient? Why is only the ground state present in this reaction? What caused these restrictions, e.g. why is the interpretation of the experimental results only qualitative?”.

The question can be formulated as “Why is that the case?”, if that is interpreted as an informative question. The main issue in explanation is “I don’t understand it”, as opposed to “I don’t accept it”, which implies argumentation. An explanation relation is a specific kind of elucidation relation. Remark that explanation does not provide an answer to the question what were the reasons for choosing a particular (experimental, theoretical, numerical, data analysis) method.

* When making an explanation relation explicit, also express the underlying causal relation.

**Notation:** 'S Is explained in $\rightarrow \leftarrow$ Explains T' is denoted in the text of S as [link type: (Is explained in); target: T], meaning "(some piece of) the module S is explained in or using the module T", and in the text of T as [link type: (Explains); target: S], meaning "that S contains a statement or other representation of information, which has to be explained, that can be explained by a the current module T."

**Example:** In the *Theoretical methods* module A08-m3c1 the relevant potential curves of sodium iodide are discussed. The basic shape of the curves is explained in the mesoscopic module on the atom-atom model MESO-m3c-mod. The explanation is made available by a link
Argumentation relations (is argued in, Provides argumentation for)

- Determine which modules or segments of modules must be referred to in order to allow readers (that are less informed and/or interested in the full details of the scientific discourse) to accept each part of the modules.
- Prototypical questions: “How can that statement be justified?” In other words, “Why is that true? Why is that plausible? Why is that acceptable? What were the reasons to do that?” The question can formulated as “Why is that the case?” if that is interpreted as a critical question. The main issue in argumentation is acceptance of the statement, as opposed to understanding it.
- Connect by a link expressing an argumentation relation the segment of the module that some readers are unlikely to accept without further argumentation to the target that should provide that argumentation.
- In the argumentation you can prove that the statement in the source is true, or justify it, if it cannot be proven rigorously. You can justify the choices that you have made in the research leading to the information represented in that statement in order to convince the reader that the information you have obtained is reliable and relevant.
- The argumentation can involve arguments supporting a standpoint given in the source module, and counterarguments refuting that standpoint. In that case, either show that these counterarguments are not strong enough to refute your standpoint, or indicate that the refuted standpoint was a hypothetical one and present and defend your modified standpoint.

Notation: The link ‘S is argued in ––– Provides argumentation for T’ is denoted in the text of S as [link type: (is argued in); target: T], meaning “T contains an argument relevant to the standpoint brought forward in here in S”, and in the text of T as [link type: (provides argumentation for); target: S], meaning that “in S a standpoint has been put forward for which T provides arguments.

Example: Berry, and Hundhausen and Pauly have done calculations that confirm the expectations of the author of A05, which is presented as an argument in favour of the reliability of the procedure of the determination of the potential well depth and the resulting parameter ‘A05-m5bi is argued in ––– Provides argumentation for RfA05.10, RfA05.14’.

Content relations

When you make a content relation explicit, check if the same link should also express one or more relations based on the communicative function: why are the link and target provided; to increase the readers understanding or their acceptance of the source?

- Dependency relations in the problem-solving process (Depends on, Is used for)
  - Identify the problem-solving dependency relations (between information units) that warrant the creation of an explicit link: determine for each
module if the information represented in it depends on the information associated to a previous step in the problem solving process, or if the information represented in it is used in a subsequent step in the problem solving process that is addressed in another module.

To identify those relations, use prototypical questions that readers may have about the relatum corresponding to the source of the link, which are to be answered by the relatum corresponding to the target of the link. Prototypical question: “What was the previous step in the problem-solving process that led to this information?”. In other words, “Where does that information depend on? What has been used to obtain this information? “

– Determine if the dependency relation is important enough to warrant the creation of a link, and if that is the case, make it explicit in a link. Present these links in the text of the modules involved, as well as in the navigation menu of each of the modules and in the Map of contents. At least include a link expressing the fact that

* the Interpretation depends on the Treated results that are interpreted;
* the Interpretation depends on the particular Theoretical methods used to interpret those results;
* the Treated results depend on the Raw data that they are based on (if available);
* the Treated results depend on the particular Methods used to generate the results;
* the Raw data depend on the particular Methods used to generate the data;
* the Findings depend on the Interpretation;
* the Findings depend on the Central problem;
* the information represented in Central problem is used in the Findings.

– If a dependency relation is not important enough to warrant the creation of a new link, but if a link has already been created to represent another type of relation between similar relata, express the dependency relation in that link as well. In particular express the dependency relation in any link that connects the Interpretation to the interpreted Treated results and to the particular Methods used in the process of interpretation, and in any link that connects the Treated results to the appropriate constituents of the Methods.

**Notation:** The link ‘S Depends on →←is used for T’, denoted in the text of S as [link type: (Depends); target: T], means that “the information represented in S depends on the information in T”, in the sense that the reader of S is supposed to be sufficiently informed of T to understand S. In the text of T [link type: (Is used for); target: S] then means that “the information given in T can be used to advance a problem-solving process to a subsequent stage, that is addressed in S”.

Example: The Treated results in A05-m4bi depend on the Experimental Methods used to generate them in module A05-m3a, and conversely the methods described in module A05-m3a can be used to get the Treated results: 'A05-m4bi Depends on \( \rightarrow \leftarrow \) ls used in A05-m3a'.

II 1.1 Transfer relations (Input from, Output to)

* Determine for each module if a particular manipulable item has been imported as input from another module, or if such an item is exported as output to another module, and if the relation is important enough to warrant the creation of a new link. Examples of such items are: formulae, figures, values of parameters.

* A transfer relation is a particular type of dependency relation in the problem-solving process. Prototypical question: "Where does that item come from?".

Notation: The link 'S Input from \( \rightarrow \leftarrow \) Output to T' is denoted in the text of S as [link type: (input from); target: T], meaning "in the module S some item from module T is used as input", and in the text of T [link type: (output to); target: S] means "a piece of information from module T is exported as output to module S".

Example: A theoretical value of the polarizability of \( K^+ \), determined by Duren and Rittner, is used as input in A05-m5bi in the process of the interpretation in which some potential parameters are calculated: 'A05-m5bi Input from \( \rightarrow \leftarrow \) Output to \( R_{\text{A05-3}}, R_{\text{A05-4}} \)'.

II 2 Elaboration relations (Is elaborated in, Elaborates)

- If some readers are likely to require further information in order to fully understand and accept the information given in a module or a particular segment of a module, provide a link to a target with an elaboration of the source.

- Elaborating on a statement can involve filling in further details, or providing more context.

- If a link labelled as 'Is elaborated in', or more specifically as 'Is detailed in' or 'More context in', does not carry a label associated to a relation based on the communicative function, that link by default expresses both an elucidation of the source and argumentation aimed at convincing the reader that the source is reliable and relevant in the situation at hand.

- Check if a link representing a particular elaboration relation should also express a synthesis relation: should a particular link labelled as 'Is summarised in' or 'More context in' also carry a label 'Is generalised in' or 'Is aggregated in'?

Notation: The link 'S Is elaborated in \( \rightarrow \leftarrow \) Elaborates T' is denoted in the text of S as [link type: (is elaborated in); target: T], meaning "the source S is 'Elaborated upon' in the module T", i.e. T provides more information on the subject than S, and in the text of T [link type: (elaborates); target: S] means that "moving from T to S the information becomes more limited", in the sense that S provides less information on the subject than T.
Example: The mesoscopic sketch of the situation provides both greater detail and a broader perspective than, i.e., an elaboration of, the microscopic Situation: 'A05-m2a is elaborated in $\rightarrow \leftarrow$-s limited in Meso-m2a'.

II 2.1 Resolution relations (Is detailed in, Is summarised in)
If some readers are likely to require further details, i.e., a finer-grained account of the subject, provide a link carrying the label 'Is detailed in' to a target with those details. A resolution relation is a specific kind of elaboration relation.

Notation: The link 'S Is detailed in $\rightarrow \leftarrow$-s summarised in T' is denoted in the text of S as [link type: (detail); target: T], meaning "the module S is 'detailed' in the module T", i.e. T provides more detailed information on the subject than S, and in the text of T [link type: (Is summarised in); target: S] means "that S summarises that information in T, in the sense that S provides fewer details on the subject than T".

Example: A module Experimental methods gives greater detail about a set-up than the abstract, which summarises the method that has been used: 'A05-m1d Is detailed in $\rightarrow \leftarrow$-s summarised in A05-m3b'.

II 2.2 Context relations (More context in, Is focused in)
If some readers are likely to require more context, i.e., more background on the subject, provide a link carrying the label 'More context in' to a target with that background. A context relation is a specific kind of elaboration relation.

Notation: The link 'S More context in $\rightarrow \leftarrow$-s focus in T' is denoted in the text of S as [link type: (More context in); target: T], meaning "the module T provides more surroundings of (some segment of) the module S", i.e. T provides more context than S, and in the text of T [link type: (Is focused in); target: S] means "that S focuses on some aspect of the information in T".

Example: Although the module Experimental methods gives greater detail about a set-up, the abstract gives a wider perspective of the situation in which the method is used. Going from the abstract to the methods module, the reader focuses on a more narrowly defined subject: 'A05-m3b More context in $\rightarrow \leftarrow$-s focused in A05-m1d'.

II 3 Similarity (Disagrees with, Is compared with, Agrees with)
- If you compare information provided in the module at hand, or a particular segment of it, to information given in another module, express the similarity of those relata in a link connecting the modules or segments of modules representing them. You can compare information represented in (a particular segment of) a module to information represented in another module of the same article or in a module that is part of another article.
- State in the text of the module in what respect the relata are similar.
- If a link representing a comparison does not carry a label associated to
a relation based on the communicative function, that link by default expresses both an elucidation of the source and an argumentation relation aimed at convincing the reader that the source is reliable and relevant in the situation at hand. For example, you can compare different results obtained for similar systems in order to convince the reader of the reliability of those results, or compare the detector that you have used to the one used in some well-known research in order to clarify your set-up and in the same time to justify that it is reliable.

- Three labels can be associated to this relation: neutral comparison, agreement and disagreement.

  * **Comparison**
    
    **Notation:** The link 'S is compared with →—Is compared with T' is denoted in the text of S as [link type: (Is compared with); target: T], meaning “the current module S is compared with module T” (using the same system and a different method or vice versa).
    
    **Example:** The authors try to compare results of a Russian group, which has reported similar experiments, with the results presented in article A03-m4b. However, the energy ranges do not overlap, so that the results are not really comparable: 'A03-m4b is compared with →—Is compared with Rf_{A03-25}'.

  * **Agreement:**
    
    **Notation:** The links S Agrees with →—Agrees with T is denoted in the text of S as [link type: (Agrees with); target: T], meaning “the opinion expressed in module S agrees with the opinion expressed in module T".
    
    **Example:** The value of the electron affinity that is obtained in the interpretation process agrees with the value suggested by Person: 'A05-m5bi Agrees with →—Agrees with Rf_{A05-2}'.

  * **Disagreement**
    
    **Notation:** The link 'S Disagrees with →—Disagrees with T' is denoted in the text of S as [link type: (Disagrees with); target: T], meaning “the opinions expressed in module S disagrees with the opinion expressed in module T".
    
    **Example:** The electron affinity A(Br₂) disagrees with the value obtained in A05 (which casts doubts on the applicability of the theory discussed in A05-m3c): 'A05-m3c Disagrees with →—Disagrees with A03-m4'.

## 4 Synthesis relations

- There are two types of asymmetric synthesis relations between individual units and synthesised units: aggregation and generalisation

- Check if a link representing a synthesis relation should also express a hierarchical relation.

### 4.1 Aggregation relations (Is aggregated in, Is segregated in)

  * Identify the asymmetric relation between the information provided
II Content relations

I Relations based on the communicative function

II 1 Dependency in the problem-solving process
(Is elaborated in, Elaborates)

II 2 Elaboration
(Is elaborated in, Elaborates)

II 3 Similarity
(Agrees with, Is compared with, Disagrees with)

II 4 Synthesis

II 5 Causality
(To cause, To effect)

I 1 Elucidation
(Is elucidated in, Elucidates)

I 1.2 Explanation
(Is explained in, Explains)

I 2 Argumentation
(Is argued in, Provides argumentation for)

II 1.1 Transfer
(Input from, Output to)

II 1.1.1 Definition
(Is defined in, Defines)

II 1.1.2 Specification
(Specifications given in, Gives specifications of)

II 1.2 Clarification
(Is clarified in, Clarifies)

II 1.2.1 Resolution
(Is detailed in, Is summarised in)

II 1.2.2 Context
(More context in, Is focused on in)

II 2.1 Resolution
(Is detailed in, Is summarised in)

II 2.2 Context
(More context in, Is focused on in)

II 2.3 Synthesis
(Is generalised in, Is specialised in)

II 3.1 Generalisation
(Is generalised in, Is specialised in)

II 3.2 Aggregation
(Is aggregated in, Is segregated in)
in modules focusing on aggregate concepts and the information represented in modules on its component concept. An aggregation relation can be expressed, for example, 1) between a microscopic module on a specific application of an entire set-up, and a mesoscopic module on a particular component of the apparatus, 2) between the complete set of theoretical methods and the component that is used for one particular step in the calculations, or the component that gives the particular approximation used to calculate a particular area.

* Identify aggregation relations in the context of hierarchical relations between constituent modules and compound modules.

* Check if a link labelled as an aggregation should also carry an elaboration label 'is summarised in' or 'more context in', and vice versa if segregation entails details and a stronger focus.

**Notation:** The link 'S is aggregated in \(\rightarrow\) is segregated in T' is denoted in the text of S as [link type: (is aggregated in); target: T], meaning "the module T is an aggregate of (some segment of) the module S", and in the text of T [link type: (is segregated in); target: S] means "that S is a component of the aggregate in T".

**Example:** The *Theoretical methods* module A08-m3c (about the calculation of the differential cross section of the reaction using an atom-atom model) contains two components: A08-m3i deals with the transition probability and subsequently A08-m3cii with the differential cross section, in which the transition probability is used. The link between the complex module and A08-m3ci carries the following label: 'A08-m3ci is aggregated in \(\rightarrow\) is segregated in A08-m3c'.

### 4.2 Generalisation relations (Is generalised, Is specialised in)

* Identify the asymmetric relation between the information provided in modules focusing on specific concepts and the information represented in modules on the generalised concept. A generalisation relation can be expressed, for example, 1) between a microscopic module on the application of a set-up in specific measurements, and a mesoscopic module on the apparatus in general, 2) between the application of a specific combination of theoretical models and approximations to particular experimental results, and the general description and discussion of those theoretical methods, 3) between the specific application of numerical methods and the general account of them.

* Identify generalisation relations in the context of hierarchical relations between constituent modules and cluster modules, in which case the link is also implicitly labelled as 'Article'.

Check if a link labelled as a generalisation should also carry a range-based label 'To wider range', or a resolution label 'is summarised in'.

**Notation:** The link 'S is generalised in \(\rightarrow\) is specialised in T' is denoted in the text of S as [link type: (is generalised in); target: T], meaning "the
central concept of module $T$ is a generalisation of a concept in the module $S$", and in the text of $T$ [link type: (Is specialised in); target: $S$] means "that $S$ represents a concept that is a special case of the general concept focused on in $T$".

**Example:** The module *Theoretical methods* A08-m3ci about transition probability in general contains two constituent modules, A08-m3ci1 and A08m-3ai2, about two different, specific types of transition probability: 'A08-m3ci1 Is generalised $\rightarrow\leftarrow$ is specialisation A08-m3ci'.

II 5. Causal relations (To cause, To effect)

- If the cause for an effect stated in the module at hand is given elsewhere, refer to that cause by means of a link expressing a causal relation.
- Check in particular whether the link expressing a causal relation can also be labelled as an explanation.

**Notation** The link 'S To cause $\rightarrow\leftarrow$ To effect T' is denoted in the text of $S$ as [link type: (To cause); target: $T$], meaning "the cause of the state of affairs or phenomenon described in $S$ is given in $T$", and in the text of $T$ [link type: (To effect); target: $S$] means "that $S$ gives an effect that is caused by something stated in $T$".

**Example:** In the *Theoretical methods* module A08-m3ci2 it is stated that only the groundstates are taken into account. The cause why only those states are present in the system is given in A08-m3ci1: 'A08-m3ci2 To cause $\rightarrow\leftarrow$ To effect A08-m3ci1'.
Appendix B

List of published material in the corpus

Ion pair formation and Molecular physics

A research programme by prof. Los et al. at the Institute for Atomic and Molecular Physics (AMOLF ) in Amsterdam

- Part A: Ion pair formation
- Part B: Collisions dynamics and vibronic transitions
- Part C: Vibronic transitions

Articles:

A02 (I) Charge transfer between alkali atoms and oxygen molecules, A.M.C Moutinho, A.P.M Baede and J. Los, Physica 51 (1971) 432-444. [INSPEC Quest Accession number and INSPEC NN not available]

A03 (I) Total cross sections for charge transfer and production of free electrons by collisions between alkali atoms and some molecules, A.P.M. Baede and J. Los, Physica 52 (1971) 422-440.
INSPEC Quest Accession number: 71054803 INSPEC NN: A71035674

INSPEC Quest Accession number: 71084148 INSPEC NN: A71055063

INSPEC Quest Accession number: 72046911 INSPEC NN: A72028223

INSPEC Quest Accession number: 73028920 INSPEC NN: A73016712

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A07 (I) Fragmentation of negative ions formed in collisions of alkali atoms and halogen molecules, A.P.M. Baede, D.J. Auerbach and J. Los, Physica 64 (1973) 134-148. INSPEC Quest Accession number: 73041892 INSPEC NN: A73026715


A17 (II) Energy transfer and differential scattering for ion pair formation in Na, K, Cs + I₂ collisions, J.A. Aten, C.W.A. Evers, A.E. de Vries and J. Los, Chem.Phys. 23 (1977) 125-134. INSPEC Quest Accession number: 77109646 INSPEC NN: A77075272

A21 (II) *Non-reactive scattering of K by Br₂ in the energy range of 0-10 eV*, C.W.A. Evers, A.E. de Vries and J. Los, Chem.Phys. 29 (1978) 399-414. INSPEC Quest Accession number: 78064279 INSPEC NN: A78042156


Letters:

INSPEC Quest Accession number: 70013028 INSPEC NN: A70006817

INSPEC Quest Accession number: 74014714 INSPEC NN: A74009417

INSPEC Quest Accession number: 79051500 INSPEC NN: A79034287

INSPEC Quest Accession number: 80036472 INSPEC NN: A80023514

INSPEC Quest Accession number: 82038448 INSPEC NN: A82024812

INSPEC Quest Accession number: 83097713 INSPEC NN: A83060897

INSPEC Quest Accession number: 86112653 INSPEC NN: A86069009

Reviews:

R1 (I) Chemi-ionization by dynamic coupling, J. Los, 8th ICPEAC, Beograd (1973) 621.


INSPEC Quest Accession number: 78103536 INSPEC NN: A78066661

INSPEC Quest Accession number: 83033730 INSPEC NN: A83021674

Theses:

T1 (Construction of the apparatus) J. Politiek, Total elastic cross sections for scattering of potassium by noble gases in the electron-volt region (alkali beams obtained by cathode sputtering) (1970)

T2 (I) A.M.C. Moutinho, Chemi-ionization in neutral-neutral collisions (1971)

T3 (I) A.P.M. Baede, Chemi-ionization by non-adiabatic transitions in atom-molecule collisions (1972)

T4 (I) G.A.L. Delvigne, Differential cross sections for chemi-ionization in alkali-halogen collisions (1973)

T5 (II) M.M. Hubers, Ion pair formation in atom-molecule collisions (1976)

T6 (II) J.A. Aten, The dynamics of ion pair formation in atom-molecule collisions (1977)


T8 (III) U.C. Klomp, Non-vertical vibronic transitions in atom-molecule collision (1982)

T9 (III) M.R. Spalburg, Studies on the dynamics of the vibronic transitions (1985)

Trajectory calculations of ion pair formation

From the research programme of the collaborating group of de Vries at the Institute for Atomic and Molecular Physics (AMOLF) in Amsterdam

Articles:

A13 (II) Total reactive cross section for K + Br₂ in the energy range of 0-4 eV, Chr.W.A. Evers, A.E. de Vries, Chem.Phys. 15 (1976) 201 - 208. [INSPEC Quest Accession number and INSPEC NN not available]

A17 (II) Trajectory surface hopping study of ionizing collisions between Na, K and Cs + I₂ in the energy range of 10-100 eV, Chris Evers, Chem.Phys. 21 (1977) 355 - 371. [INSPEC Quest Accession number and INSPEC NN not available]

A22 (II) Total cross sections for K + Br₂ at relative energies between 0 and 800 eV, C.W.A. Evers, Chem.Phys. 30 (1978) 27 - 32. [INSPEC Quest Accession number and INSPEC NN not available]
Theses:

T10 A. van der Meulen, *The reaction K + Br₂ → KBr + Br in the electronvolt energy region* (1974)

Appendix C

Modularised articles

C.1 Legenda

C.1.1 Characterisation of the modules

Unique identification of the modules

In the examples, the modules carry a corpus-specific unique identification. This minimal identification encodes the conceptual function and the level of the information. For microscopic modules, it also encodes which article the module is a component of. The modularised articles in the examples are identified as respectively A05 and A08. The identification distinguishes between different domain-oriented labels, without encoding them. The other bibliographic data characterising a module, such as the author names and the publication dates, apply to the article as a whole. Therefore these bibliographic data are indirectly encoded in the article number.

The root of the characterisation of the modules is ‘PUB-my’, in which PUB identifies the publication of which the module is a part and my identifies the module as it is distinguished from the conceptual function and the physics point of view.

Identifying the publication

The number of the article is given in the bibliography of the corpus in Appendix B. The articles and the publications in Letters journals, both of the core of the corpus and the related research, are numbered chronologically. The review papers and the thesis are identified separately as Rx and Tx respectively.

The meso- and macroscopic modules carry a label containing ‘MESO-my’ (abbreviated as ME-my) or ‘MACRO-my’ (MA-my). As these modules do not directly correspond to original articles, they are not distinguished by the standard bibliographical data. In order to make the identification somewhat more intuitive, the physics characterisation of these modules is encoded

<table>
<thead>
<tr>
<th>PUB</th>
<th>The publication that the module is part of</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ax</td>
<td>= Article number x</td>
</tr>
<tr>
<td>Rx</td>
<td>= Review number x</td>
</tr>
<tr>
<td>Tx</td>
<td>= Thesis number x</td>
</tr>
<tr>
<td>MESO = ME</td>
<td>= The collection of mesoscopic modules we created</td>
</tr>
<tr>
<td>MACRO = MA</td>
<td>= The collection of macroscopic modules we created</td>
</tr>
</tbody>
</table>
m1 = Meta-information
m1a = Bibliographic information
m1b = Physical index terms
m1c = 'Map of contents'
m1d = Abstract
m1e = List of References
m1f = Acknowledgements
m2 = Positioning
m2a = Situation
m2b = Central problem
m3 = Methods
m3a = Experimental methods
m3b = Numerical methods
m3c = Theoretical methods
m4 = Results
m4a Raw data
m4b = Treated results
m5 = Interpretation
m5a Qualitative interpretation
m5b Quantitative interpretation
m6 = Outcome
m6a = Findings
m6b = Leads for further research

Table C.1
Modules distinguished by the conceptual function

in an abbreviation. For example, MESO-m3c-mod identifies the mesoscopic Theoretical methods module on the atom-atom model for molecular collisions.)

Identifying the module by conceptual function and physics content: my

For the identification A-z-my, the number of the module my is determined firstly by the conceptual function as given in Table C.1.

Constituent modules based on a differentiation in the physics characterisation are indicated as A-z-my-z, where z enumerates the constituent modules (i,ii,iii,...), and further differentiation as A-z-my-z-a, where a enumerates the constituent modules of the constituent modules (1,2,3,...).

For example, the Treated results in [Delvigne and Los, 1973] are identified with the code A08-m4b, the experimental component of those Treated results with A08-m4bi and the particular treated results on the experimental cross section with A08-m4bil.

External references: Rf_Az,y

External references, to particular modules or articles outside the corpus, are encoded as Rf_Az,y, where Az is the code of the article in which the reference is given, and y the number of that reference in the list of references.

A reference to an entire article corresponds to a reference to its module Meta-information m1. We indicate a reference to a module that is not available in modularised articles as 'm*'.

Labels

The characterisation of each module is given in a table that remains accessible (either hidden or visible) when the reader consults the module. Example:

<table>
<thead>
<tr>
<th>Characterisation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Conceptual function:</td>
<td>Goal</td>
</tr>
<tr>
<td>Range:</td>
<td>Microscopic</td>
</tr>
<tr>
<td>Physics:</td>
<td>[terms]</td>
</tr>
<tr>
<td>Bibliographic:</td>
<td>Delvigne, Los [AMOLF]; Physica [1972]</td>
</tr>
<tr>
<td>Identification:</td>
<td>A05-m12</td>
</tr>
</tbody>
</table>
C.1. LEGENDA

Organisational relations:

Hierarchical: S contains, en → part of, pt T
Proximity: S external, ext → external, ext T
S project, pj → project, pj T
Range-based: S to (a module with a) narrower range, nr → to (a module with a) wider range, wr T
Administrative: S to the meta-information, meta → to the context, info T
Sequential: Complete path: S sq<next, sq< → → sq<back, sq<b T
Essay-path: S sq<next, sq< → → sq<back, sq<b T

Scientific discourse relations:

Based on the communicative function: Elucidation: S elucidated in, elu → elucidates, use T
Clarification: S clarified in, cl → clarifies, use T
Definition: S defined in, def → defines, use T
Specification: S specifications given in, spc → gives specifications, use T
Explanation: S explained in, exp → explains, use T
Argumentation: S argued in, arg → to standpoint, stop T
Content
Dependency: S depends on, dp → used for, use T
Transfer: S gets input from, in → provides output into, out T
Elaboration: S elaborated in, elb → limited in, lim T
Resolution: S summarised in, sum → detailed in, det T
Context: S focused on in, fo → more context, con T
Similarity: S compared to, com → compared to, com T
S agrees with, agr → agrees with, agr T
S disagrees with, dis → disagrees with, dis T
Synthesis:
Aggregation: S aggregated in, ag → ; segregated in, sq T
Generalisation: S generalised in, gen → ; specialised in, sp T
Causality: S To cause, ca → To effect, ef T

Table C.2
Notation (and occurring abbreviations) of the types of relations that can be represented in links, with organisational relations (in italic) and scientific discourse relations (see section 4.3)

C.1.2 Navigation

The main navigation menu, with links between module in the same or other article remains accessible (either hidden or visible) when the reader consults the module. An example of a navigation menu:

<table>
<thead>
<tr>
<th>Referred to from:</th>
<th>Navigation menu</th>
<th>Referring to:</th>
</tr>
</thead>
<tbody>
<tr>
<td>map mlc</td>
<td>-inf→ -meta</td>
<td>←meta → ←inf→ meta mlc</td>
</tr>
<tr>
<td>Ax-mu</td>
<td>su-ex→ su-ex</td>
<td>←su→ex→ ←su→ex Ax-mu</td>
</tr>
<tr>
<td></td>
<td></td>
<td>This module</td>
</tr>
<tr>
<td></td>
<td>su-ex//sum//su-bck→ ←rnt//detl//su-ex→ ←rnt//detl//su-ex→ mu</td>
<td>←su-ex//sum//su-bck→ [Ax-mu]</td>
</tr>
</tbody>
</table>

In the navigation menu, the links leading to this module as a target are indicated on the left-hand side. On the right-hand side, the links starting from this module as a source are listed. Targets that are referred to from the text are enclosed in [brackets], contrary to targets that are only referred to from the navigation menu, such as the standard meta-information.

The vertical position of other modules with respect to the current one, Ax-mu indicates the relative 'position' of that module in the problem-solution pattern with respect to this one (i.e.
APPENDIX C. MODULARISED ARTICLES

\begin{tabular}{llll}
ag & = Aggregated in (aggregation) & in & = Input from (transfer) \\
agr & = Agrees with (similarity relation) & info & = To content (administrative) \\
arg & = Argued in (argumentation) & meta & = To meta-information (administrative) \\
chr & = Clarified in (clarification) & mr & = To narrower range (range-based) \\
cm & = Contains (hierarchical) & lm & = Limited in (elaboration) \\
com & = Compared to (similarity) & pln & = Explains (explanation) \\
cx & = More context in (context) & pt & = Part of (hierarchical) \\
def & = Defined in (definition) & out & = Output to (transfer) \\
d & = Disagrees with (similarity) & sg & = Segregated in (aggregation) \\
dp & = Depends on (dependency) & sm & = Summarised in (resolutions) \\
dt & = Detailed in (resolutions) & sp & = Specialised in (generalisation) \\
eff & = To effect (causal) & sq-b & = Step back (complete path) \\
elb & = Elaborated in (elaboration) & sq-n & = Next step (complete path) \\
elsb & = Step back (essay-type path) & stp & = Provides arguments for (argumentation) \\
elsn & = Next step (essay-type path) & unc & = Clarifies (clarification) \\
exp & = Explained in (explanation) & und & = Defines (definition) \\
ext & = External (proximity) & une & = Elucidates (elucidation) \\
fc & = Focused on in (context) & uns & = Gives specifications (specification) \\
gn & = Generalised in (generalisation) & usd & = Used for (dependency) \\
wd & = To wider range & & (range-based) \\
\end{tabular}

Table C.3

Index of the abbreviations of the labels associated to the various types of relations:

it indicates if the link points forward or backward in the problem-solution pattern).

In the text of the module, the hyperlinks relating the different modules are indicated as follows: [A brief description of the link and its target (link type: [link type]; target: [identification number]).

That text is hidden until the appropriate icon is pointed at or clicked. In the link type, the relation that presumably matters most for the reader (and that mainly prompted the author to create the link) is capitalised.

C.1.3 Text

In the modular version of A05, we have indicated typographically how the module has been created from the original version:

- Ordinary times roman = literally copied from an original article; by default from the article at hand. The source of information copied from another article is indicated in a marginal note.
- Small text = a rephrasing of the original text with the same information content.
- Slanted text = supplied manually, i.e. it does not originate from the linear version. More than just a light rephrasing has taken place. Addition of some information to the module is necessary to make the module complete and coherent.

Also in [module]
- Sans serif = overlapping information: the same information is included in more than one module, stated in a marginal note.
- Footnotesize text is hidden from view until activated.

Hyperlinks and elaborate details are presented using footnotesize text and therefore supposed to be hidden from first view. Details that are hidden can be ‘unfolded’ by clicking and thus included in the running text. Those ‘unfolded details’ are indicated as follows:
Details:
(Mathematical) details can be hidden from first view for practical reasons, namely to preserve clearly the line of reasoning without encumbering the reader with all details.

Likewise, the reader can enlarge the figures, which are rather small in the ‘basic’ presentation, to avoid overcrowding the screen (and in the case of the printed appendix, to avoid overcrowding the pages).

**Comments on Module=Ax-my:**

- Comments on the modularised article and the modularisation process are itemised in a box, at the end of the module.
C.2 The modularised version of A05

**META-INFORMATION = A05-m1**

<table>
<thead>
<tr>
<th>Characterisation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Conceptual function:</strong></td>
<td>Meta-information</td>
</tr>
<tr>
<td><strong>Range:</strong></td>
<td>Microscopic</td>
</tr>
<tr>
<td><strong>Physics:</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Bibliographical:</strong></td>
<td>Deligne, Les [AMOLF]; Physica [1972]</td>
</tr>
<tr>
<td><strong>Identification:</strong></td>
<td>A05-m1</td>
</tr>
</tbody>
</table>

This module *Meta-information* contains

1. Bibliographical information = A05-m1a  [[link type: ‘CONTAINS’; target: A05-m1a]]
2. Physics terms = A05-m1b  [[link type: ‘CONTAINS’; target: A05-m1b]]
3. Map of contents = A05-m1c  [[link type: ‘CONTAINS’; target: A05-m1c]]
4. Abstract = A05-m1d  [[link type: ‘CONTAINS’; target: A05-m1d]]
5. References = A05-m1f  [[link type: ‘CONTAINS’; target: A05-m1f]]
6. Acknowledgement = A05-m1e  [[link type: ‘CONTAINS’; target: A05-m1e]]

[A starting point of the essay-type path: Situation [link type: ‘ESSAY-NEXT/information’; target: A05-m2a]]

[Start of the complete sequential path: Bibliographical information [link type: ‘SEQ-NEXT/contains’; target: A05-m1a]]

**Comments on Meta-information=A05-m1:**

- This is a compound module in which six components are aggregated. A modular summary of these constituent modules is given in the form of a table of contents. All constituents are connected to this complex module by means of a link, which is indicated in the text as, for example,  [[link type: ‘CONTAINS’; target: A05-m1a]].

- This module is the first module encountered by readers who consult the article as a whole; it is a starting point of both the complete sequential path and the essay-type path. There is a second starting point of the essay-type sequential path in the Abstract m1d.

- All meta-modules (and constituent modules) are connected to all ‘scientific content modules’ (and constituent modules) in the article by means of a link expressing an administrative relation: ←_metaInfo_ →.
Bibliographic information = A05-m1a

<table>
<thead>
<tr>
<th>Characterisation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Conceptual function:</strong></td>
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<td><strong>Range:</strong></td>
</tr>
<tr>
<td><strong>Physics:</strong></td>
</tr>
<tr>
<td><strong>Bibliographic:</strong></td>
</tr>
<tr>
<td><strong>Identification:</strong></td>
</tr>
</tbody>
</table>

**Title**

*The differential cross section for chemi-ionization in alkali atom–halogen molecule collisions. Classical interpretation*

**Journal**

Physica

**Identification of the article**

A05

**Authors**

C.A.L. Delvigne

**Affiliation:**

F.O.M.-Instituut voor Atoom- en Molecuulfysica, Amsterdam, The Netherlands

address: Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

**Current address:**

unknown

J. Los:

**Affiliation:**

F.O.M.-Instituut voor Atoom- en Molecuulfysica, Amsterdam, The Netherlands

address: Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

**Current address:** AMOLF, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands

**Dates**

Date received: 25 November 1971

[Next step on the complete sequential path: Physics index terms (link type: 'SEQ-NEXT'; target: A05-m1b)]

[Step back on the complete sequential path: Meta-information (link type: 'SEQ-BACK/is part of'; target: A05-m1)]

**Comments on Bibliographic data=A08-m1a:**

- The original article is uniquely characterised by the journal name, volume, year of publication and page numbers: Physica 59 (1972) 61-76. It also provides names and affiliations of the author, the title and the date at which the manuscript was received by the publisher. The current addresses of the authors are not provided in the original article.
### Physics index terms = A05-m1b

<table>
<thead>
<tr>
<th>Characterisation</th>
<th>Meta-information: Physics index terms</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Conceptual function</strong></td>
<td>Microscopic</td>
</tr>
<tr>
<td><strong>Range</strong></td>
<td>-</td>
</tr>
<tr>
<td><strong>Physical</strong></td>
<td>-</td>
</tr>
<tr>
<td><strong>Bibliographic</strong></td>
<td>Delvigne, Los (AMOLF); Physica (1972)</td>
</tr>
<tr>
<td><strong>Identification</strong></td>
<td>A05-m1b</td>
</tr>
</tbody>
</table>

#### POSITIONING

**A05-m2** Harpoon model  
Charge transfer - chemi-ionization = ion-pair formation  
Differential cross section [chemi-ionisation; alkali atom, halogen molecule; eV]  
Atom-atom model  
Electrovolt beams

#### Situation

**A05-m2a** Harpoon model  
Charge transfer  
Scattering  
Electrovolt beams

#### Central question

**A05-m2b** Differential cross section [chemi-ionisation; alkali atom, halogen molecule; eV]  
Atom-atom model

#### METHODS

**A05-m3** Atom-atom model  
Molecular beam scattering

**A05-m3c** Binary collisions  
Classical trajectory calculations  
Landel-Zener  
Impact parameter approximation  
Isotopic potential

#### Experimental methods

**A05-m3a** Molecular beam techniques  
Scattering [source: Sputtering; selection: Skotted disc; Surface ionization; interaction: Static gas analysis; Electrostatic lenses; detection: Channel electron multiplier]

#### RESULTS

**A05-m4** Differential cross section [chemi-ionisation; alkali atom, halogen molecule; eV].

**Raw data**

**A05-m4a** Differential cross section [chemi-ionisation; alkali atom, halogen molecule; eV]  
**A05-m4a1** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  
**A05-m4a1i** Differential cross section [chemi-ionisation; Li, Br2; 11.25 eV]  
**A05-m4a1ii** Differential cross section [chemi-ionisation; K, Cl2; 11.25 eV]  
**A05-m4a1iii** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  
**A05-m4a1iv** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  
**A05-m4a1v** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  

**Treated results**

**A05-m4b** Differential cross section [chemi-ionisation; alkali atom, halogen molecule; eV]  
**A05-m4b1** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  
**A05-m4b1i** Differential cross section [chemi-ionisation; Li, Br2; 11.25 eV]  
**A05-m4b1ii** Differential cross section [chemi-ionisation; K, Cl2; 11.25 eV]  
**A05-m4b1iii** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  
**A05-m4b1iv** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  
**A05-m4b1v** Differential cross section [chemi-ionisation; K, Br2; 6.9, 10.35 eV]  

#### INTERPRETATION

**A05-m5** Classical trajectory calculations;  
Crossing diabatic potentials

**Qualitative interpr.**

**A05-m5a** Atom-atom model  
Classical trajectory calculations.  
Differential cross section [chemi-ionisation; K, Br2; eV].
C.2. THE MODULARISED VERSION OF A05

Qualitative

**A05-m5ai** Differential cross section[chemi-ionisation; K, Br2; eV]; Classical trajectory calculations; Atom-atom model

Quantitative interpretation

**A05-m5b** Classical trajectory calculations, Differential cross section[chemi-ionisation; K, Br2; eV]; Quantitative

**A05-m5bi** Rüttner potential V(r)K+Br2

ENDOTHERMICITY ΔE:

Electron affinity EA(Br2);

Orientation αBr2

Crossing distance \( \bar{R}_c \);

Resonance energy \( \mathcal{H}_{12} \);

Ionic-well depth \( c \);

Repulsive steepness coefficient \( \rho \);

Deflection function

**A05-m5bi** Differential cross section[chemi-ionisation; K, Br2; eV]; Deflection function

Calculation

Atom-atom model

Landau-Zener

OUTCOME

**A05-m6** Differential cross section[chemi-ionisation; alkali atom; halogen molecule; eV range]; Atom-atom model

Classical trajectory calculations

Findings

**A05-m6a** Differential cross section[chemi-ionisation; alkali atom; halogen molecule; eV range]; Atom-atom model

Classical trajectory calculations

Qualitative

**A05-m6b** Differential cross section[chemi-ionisation; alkali atom; halogen molecule; eV range]

Quantitative

High resolution

[Next step on the complete sequential path: Map of contents (link type: 'SEQ-NEXT'; target: A05-m1c)]

[Step back on the complete sequential path: Bibliographical information (link type: 'SEQ-BACK'; target: A05-m1a)]

**Comments on the List of index terms**

- The physics terms assigned to this article by INSPEC are:
  - Controlled Terms: ATOMIC COLLISION PROCESSES; BROMINE; IODINE; IONISATION; LITHIUM; MOLECULAR COLLISION PROCESSES; POTASSIUM
  - Uncontrolled Terms: differential cross section; potential parameters; crossing distance; resonance energy; chemi ionization; pseudocrossing; K+Br2 producing K++Br+Br; K+I2 producing K++I+I; Li+Br2 producing Li+Br+Br; inelastic collisions; alkali atom halogen molecule collisions
  - Classification Codes: A3420 Interatomic and intermolecular potentials and forces; A3440 Elastic scattering of atoms and molecules; A3450 Inelastic scattering of atoms and molecules; A8230 Specific chemical reactions; reaction mechanisms
Figure C.1. All – elementary and complex - microscopic modules are given, as well as links expressing dependency relations (including the more specific transfer relations) and links expressing the essay-type sequential path (dashed line).

[Next step on the complete sequential path: Abstract (link type: ‘SEQ-NEXT'; target: A05-m1d)]

[Step back on the complete sequential path: Physics index terms (link type: ‘SEQ-BACK'; target: A05-m1b)]
Comments on Map of contents=A05-mlc:

- The ‘map of contents’ is intended to provide the reader with an overview of the article allowing for efficient navigation and for insight in the coherence of the article.

- In an electronic environment the map is interactive: the representations of the modules in the map are linked to the modules themselves via hyperlinks. The level of detail of the map can be determined by the reader. The default presentation includes all the modules of the article and no relations between them (except maybe the main sequential path). The reader can also hide the component modules concentrating on the main modules, or add more details such as all or some specified types of relations between all or some specified modules, such as the mesoscopic modules linked to the modules of the article, and such as the full physics characterisation of modules.

- In this map the modules of the article are presented with a few physics terms, the ‘essay-type’ sequential path linking the modules, the directly related mesoscopic and macroscopic modules and the corresponding ‘wider range’ links, as well as some of the most important links representing ‘problem solving dependency’, in order to illustrate the relations aspect of the modular structure.
Abstract = A05-m1d

For the inelastic-collision processes \( M + X_2 \rightarrow M^+ + (X + X^-) \) [Positioning [link type: elaborated in/info; target: A05-m2]], where the transition to the ionic state takes place via pseudocrossing of the neutral and ionic ground states, the relative differential cross section has been measured using molecular beam techniques [Experimental methods [link type: INFO/detailed in/focused on in; target: A05-m4]] at a kinetic energy of the colliding particles in the eV range. Results [Result [link type: INFO/detailed in/focused on in; target: A05-m4]] are shown for the systems K + Br₂, K + I₂ and Li + Br₂. The measurements on K + Br₂ are compared [Interpretation [link type: INFO/detailed in/focused on in; target: A05-m5]] with calculations based on a simple classical model [Theoretical methods [link type: INFO/detailed in/focused on in; target: A05-m3a]] using the impact-parameter approximation, an isotropic intermolecular potential and neglecting the internal states of the \( X_2 \) molecule. These measurements seem to be suitable for the determination of potential parameters, crossing distance and resonance energy at the crossing point [Interpretation [link type: INFO/detailed in/focused on in; target: A05-m5a]]. The classically calculated differential cross sections [Details on the calculation are given in an Interpretation module [link type: INFO/detailed in/focused on in; target: A05-m5a]] are only in qualitative agreement with the measurements [Outcome [link type: INFO/detailed in/focused on in; target: A05-m6]].

Comments on Abstract=A05-m1d:

- We have used the abstract provided in the original article, only adding links to it. The question how abstracts can be improved, in particular in an electronic and modular environment, is addressed in [Van der Tol, 1999].

- Because the abstract provides an important overview of the article as a whole, we have created a starting point of the essay-type in this module, in addition to the starting point at 'the top of the article', in the module Meta-information m1.
References = A05-m1e

<table>
<thead>
<tr>
<th>Characterisation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Conceptual function:</strong></td>
</tr>
<tr>
<td><strong>Range:</strong></td>
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<tr>
<td><strong>Physics:</strong></td>
</tr>
<tr>
<td><strong>Bibliographic:</strong></td>
</tr>
<tr>
<td><strong>Identification:</strong></td>
</tr>
</tbody>
</table>

References in the article

A01 A.P.M. Baede, A.M.C. Moutinho, A.E. de Vries and J. Los, Chem. Phys. Lett. 3 (1969). [in A05-m2a] [link to occurrence(s) in text]

A02 A.M.C Moutinho, A.P.M. Baede and J. Los, Physica 51 (1971) [in A05-m2a] [link to occurrence(s) in text]

A03 A.P.M. Baede and J. Los, Physica 52 (1971) 422. [in A05-m2a,3a,5bi] [link to occurrence(s) in text]

A04 A.M.C. Moutinho, J.A. Atan and J. Los, Physica 53 (1971). [in A05-m2a] [link to occurrence(s) in text]

A06 G.A.L. Delvigne and J. Los, to be published. [in A05-m5bi] [link to occurrence(s) in text]

T2 A.M.C. Moutinho, Thesis, Amsterdam (1971). [in A05-m2a] [link to occurrence(s) in text]

RfA07 1a R.K.B Hofking and E.W. Rothe, J. Chem. Phys. 51 (1969) 1607. [in A05-m2a] [link to occurrence(s) in text]


RfA07 1e J. Weiser, W.B. Peatmanns, and R.S. Berry, Phys. Rev. Lett. 25 (1970) 79. [in A05-m2a] [link to occurrence(s) in text]

RfA07 1f J.T. Moseley, W.H. Abersh, and J.R. Peterson, VIICPEAC, Amsterdam (1971). [in A05-m2a] [link to occurrence(s) in text]

RfA07 2 W.B. Person, J. Chem. Phys. 38 (1963) 109. [in A05-m3c,5bi] [link to occurrence(s) in text]

RfA07 3 R. Dürren, Private communication. [in A05-m3c,5bi] [link to occurrence(s) in text]

RfA07 4 E.S. Rittner, J. Chem. Phys. 19 (1951) 1030. [in A05-m4bi,5bi] [link to occurrence(s) in text]

MESO-m3a-sput A.M.C. Moutinho, P.G. Besaar, J. Los and J. Kistemaker, Nucl. Instrum. Methods 71 (1969) 56. [in A05-m3a,6b] [link to occurrence(s) in text] (=RfA06)

MESO-m3a-surf J. Politiek and J. Los, Rev. Sci. Instrum. 40 (1969) 1576. [in A05-m3a] [link to occurrence(s) in text] (=RfA07)

RfA07 8 F.T. Smith, R.P. Marchi and K.G. Dedrick, Phys. Rev. 150 (1966) 79. [in A05-m5bi] [link to occurrence(s) in text]

RfA07 9 Handbook of Chemistry and Physics. [in A05-m5bi,ii] [link to occurrence(s) in text]

RfA07 10 M.V. Berry, Proc. Phys. Soc. 89 (1966) 479. [in A05-m5bi] [link to occurrence(s) in text]

RfA07 11 B.S. Duchart, M.A.D. Fluendy and K.P. Lawley, VIIICPEAC, Amsterdam (1971). [in A05-m5bi] [link to occurrence(s) in text]

RfA07 12 K.W. Ford and J.A. Wheeler, Ann. Phys. 7 (1959) 259, 287. [in A05-m5aii] [link to occurrence(s) in text]

RfA07 13 R.B. Bernstein, Adv. Chem. Phys. 10 (1966) p.75. [in A05-m5aii] [link to occurrence(s) in text]

RfA07 14 E. Hundhausen and H. Pauly, Z. Phys. 187 (1965) 305. [in A05-m5bi] [link to occurrence(s) in text]

MESO-m2a Situation [in A05-m2a] [link to occurrence(s) in text]

MESO-m2b Central problem (contextualised in/wider range) [in A05-m2b,6b] [link to occurrence(s) in text]

MESO3a-surf Theoretical methods, atom-atom model [in A05-m2a,3a,5ai,5aii,5bi] [link to occurrence(s) in text]

MESO3a-def Th. meth. Deflection function (contextualised in/wider range) [in A05-m4bi-iii,5ai,6b,ii] [link to occurrence(s) in text]
MESO-m3c-treat the method Data analysis and presentation technique [detailed in wider range] [in A05-m4bi-iii] [link to occurrence(s) in text]

MESO-m3a-charge exp. meth Charge transfer [in A05-m6b] [detailed in wider range, focus]

MESO-m3a's Other experimental methods [in A05-m3a] [detailed in focus/wider range] [link to occurrence(s) in text]

References per module

POSITIONING = A05-m2 [-]

Situation = A05-m2a

RF_A051a R.K.B Holling and E.W. Rothe, J. Chem. Phys. 51 (1969) 1607, (external/ elaborated in); [link to occurrence(s) in text]

T2 A.M.C. Moutinho, Thesis, Amsterdam (1971), (project/elaborated in/wider range); [link to occurrence(s) in text]

A03 A.P.M. Baede and J. Los, Physica 52 (1971) 422, (project/elaborated in); [link to occurrence(s) in text]

RF_A051d R.N. Compton, S.J. Nailey, H.C. Schweinler, and V.E. Anderson, VII ICPEAC, Amsterdam (1971), (external/elaborated in); [link to occurrence(s) in text]

RF_A051le J. Weiner, W.B. Pratmann, and R.S. Berry, Phys. Rev. Lett. 25 (1970) 79, (external/elaborated in); [link to occurrence(s) in text]

RF_A051f J.T. Moseley, W.H. Abers, and J.R. Peterson, VII ICPEAC, Amsterdam (1971), (external/elaborated in); [link to occurrence(s) in text]

A01 A.P.M. Baede, A.M.C. Moutinho, A.E. de Vries and J. Los, Chem.Phys.Lett. 3 (1969), (project/elaborated in); [link to occurrence(s) in text]

A02 A.M.C. Moutinho, A.P.M. Baede and J. Los, Physica 51 (1971), (project/elaborated in); [link to occurrence(s) in text]

A04 A.M.C. Moutinho, J.A. Aten and J. Los, Physica 53 (1971), (project/elaborated in); [link to occurrence(s) in text]

MESO-m2a Situation, (project/elaborated in/wider range); [link to occurrence(s) in text]

MESO-m3c-mod Theoretical methods: Atom-atom model, (project/detailed in/focused on in/wider range); [link to occurrence(s) in text]

MESO-m3a Experimental methods, (project/detailed in/focused on in/wider range); [link to occurrence(s) in text]

Central question = A05-m2b

MESO-m2b Central problem, (project/elaborated in/wider range); [link to occurrence(s) in text]

METHODS = A05-m3 [-]

Theoretical methods = A05-m3c

RF_A052 W.B. Person, J. Chem. Phys. 38 (1963) 109, (external/input from/explained in/argued in); [link to occurrence(s) in text]

A03 A.P.M. Baede and J. Los, Physica 52 (1971) 422, (project/disseminates with/arguments found in); [link to occurrence(s) in text]

RF_A053 R. Düren, Private communication. [in A05-m3c,5b], (external/arguments found in); [link to occurrence(s) in text]

MESO-m3c-mod Theoretical methods: Atom-atom model [detailed in/wider range/project] [link to occurrence(s) in text]

MESO-m3c-def Theoretical methods: Deflection function and differential cross section [detailed in/wider range/project] [link to occurrence(s) in text]

Experimental methods = A05-m3a

MESO-m3a-sputt = Moutinho A.M.C. Moutinho, P.G. Ikelaar, J. Los and J. Kistemaker, Nucl. Instrum. Methods 71 (1969) 56, (project/wider range/detailed in/focused on in); [link to occurrence(s) in text]

MESO-m3a-surf = Politek J. Politek and J. Los, Rev. Sci. Instrum. 40 (1969) 1576, (project/wider range/detailed in/focused on in); [link to occurrence(s) in text]

MESO-m3a-IR Experimental method: IR detector, (project/wider range/detailed in/focused on in); [link to occurrence(s) in text]
C.2. THE MODULARISED VERSION OF A05

MES0-m3a-dsk Experimental method: Slotted disk. (project/wider range/detailed in/focussed on in); [link to occurrence(s) in text]

MES0-m3a's Other experimental methods. (project/wider range/detailed in/focussed on in); [link to occurrence(s) in text]

RESULTS = A05-m4 [-]

Raw data = A05-m4a [-]

Treated results = A05-m4b [-]

Treated results = A05-m4b/i

MES0-m3c-treat Theoretical methods: Data analysis and presentation technique. (detailed in/depends on/wider range/project); [link to occurrence(s) in text]

MES0-m3c-def Theoretical methods: Deflection function and differential cross section (detailed in/explained in/wider range/project); [link to occurrence(s) in text]

Treated results = A05-m4bi

Ref 1 E.S. Ritter, J. Chem. Phys. 19 (1951) 1030. (external/input from); [link to occurrence(s) in text]

MES0-m3c-treat Theoretical methods: Data analysis and presentation technique. (detailed in/depends on/wider range/project); [link to occurrence(s) in text]

MES0-m3c-def Theoretical methods: Deflection function and differential cross section (detailed in/explained in/wider range/project); [link to occurrence(s) in text]

INTERPRETATION = A05-m5

MES03a-mod Theoretical methods: Atom -atom model (depends on/detailed in/wider range/project); [link to occurrence(s) in text]

Qualitative interpretation = A05-m5a [-]

Qualitatief = A05-m5ai

MES03a-mod Theoretical methods: Atom -atom model (depends on/detailed in/wider range/project); [link to occurrence(s) in text]

MES03a-def Theoretical methods: Deflection function and differential cross section (detailed in/wider range/project); (input from/wider range/project) [link to occurrence(s) in text]

Qualitatief = A05-m5aii

Ref 12 K.W. Ford and J.A. Wheeler, Ann. Phys. 7 (1959) 259, 287. (elaborated in/wider range/project) [link to occurrence(s) in text]

Ref 13 R.B. Bernstein, Adv. Chem. Phys. 10 (1966) 75. (input from/elaborated in/wider range/project) [link to occurrence(s) in text]

MES03a-def Theoretical methods: Deflection function and differential cross section (detailed in/input from/project/wider range); [link to occurrence(s) in text]

Quantitatief = A05-m5b [-]

Quantitatief = A05-m5bi

Ref 14 W.R. Person, J. Chem. Phys. 38 (1963) 109. (agrees with/external) [link to occurrence(s) in text]

A06 G.A.L. Delville and J. Los, to be published, depends on/detailed in/project; [link to occurrence(s) in text]

A05-m4b Baede, Los (agrees with/project);[link to occurrence(s) in text]

Ref 15 R. Düren, Private communication. (input from/external); [link to occurrence(s) in text]

Ref 16 E.S. Ritter, J. Chem. Phys. 19 (1951) 1030. (input from/external); [link to occurrence(s) in text]

Ref 17 Handbook of Chemistry and Physics. (input from/external); [link to occurrence(s) in text]

Ref 18 F.T. Smith, R.P. Marchi and K.G. Dederick, Phys. Rev. 150 (depends on/external) [link to occurrence(s) in text]
MESO3a-deff Theoretical methods: Deflection function and differential cross section (wider range/detailed in/put from) [link to occurrence(s) in text]

Quantitative = A05-m5bi

MESO3a-mod Theoretical methods: Atom-atom model (detailed in/put from/wider range/project) [link to occurrence(s) in text]

MESO3a-deff Theoretical methods: Deflection function and differential cross section (detailed in/put from/wider range/project) [link to occurrence(s) in text]

**OUTCOME = A05-m6 [-]**

**Findings = A05-m6a [-]**

**Leads for further research = A05-m6b**

MESO-m2b-prob Central problem (detailed in/wider range)

M6 A.M.C. Moutinho, P.G. Ikelaar, J. Los and J. Kristensen, Nucl. Instrum. Methods 71 (1969) 56. (detailed in/wider range/focus) [link to occurrence(s) in text] (= MESO-m3a-putt)

MESO-m3a-charge Experimental methods: Charge transfer(detailed in/wider range/focus)

[Next step on the complete sequential path: Acknowledgements [link type: 'SEQ-NEXT'; target: A05-m1f]]

[Step back on the complete sequential path: Abstract [link type: 'SEQ-BACK'; target: A05-m1d]]

**Comments on Lists of references=A05-m1e:**

- In this module, we list the references to modules outside the article at hand, i.e. to mesoscopic and macroscopic modules, to particular modules written by authors working on the same research project or by others, and to entire articles (where an article is a special case of a complex module).

- In principle, this modular article is embedded in a network of modularly published articles. Here, however, only corpus articles are in modular form. Therefore, we could only specify the target article of the external links to articles that are not part of the corpus, not the particular module that would have been referred to if it had been available. We indicate such a target as Ax-m*.

- The references are listed in two ways: in a complete list of all references in the entire article, and in separate lists of the references in each particular module. These lists given the reader an overview of the embedding in the literature of respectively the article and the module. Creating these lists by hand, as we did, is a lot of work. Therefore, this process has to be automated to meet the requirements of authors of new modular articles.
Acknowledgements = A05-m1f

This work is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (Foundation for Fundamental Research on Matter) and was made possible by financial support from the Nederlandse Organisatie voor Zuiver Wetenschappelijk Onderzoek (Netherlands Organization for the Advancement of Pure Research).

[Next step on the complete sequential path: Positioning [link type: ‘SEQ-NEXT'; target: A05-m2]]
[Step back on the complete sequential path: Lists of references [link type: ‘SEQ-BACK'; target: A05-m1e]]

Comments on Lists of references=A05-m1e:

- The acknowledgements given in the original article have been recast directly into this module.


**POSITIONING = A05-m2**

<table>
<thead>
<tr>
<th>Characterisation</th>
</tr>
</thead>
<tbody>
<tr>
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<tr>
<td><strong>Range:</strong></td>
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<tr>
<td><strong>Physics:</strong></td>
</tr>
<tr>
<td><strong>Bibliographic:</strong></td>
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<td><strong>Identification:</strong></td>
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<th>situation m2a</th>
<th>problem m2b</th>
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<td>$v/\text{m}/\text{m}$ $\rightarrow$ $-e_\text{m}/\text{ag}/\text{m}$</td>
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</tbody>
</table>

In the context [More details on the context in the constituent module Situation (link type: ‘CONTAINS/is segregated in/detailed in’); target: A05-m2a] of the harpoon model, the central problem [More details on the central problem in the constituent module Central problem (link type: ‘CONTAINS/is segregated in/detailed in’); target: A05-m2b] addressed in this article is the measurement of the relative differential cross section of some alkali atom-halogen molecule charge-transfer collisions in the electronvollt range and the interpretation in terms of a simple classical atom-atom model for ion-pair formation in molecular collisions.

**Comments on Positioning=A05-m2:**

- The **Positioning** is an aggregate, compound module containing two constituent modules, the **Situation** and the **Central problem**.

- This module is based on section 1.Introduction in the printed article. In that section, a lot of details were given about the theories used in the article. These details are represented in the modular version in the **Theoretical methods** module A05-m3c and the mesoscopic **Theoretical methods** modules cited in that module.

- In this module we state, more explicitly than the original section 1. Introduction, what is the problem of the research project in general and of the article in particular, and how that problem is addressed using experimental and theoretical methods.

- In the navigation menu, the links leading to this module as a target are indicated on the left-hand side. On the right hand side, the links starting from this module as a source are listed. Targets that are referred to from the text are enclosed in brackets, contrary to targets that are only referred from the navigation menu. The types of relations that are expressed in each link are indicated by an abbreviation. A legend for these abbreviations is given in the appendix.

- The text is coded typographically, to indicate text supplied manually, rephrased text and text overlapping with other modules (see legend). In the margins we have indicated in which module a particular piece of overlapping text appears as well.
### C.2. THE MODULARISED VERSION OF A05

#### Situation = A05-m2a

**Characterisation**

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<td><strong>Physics:</strong></td>
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<td><strong>Bibliographic:</strong></td>
<td>Delvigne, Los [AMOLF]; Physica [1972]</td>
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<td><strong>Identification:</strong></td>
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<tr>
<td>prb.m2b</td>
<td>$- \text{ps} / \text{cm} / \text{m} / \text{at} \rightarrow - \text{cm} / \text{ag} / \text{sm}$</td>
<td>prb.m2b</td>
</tr>
</tbody>
</table>

In recent years several measurements have been performed for total cross sections for chemi-ionisation in the inelastic-collision processes $A + B \rightarrow A^+ + B^-$ as well as for the inverse neutralization $[\text{link type: 'elaborated in/external'; target: RA05.1a-m1, RA05.1d-m1, RA05.1e-m1, RA05.1f-m1 [elaborated in/wider range/project'; target: T2}]. In the research programme from which this article issues [More on the situation in a mesoscopic module (link type: 'elaborated in/wider range/project'; target: MESO-m3a), total cross sections have been measured, using electronvolt molecular beam techniques [link type: 'detailed in/focussed on in/wider range/project'; target: MESO-m3a]], for collisions between alkali atoms and halogen molecules $[\text{link type: 'elaborated in/project'; target: A01-m1}], alkali atoms and $O_2$ $[\text{link type: 'elaborated in/project'; target: A02-m1}], alkali atoms and $Br_2$, $Cl_2$, $N_2$, $NO_2$, $N_2$ and $CO_2$ $[\text{link type: 'elaborated in/project'; target: A03-m1}]$. The total cross sections of alkali atoms and $Cl_2$ and $Br_2$ have also been measured as a function of the secondary beam temperature $[\text{link type: 'elaborated in/project'; target: A04-m1}]$.

These cross sections are interpreted tentatively in terms of a simple atom-atom model $[\text{link type: 'detailed in/focussed on in/wider range/project'; target: MESO-m3c-mod}], according to which the transition to the ionic state takes place via a crossing of the neutral and ionic ground states, which is passed twice in a collision. The transition probability is given by the Landau-Zener formula.

Here we report the relative differential cross sections of some alkali atom-halogen molecule charge-transfer collisions $[\text{The central problem in this situation is focussed on in the module Central problem [link type: 'focussed on in/used in/sq-next/essay-next'; target: A05-m2b]}]. Also in m3a Also in m3c,5 Also in m2

[Next step on the essay-path: Central problem [link type: 'sq-next/essay-next/used for/focussed on in; target: A05-m2b]]
[Back to a beginning the essay-path: Meta-information [link type: 'essay-back/meta'; target: A05-m1]]
[Back to a beginning the essay-path: Abstract [link type: 'essay-back/meta'; target: A05-mld]]
Comments on Situation=A05-m2a:

- We have included in this module a brief summary of the state of affairs of the research project from which this article is issued. The original text refers to an article (A03) and a PhD thesis (T2) in the same project.

- The links to previous work refer to the articles as a whole. Therefore the links lead to the Meta-information of the cited articles.

- A more elaborate account of the development of the domain in science and of the relevance of this particular research project within the domain is given in the mesoscopic module MESO-m2a.
**C.2. THE MODULARISED VERSION OF A05**

**Central problem = A05-m2b**

**Characterisation**

<table>
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<th>Positioning, central problem</th>
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**Navigation menu**

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<tr>
<td><strong>methods m3</strong></td>
<td><strong>m2b</strong></td>
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<td>-c(a)_x/(a)_x \rightarrow +c(a)/c(a)_x)</td>
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<td><strong>findings m6a</strong></td>
<td><strong>finds m6a</strong></td>
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</table>

We study alkali atom-halogen molecule charge-transfer collisions. [More on this central problem in the mesoscopic module [link type: 'elaborated in/wider range/project'; target: Meso-m2b], [The Findings depend on this central problem [link type: 'used in'; target: A05-m6a]]].

**We measure in eV molecular beam experiments** [Details in the module Experimental methods [link type: 'detailed in/focussed on in'; target: A05-m3a]] the relative differential cross sections for chemi-ionisation of the systems K + Br\(_2\) at initial relative kinetic energies of 10.35 and 6.9 eV, K + I\(_2\) at 11.15 eV and Li + Br\(_2\) at 6.25 eV.

*Then we try to explain the measurements on the process K + Br\(_2\) \rightarrow K\(^+\) + (Br...Br\(^-\))* with simple classical atom-atom model, using the impact-parameter approximation, an isotropic intermolecular potential and neglecting the internal states of the X\(_2\) molecule [Details in the module Theoretical methods [link type: 'detailed in/focussed on in'; target: A05-m3c]] , both qualitatively [Details in the Qualitative interpretation [link type: 'detailed in/focussed on in'; target: A05-m5a]] and quantitatively by comparing them to calculations based on the model [The details on this interpret are given in a module Quantitative interpretation [link type: 'detailed in/focussed on in'; target: A05-m5b]].

[Next step on the essay-path: Experimental methods [link type: 'essay-next/detailed in'; target: A05-m3a]]

[Step back on the essay-path: Situation [link type: 'essay-back/sq-back/depends on'; target: A05-m2a]].
Comments on Central problem=A05-m2b:

- In the corpus articles (in the original as well as in the modularised version), the central problem is formulated in terms of a well-defined goal. The course of action at the microscopic level is sufficiently clear to define such a goal. In the original text of A05 the central problem is described in section 1.Introduction and in the abstract.

- In theory, the method used to solve the central problem should not be mentioned when that problem is stated. However, in this domain of experimental research on molecular dynamics, we do name the method in the description of the problem. In this type of research, the methods (scattering) are an integral part of the central problem. The experimental method, in particular, determines the choice of problem and the solution, as well as the community of peers in which the research is embedded. Thereby, it more or less defines the domain of the research.

In A05 it is made clear that the article has an experimental component, which is valuable on its own, and a theoretical component in which the experimental results are interpreted. Therefore both aspects are reflected in the Central Problem.

- The module Central problem overlaps a lot with the module m6a Findings, where an answer to the central question is formulated. This module also shares information with other modules, announcing the response to the problem at hand, which is elaborated in these other modules: the Central problem is a ‘summarising module’.
Methods = A05-m3

In order to solve the problem of the measurement and interpretation of the chemi-ionisation in alkali atom-halogen molecule collisions, eV molecular beam techniques [Specific details in the module Experimental methods (link type: 'contains/specified in/detailed in'; target: A05-m3a)] were used to determine the experimental differential cross sections. The theoretical 'toolbox' contained a simple classical atom-atom model for ion-pair formation in molecular collisions [Details of the model in the module Theoretical methods (link type: 'contains/specified in/detailed in'; target: A05-m3a)]

Comments on Methods—A05-m3:

- Methods is a compound module, in which the specific (experimental and theoretical) methods are generalised as ‘methods in general’.
- This is a complex module in which the experimental methods and the theoretical methods are brought together. The module summary overlaps a lot with its constituent modules, with the results, with the module summary if the Interpretation (coherence) and with the 'summarising' modules Central problem and Findings. In fact this module summary provides an abstract of the article as a whole, emphasising the method aspect.
- In the original text, the authors speak of a ‘simple classical model’. We have specified that model in the running text as a ‘atom-atom model for ion-pair formation in molecular collisions’.

**Experimental methods = A05-m3a**

**Characterisation**

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**Physics:** Molecular beam techniques. Scattering [source: Sputtering; selection: Slotted disk; Surface ionization; interaction: Static gas; analysis: Electrostatic lenses; detection: Channel electron multiplier].

**Bibliographic:** Dévigné, Los [AMOLF]; Physica (1972)

**Identification:** A05-m3a

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### Also in:

- A05-m2a
- m2b, m4b

**Molecular beam techniques** provide a powerful tool for the study of molecular dynamics. Fig. A05-m3a-F1 shows schematically the apparatus we have used to measure the relative differential cross sections of chemi-ionization of the systems K + Br₂ at initial relative kinetic energies of 6.9 and 10.35 eV [The apparatus is used to generate raw data and, subsequently, experimental results (link type: ‘used for’; target: A05m4b)]. Li + Br₂ at 6.25 eV and K + I₂ at 11.25 eV [The apparatus is used to generate raw data and, subsequently, experimental results (link type: ‘used for’; target: A05m4b)].

The sputtering source consists of an Ar⁺ ion source (1). By bombardment of the alkali target (2) by 15 keV Ar⁺ ions, alkali atoms are formed with a kinetic energy in the eV range. [This component is discussed in detail in a mesoscopic module Experimental methods (link type: ‘detailed in/focussed on in/is segregated in/wider range/project’; target: MESO-m3a)]

The beam is collimated by two slits of 0.6 × 6 mm² and velocity-selected by a slotted-disk selector (3) with an energy spread of about 20 percent fwhm. [This component is discussed in detail in a mesoscopic module Experimental methods (link type: ‘detailed in/focussed on in/is segregated in/wider range/project’; target: MESO-m3a)]

Figure A05-m3a-F1. Scheme of the apparatus. An explanation is given in the text.
range/project; target: MESO-m3a].

The relative beam intensity is measured continuously by a surface-ionization detector (4), the detection efficiency of which is expected to be slightly energy-dependent [This component is discussed in detail in a mesoscopic module Experimental methods (link type: 'detailed/focussed on in/is segregated in/wider range/project'; target: MESO-m3a].

The beam is lead into a big collision chamber (5) filled with a static halogen gas at room temperature at a pressure of about $5 \times 10^{-5}$ torr; this pressure is low enough to neglect double collisions [This component is discussed in detail in a mesoscopic module Experimental methods (link type: 'detailed/focussed on in/is segregated in/wider range/project'; target: MESO-m3a].

Positive alkali ions formed in the collision region may enter a rotating detector chamber (6-9), which has an angular resolution of 0.5° for scattering angles less than 30° and 2.5° for large scattering angles [This component is discussed in detail in a mesoscopic module Experimental methods (link type: 'detailed/focussed on in/is segregated in/wider range/project'; target: MESO-m3a].

A grid (10) screens the electric field of the lenses and channeltron to avoid as much as possible distortion of the ion paths between collision region and the second detector diaphragm. Other sources of distortion are contact potentials and electrostatic charged spots; therefore all relevant instruments have been made of the same nonmagnetic stainless steel, coated with a thin layer of graphite. [This component is discussed in detail in a mesoscopic module Experimental methods (link type: 'detailed/focussed on in/is segregated in/wider range/project'; target: MESO-m3a].

We measured differential cross-section curve in runs on either side of the $\theta = 0$ axis (symmetry test). The measuring time for one run is about four hours.
Comments on Experimental methods: A05-m3a:

- The components of the general set-up have been used in previous articles. Therefore details can be found in mesoscopic modules. In this module, a brief overview is given for the sake of coherence.

- The microscopic, article-dependent details are provided here. The size of the slit varies in the course of the corpus and is therefore microscopic information. This type of detector and its energy dependence have been discussed before. Therefore all details can be found in the mesoscopic module. The sample and the pressure within the collision chamber vary in the course of the corpus and are therefore microscopic information.

- The components aggregate into the set-up as a whole. Therefore, the links provided in this module to components of the mesoscopic module MESO-m3a are typed with the inverse of aggregation: [link: is segregated in].

- This module corresponds quite closely to the section 2. Experimental.

- The methods modules are relatively small (w.r.t. the results and especially the interpretation). However, is the case because most of the information on the experimental methods is general and presented in mesoscopic modules.

- In the original two articles by the same group (Moutinho and Politiek) that are not part of the corpus are cited. These references have been replaced by references to mesoscopic modules Experimental Methods, ‘MESO-m3a-sputt’ and ‘MESO-m3a-surf’ about the sputtering source and surface ionisation detection.

- Part of the Experimental Methods is the measurement, i.e. the usage of the set-up: what is measured (sample) at what energy range, at what pressure etc

- The sources of errors are supposed to be linked to the error discussion in the Results module, where the impact of the errors that occur in the methods and tools on the final results is determined. The discussion of the apparatus however seems to be incomplete in A05 - the results refer to ‘apparatus effects’ in general, rather than specific restrictions.
Theoretical methods = A05-m3c

The experimental differential cross sections for chemi-ionization in $M + X_2 \rightarrow M^+ + X_2^-$ are analyzed using a simple classical atom-atom model for ion-pair formation in molecular collisions [The model is discussed in detail in a mesoscopic Theoretical methods module (link type: 'detail/wider range/project'); target: MESO-m3c-mod: the transition to the ionic state takes place via crossing of the neutral and ionic ground states. The electron transition probability is calculated applying the Landau-Zener approximation; trajectories are calculated using the impact parameter approximation [The calculation method is discussed in detail in a mesoscopic Theoretical methods module (link type: 'detailed in/wider range/project'); target: MESO-m3c-defl]. We assume an isotropic intermolecular potential and neglect the internal states of the $X_2$ molecule.

Applicability of the model to the measured collision:
If we apply this model to the system of $K - Br_2$, we assume that the following simplifications are valid

Simplification 1: no internal states Br$_2$
We simplify the potential surfaces by neglecting the vibrational-state distribution and describe the collision as a two-body problem.

Actually the interatomic $M - X - X$ potential should be described by hypersurfaces to include for instance the vibrational states of the $X_2$ and $X_2^-$ molecules. However, we cannot resolve the vibrational structure from the differential cross section, so these effects only have an averaging effect on the measurements.

Unfortunately the effect of vibrational excitation is rather large for the collisions of interest. From the semi-empirical Br$_2$ and Br$_2^-$ interatomic-potential curves of Person [link type: 'explained in/argued in/input from/external'; target: Rf$_{A05}$-m3*] it can be seen that even at a very restricted low vibrational-state distribution of Br$_2$, the exothermic Br$_2 \rightarrow Br_2^-$ transition can cause a high vibrational excitation or even dissociation of the Br$_2^-$ molecule, giving a wide range of possible values of the electron affinity $A(\text{Br}_2)$. As

$$\Delta E = I(M) - A(X_2), \quad (C.1)$$

where $I(M)$ represents the ionization potential of the alkali atom and $A(X_2)$ the electron
affinity of the halogen molecule, this means that in a chemi-ionization process \( \Delta E \) is very dependent on the vibrational state of the halogen molecule before and after the collision.

Indeed, the largest possible bromine-electron affinity \( A(\text{Br}_2) \), as measured by Baede and Los \([\text{link type='arguments in/disagrees/project'; target=A03-m4bi]}\), 2.8 eV, is very different from our value of 1.2 eV for the vertical electron affinity \([\text{The value for the electron affinity, obtain in the Quantitative interpretation, is input into this module [link type='arguments in/input from'; target=A05-m5bi]}\].

Therefore this simplification is not really valid.

**Simplification 2: isotropic intermolecular potential**

Another simplification is made by neglecting anisotropy effects. The anisotropic potentials will also have an averaging effect on the measurements. \([\text{link type='arguments in/external'; target=R6a05]}\] has determined by classical trajectory calculations the chemi-ionization differential cross section of \( K + \text{Br}_2 \) taking into account a nonspherical bromine molecule. His results for collinear and perpendicular collisions are quite different.

Therefore this simplification is not really valid either.
Comments on Theoretical methods=A05-m3c:

- A05-m3c argues and explains that the model is not really applicable in the present situation. That is not a conclusion of the article: the authors were already aware it and stated it in the Introduction of the original article. The authors tried how far they could get using this admittedly inadequate theoretical model. In article A08 this problem is addressed, by considering a more simple system for which the assumptions are valid.

- Person’s interatomic potential curves are used to explain and argue that the vibrational excitation plays an important role, and therefore the link to Person is typed as ([link: ‘explained in/argued in’]). If Person’s article were modularised, the reference would point to a specific module m*: a particular figure is used as input in the line of reasoning presented in this module; this fact is typed in the link as ([link type: ‘input from’]). The value for the electron affinity reported in A03-m4b is also imported into this line of reasoning: the fact that the values disagrees with the value found here is used as an argument: ([link: ‘argued in’]).

- In this module the value of the electron affinity that is only calculated ‘later on’ in the problem-solution pattern (and later on in the original article) is used as an argument supporting the standpoint that the effect of vibration is large in this reaction. The line of reasoning in the article is not linear. In a modular, non-linear structure, such a ‘forward reference’ can be made explicit in a link labelled ‘Input from’ to the Interpretation module.

- This theoretical model does not depend on the experimental results, although its presentation in the original article does so (the model is explained using a figure containing experimental results). In fact the model is only concerned with general shapes and not with the exact results.

- This Theoretical methods module is relatively small (with respect to the results and especially the interpretation). However, that is only the case because the account of the theoretical models used in this article is general information that is presented in mesoscopic modules that allows for multiple use. A brief summary of the theoretical methods is given. The discussion of the applicability to the reactions at hand is ‘new information’, which is not part of the mesoscopic modules.

- A lot of information that we classified as Theoretical methods was presented in the Introduction of the original article.

- In principle, this modular article is embedded in a network of modularly published articles. Here, however, only corpus articles are in modular form. Therefore, we could only specify the target article of the external links to articles that are not part of the corpus, not the particular module that would have been referred to if it had been available. We indicate such a target as A.x-m*.
RESULTS = A05-m4

The differential scattering cross section for chemi-ionization has been measured in the eV range for alkali atom-halogen molecule collisions, using a molecular beam set-up. These results depend on the experimental methods (link type: 'depends on'; target: A05-m3a).

Thus raw data [To the Raw data (link type: 'contains/specified in'; target: A05-m4a)] and treated results [To the Treated results (link type: 'contains/specified in'; target: A05-m4b)] have been obtained for:

- K + Br₂ → K⁺ + (Br + Br⁻) at 6.9 eV and 10.35 eV [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4a)], [To the Treated results (link type: 'contains/specified in/detailed in'; target: A05-m4b)]
- Li + Br₂ → Li⁺ + (Br + Br⁻) at 6.25 eV and K + I₂ → K⁺ + (I + I⁻) at 11.25 eV [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4a)], [To the Treated results (link type: 'contains/specified in/detailed in'; target: A05-m4b)].

This module also contains a copy of 'theoretical data and results' obtained as intermediary results in the course of the interpretation [Input from the module Quantitative interpretation (link type: 'input from'; target: A05-m5b)]. These results are the potential, the deflection function and the theoretical cross section of K + Br₂ [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4a)], [To the Treated results (link type: 'contains/specified in/detailed in'; target: A05-m4b)].
Comments on Results=A05-m4:

- **Results** is a generalising compound module in which the specific results of the article are brought together. Therefore the links to the specific results are typed as [link: specified in].

- In an earlier version of this module, four constituent modules have been distinguished in the Raw data and the Treated results, in which the results for reactions of K + Br₂ at 6.9 eV, K + Br₂ at 10.35 eV, K + I₂ at 11.25 eV, and Li + Br₂ at 11.25 eV were represented separately, because we assumed that the authors and readers of this module would consider each such reaction as a different concept. However, based on discussion with prof. Los, we have changed that assumption; now it is assumed that the results on reactions between different kinds of alkali-atoms and halogen molecules, at different energies in general form a single conceptual unit. Different constituent modules can be distinguished to emphasise a particular reaction. In this module, the K + Br₂ reactions are isolated, because these are the reactions that are considered in the Interpretation. In the original article the results were also grouped thus: K + Br₂ at 6.9 eV and 10.35 eV in one figure, and K + I₂ and Li + Br₂ at 11.25 eV in another figure.

- In the Interpretation intermediary results are generated. We have characterised these explicitly as Results by copying them to this module. The results in m4aiii/biιi are copies from the Quantitative interpretation module A05-m5b. They are incorporated in the sequential paths via that Interpretation, not via the Results.

- All results (i.e. all complex modules and constituent modules) are linked to the methods used to obtain them, because they depend on them quite strongly.

- There is massive overlap in the Results module: the module summaries does not contain any new information, but it describes the constituent modules. These module summaries are of course avoided by the essay-type path with simulates the ‘traditional’ flow of the article.
Raw data = A05-m4a

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The differential scattering cross section for chemi-ionization has been measured in the eV range for alkali atom-halogen molecule collisions, using a molecular beam set-up [These results depend on the Experimental methods (link type: 'depends on'; target: A05-m3a)].

**Thus raw data that have been obtained for:**

- K + Br$_2$ $\rightarrow$ K$^+$ + (Br + Br$^-$) at 6.9 eV and 10.35 eV [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4a)]
- Li + Br$_2$ $\rightarrow$ Li$^+$ + (Br + Br$^-$) at 6.25 eV and K + I$_2$, $\rightarrow$ K$^+$ + (I + I$^-$) at 11.25 eV [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4a)]

This module also contains a copy of 'theoretical data' obtained as intermediary results in the course of the interpretation [Input from the Quantitative interpretation (link type: 'input from'; target: A05-m3b)]. These results are the potential, the deflection function and the theoretical cross section of K + Br$_2$ [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4a)].

**Comments on Raw data=A05-m3a:**

- I've created this empty module for the raw data as an indication; in principle, raw data could be provided in this module. However, I cannot do so in this modularised version of a corpus article. The raw data are not available, as they have not been stored. In this module, output of the detector could be provided, as well as raw numbers generated in calculations.

- The raw data are not suitable for sequential reading by human readers. Sequential readers can in practice choose, for example, in the complex module Results m4 to skip directly to the Treated results. The complete sequential path however does lead through these modules.
Treated results = A05-m4b

The differential scattering cross section for chemi-ionization has been measured in the eV range for alkali atom-halogen molecule collisions, using a molecular beam set-up. These results depend on the Experimental methods (link type: 'depends on'; target: A05-m3a).

Thus we have a graphical representation of the results that have been obtained for:

- \( \text{K} + \text{Br}_2 \rightarrow \text{K}^+ + (\text{Br} + \text{Br}^-) \) at 6.9 eV and 10.35 eV [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4b)]

- \( \text{Li} + \text{Br}_2 \rightarrow \text{Li}^+ + (\text{Br} + \text{Br}^-) \) at 6.25 eV and \( \text{K} + \text{I}_2 \rightarrow \text{K}^+ + (\text{I} + \text{I}^-) \) at 11.25 eV [To the Raw data (link type: 'contains/specified in/detailed in'; target: A05-m4b)]

This module also contains a copy of 'theoretical data' obtained as intermediary results in the course of the interpretation [Input from the module Quantitative interpretation (link type: 'input from'; target: A05-m5b)]. These results are the potential, the deflection function and the theoretical cross section of \( \text{K} + \text{Br}_2 \) [To the Treated results (link type: 'contains/specified in/detailed in'; target: A05-m4b)].

[Next step on the complete path: Treated results (link type: 'sq/contains/specialised in/detailed in'; target: A05-m4b)]
[Step back on the complete path: Raw data (link type: 'sq-back/depends on'; target: A05-m3a)]
**Comments on Treated results—A05-m4b:**

- In order to relate the restrictions on the results directly to the restrictions on the methods, the notions of ‘apparatus effects’ in A05 should be specified in a more elaborate description or argumentation of the reliability of the results.

- Many details on the analysis and treatment of the raw data are mesoscopic and included in MESO-m3a-treat via [Details on the methods in a mesoscopic module (link type: 'detailed in/wider range'; target: MESO-m3a-treat)].

- There is massive overlap between the ‘parallel’ results modules (the same type of results, for different systems): The modules contain almost the same text; the figures however are very important here and those differ. The overlap between the parallels is a direct consequence of the definition of modularity: modules can be consulted separately. Those overlapping texts can be hidden from first view, to accommodate those who consult more than one of the parallel modules.

- The treated results contain intermediary results copied from the *Interpretation*, in order to allow for a search by the label ‘results’. These are direct copies and as such overlap completely with the *Interpretation* modules where they came from.
C.2. THE MODULARISED VERSION OF A05

Experimental treated results (KBr₂) = A05-m4bi

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The differential scattering cross section for chemi-ionization has been measured in the eV range for alkali atom-halogen molecule collisions, using a molecular beam set-up. [These results depend on the Experimental methods (link type: 'depends on'; target: A05-m3a).

Thus we have a graphical representation of the results that have been obtained for:

- \( K + Br₂ → K^+ + (Br + Br^-) \) at 6.9 eV and 10.35 eV [To the Treated results (link type: 'contains/specifies in/detailed in'; target: A05-m4bi)]

- \( Li + Br₂ → Li^+ + (Br + Br^-) \) at 6.25 eV and \( K + I₂ → K^+ + (I + I^-) \) at 11.25 eV [To the Treated results (link type: 'contains/specifies in/detailed in'; target: A05-m4bi2)]

[Next step on the complete sequential path: Treated results (link type: ‘SEQ-NEXT/contains/is specialised in’; target: A05-m4bi1)]

[Step back on the complete sequential path: Treated results (link type: ‘SEQ-BACK/is part of/is aggregated in’; target: A05-m4b)]

Comments on Treated results, experimental = A05-m4bi:

- This is a cluster module with experimental results, which contains two components: an elementary module focusing specifically on collisions between K and Br₂, and one about LiBr₂ and KI₂. By synthesizing these elementary modules into a cluster module, we emphasize that they are related more strongly to each other than to the other elementary module that is part of the complex module Treated results: the module A05-m4bi represents theoretical results.
Experimental treated results (KB\textsubscript{2}) = A05-m4bi1

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- exp.m3a
- res. m4
- data m4ai
- tr.res.m4bi
- int.m5a, ai

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Also in m4/4b/2a/3b

Figure A05-m4bi1-F1 shows the polar differential scattering cross section (CM system) for chemi-ionization of K + Br\textsubscript{2} at initial relative kinetic energies of 6.9 eV and 10.35 eV that has been measured [These results depend on the Raw data (link type: 'depends on'; target: A05-m4ai)] using a molecular beam set-up [These results depend on the Experimental methods (link type: 'depends on'; target: A05-m3a)].

Each measured differential cross-section curve is a superposition of four runs: two runs on either side of the \(\theta = 0\) axis (symmetry test) [Details on the method in a mesoscopic module (link type: 'detailed in/depends on/wider range/project'; target: MESO-3c-treat)]. Equal units have been used on the ordinate. The \(\tau\) scale changes beyond 300 eV - degree.

**Reliability** The results for \(\theta < 2^\circ\) are less reliable due to apparatus effects [The restrictions on the results depend on those of the Experimental methods (link type: 'depends on/detailed in'; target: A05-m3a)] and the difficulty of determining the scattering volume exactly. The fact that the differential cross section for \(\tau \rightarrow 0\) seems to go to zero is probably due to these effects.

The symmetry test indicated that the measured differential cross section is indeed symmetric, as was expected from the fact that only the absolute value of the angle is experimentally relevant. [This is explained in a mesoscopic module (link type: 'detailed in/explained in'; target: MESO-3c-defl)].

Also in m4b2

- Next step on the essay-path: [Treated results (link type: 'essay-next/sq-next'; target: A05-m4bi1)]
- Step back on the essay-path: [Experimental methods (link type: 'essay-back/depends on'; target: A05-m3a)]

![Figure A05-m4bi1-F1. K + Br\textsubscript{2}, chemi-ionization differential cross section (CM system), measured at colliding energies of 6.9 and 10.35 eV.](image-url)
Comments on Treated results, experimental=A05-m4bi1:

- This elementary module focuses on collisions between K and Br₂. We have represented these results in a separate elementary module, because the discussion in the module Interpretation concentrates on KBr₂. Therefore we assume that readers wish to consult this module separately from the module A05-m4bi2 representing the results on LiBr₂ and KI₂.

- The details on the data analysis and the reliability of the results are identical in the next module A05-m4bi2. We have hidden from first view to spare, in particular, the sequential reader this overlap.
Experimental treated results (LiBr$_2$ at 6.25 eV and KI$_2$ at 11.25 eV) = A05-m4bi2

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Figure A05-m4bi2-F1 shows the polar differential scattering cross section (CM system) for chemi-ionization of Li + Br$_2$ at initial relative kinetic energies of 6.25 eV and K + I$_2$ at 11.15 eV that has been measured. These results depend on the raw data [link type: ‘depends on’; target: A05-m4ai] using a molecular beam set-up [These results depend on the Experimental methods [link type: ‘depends on’; target: A05-m3a].

[unfold details on the data analysis and the reliability of the results] Each measured differential cross-section curve is a superposition of four runs; two runs on either side of the $\theta = 0$ axis (symmetry test) [Details on the treatment of the results in a mesoscopic mode (link type: ‘detailed in/depends on/wider range/project’; target: MESO-m3c-treat].

Reliability The results for $\theta < 2^\circ$ are less reliable due to apparatus effects [Restrictions on the results depend on those on the Experimental methods (link type: ‘depends on’; target: A05-m3a) and the difficulty of determining the scattering volume exactly. The fact that the differential cross section for $\tau \rightarrow 0$ seems to go to zero is probably due to these effects.

The symmetry test indicated that the measured differential cross section is indeed symmetric, as was expected from the fact that only the absolute value of the angle is experimentally relevant. [In the mesoscopic description of the deflection function and differential cross section, it is explained why only the absolute angle is relevant (link type: ‘detailed in/explained in’: target: MESO-m3c-def).

![Graph](image)

Figure A05-m4bi2-F1. Li + Br$_2$ at 6.25 eV and K + I$_2$ at 11.25 eV, chemi-ionization differential cross section (CM system). The units on the ordinate are not related.
C.2. THE MODULARISED VERSION OF A05

Comments on Treated results, experimental=A05-m4bi2:

- This elementary module represents the experimental results on LiBr₂ and KI₂. At first, we had created separate elementary modules for the three different types of collision partners: LiBr₂, KI₂ and KBr₂. However, this distinction turned out to be too fine-grained. Following the expert opinion of prof. Los, we assume that readers do not consider collisions between different but comparable collision partners to be different subjects, so that readers will not be interested in consulting the different results separately. The reason why we still have represented the results on KBr₂ in a separate elementary module, is that in the Interpretation those results are used as an example to make the discussion concrete.
Treated results = A05-m4bii

Characterisation

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Also in m5bi, MESO-
m3c-mod

The ionic potential for the system K + Br\(_2\) \rightarrow K\(^+\) + Br\(^-\) is given by a Rittner potential of the form \([\text{link type: 'input from'; target: RfA064-m*]}\):

\[
U_{\text{ion}}(R) = -\frac{e^2}{R} - \frac{e^2(\alpha_{M^+} + \alpha_{X^-})}{2(R^4 + \alpha^4)} - \frac{2e^2\alpha_{M}\alpha_{X^-}}{R^2} \tag{C.2}
\]

\[
-\frac{C_{\text{ion}}}{R^6} + A_{\text{ion}} e^{-R/\rho_{\text{ion}}} + \Delta E.
\]

(a coulombic term, a screened polarization term, dipole-dipole interaction and the endothermicity \(\Delta E\)) and the covalent potential is given by a Van der Waals term and the repulsive term:

\[
U_{\text{ovv}}(R) = -(C_{\text{ovv}}/R^6) + A_{\text{ovv}} e^{-R/\rho_{\text{ovv}}}, \tag{C.3}
\]

with the following values determined in module A05-m5bi \([\text{link type: 'input from') quantitative interpretation m5bi]}\):

\[
\Delta E = 3.1 \text{ eV},
\alpha_{\text{Br}^-} = 150 \text{ Å}^3,
\varepsilon = 1.8 + 3.1 \text{ eV},
\]

Figure A05-m4bii-F1. K–Br\(_2\), ionic and covalent potential curves.
\[ \rho = 0.3 \text{Å}, \]
\[ A = 5 \times 10^5 \text{ eV}, \]
\[ H_{12} = 4.5 \times 10^{-2} \text{ eV}, \]

and the values

\[ \alpha_{K^+} = 0.94 \text{ Å}^3 \]  
\[ C = 10^5 \text{ eV Å}^6, \text{ (arbitrary)} \]
\[ a = 5 \text{ Å}, \text{ (arbitrary)} \]

The resulting potential is presented in figure A05-m4bi-F1.

For a system with the potential given above, the deflection function turns out to be closed. Figure A05-m4bi-F1 represents the deflection curves for chemi-ionization scattering of K + Br\textsubscript{2} (CM system).

The full curves represent the classically calculated scattering angle for “ionic” and “covalent” scattering at colliding energies of 10.35 and 6.9 eV, determined [input from the Quantitative interpretation (link type: ‘input from’; target: A05-m5bi)] using a simple classical model and measurements of the differential cross section in a molecular beam experiment. The dashed curves show the “pure inelastic” scattering-angle contribution to the full-line curves.

The differential cross section calculated based on the deflection function given above has the following shape: Figure A05-m4bi3 represents the classically calculated determined [input from the Quantitative interpretation (link type: ‘input from’; target: A05-m5bi)] chemi-ionization differential cross section of K + Br\textsubscript{2} (CM system) at colliding energies of 6.9 and 10.35 eV and convoluted with the energy spread of the velocity selector.

For both energies equal units have been used on the ordinate. The dotted lines indicate the \( \rho \) dependence of the slope steepness for “covalent” scattering. At \( E_1 = 10.35 \text{ eV} \) and different values of the polarizability \( \alpha_{Br^2-} \), and the ionic-well minimum \( \varepsilon \) the positions of the scattering angle for \( b = R_c \) scattering respectively the classical rainbow angle have been indicated along the abscissa. The values used in the calculations have been underlined.

![Figure A05-m4bi-F2. K + Br\textsubscript{2}, deflection curves for chemi-ionization scattering (CM system).](image-url)
Figure A05-m4bii-F3. $K + Br_2$, classically calculated chemi-ionization differential cross section (CM system) at colliding energies of 6.9 and 10.35 eV.

**Comments on Treated results, theoretical=A05-m4bii:**

- These are ‘qualitative theoretical results’: for this type of reactions, the potential, the deflection function and the differential cross section have the given form. Making the theoretical values exact would take place via fitting. However, it is concluded in the article that there is no quantitative agreement between the theoretical and the experimental values.

- The closed shape of the deflection function was a new result: other deflection functions were open, i.e. not bounded by the maximum distance $b = R_c$. For closed deflection functions there is more than one contribution to a scattering angle, such that interference may occur.

- The general shape of the deflection function was ‘promoted’ to the mesoscopic level, because the deflection function plays an important role in the calculation of the differential cross section. However, this figure turned out to be distorted by the fact that a collision between an atom and a molecule is treated as a binary collision. In A08 the deflection function is determined for an atom-atom collision and that, more reliable, deflection function than replaced the figure obtained here in the mesoscopic module.
### INTERPRETATION = A05-m5

**Characterisation**

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**Range:** Microscopic

**Physics:** Classical trajectory calculations; Crossing diabatic potentials

**Bibliographic:** Deligne, Los [AMOLF]; Physica [1972]

**Identification:** A05-m5

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The differential cross sections [This interpretation depend on the Treated results (link type: 'depends on'; target: A05-m5b) for chemi-ionization in M + X_2 → M^+ + X_2 collisions, in particular in K + Br_2 → K^+ + Br_2, are explained qualitatively [Details in the module Qualitative interpretation (link type: 'detailed in/contains'; target: A05-m5a)] with a simple classical atom-atom model for ion-pair formation in molecular collisions [This interpretation depends on the model given in the Theoretical methods (link type: 'depends on'; target: A05-m3c). [Details on this model in a mesoscopic module (link type: 'depends on/detailed in/wider range/project'; target: MESO-m3c-mod)] via the general shape of the deflection function. A quantum mechanical explanation is suggested for the small angles in which the classical interpretation is not valid [Details in the module Qualitative interpretation (link type: 'contains/specified in/detailed in'; target: A05-m5a, qnt.m5a)] in A05-m5a, qnt.m5a, qnt.m5b, qnt.m5bii, qnt.m5biiii.

In order to interpret the results more quantitatively [The interpretation is specified in a Quantitative interpretation (link type: 'contains/specified in'; target: A05-m5bi), the potential parameters and the classical deflection function of the system are determined via fitting the results calculated according to the classical model with the experimental results [Specific details in a module Quantitative interpretation (link type: 'contains/specified in/detailed in'; target: A05-m5bi)]. Based on the potential parameters and the deflection function thus determined, the differential cross section of the collision is calculated and compared to the measurements [Specific details in a module Quantitative interpretation (link type: 'contains/specified in/detailed in'; target: A05-m5bi)]. However, quantitative agreement is poor.

[Next step on the complete path: Qualitative interpretation (link type: 'sq/contains'; target: A05-m5a)]
[Step back on the complete path: Treated results (link type: 'sq-back'; target A05-m5bii)]
Comments on Interpretation—A05-m5:

- The theory or theories and technique(s) used for the interpretation are described and discussed (with respect to their reliability and applicability) in the *Theoretical methods* module m3c. The description and discussion of the resulting interpretation(s) in terms of physical phenomena is put in this module.

- The discussion of the experimental curve given in A05-m4b takes place in A05-m5, especially in the qualitative interpretation m5a, more especially in the classical one in A05-m5ai.

- For the sake of clarity I have firstly separated the qualitative from the quantitative interpretation using the conceptual function, and then subdivided the resulting modules based on their physics content. I think that in A05 these are ‘full-blown independent information units’, rather than just parts of a single elementary module. The *Interpretation* module thus has been allotted optional constituent modules: *Qualitative interpretation* and *Quantitative interpretation*.

- Most of the external references to other work appear in the *Interpretation* modules.
C.2. THE MODULARISED VERSION OF A05

Qualitative interpretation = A05-m5a

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The differential cross section for chemi-ionization in

\[ K + Br_2 \rightarrow K^+ + Br_2^- \]  \hspace{1cm} (C.4)

collisions [This interpretation depends on the Treated results [link type: 'depends on'; target: A05-m4bi]] is interpreted qualitatively in this module with a simple classical atom-atom model for ion-pair formation in molecular collisions, with the impact parameter approximation [This interpretation depends on the Theoretical methods [link type: 'depends on/detailed in'; target: A05-m3c], via the general shape of the deflection function.

Most of the general shape of the experimental \( K + Br_2 \) cross-section curve can indeed be explained using the classical model [Details on the classical interpretation [link type: 'detailed in/contains/specified in'; target: A05-m5ai]]. For small angles a quantum mechanical explanation is suggested [Details in the quantum interpretation [link type: 'contains/specified in/detailed in'; target: A05-m5aia]].

[Next step on the complete path: Qualitative interpretation [link type: 'sq/contains/specialised in/detailed in'; target: A05-m5ai]]

[Step back on the complete path: Treated results [link type: 'sq-back/part of'; target A05-m5]]

**Comments on Qualitative interpretation=A05-m5a:**

- This is a cluster module, containing two elementary modules that focus on two specific qualitative interpretations: a classical one and a quantum mechanical one.
Qualitative interpretation: classical = A05-m5ai

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We have tried to interpret measured cross sections with a simple classical atom-atom model for ion-pair formation in molecular collisions [Details in this model in a mesoscopic module (link type: 'depends on/detailed in/wider range/project'; target: MESO-m3x-mod)]. The transition to the ionic state takes place via crossing of the neutral and ionic ground states. The electron transition probability is calculated applying the Landau-Zener approximation; trajectories are calculated using the impact parameter approximation.

At least qualitatively the shape of the measured differential cross sections in M + X₂ → M⁺ + X₂⁻ collisions can indeed be understood from the general shape of the deflection curve as sketched in figure A05-m5ai-F1 [This figure is exported to a mesoscopic module (link type: 'output to/wider range/project'; target: MESO-m3x-defl[figure,full text]) and the equation for the differential cross section [The equation is obtained from a mesoscopic module (link type: 'input from/detailed in/wider range/project'; target: MESO-m3x-defl[equation,full text])]

\[
I(\theta) = \frac{1}{\sin \theta} \sum_{i=1,2,...} P_i \left( 1 - P_i \right) \frac{\partial \theta}{\partial \theta_i}.
\]

(C.5)

Figure A05-m5ai-F1. The deflection function.
In order justify that statement, we compare as an example the measured K + Br₂ cross-section curve (figure A05-m4bii-F1 [The figure is input from the module Treated results (link type: 'input from'; target: A05-m4bii)]) with that to be expected classically, assuming that the value of $P_b(1 - P_b)$ does not change very much over the greater part of the $b$ range; only in a very narrow region at $b \approx R_e$ the ionization probability rapidly goes to zero.

For $\tau > 300$ eV degree the small differential cross section is due to the two small contributions of net repulsive scattering where $db/d\Theta$ is small.

With decreasing $\tau$ the classical rainbow angle where $db/d\Theta \to \infty$ gives rise to the rainbow structure at $\tau \lesssim 300$; the minimum at $\tau \approx 150$ is caused by the vanishing contribution for $b \approx R_e$ because then $db/d\Theta$ as well as $P_b$ tend to zero.

On account of the large value of $db/d\Theta$ around the inflection point on the “covalent” part of the deflection curve, a maximum is expected, seen indeed at $\tau \approx 100$.

At last it can be seen from the $b - \tau$ curve that the small-angle cross section consists of four small contributions; the polar differential cross section in this region had to be at least two times the large-angle value for $\tau > 300$, in agreement with the measurements. However, the small maximum in this small-angle region, seen in all cross-section curves, cannot be explained by this classical model. (The small-angle errors mentioned above are not important enough to cause the maxima.) [link forward quantum A05-m5bii]

Thus the general shape of the measured differential cross section can indeed be explained using a simple classical harpoon model, except for small angles.

Assumption

We assume that the value of $P_b(1 - P_b)$ does not change very much over the greater part of the $b$ range; only in a very narrow region at $b \approx R_e$ the ionization probability rapidly goes to zero. This assumption is justified for $H_{12} = 4.5 \times 10^{-2}$eV, which is the estimated value for this system given in the Quantitative interpretation [The value is input from the Quantitative interpretation [link type: 'input from'; target: A05-m5ai]].

[Next step on the essay-path: Quantummechanical qualitative interpretation (link type: 'essay-next/sq-next'; target: A05-m5ai)]

[Step back on the essay-path: Treated results (link type: 'essay-back'; target A05-m4bii)]

![Figure A05-m4bii-F1. K + Br₂, chemi-ionization differential cross section (CM system), measured at colliding energies of 6.9 and 10.35 eV. For both energies equal units have been used on the ordinate. The $\tau$ scale changes beyond 300 eV · degree. Also in A05-m4bl.](image-url)
**Comments on Qualitative interpretation=A05-m5ai:**

- The figure of the deflection function is used to give a basic explanation of experimental results. The general shape of that figure has been determined without input from the experimental results. The precise form is obtained via fitting of the experimental differential cross section with a theoretical differential cross section calculated based on this deflection function. This fitting procedure takes place in the *Quantitative interpretation*.

- The graphical presentation of the experimental results from A05-m4bi has been copied to this module, in order to make it complete: for a clear discussion of the curve, the curve itself has to be visible.

- Here we have a non-linearity in the original article in terms of a ‘forward reference’: an assumption is made which is known to be satisfied only when the resonance energy for this system has been determined in A05-m5bi.
C.2. THE MODULARISED VERSION OF A05

Qualitative interpretation: quantum mechanical = A05-m5a1i

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In the measured differential cross section of the chemi-ionization reaction \( \text{M} + \text{X}_2 \rightarrow \text{M}^+ + \text{X}_2^- \) a small maximum is observed in the small-angle region, seen in all cross section curves,

[click to show the figure of the cross sections given in A05-m4bi [link type: 'input from/contextualised in'; target: A05-m4bi]]

that cannot be explained [Compare to the classical Qualitative interpretation [link type: 'compare/sq-back'; target: A05-m5a1i] by a classical model stating the **general shape of the deflection curve as sketched in figure A05-m5a1i-F1**]

[click to show the figure of the deflection function given in MESO-m3c-defl [This figure is obtained from a mesoscopic module [link type: 'input from/contextualised in/wider range/project'; target: MESO-m3c-defl]]

and the equation for the differential cross section [Move on the deflection function in a mesoscopic module [link type: 'elaborated in/wider range/project'; target: MESO-m3c-defl]]

\[
I(\theta) = \frac{1}{\sin \theta} \sum_{i=1,2,...} P_b \left( 1 - P_b \right) b_i \left| \frac{\text{d} b_i}{\text{d} \theta} \right|.
\] (C.6)

Quantum mechanically this phenomenon can be explained by constructive interference of some contributions, for instance the contributions of the two net repulsive branches of the \( b-\tau \) curve. Because of the nearly equal slopes and about equal collision parameters of these branches at small scattering angles, the wavelength of the interference is rather long.

Figure A05-m4bi1-F1-m5a1i. Differential cross section K + Br₂ from A05-m4bi.
a rough estimate has shown that the wavelength has a value of a few degrees at the energies used, which is of the same order of magnitude as the widths of the measured maxima.

[unfold details estimation:]

Quantum mechanically the simple addition of contributions to the differential cross section according to Eq. (C.6) must be replaced by a formula adding the scattering amplitudes. Especially in the case of an interference structure with a long wavelength the differential cross sections, calculated classically and quantum mechanically could be very different. The composition of the steep "repulsive" branches of the deflection curve (see Fig. A05-m5aii-F1) it is expected to give such a long-wavelength structure on the differential cross section. Now we shall give a rough estimation of this wavelength. Following the Ford and Wheeler [[link type: 'external/input from'; target: RF00102] semiclassical treatment of the scattering amplitude and using the notation of Bernstein [[link type: 'external/wider range/input from/elaborate'; target: RF00103] the amplitudes of the contributions for repulsive scattering to the differential cross section is given by

\[
f_{1,2}(\theta) = \frac{1}{k(2 \sin \theta)^{1/2}} \left( \frac{L_{1,2}}{-\eta''_{1,2}} \right)^{1/2} \times \exp \left[ i(2\eta_{1,2} - L_{1,2}\theta - \frac{1}{2} \pi) \right],
\]

where the indices 1 and 2 indicate the "covalent" and "ionic" contributions. The combined amplitude of these two contributions can be written by

\[
f(\theta) = f_1(\theta) + f_2(\theta).
\]

From Fig. A05-m5aii-F1 it can be seen that the branches for net repulsive scattering have about equal values of \( b \) and about equal slopes \( db/d\theta \) for a certain value of \( \theta \). Considering the relations

\[
b = L/k \quad \text{and} \quad \eta'' = d\theta/2dL,
\]

we conclude \( L_1 \approx L_2 \equiv L_0 \) and \( \eta''_{L_1} \approx \eta''_{L_2} \equiv \eta''_0 \) from which we obtain directly

\[
f(\theta) \approx \frac{1}{k} \left( \frac{L_0}{-2\eta''_0 \sin \theta} \right)^{1/2} \times \exp \left[ i(2\eta_{L_1} - L_1\theta - \frac{1}{2} \pi) \right]
\]

Figure A05-m5aii-F1. Deflection function from MESO-m3c-defl.
\[ + \exp \left[ \left( 2\eta L_3 - L_2 \theta - \frac{1}{2}\pi \right) \right]. \]

In an elementary way the intensity can be found as follows:

\[
I(\theta) = \frac{2L_0}{-k^2\eta^2\sin \theta} \\
\times \cos^2 \left[ \eta L_1 - \eta L_2 - \frac{1}{2} \theta (L_1 - L_2) \right],
\]

and, according to \( \eta_L = \frac{1}{2} \theta_L, \)

\[
I(\theta) = \frac{2L_0}{-k^2\eta^2\sin \theta} \\
\times \cos^2 \left[ \frac{1}{2} L_1 \int_{-\infty}^{\infty} \Theta(l_1)dl \\
- \frac{1}{2} L_2 \int_{-\infty}^{\infty} \Theta(l_2)dl - \frac{1}{2} \theta (L_1 - L_2) \right].
\]

Now we compare two scattering angles \( \theta_p \) and \( \theta_q \). Then the difference \( \Delta \) in the argument of the cosine is given by:

\[
\Delta = \frac{1}{2} \int_{-\infty}^{\infty} \Theta(l_1)dl - \frac{1}{2} \int_{-\infty}^{\infty} \Theta(l_2)dl \\
- \frac{1}{2} \theta_p (L_{1p} - L_{2p}) + \frac{1}{2} \theta_q (L_{1q} - L_{2q}).
\]

Fig. A05-5a11-F1 shows that in the interesting region the curves are about straight lines so we simplify the last equation into

\[
\Delta \approx \frac{1}{4} (L_{1p} - L_{1q})(\theta_p - \theta_q) \\
- \frac{1}{4} (L_{2p} - L_{2q})(\theta_p - \theta_q) \\
- (L_{1p} - L_{2p}) \frac{1}{2} \theta_p + (L_{1q} - L_{2q}) \frac{1}{2} \theta_q \\
= \frac{1}{4} (\theta_p + \theta_q)(L_{2p} - L_{1p} + L_{2q} - L_{1q}) \\
+ \theta_q (L_{1q} - L_{2q}).
\]

For two not very different scattering angles \( \theta_p \) and \( \theta_q \) we can roughly estimate a value of \( \Delta \) by \( \theta_p \approx \theta_q \equiv \theta_0 \). Then

\[
\Delta = \frac{1}{2} \theta_0 (L_{1q} - L_{2q} + L_{2p} - L_{1p}).
\]

Using the relation \( b = L/k \) (where \( k \approx 400 \text{ Å}^{-1} \) for K + Br at 10.35 eV) it can be seen graphically that at small positive scattering angles the interference of these two contributions has a wavelength of the order of a few degrees at colliding energies of about 10 eV.

Although we have only considered a two-contribution interference instead of four contributions, this interference can explain the observed bump in the differential cross section at small angle.
Comments on Qualitative interpretation=A05-m5aii:

- The mathematical details of this qualitative quantum estimation are available to those who need some further explanation and justification. They are hidden from first view for the clarity of the main line of reasoning and to spare the reader who is not interested in the full digression. The mathematical elaboration does not form an information unit that can be consulted separately and therefore does not form a separate module.

- Most of the quantum interpretation was presented in an appendix in the original article.

- In the corpus, Bernstein’s publication in Advances in Chemical Physics (RfA05.13) is used as a standard work on quantum effects in molecular scattering. Therefore, we consider it to be macroscopic. The information referred to in this module, which is presented in section V. The Scattering Amplitude, could be recast in a macroscopic module Theoretical methods.
# C.2. The Modularised Version of A05

## Quantitative interpretation = A05-m5b

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**In order to interpret measured differential cross sections of K + Br2 chemi-ionization [This also in A05-m5]**

Interpretation depends on Treated results [link type: 'depends on/detailed in'; target: A05-m5b] [This interpretation depends on Treated results [link type: 'depends on/detailed in'; target: A05-m5b] more quantitatively, the potential parameters and the classical deflection function of the system are determined via fitting the results according to the classical atom-atom model [The interpretation depend on the Theoretical methods [link type: 'depends on/detailed in'; target: A05-m3c]] with the experimental results [Details link type: 'contains/specified in/detailed in'; target: A05-m5bii]. Based on the potential parameters and the deflection function thus determined, the differential cross section of the collision is calculated and compared to the measurements [Details in a module: Quantitative interpretation [link type: 'contains/specified in/detailed in'; target: A05-m5bii]]. However, quantitative agreement is poor.

### Comments on Quantitative interpretation = A05-m5b:

- Completely overlapping with the summary in m5.
- Intermediary results in the process of interpretation are copied to the Results module.
- The two constituent modules making up the quantitative interpretation both contain information about the calculation of some theoretical results that can be consulted separately. Together, they form the two steps towards the quantitative interpretation.
Potential and deflection function = A05-m5bi

Characterisation

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<td>Range</td>
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<tr>
<td>Physics:</td>
<td>Rüttner potential, Endothermicity, Electron affinity, Polarizability, Crossing distance, Resonance energy, Ionic-well depth, Repulsive steepness, Deflection function</td>
</tr>
<tr>
<td>Bibliographic:</td>
<td>Dévogué Los (AMOLF); Physics [1972]</td>
</tr>
<tr>
<td>Identification:</td>
<td>A05-m5bi</td>
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</table>

We calculate with a simple classical atom-atom model [link type: 'depends on/detailed in'; target: A05-m3c] some potential parameters of the K-Br₂ system by fitting calculated deflection functions with specific features of the measured differential cross section [link type: 'depends on/detailed in'; target: A05-m4bi], thus determining simultaneously the exact shape of the deflection function.

The ionization deflection function can be calculated from the potential-energy curves [link type: 'detailed in/wider range/project'; target: MESO-m3c-defl]. Choosing potential parameters by trial and error, the scattering function has been calculated via fitting with the measured differential cross section for the K+Br₂ case by a new method [link type: 'external/depends on/detailed in'; target: A06]. The numerical calculation of the classical deflection angle is performed with a well-known error. For the calculation we have used the crossing potential curves with the assumption that the charge exchange occurs exactly at the crossing point.

Because the colliding particles are rather heavy and the kinetic energy is not very low, it will be reasonable to compare the measurements primarily with classical calculations. Small quantum-mechanical interference structures on the differential cross-section curves will be washed out by the large energy spread of the alkali beam, the averaging effect of the internal state distribution and the anisotropy of the halogen molecule, the extent of the crossing region and the finite angular resolution of the detector.

For the ionic-potential curve we have chosen a Rüttner potential [link type: 'input from'; target: RfA00-4] of the form:

\[ U_{\text{ion}}(R) = -\frac{e^2}{R} - \frac{e^2(\alpha_M^+ + \alpha_X^-)}{2(R^4 + a^4)} - \frac{2e^2\alpha_M\alpha_X^-}{R^2} - \frac{C_{\text{ion}}}{R^6} + A_{\text{ion}} e^{-R/\rho_{\text{ion}}} + \Delta E. \]  

(C.7)

The covalent potential is given by:

\[ U_{\text{cov}}(R) = -(C_{\text{cov}}/R^6) + A_{\text{cov}} e^{-R/\rho_{\text{cov}}}. \]

(C.8)
Because we use for the ionic and covalent potential formulas many parameters we have looked for effects in the differential cross section that are mainly due to only one of these parameters. The parameters that can be determined rather directly in this way are the endothermicity of the collision $\Delta E$, the polarizability of the bromine ion $\alpha_{\text{Br}^+}$, the crossing distance $R_c$, the resonance energy $H_{12}$, the repulsive steepness coefficient $\rho$ and the ionic-well depth $\varepsilon$.

Firstly $\Delta E$ and the electron affinity of $\text{Br}_2$ are determined via fitting of the relative shifts of the maxima and the small-angle deflection slopes of the deflection function at different energies with the measured shifts. They are found to be $\Delta E = 3.1$ eV and $A(\text{Br}_2) = 1.2$ eV.

[unfold details:]

$\Delta E$ determination

The rule $\tau = C(b)$ is a well-known approximation for elastic scattering, indicating that the scattering angle multiplied by the kinetic energy is in first-order approximation only a function of the impact parameter $b$. The use of this rule for inelastic scattering might be a method to determine the inelasticity $\Delta E$. However, even for elastic scattering the reduced scattering angle $\tau$ only in a first approximation \cite{link:external/is argued in Ref[An9]} is independent of the kinetic energy. Fig. A05-m5aii-F1 shows the calculated scattering-angle curves for two different values of $E_i$. So the very obvious shift of the "covalent" as well as of the "ionic" parts of the deflection curves relative to each other along the "reduced" angle $\tau$ scale is not only due to the inelasticity of the collision, but partly to the incorrectness of the elastic $\tau = C(b)$ rule. To fix a value of $\Delta E$ from this shift we had to separate carefully these two effects. Therefore we separate the total collision into an elastic and a "purely inelastic" part. Up to the second passing of $R_c$ the collision process is elastic because at $R_c$ we are again at zero level of the potential energy due to the flatness of the covalent potential curve for $R > R_c$. The part of the collision from the second passing of $R_c$ up to infinity we call purely inelastic scattering. The dashed curves of A05-m5aii-F1 show for the two relevant different initial energies the pure inelastic contribution to the total scattering angle, that is the hypothetical deflection curve for particles following a straight line until the second crossing where ionization takes place. As already stated, this scattering angle as a function of $b$ is a contribution due especially to the inelasticity, irrespective of whether the diabatic transition takes place in the incoming or in the outgoing branch of the collision. The elastic contributions can be found by subtracting the total and pure inelastic scattering angle. Comparing the relative total scattering-angle shift and the pure inelastic scattering-angle shift it is obvious that generally the larger part of the former one is due not to the inelastic effect but to the incorrectness of the $\tau = C(b)$ rule, seen most clearly at small values of $b$ where indeed higher-order terms become important. Only for "covalent" scattering with $b > 4.5$ Å (about straight line trajectories up to the second passing of $R_c$) the shift is mainly due to the inelasticity, so the measured differential cross sections of covalent scattering at scattering angles belonging to this $b$ range ($\tau \approx 100$ eV degrees range) are suitable to determine $\Delta E$. Fortunately, the interesting contribution from this range to the scattering-angle region is dominant over the three other contributions originating from smaller impact parameters. The calculated relative shifts of the maxima and small-angle slopes of the "covalent" differential cross section as a function of $E_i$, fit the measured shifts if we take $\Delta E = 3.1$ eV. Because $\Delta E = I(K) - A(\text{Br}_2)$ and the ionization potential of potassium is known to be 4.3 eV \cite{link:external/input from; target: Ref[An9]}, the electron affinity of Br$_2$ had to be $A(\text{Br}_2) = 1.2$ eV, the same value as the one suggested by Petkin\cite{link:external/agrees with; target: Ref[An9]} for the vertical electron affinity.

Then $\alpha_{\text{Br}^+}$ is determined via fitting the scattering angle for collisions with $b = R_c$ with the measured minimum: $\alpha_{\text{Br}^+} \approx 150$ Å$^2$.
\[ \alpha_{\text{Br}_2} - \text{determination} \]
Assuming
\[ U_{\text{ion}}(R \geq R_c) \approx -\frac{e^2}{R} - \frac{e^2(\alpha_{K^+} + \alpha_{\text{Br}_2}^{-})}{2(R^4 + a^4)} + \Delta E, \]
where \( \Delta E = 3.1 \text{ eV} \), the value \( \alpha_{K^+} + \alpha_{\text{Br}_2}^{-} = 150 \text{ Å}^3 \) fits the calculated scattering angle for collisions with \( b = R_c \) with the measured minimum at \( t \approx 140 \). The place of the minimum is only weakly dependent on the value of \( \Delta E \) and \( a \), but strongly dependent on the value of \( \alpha_{K^+} + \alpha_{\text{Br}_2}^{-} \). A theoretical value of the polarizability of \( K^+ \) is \( \alpha_{K^+} = 0.94 \text{ Å} \) \( \text{[link type: } \text{external/input from: RfA03,RfA05]} \text{, from which follows then } \alpha_{\text{Br}_2}^{-} \approx 150 \text{ Å}^3 \).

substituting the obtained values of \( \alpha_{K^+} + \alpha_{\text{Br}_2}^{-} \) and \( \Delta E \) in the assumed potential, \( R_c \) can be determined to be \( R_c = 5.8 \text{ Å} \).

\[ R_c - \text{determination} \]
Assuming the ionic potential is given by Eq. (C.9) and \( U_{\text{cav}} \approx 0 \) both for \( R \geq R_c \), then, substituting the determined values of \( \alpha_{K^+} + \alpha_{\text{Br}_2}^{-} \) and \( \Delta E \), the crossing distance \( R_c \) can be calculated. The dependence on the screening parameter \( a \) is rather weak and for an arbitrary value at of \( a = 5 \text{ Å} \) five find \( R_c = 5.8 \text{ Å} \).

The well depth of the potential curve is determined using the classical rainbow angle:
\[ \varepsilon = 1.8eV \]

\[ \varepsilon - \text{determination} \]
In the case in which the character of the potential curve is known (here we have chosen the Rittner formula for the ionic potential), the classical rainbow angle is a good indication of the well depth of the potential curve. By calculating the value of \( (d^2\Omega/dk^2)_{\text{rainbow}} \) from the curve of A05-m5a11-F1, the rainbow parameter \( q \) defined by
\[ q = \frac{\hbar^2}{4\mu E_0} \left( \frac{d^2\Omega}{dk^2} \right)_{\text{rainbow}}, \]
can be calculated to be about \( 0.2 \times 10^{-5} \) for \( E_0 = 10.35 \text{ eV} \). The Airy approximation of the rainbow structure needs the parameter \( q \) and predicts a spacing between the supernumerary rainbows of about \( 8 \text{ eV} \cdot \text{degree} \) and a spacing of about \( 15 \text{ eV} \cdot \text{degree} \) between the first maximum and the first supernumerary. In the measurements, the energy spread of 20 percent of the alkali beam prevents the resolution of the supernumeraries; only a hint can be found, particularly from the Li + Br₂ differential cross-section measurements in Fig. A05-m4b12-F1. For \( K + \text{Br}_2 \) (Fig. A05-m4b11-F1) the differential cross section between \( \tau = 150 \) and \( \tau = 300 \) is expected to be the envelope of the rainbow structure with a principal maximum of low intensity while the intensities of the supernumeraries increase. However, the Airy approximation predicts a continuous decrease of the intensity but the simple Airy method is only a good approximation if the deflection curve is nearly parabolic near the classical rainbow point; our calculated deflection function deviates from parabolic too much to use this approximation. It has been shown by Berry \( \text{[link type: } \text{external/arguments found in/compared with: RfA05.10]} \) for a special case (Lennard-Jones potential) that the intensities of the supernumeraries increase calculating the rainbow structure with the uniform approximation or with exact calculations of Hundhausen and Pauly \( \text{[link type: } \text{external/arguments found in/compared with: RfA03.14]} \). However, in all calculations the distances between the maxima are nearly the same.
C.2. THE MODULARISED VERSION OF A05

Taking into account the supernumerary spacings and convolution effects, the classical rainbow can be expected at \( \tau \approx 275 \text{ eV} \cdot \text{degree} \) on the K + Br\(_2\) cross-section curve. A Rittner potential with a minimum at \(-1.8 \text{ eV}\) gives the same calculated classical rainbow angle.

**reliability calculated value:**

Very recently we have resolved the rainbow structure of the K + Br\(_2\) differential cross section (Fig. A05-m5bi-F1) by using a potassium beam of about 15 eV with a very small energy spread. The results have not been used in the calculations described here but the resolved rainbow structure indicate indeed a classical rainbow at \( \tau \approx 275 \text{ eV} \cdot \text{degree} \) and a supernumerary spacing of about 10 eV \cdot \text{degree} \). This spacing at a kinetic energy of 15 eV is in agreement with the predicted spacing of 8 eV \cdot \text{degree} at 10.35 eV by virtue of the proportionality to \( E^{1/3} \).

**The repulsive steepness coefficient is determined via a doubtful classical fit:** \( \rho = 0.3 \text{ Å} \)

[unfold details:]

**\( \rho \) determination**

Figs. A05-m5bi-F2, A05-m5bi-F3 and Eq. (C.10), i.e.

\[
I(\theta) = \frac{1}{\sin \theta} \sum_{i=1,2,\ldots} P_b (1 - P_b) b_i \left| \frac{d\Phi_i}{d\Theta} \right|. \tag{C.10}
\]

indicate, that with increasing steepness of the potential, the steepness of the deflection curve for small \( b \) also increases and consequently the contribution of these parts to the differential cross section decreases. On the other hand the steepness of the repulsive potential has nearly no influence on the large contribution of “covalent” scattering to the differential cross section at \( \tau \approx 100 \text{ eV} \cdot \text{degree} \), but it does influence the decrease to the small value at \( \tau \gtrsim 50 \). Summarizing, the value of the cross section at \( \tau \approx 100 \) relative to the small values at \( \tau < 50 \) and \( \tau > 300 \) and the slope at \( 50 < \tau < 100 \) might be suitable to determine a value for \( \rho \), in our classical consideration. However, it can be expected that the difference between classical and quantum calculations could be large especially for the quantitative calculation of the differential cross section. Therefore the value of \( \rho = 0.3 \text{ Å} \) that gives the best classical fit (supposing equal values of \( \rho \) for the covalent as well as the ionic potential) is rather doubtful, in spite of the fact that the classical calculated cross sections are very sensitive to the value of \( \rho \). At any rate the value \( \rho = 0.3 \text{ Å} \) for K + Br\(_2\) is a very realistic one compared with other molecules with a known value of \( \rho \).
The resonance energy is determined by fitting the curve height ratio and found to be $H_{12} = 4.5 \times 10^{-2}$ eV.

**$H_{12}$ determination**

The differential cross sections of Fig. A05-m4bi-F1 indicate equal total cross sections for chemi-ionization of K + Br$_2$ at energies of 10.35 and 6.9 eV, in agreement with total cross-section measurements of Baede and Los. However, the remarkable shift of the curve-height ratio as a function of

$$
\tau, R(\tau) = (I \sin \theta/10.35)/(I \sin \theta/6.9)
$$

is mainly due to the dependence of $P_b(1 - P_b)$ on $E_1$ and $b$ and partly due to the unequal values of the quantity ($dB/dr$) for the two energies. The curve-height ratio does not give a value of the resonance energy $H_{12}$ directly, because this ratio is also a function of the potential curves. Eq. (C.12) for the transition probability requires explicitly the slopes of the crossing potential curves at $R_c$, while moreover the exact shapes of the potential curves are important to know the collision parameter $b$ for a certain scattering angle $\tau$. We have calculated the ratios $R(120) = 1.092$, $R(40) = 0.84$, and $R(400) = 0.7$ using the given potential parameters and a resonance energy $H_{12} = 4.5 \times 10^{-2}$ eV. Of course there is the difficulty of the ambiguous $\tau \rightarrow b$ relation but in the examples considered the scattering at $\tau \approx 120$ has one strongly dominating contribution and scattering at $\tau \approx 40$ and $\tau \approx 400$ has, respectively, four and two contributions with about equal values of $b$. The ratio at $\tau \approx 120$ is the most important one for the derivation of $H_{12}$ because [on account of the flat long-range covalent potential curve and the simple form of $U_{el}(R \gtrsim R_c)$] the value of $R(120)$, where $b$ is only a little bit smaller than $R_c$, is only a function of ($a_{K^+} + a_{Br_2}^{-}$) and $\Delta E$. A second point for the importance of $R(120)$ is, that this ratio is most sensitive with respect to the variation of trial values of $H_{12}$. The calculated ratios given above are in very good agreement with the measurements. This method to fix $H_{12}$ seems to be rather sensitive: a resonance energy of $6.5 \times 10^{-2}$ eV would predict the quite different ratios 1.44, 0.95 and 0.73, respectively. The value $H_{12} = 4.5 \times 10^{-2}$ eV is in rather good agreement with the value of Ref. 1c which would be about $6 \times 10^{-2}$ eV if the same polarizability is taken.

Summarizing, we have determined for the K−Br$_2$ system most of the potential parameters; the missing parameters have been chosen to construct the potential curves in Fig. A05-m5bi-F2 and the deflection functions in Fig. A05-m5bi-F3. The values used are:

$$
\begin{align*}
\Delta E &= 3.1 \text{ eV}, \\
\alpha_{K^+} &= 0.94 \text{ Å}^3
\end{align*}
$$

([link type: ‘input from’; target: RFa04i4])
\[ \epsilon = 1.8 + 3.1 \text{ eV}, \quad C = 10^3 \text{ eV} \cdot \text{Å}^6, \quad (\text{arbitrary}), \]
\[ H_{12} = 4.5 \times 10^{-2} \text{ eV}, \quad a = 5 \text{ Å}, \quad (\text{arbitrary}), \]
\[ \rho = 0.3 \text{ Å}, \quad A = 5 \times 10^5 \text{ eV}, \]
\[ \alpha_{\text{Br}_2} = 150 \text{ Å}^3, \]

where the value for \( A \) has been fixed after the choice of \( C \) and \( a \), by requiring the ionic well minimum at \(-1.8 \text{ eV}\). For simplicity the Van der Waals term and repulsive term of both potential curves are supposed to be the same.

Based on the potential curves of the system, the classical deflection function is calculated [This calculation depends on theoretical methods given in a mesoscopic module (link type: ‘depends on/wider range/project’; target: MESO-m3c-defl)]; [This calculation depends on numerical theoretical methods given in another article (link type: ‘depends on/project’; target: A06-m3c)]; For collisions with two channels, a covalent one and an ionic one [These trajectories are given in a mesoscopic module (link type: ‘wider range/project/elaborated in’; target: MESO-m3c-mod#trajectories], the deflection function consists of a covalent and an ionic branch which are joined at the crossing radius \( R_c \), as is shown in figure A05-m5bi-F3, forming a closed deflection curve.

From the deflection function then, the differential cross section can be calculated [The deflection function is used for that purpose in the Quantitative interpretation (link type: ‘used in’; target: A05-m5bi)].
Comments on Quantitative interpretation A05-m5bi:

- The details of this quantitative estimation are available to those who need some further explanation and justification. They are hidden from first view for the clarity of the main line of reasoning. The mathematical elaboration does not form an information unit that can be consulted separately and therefore does not form a separate module.

- In this module we aim for an exact expression of the potential and the deflection function, not yet for the differential cross section. Especially the potential may be of interest separately. The results of this module will also be used as input in A05-m5bii, where the theoretical differential cross section will be calculated. The potential curves (including the parameters) and deflection functions that are determined here can be seen as ‘theoretical results’. As such, they are be copied to the Results module. They could also be provided with an extra label in some other way, that permits interested readers to locate them. The determination of the potential parameters is almost entirely copied from the section 4. Discussion in the original article. The deflection function was already presented in the Introduction, with forward pointers to the potential given in that section 4. Discussion. However, in the Introduction only the general shape of the deflection curve was referred to. That general shape has been presented in the modular version in MESO-m3a-defl.]

- I suppose that in Rittner’s cited article details are provided on these potentials, including assumptions of terms that can be neglected, justifying and explaining the choice of this potential.

- Target of a ‘forward reference’: the theoretical methods m3c refer to the value of the electron affinity of the system which is calculated here.
C.2. THE MODULARISED VERSION OF A05

Theoretical cross sections = A05-m5bii

Characterisation

Conceptual function: Interpretation

Range: Microscopic

Physics: Landau-Zener model; Differential cross section[chemi-ionization,K,Br2,eV] deflection function; Calculation

Bibliographic: Delignet,Los (AMOLF); Physica (1972)

Identification: A05-m5bii

Using a simple classical atom-atom model for ion-pair formation in molecular collisions
[Depends on the Theoretical methods (link type: ‘depends on/detailed in’; target: A05-m3c), we interpret the experimental differential cross section for chemi-ionization in alkali halide systems, by comparing the experimental cross sections to theoretical cross sections calculated with the model.

The differential cross sections for chemi-ionization of K + Br2 at colliding energies of 10.35
and 6.9 eV have been calculated [Depends on the theoretical methods given in a mesoscopic module (link type: ‘depends on/wider range/project’; target: MESO-m3c-def)], in a procedure in which the differential cross section is determined via the potential curves of the system and the classical deflection function[The calculated curves are input from a module Quantitative interpretation (link type: ‘input from’; target: A05-m5bii)], by fitting the calculated cross section with the experimental one [The calculated curves are input from a module Treated results (link type: ‘depends on/input from’; target: A05-m4bii)].

The theoretical cross section is expressed by [The equation is input from a mesoscopic module (link type: ‘input from/detailed in/wider range/project’; target: MESO-m3c-def)]

\[
I(\theta) = \frac{1}{\sin \theta} \sum_{i=1,2,...} P_b (1 - P_b) b_i \left| \frac{d\theta_i}{d\theta} \right| .
\] (C.11)

in terms of the deflection function \(\theta(b)\) and the Landau-Zener transition probability given by [The equation is input from a mesoscopic module (link type: ‘input from/detailed in/wider range/project’; target: MESO-m3c-mod)]

\[
P_b = \exp \left( -2\pi H_{12}^2 \right) \times \left\{ h(2\mu^{-1} E_i (E_{Rc}/E_i - b^2/R^2_c)) \right\}^{1/2} \times \frac{d}{dR} \left( H_{11} - H_{22} \right) \left( \frac{1}{R_c} \right) ^{-1/2} ,
\] (C.12)

where \(E_i\) represents the initial relative kinetic energy, \(\mu\) the reduced mass of the colliding particles, \(dH_{11}/dR\) and \(dH_{22}/dR\) the slopes of the diabatic potential curves at the crossing
Figure A05-m5bii-F1. K + Br₂, classically calculated chemi-ionization differential cross section (CM system) at colliding energies of 6.9 and 10.35 eV and convoluted with the energy spread of the velocity selector. For both energies equal units have been used on the ordinate. The dotted lines indicate the $\rho$ dependence of the slope steepness for “covalent” scattering. At $E = 10.35$ eV and different values of the polarizability $\alpha_{Br_2}^+$, and the ionic-well minimum $\varepsilon$ the positions of the scattering angle for $b = R_c$ scattering respectively the classical rainbow angle have been indicated along the abscissa. The values used in the calculations have been underlined.

The resulting classically calculated chemi-ionization differential cross section for K + Br₂ are shown in Fig. A05-m5bii-F1.

The general shape of this calculated differential cross section agrees with the measured cross section, and therefore the simple classical atom-atom model [Details in the module Qualitative interpretation (link type: 'detailed in'; target: A05-m5a] gives a qualitative interpretation of the measurements.

**reliability interpretation**

The qualitative agreement between the calculated curves with the measured curves [The curves are given in the Treated results (link type: ‘input from’; target: A05-m5bii] [The curves are given in the Treated results (link type: ‘input from’; target: A05-m4bii] is good but there is only a poor quantitative agreement.

Of course, a bad agreement for the “ionic” part of the differential cross section is expected because of the very different results for the rainbow structure as calculated classically and quantum mechanically. Due to the choice of $\Delta E$ and $H_{12}$, Fig. A05-m5bii-F1 shows the agreement of the inelasticity shifts and curve ratio; at the same time the sensitivities of the determination of the parameters $\alpha_{Br_2}^+$, $\rho$ and $\varepsilon$ are shown.

For the the estimated value of $H_{12}$, the value of $P_0(1 - P_0)$ does not change very much over the greater part of the $b$ range; only in a very narrow region at $b \approx R_c$ the ionization probability rapidly goes to zero.

Now let us make a comparison between the differential cross section of K + Br₂ and the measured one of Li + Br₂. A few estimates can be made easily. For Li + Br₂ the minimum in the cross-section curve for $b = R_c$ scattering occurs at $\tau \approx 175$ as compared to 135 eV · degree for K + Br₂. Because $\alpha_{K^+} + \alpha_{Br_2}^- \approx \alpha_{Li^+} + \alpha_{Br_2}^-$ the inelasticity of the Li + Br₂ collision will be larger. Indeed the endothermicity must be 1.1 eV larger due to the differences of ionization potential: $I(Li) = 5.4$ eV [link type: ‘input from’; target: RfAg9] and $I(K) = 4.3$ eV. The classical rainbow at $\tau \approx 400$ indicates a larger well depth of the ionic potential curve of Li–Br₂.
The relative differential cross sections of K + Br$_2$ and K + I$_2$ are nearly completely identical so a good similarity of the molecular constants can be expected. Duchart et al. [link type: 'agrees with/external'; target: Duchart] have measured the K + I$_2$ differential cross section for elastic scattering at a kinetic collision energy of 100 eV. The distances between the maxima of their resolved rainbow are equal to the supernumerary spacing that we should predict for K + Br$_2$ ionization scattering at 100 eV.

Thus the potential parameters determined in module A05-m5bi [Details in a module Quantitative interpretation [link type: 'detailed in'; target: A05-m5bi]] are rather reliable.

[Next step on the essay-path: Findings [link type: 'essay-next/sq-next'; target: A05-m6a]]
[Step back on the essay-path: Quantitative interpretation [link type: 'essay-back/sq-back'; target: A05-m5bi]]
Comments on Quantitative interpretation A05-m5bii:

- The theoretical differential cross sections can be seen as ‘theoretical results’. As such, they are be copied to the Results module. They could also be provided with an extra label in some other way, that permits interested reader to locate them.

- We consider the theoretical differential cross section as an ‘interpretation’ of the experimental one, and the comparison of the theoretical to the experimental cross sections as part of the discussion on the reliability of the interpretation. As such the description of the interpretation itself (i.e. the theoretical results of the calculation of the cross section) and the argumentation on its reliability are part of the same module according to the modular model.

- This justifies the assumption used in the Interpretation A05-m5ai; only in a very narrow region at \( b \approx R_c \) the ionization probability rapidly goes to zero.

- In the module Quantitative interpretation the authors try to give a quantitative explanation of the experimental results, but conclude that this is not possible in the current work: in A05-m5bii it is stated that there is poor quantitative agreement.

- The theoretical differential cross section, which is to be compared to the experimental cross section in order to see if they agree, depends on the classical deflection function, which in its turn depends on the potential of the system. Thus the calculation of the cross section takes place in three steps. However, these steps cannot be taken in a linear manner: everything is determined “iteratively” via fitting. This means that the steps, and the two constituent modules of the Quantitative interpretation are not at all clear cut.
OUTCOME = A05-m6

Characterisation

Conceptual function: Outcome

Range: Micrometric

Physics:
Differential cross section of chemi-ionisation of alkali atom, halogen molecule energy range, Atom-atom model, Classical trajectory calculations

Bibliographic:
Delvigne, J. (AMOLF); Physica (1972)

Identification:
A05-m6

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This module contains/specified in:

- Findings [[link type: 'contains/specified in/is segregated in'; target: A05-m6a]]
- Leads for further research [[link type: 'contains/specified in/is segregated in'; target: A05-m6b]]

Comments on Outcome=A05-m6:

- The original article did not have a Conclusions section. However, the information found at the end of the article where such a section could have been made explicit is included in this module.
- This module summary in this complex module does not add anything for the sequential reader, except a table of contents without particular interest. However, the complete sequential path passes by for the sake of completeness.
Findings = A05-m6a

**Characterisation**

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The relative differential cross sections for chemi-ionisation of the systems K + Br$_2$ at initial relative kinetic energies of 10.35 and 6.9 eV, K + I$_2$ at 11.15 eV and Li + Br$_2$ at 6.25 eV have been measured [The interpretation depends on the Treated results (link type: ‘depends on/detailed in’; target: A05-m6b) in molecular beam experiments [Details on the Experimental methods (link type: ‘depends on/detailed in’; target: A05-m3a)].

The general shape of the measured cross sections can be explained qualitatively using a classical atom-atom-Zener model, via the general shape of the deflection function [link type: ‘arguments found in’] qualitative interpretation m5aj. A classical explanation suffices, except for small angles, where a quantum explanation is necessary [Arguments found in a module Qualitative interpretation (link type: ‘argued in’; target: A05-m5bi)].

The relative differential cross section has been calculated for the inelastic-collision process K + Br$_2$ → K$^+$ + (Br + Br$^-$). The calculation is based on a simple classical model, using impact-parameter approximation, an isotropic intermolecular potential and neglecting the internal states of the X$_2$ molecule [The details are given in the module Theoretical methods (link type: ‘depends on/detailed in’; target: A05-m3c)], and based on the potential of the system which has been determined via fitting.

These measurements do seem to be suitable for the determination of potential parameters, crossing distance and resonance energy at the crossing point [link type: ‘arguments found in’; target: A05-m5b].

However, the classically calculated differential cross sections are only in qualitative agreement [Arguments for this standpoint are given in a module Quantitative interpretation (link type: ‘argued in’; target: A05-m5bi)] with the measurements [This interpretation depends on the Treated results (link type: ‘depends on’; target: A05-m4b)]. Quantitative agreement is poor, because the assumed simplifications of an isotropic potential and the absence of internal state are invalid for the systems at hand.

Thus, in answer to the central question of this article [The question is detailed in the module Central problem (link type: ‘depends on/detailed in’; target: A05-m2b)], the differential cross section of chemi-ionisation of alkali halides have been measured and explained qualitatively using a simple classical system, but a quantitative explanation of the reaction dynamics has not been found.
Comments on Findings=A05-m6a:

- This module contains a brief recapitulation of what has been achieved in this article. The bottom line is of A05 is: Is the simple classical model a good explanation of the reaction? No it isn’t. In article A08 this problem is addressed by experimenting on a more simple system and by using a more complex model.

- *Findings* is a ‘summarising module’ and therefore a lot of modules overlap with it.
Leads for further research = A05-m6b

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A simple classical atom-atom model qualitatively explains the relative differential cross sections of chemi-ionization processes \( M + X_2 \rightarrow M^+ + (X + X^-) \). However, there is still no reliable quantitative explanation [More about the goal of this research in a mesoscopic module Central problem (link type: 'detailed in/wider range/project'; target: Meso-m2b)]. A simple classical atom-atom model is not sufficient for the explanation of ion-pair formation in molecular collisions.

It has already been found [Input from Findings of an earlier article (link type: 'input/project'; target: A04-m6a)] that the total cross sections of collisions between Li or Na atoms and I atoms can be described using the Landau-Zener transition probability. The question is whether the differential cross section of such a simpler system can also be explained using the Landau-Zener model.

[click for note added in hindsight]

The differential cross section of the collision process \( Na + I \rightarrow Na^+ + I^- \) have been determined in a later article and it was found that the cross section is indeed described by the simple atom-atom model with the Landau-Zener transition probability [Compare these findings to the ones in the subsequent article (link type: 'compared'; target: A08-m6a)].

For a more detailed study the experimental resolution should be enhanced. Recently we have replaced the sputtering source [The source is described in detail in a mesoscopic Experimental methods module (link type: 'detailed in/focussed on in/wider range/project'; target: Meso-m3a)] by a charge-exchange source [The source is described in detail in a mesoscopic Experimental methods module (link type: 'detailed in/focussed on in/wider range/project'; target: Meso-m3a)]. In the near future we shall determine the potential parameters of some alkali atom-halogen molecule potential curves by quantum-mechanical calculations and with the help of better resolved differential cross sections.

**Comments on Leads for further research=A05-m6b:**

- When new problems specified here are addressed in later articles, a link to that later article is added in hindsight.
C.3 The modularised version of A08

**Meta-information=A08-m1**

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2. List of physics terms=A08-m1b [[link type: ‘contains/detailed in’; target: A08-m1b]]
3. Map of contents=A08-m1c [[link type: ‘contains/detailed in’; target: A08-m1c]]
4. Abstract=A08-m1d [[link type: ‘contains/detailed in’; target: A08-m1d]]
5. Lists of references=A08-m1e [[link type: ‘contains/detailed in’; target: A08-m1e]]
6. Acknowledgement=A08-m1f [[link type: ‘contains/detailed in’; target: A08-m1f]]

[Start essay-type path: Situation [link type: ‘essay-next/information’; target: A08-m2a]] [Start of the complete sequential path: Bibliographical information [link type: ‘SEQ-NEXT/contains’; target: A08-m1a]]

**Comments on Meta-information=A08-m1:**

- This is a compound module in which six components are aggregated. A modular summary of these constituent modules is given in the form of a table of contents. All constituents are connected to this complex module by means of a link, which is indicated in the text as, for example, [[link type: ‘contains/detailed in’; target: A08-m1a]].

- This module is the first module encountered by readers who consult the article as a whole; it is a starting point of both the complete sequential path and the essay-type path. There is a second starting point of the essay-type sequential path in the Abstract m1d.

- All ‘meta-modules’ (the Meta-Information and its constituent modules) are coupled to all ‘content modules’ in the article by means of a link expressing an administrative relations: \( \leftarrow_{\text{meta}} \rightarrow \) (see the legend in appendix C.1.2.).
Bibliographic information=A08-m1a

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Title
Rainbow, Stueckelberg oscillations and rotational coupling on the differential cross section of Na + Cl → Na⁺ + Cl⁻

Journal
Physica

Identification of the article
A08

Authors
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Dates
Date received: 7 March 1973

[Next step on the complete sequential path: Physics index terms (link type: 'SEQ-NEXT'; target: A08-m1b)]

[Step back on the complete sequential path: Meta-information (link type: 'SEQ-BACK/part of'; target: A08-m1)]

Comments on Bibliographic data=A08-m1a:

- The original article is uniquely characterised by the journal name, volume, year of publication and page numbers: 67 (1973) 166-196. It also provides names and affiliations of the author, the title and the date at which the manuscript was received by the publisher. The current addresses of the authors are not provided in the original article.
## C.3. THE MODULARISED VERSION OF A08

### Physics index terms = A08-m1b

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**POSITIONING**  
* A08-m2: Harpoon model  
  Charge transfer - chemi-ionization = ion-pair formation  
  Differential cross section [chemi-ionisation; Na, l; eV]  
  Atom-atom model  
  Electrons beams  

**Situation**  
* A08-m2a: Harpoon model  
  Charge transfer  
  Scattering  
  Electrons beams  

**Central problem**  
* A08-m2b: Differential cross section [chemi-ionisation; Na, l; eV]  
  Semi-classical atom-atom model  
  Electrons beams  

**METHODS**  
* A08-m3: Atom-atom model  
  Semi-classical  
  Electrons beams  

**Experimental methods**  
* A08-m3a: Molecular beam techniques  
  Scattering [source: Charge-exchange; selection: Slotted disc; interaction: Static gas, Crossed beam; analysis: Multi-channel, Electrostatic lenses; detection: Surface ionisation, Channel electron multiplier]  

**Theoretical methods**  
* A08-m3c: Atom-atom model  
  Landau-Zener  
  Rotational coupling  
  Semi-classical  
  Impact parameter approximation  
  Lowest-order stationary phase approximation  
  Uniform rainbow approximation  
  JWKB phase shifts  

**Theoretical methods**  
* A08-m3c1: Atom-atom model  
  Transition probabilities  
  Landau-Zener  
  Rotational coupling  

**Theoretical methods**  
* A08-m3c2: Atom-atom model  
  Transition probabilities  
  Landau-Zener  
  Rotational coupling  

**Theoretical methods**  
* A08-m3c3: Atom-atom model  
  Semi-classical differential cross section  
  Impact parameter approximation  
  Lowest-order stationary phase approximation  
  Uniform rainbow approximation  
  JWKB phase shifts  

**RESULTS**  
* A08-m4: Differential cross section [chemi-ionisation; Na, l; 13.85 eV]  
* A08-m4b: Measurement  
  Measurement  
  Rainbows structure  
  Repulsive interference  
  Differential cross section [chemi-ionisation; Na, l; 13.85 eV]  
  Measurement  
  A08-m4b1: Differential cross section [chemi-ionisation; Na, l; 13.85 eV]  
  Calculation  
  Potential Na+1  
  Deflection function [chemi-ionisation; Na, l; 13.85eV]  
  Calculation  
  A08-m4b2: Differential cross section [chemi-ionisation; Na, l; 13.85eV]  
  Calculation
**APPENDIX C. MODULARISED ARTICLES**

*A08-m1**

Rainbow structure

Differential cross section [chemi-ionisation; Na; I; 13-63 eV]

Calculation

**INTERPRETATION**

*A08-m5*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Lanzlau-Zener

**Qualitative interp.**

*A08-m5a*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Rainbow

Stueckelberg

**Quantitative interp.**

*A08-m5b*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Lanzlau-Zener

Rotation

*A08-m5bi*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Ritter potential $V(r)_{Na+I}$ [Endothermicity $\Delta E$,

Electron affinity $EA(Br_2)$, Polarizability $\alpha_{Br^-}$,

Crossing distance $R_c$, Resonance energy $H_{12}$,

Ionic-well depth $\epsilon$, Repulsive steepness coefficient $\rho$]

Deflection function

*A08-m5bi*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Lanzlau-Zener

Rotation

*A08-m5bi*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Lanzlau-Zener

Rainbow

Stueckelberg

*A08-m5bi*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Lanzlau-Zener

Rotational coupling

**OUTCOME**

*A08-m6*

Atom-atom model;

chemi-ionization

Lanzlau-Zener

Rotation

**Findings**

*A08-m6a*

Differential cross section [chemi-ionisation; Na; I; 13-85 eV]

Semi-classical atom-atom model for ion-pair formation in molecular collisions

Lanzlau-Zener

Rotational coupling

**Leads further research**

*A08-m6b*

Vibration

[Next step on the complete sequential path: Map of contents (link type: ‘SEQ-NEXT’; target: A08-m1c)]

[Step back on the complete sequential path: Bibliographical information (link type: ‘SEQ-BACK’; target: A08-m1a)]
Comments on Physics index terms=A08-m1b:
Terms assigned to the article by INSPEC:

- Controlled Terms: ATOMIC COLLISION PROCESSES; ATOMIC FORCES; IODINE; IONISATION OF ATOMS; SODIUM

- Uncontrolled Terms: rainbow oscillations; atom-atom collision; Na; I; 13 to 85 eV kinetic energies; potential curve crossing; lowest order stationary phase approximation; Landau Zener transition probability; Stueckelberg oscillations; rotational coupling; differential cross sections; interference of scattering; ionic interatomic potential; covalent potential parameters; pseudocrossing parameter; semiclassical differential cross sections; JWKB phase shifts; impact parameters; relative intensities; oscillation wavelengths; rotational coupling

- Classification Codes: A3440 Elastic scattering of atoms and molecules; A3450 Inelastic scattering of atoms and molecules
Map of contents=A08-m1c

Figure C.16. Fig.A08-m1c-F1: The general map of contents, overview of the modules.
Figure C.17. Fig A08-m1c-F2: The essay-oriented map of contents, emphasising the essay-type path.
Figure C.18. Fig.A08-m1c-F3: A ‘fish-eye’ map of contents, emphasising the \textit{Theoretical methods} module A08-m3c1.

\textbf{Comments on Map of contents=A05-m1c:}

- The ‘map of contents’ is intended to provide the reader with an overview of the article allowing for efficient navigation and for insight in the coherence of the article.

- We have given three kinds of maps, reflecting three ways of looking at the article:
  
  - a full map of all modules in the article arranged by main module, in order to provide a general overview of all modules (see figure A08-m1c-F1),
  
  - a map of the modules arranged following the essay-type route (figure A08-m1c-F2), highlighting only the modules that are visited by that route, and the links expressing the sequential routes,

  - a map focusing on the \textit{Theoretical methods} module A08-m3c1 (figure A08-m1c-F3), which presents A08-m3c1, with its full characterisation, structure and emphasis.
C.3. THE MODULARISED VERSION OF A08

Lists of references=A08-m1e

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References in the article

A02 A.M.C. Moutinho, A.P.M. Baede and J. Los, Physica 51 (1971) 432-444. [link to occurrence(s) in text]

A03 A.P.M. Baede and J. Los, Physica 52 (1971) 422-440. [link to occurrence(s) in text]


A05 G.A.L. Delvigne and J. Los, Physica 59 (1972) 61-76. [link to occurrence(s) in text]

A06 G.A.L. Delvigne and J. Los, Physica 63 (1973) 339-350. (is detailed in/genera) [link to occurrence(s) in text]

A07 A.P.M. Baede, D.J. Auerbach and J. Los, Physica 64 (1973) 134-148. [link to occurrence(s) in text]

R[A002] J.A. Aten, G.A.L. Delvigne, and J. Los, to be published. [in A08-m2a] [link to occurrence(s) in text]


R[A005] A. Russek, Phys. Rev. A 4 (1971) 1918. [in A08-m2a] [link to occurrence(s) in text]


R[A011] M.M. Patel and V.B. Gohel, Z. Naturforsch. 27a (1972) 1227. [link to occurrence(s) in text]


R[A018] Landolt-Börnstein, Zahlenwerte und Funktionen, I. Band, I. Teil, (Springer-Verlag, Berlin, 1950). [link to occurrence(s) in text]

R[A019] G.A.L. Delvigne and J. Los, Physica 63 (1973) 339. [link to occurrence(s) in text]

References in the modules

**POSITIONING** = A08-m2
**Situation** = A08-m2a

**ME-m2a** mesonic *Situation (elaborate/project/wider range)* [link to occurrence(s) in text]

**ME-m3a-mod** mesonic *Experimental methods* [link to occurrence(s) in text]

**MA-m33-Bern** R.B. Bernstein, Adv. Chem. Phys. 10 (1966) p.75. [in A08-m2a,2b,3ci] [link to occurrence(s) in text]

**References**

A02 A.M.C. Moutinho, A.P.M Baede and J. Los, Physica 51 (1971) 432-444. (elaborate/project) [link to occurrence(s) in text]

A03 A.P.M. Baede and J. Los, Physica 52 (1971) 422-440. (elaborate/project) [link to occurrence(s) in text]

A04 A.M.C. Moutinho, J.A. Aten, and J. Los, Physica 53 (1971) 471-492. (elaborate/project) [link to occurrence(s) in text]

A05 G.A.L. Delvigne and J. Los, Physica 59 (1972) 61-76. (elaborate/project) [link to occurrence(s) in text]

A06 G.A.L. Delvigne and J. Los, Physica 63 (1973) 339-350. (as detailed in/project) [link to occurrence(s) in text]

A07 A.P.M. Baede, D.J. Auerbach and J. Los, Physica 64 (1973) 134-148. (elaborate/project) [link to occurrence(s) in text]

A082 J.A. Aten, G.A.L. Delvigne, and J. Los, to be published. (argumentation in/project) [link to occurrence(s) in text]

A083 See for example: D. Coffey, D.C. Lents and F.T. Smith, Phys. Rev. 187 (1969) 201. (as elaborated in/external) [link to occurrence(s) in text]

A084 See for example: M. Barat, J. Baudon, M. Abignoli and J.C. Houver, J. Phys. B 3 (1970) 230 (as elaborated in/external) [link to occurrence(s) in text]
C.3. THE MODULARISED VERSION OF A08

\[ \text{RefA08} \] A. Russek, Phys. Rev. A 4 (1971) 1918. (elaborated in/external) [link to occurrence(s) in text]

Central question=\text{A08-m2b}

ME-m2b mesoscopic Central problem (is elaborated in/project/wider range) [link to occurrence(s) in text]

MA-m3c-Bern#Stock R.B. Bernstein, Adv. Chem. Phys. 10 (1966) p.75. (is elaborated in/wider range/external) [link to occurrence(s) in text]

\text{METHODS=\text{A08-m3}}

Experimental methods=\text{A08-m3a}

ME-m3a mesoscopic Experimental methods (is detailed in/generalized in/project/wider range) [link to occurrence(s) in text]

ME-m3a-I mesoscopic Experimental methods (is detailed in/focused on in/generalized in/segregated in/project/wider range) [link to occurrence(s) in text]

ME-m3a-Ir mesoscopic Experimental methods (is detailed in/focused on in/generalized in/segregated in/project/wider range) [link to occurrence(s) in text]

1. Other experimental methods MESO-m3a's (is detailed in/focused on in/generalized in/segregated in/project/wider range) [link to occurrence(s) in text]

\[ \text{RefA08} \] R.K.B. Helbing and E.W. Rothe, Rev. Sci. Instrum. 39 (1968) 1948. (compared to/external)[link to occurrence(s) in text]

Theoretical methods=\text{A08-m3c}

ME-m3c-mod mesoscopic Theoretical methods (is detailed in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-defl mesoscopic Theoretical methods (is detailed in/focused on in/general/project/wider range) [link to occurrence(s) in text]

\text{Theoretical methods=\text{A08-m3ci}}

ME-m3c-mod mesoscopic Theoretical methods (is detailed in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-defl mesoscopic Theoretical methods (is detailed in/focused on in/general/project/wider range) [link to occurrence(s) in text]

A04 \[ =\text{[RefA08]} \] A.M.C. Moutinho, J.A. Aten, and J. Los, Physica 53 (1971) 471-492. (input from/project)[link to occurrence(s) in text]

\text{Theoretical methods=\text{A08-m3ci1}}

ME-m3c-mod mesoscopic Theoretical methods (is detailed in/general/project/wider range) [link to occurrence(s) in text]

\[ \text{RefA08} \] Values from Henschbach, D. and Grice, R., tabulated by Ewing, J.J., Milstein, R. and Berry R.S., J. Chem. Phys. 54 (1971) 1752. (input/external) [link to occurrence(s) in text]

\[ \text{RefA08} \] R.E. Olson, P.T. Smith, and E. Bauer, Appl. Optics 10 (1971) 1848. (input/external) [link to occurrence(s) in text]

\[ \text{RefA08} \] E.E. Dikitin and A.I. Reznikov, Phys. Rev. A6 (1972) 522. (agreed in/external) [link to occurrence(s) in text]

\text{Theoretical methods=\text{A08-m3ci2}}

ME-m3c-mod mesoscopic Theoretical methods (is detailed in/elaborated in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-mod mesoscopic Theoretical methods (input/defined in/general/project/wider range) [link to occurrence(s) in text]

\[ \text{RefA08} \] A. Russek, Phys. Rev. A 4 (1971) 1918. (detailed in/general/project/wider range)[link to occurrence(s) in text]

\text{Theoretical methods=\text{A08-m3ci}}

ME-m3c-defl mesoscopic Theoretical methods (elaborated in/elaborated in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-defl mesoscopic Theoretical methods (defined in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-defl mesoscopic Theoretical methods (input/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-defl mesoscopic Theoretical methods (defined in/input/general/project/wider range) [link to occurrence(s) in text]
APPENDIX C. MODULARISED ARTICLES

RF\textsubscript{A08-21} K.W. Ford and J.A. Wheeler, Ann. Physics 7 (1959) 259, 287. (detailed in/omitted in/external) [link to occurrence(s) in text]

RF\textsubscript{A08-22} G.B. Airy, Proc. Cambridge Philos. Soc. 6 (1838) 379. (detailed in/omitted in/external) [link to occurrence(s) in text]

RF\textsubscript{A08-23} M.V. Berry, Proc. Soc. 89 (1966) 479. (detailed in/argued in/omitted in/external) [link to occurrence(s) in text]


RESULTS=A08-m4

\begin{itemize}
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  \item Treated results=A08-m4bi
  \item Treated results=A08-m4bi1
\end{itemize}

ME-m3a-1 mesoscopic Experimental methods (depends on/detailed in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-treat mesoscopic Theoretical methods (clarified in/argued in/general/project/wider range) [link to occurrence(s) in text]

ME-m3c-defl mesoscopic Theoretical methods (explained in/to cause/general/project/wider range) [link to occurrence(s) in text]

\begin{itemize}
  \item Treated results=A08-m4bi
  \item Treated results=A08-m4bi1
  \item Treated results=A08-m4bi2
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ME-m3c-mod mesoscopic Theoretical methods (input/general/project/wider range) [link to occurrence(s) in text]

\begin{itemize}
  \item Treated results=A08-m4bi3
  \item INTERPRETATION=A08-m5
  \item Qualitatief=A08-m5a
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ME-m3c-defl mesoscopic Theoretical methods (detailed in/input/general/project/wider range) [link to occurrence(s) in text]

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ME-m3c-mod mesoscopic Theoretical methods (detailed in/depends on/general/project/wider range) [link to occurrence(s) in text]

RF\textsubscript{A08-13} E.S. Rittner, J. Chem. Phys. 19 (1951) 1030. (input/external) [link to occurrence(s) in text]

\begin{itemize}
  \item Quantitatief=A08-m5bi
  \item Quantitatief=A08-m5bi1
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ME-m3c-defl mesoscopic Theoretical methods (detailed in/depends on/general/project/wider range) [link to occurrence(s) in text]

\begin{itemize}
  \item Quantitatief=A08-m5bi2
\end{itemize}

ME-m3c-mod mesoscopic Theoretical methods (detailed in/depends on/general/project/wider range) [link to occurrence(s) in text]

A04 =RF\textsubscript{A08-4} A.M.C. Moumindo, J.A. Aten, and J. Los, Physica 53 (1971) 471-492. (input/project) [link to occurrence(s) in text]

OUTCOME=A08-m6 [ - ]

Findings=A08-m6a [ - ]

Leads for further research=A08-m6b

ME-m3c-mod mesoscopic Theoretical methods (is detailed in/general/project/wider range) [link to occurrence(s) in text]
In this module, we list the references to modules outside the article at hand, i.e. to mesoscopic and macroscopic modules, to particular modules written by authors working on the same research project or by others, and to entire articles (where an article is a special case of a complex module).

In principle, this modular article is embedded in a network of modularly published articles. Here, however, only corpus articles are in modular form. Therefore, we could only specify the target article of the external links to articles that are not part of the corpus, not the particular module that would have been referred to if it had been available. We indicate such a target as Ait x-m#.

The references are listed in two ways: in a complete list of all references in the entire article, and in separate lists of the references in each particular module. These lists given the reader an overview of the embedding in the literature of respectively the article and the module. Creating these lists by hand, as we did, is a lot of work. Therefore, this process has to be automated to meet the requirements of authors of new modular articles.
Acknowledgements=A08-m1f

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<td>A08-m1f</td>
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We are pleased to acknowledge the valuable help of H.P. Alberda for developing the automatic scanning and data assembling.

This work part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (Foundation for Fundamental Research on Matter) and was made possible by financial support from the Nederlandse Organisatie voor Zuiver-Wetenschappelijk Onderzoek (Netherlands Organization for the Advancement of Pure Research).

[Next step on the complete sequential path: Positioning (link type: ‘SEQ-NEXT’; target: A05-m2)]
[Step back on the complete sequential path: Lists of references (link type: ‘SEQ-BACK’; target: A05-m1e)]

Comments on Lists of references=A05-m1e:

- The acknowledgements given in the original article have been recast directly into this module. In addition to the standard financial acknowledgement, a scientific contribution by a non-author is acknowledged.
C.3. THE MODULARISED VERSION OF A08

POSITIONING=A08-m2

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<td>Range: Microscopic</td>
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<tr>
<td>Physics: Harpoon model; Charge transfer/Chem reaction/ion-pair formation; Differential cross section [chem-ionisation; Na atom, I atom; eV]; Atom-atom model; Electronvolt beams</td>
</tr>
<tr>
<td>Bibliographic: Delvigne,Los [AMOLF]; Physics (1973)</td>
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<td>Identification: A08-m2</td>
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</table>

In the context [link type: 'detailed in[contains/segregated in]/seq-next'; target: A08-m2a] of the harpoon model, the central problem [link type: 'detailed in[contains/segregated in'; target: A08-m2b] addressed in this article is the measurement in the electronvolt range of the relative differential cross section of Na atom - I atom charge-transfer collisions and the interpretation in terms a semiclassical model, taking into account rainbow and Stueckelberg oscillations.

[Next step on the complete sequential path: Situation [link type: 'SEQ-NEXT/contains/segregated in/detailed in'; target: A08-m2a]]

[Step back on the complete sequential path: Acknowledgements [link type: 'SEQ-BACK/meta-information'; target: A08-m1f]]

**Comments on POSITIONING=A08-m2:**

- This is a compound module in which two components are aggregated. An overview of these constituent modules is given in a brief module summary.

- This module corresponds to the *Introduction* in the original article, without coinciding entirely with it. The details on the theoretical methods included in the *Introduction* are omitted from the module *Positioning*, as well as the announcement that a discrepancy has been found between the measurements and the calculations and that this problem could be solved by taking into account rotational coupling. We have expanded the references to previous articles from the same research project.
A08-m2a Situation

Characterisation

Conceptual function: Positioning situation

Range: Microscopic

Physics: Harpoon model; Charge transfer; Scattering; Electronvolt beams

Bibliographic: Delvigne, L. (AMOLF); Physica [1973]

Identification: A08-m2a

In the research program from which this article issues [More about the situation in a mesoscopic module [link: ‘elaborated in/project/wider range’; target: MESO-m2a] , total and differential cross sections have been measured for collisions between electronegative and electron positive atoms and molecules, using molecular beam techniques [Particulars on those techniques in the mesoscopic Experimental methods module [link type: ‘detailed in/focused on in/project/wider range’; target: MESO-m3a] . These cross sections have been interpreted tentatively in terms of a simple classical atom-atom model for ion-pair formation in molecular collisions [Particulars on that model in a mesoscopic Theoretical methods module [link type: ‘detailed in/focused on in/project/wider range’; target: MESO-m3c-mod] , according to which the transition to the ionic state takes place via crossing of the neutral and ionic ground states, with a probability given by the Landau-Zener approximation.

We have studied total cross sections for collisions between alkali atoms and O_2 [link type: ‘project/elaborated in’; target: A02-m1] , alkali atoms and Br_2, Cl_2, Cl_2, NO_2, N_2 and CO_2 [link type: ‘project/elaborated in’; target: A03-m1] . The total cross section of alkali atoms and Cl_2 and Br_2 has also been measured as a function of the secondary beam temperature [link type: ‘project/elaborated in’; target: A04-m1] and taking into account the fragmentation of the negative ion [link type: ‘project/elaborated in’; target: A07-m1].

We have also published measurements on the differential cross section for chemi-ionization in some alkali atom–halogen molecule collisions in an earlier paper [link type: ‘project/elaborated in’; target: A05-m1] . The measurements have been compared with classical calculations, using the two-state approximation and the Landau-Zener theory to describe diabatic transitions at the crossing of the ionic and covalent potential surfaces [particulars on the model used for these calculations in a mesoscopic Theoretical methods module [link type: ‘detailed in/focused in/project/wider range’; target: MESO-m3c-mod] ]
C.3. THE MODULARISED VERSION OF A08

via the determination of the deflection function using the numerical method described in [link
type: 'project/elaborated in'; target: A06-m*]].

As a stringent simplification we have considered the diatomic halogen molecule as a single
particle, forming with the alkali atom an isotropic potential field with an isotropic crossing
of ionic and neutral potential surfaces. The consequence of the simplification is the neglect of
rotation and vibration of the halogen molecule and an application of the Landau–Zener transition
formula independent of the angular position of the halogen molecule with respect to the radius
vector between the two collision partners. A comparison of measurements and calculations has
shown that the quantitative agreement is very poor [link type: ‘project/depends on'; target: Findings A05-
m6a]. Moreover, a semiclassical approximation with the same simplification does not improve
the agreement [reasons for this are given in a subsequent article [link type: 'elucidated in/to cause/external '; target: RfA082-m*]] .

Because at that time the lack of agreement was not well understood, we started measurements
on atom–atom scattering of the same type to test the semiclassical calculation method and the
suitability of the Landau–Zener theory for this type of collision processes.

We have studied the Na + Cl → Na+ + Cl− collision process. Of course this process does not need
the simplifications described above. Moreover, this process is convenient for calculating the
differential cross section because at least the shape of one of the potential curves, the ionic
Na+Cl− curve, is well known while the measurements allow estimations of the covalent NaI
curve.

We use atomic beam techniques allowing for the experimental resolution of interferences of
two types, viz. the rainbow structure and the Stueckelberg oscillations [Bernstein elucidates rainbow
and Stueckelberg oscillations in a macroscopic publication [link type: 'elucidated in/elaborated in/wider range/external';
target: RfA0813]] . Stueckelberg oscillations have been observed before at elastic and inelastic
scattering from noble–gas ion on noble–gas atom collisions, by Lorents and Smith et al. [link type:
'external/elaborate'; target RfA085-m*] and by Barat et al. [link type: 'external/elaborate'; target: RfA085-m*] .

We also consider rotational coupling in our calculations. Rotational coupling couples a
covalent state with the ionic state and is generally expected to be most effective for collisions
with large impact parameters. A theoretical description of this phenomenon has been given, for
example, by Russek [link type: 'external/elaborate'; target: RfA085-m*] , but rotational coupling has not
yet been observed in combination with Landau–Zener transitions.

[Next step on the essay-path: Central problem [link type: 'essay-next/seq-next/used for/focused on in'; target: A08-m2b]]
[Next step on the complete sequential path: Central problem [link type: 'seq-next/essay-next/used for/focused on in'; target: Central problem A08-m2b]]
[Back to beginning of the path [link type: 'essay-back/meta-information'; target: Meta-information A08-m1]]
[Step back on the complete sequential path: Positioning [link type: 'sq-back/part of/aggregated in/summarised in'; target: A08-m2]]
Comments on A08-m2a Situation:

- Most of the embedding is derived from the section 1. Introduction, though the sequence of the paragraphs has been changed to form a more coherent module.

- In this Situation module, like in the original 1. Introduction section, the article is explicitly linked to the previous article A05 on differential cross sections, in which unwarranted simplifications were made. In this article the authors take a step back and explore a simpler system for which the necessary assumptions are valid. Central issue of the article.

Like in the original Introduction, the findings of the previous article A05 are summarised here. This summary could, for the sake of efficiency, be reduced to a mere pointer to the Findings of A05. However, we have repeated that information, for the sake of completeness, in this Situation module, because it serves as an argument for the relevance of the research reported on in this article: article A08 provides a necessary step following article A05.

- Following the definition of the Situation module, this module contains the argumentation on the relevance, in the given situation, of the central problem addressed in the article.

- Rainbow and Stueckelberg oscillations, rotational coupling, the application of the semiclassical approximation and the Landau-Zener approximation are embedded via references to other work. We have created a mesoscopic module presenting information about the Landau-Zener approximation.

- Reference RfA08.2 is a ‘broken link’: J.A. Aten, G.A.L. Delvigne, and J. Løe had planned to write that article, but it has never been published.
Central problem = A08-m2b

Characterisation

Conceptual function: Positioning central problem

Range: Microscopic

Physics: Differential cross section [chemi-ionisation; Na, IeV]; Semi-classical atom-atom model; Electronvolt beams

Bibliographic: Delvigne, Los [AMOLF]; Physica [1973]

Identification: A08-m2b

In order to test the semiclassical calculation method [That method is given in the Theoretical methods [link type: 'detailed in/focused in'; target: A08-m3cii]] and to test the suitability of the Landau-Zener theory for chemi-ionization in collision processes [That theory is given in the Theoretical methods [link type: 'focused in'; target: A08-m3ci]], the Na + Cl → Na⁺ + Cl⁻ collision process is studied [More on the context of this research in the Situation module [link type: 'context in/essay-back/sq-back'; target: A08-m2a]] [More on the goal of the research in the microscopic Central problem module [link type: 'elaborated in/project/wider range'; target: MESO-m2b]] [An answer to this central question in the Findings module [link type: 'used in'; target: A08-m6a]].

For that purpose, relative differential cross sections are measured for the atom-atom collision process Na + Cl → Na⁺ + Cl⁻ at kinetic energies from 13 to 85 eV, using atomic beam techniques [Particulars on those techniques in the Experimental methods [link type: 'detailed in/focused in/essay-next'; target: A08-m3a]] allowing for the experimental resolution of interferences of two types, viz. the rainbow structure and the Stueckelberg oscillations [More on the rainbow and Stueckelberg oscillations in Bernstein [link type: 'external/elaborated in/wider range'; target: MACRO-m3c-Bern]].

The measurements are then compared with semiclassical differential cross sections for the chemi-ionization calculated via the deflection curves, the Landau–Zener transition probability, the stationary-phase approximation and JWKB phase shifts, using estimations of the covalent potential parameters and the pseudocrossing parameter $H_{12}$ based on the measurements. Calculations are performed both with and without taking into account the phenomenon of rotational coupling.

[Next step on the essay-path: Experimental methods [link type: 'essay-next/focused on in/detailed in'; target: A08-m3a]]

[Next step on the complete sequential path: Methods [link type: 'seq-next'; target: A08-m3]]

[Step back on the essay-path: Situation [link type: 'essay-back/sq-back/depends on/context in'; target: A08-m2a]]

[Step back on the complete sequential path: Situation [link type: 'sq-back/essay-back/depends on/context in'; target: A08-m2a]]
Comments on Central problem=A08-m2b:

- The central problem addressed in this article is the applicability of the theoretical methods, in particular the Landau-Zener theory, to the explanation of chemionisation in collision processes. In order to solve that problem, a specific goal is formulated: the measurement and calculation of the different cross sections for those processes.

- The central problem is derived from the abstract and the section Introduction, which explicitly states why the current collision process was studied. We have rephrased the text, to make it coherent.

- All information represented in this module is also represented (in different words) in the Situation module or in the Methods module.
C.3. THE MODULARISED VERSION OF A08

Methods = A08-m3

Characterisation

Conceptual function: Methods

Range: Microscopic

Physics: Atom-atom model; Semiclassical; Electronvolt beams

Bibliographic: Delignes, Los (AMOLF); Physica (1973)

Identification: A08-m3

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Methods

Atomic beam techniques [Particulars on this technique in the Experimental methods [link type: 'contains/regulated in/detailed in/focused in/sq-next': target: A08-m3a]] are used to measure the experimental differential cross sections of the chemi-ionization in sodium atom-iodine atom collisions in the electronvolt range.

We interpret the experimental methods thus obtained using the following theoretical methods. [These methods are grouped in the module Theoretical methods [link type: 'contains/regulated in': target: A08-m3c]]. We try to explain this chemi-ionization process by means of a semiclassical atom-atom model for ion-pair formation [Particulars on the model in the Theoretical methods [link type: 'contains/regulated in/detailed in/focused in': target: A08-m3ci]], which is based on transitions between electronically coupled states of the system, in particular Landau-Zener transitions [Focus on the LZ transitions in a Theoretical methods module [link type: 'contains/regulated in/specialised in/detailed in/focused in': target: A08-m3ci2]]. In addition, the phenomenon of rotational coupling is taken into account [Focus on rotational coupling in a Theoretical methods module [link type: 'contains/regulated in/specialised in/detailed in/focused in': target: A08-m3ci2]].

The differential cross sections are calculated, from the states of the system, via the deflection function, using the stationary phase approximation, the uniform approximation and JWKB phase shifts [Particulars on the calculation methods in the Theoretical methods [link type: 'contains/regulated in/detailed in/focused in': target: A08-m3ci]].

[Next step on the complete sequential path: Experimental methods [link type: 'seq-next/contains/regulated in/detailed in/focused on': target: A08-m3a]]

[Step back on the complete sequential path: Central problem [link type: 'sq-back/depends on': target: A08-m2b]]
Comments on Methods=A08-m3:

- This is a complex module containing three different levels of constituent modules. In the first place, this module two components are aggregated: Experimental methods and Theoretical methods.

In the second place, the Theoretical methods in its turn also has two components: one about the transition probability in general and one about the calculation of the differential cross section.

In the third place, that module about the transition probability is a cluster module containing two constituent modules about specific types of transition probabilities. An overview of these constituent modules is given in a brief module summary.

- The concepts of this particular reaction studied (differential cross section of chemi-ionization of sodium atoms-iodine atoms), of this particular experimental method used to do so (beam techniques), and of this particular theory (semiclassical model) are included in almost every module in the article, in different combinations and in more or in less detail - in particular in the Central problem and the Situation and in the appropriate (experimental or theoretical) constituent modules of this complex Methods module. However, the actual phrasing of the module summary is ours. It doesn’t occur literally in other modules, so that the overlap is kept from getting annoying.
C.3. THE MODULARISED VERSION OF A08

Experimental methods = A08-m3a

Characterisation

Conceputal function: Methods, experimental methods

Range: Microscopic

Physics: Molecular beam techniques, Scattering [source: Charge-exchange; selection: Slotted disc; interaction: Static gas/Crossed beam; analysis: Multi-channel, Electrostatic lenses; detection: Surface ionisation, Channel electron multiplier]

Biographical: Delville, Les [AMOLF]; Physica [1973]

Identification: A08-m3a

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<tr>
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<td><em>s/a</em> → <em>s/a</em></td>
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<tr>
<td>res. m4bi</td>
<td><em>s/a</em> → <em>s/a</em></td>
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</table>

Beam techniques provide a powerful tool for the study of molecular dynamics. The general shape of the setup for beam experiments is given in [Details on the general Experimental methods are given in a mesoscopic module [link type: ‘detailed in/generalised in/project/wider range’; target: MESO-m3a]] . A scheme of the apparatus we have used to measure relative differential cross sections for the atom–atom collision process Na + Cl → Na⁺ + Cl⁻ at kinetic energies from 13 to 85 eV [These methods are used to generate experimental results [link type: ‘used for’; target: A08-m4bi]] is given in Fig. A08-m3a-F1

The charge-exchange source of the sodium beam (1) is of the same type as constructed by Helbing and Rothe [Compare with the set-up of others [link type: ‘compare/external’; target: RaO87-m8]] and has been described elsewhere [link type: ‘detailed in/focused on in/clarified in/generalised in/segregated in/wider range/project; target: RaO88-MESO-m3a-charg].

For selection of the state of the Na atoms of the beam a pulsed voltage over the directly heated ionization cathode and a chopped-detection technique [General details of this technique are given in a mesoscopic module [link type: ‘detailed in/’ is focused in/clarified in/generalised in/segregated in/wider range/project; target: MESO-m3a-chop]] have been used to avoid energy spread of the beam caused by the potential drop over the cathode. The total energy spread is about 0.5 eV FWHM. The neutral beam is collimated by the exit slit of the source and a second slit (2) placed at a distance of 35 cm. The slits have equal dimensions of 0.5 × 3 mm².

This primary sodium beam interacts with iodine gas, which is generated in an oven (4) described in more detail in [link type: ‘detailed in/is focused in/clarified in/generalised in/segregated in/wider range/project; target: MESO-m3a-1’] .

At working conditions the iodine pressure in the collision region is estimated to be about 3 × 10⁻⁴ torr; while the temperature of the oven was about 1200°C to ensure complete dissociation. Because the oven rotates simultaneously with the detector, the slots in the tantalum cylinders and heat shields to the detector are only 7 × 2.5 mm². The entrance slots of the sodium
beam are $7 \times 8$ mm$^2$, which enables the measurements of scattered particles up to a laboratory angle of 22 degrees.

The reaction products are analyzed in the differentially pumped detection chamber (5), which they enter via a pumping resistance (6) with identical discs on both ends and with eleven rectangular diaphragms with widths of 0.25, 0.50, 1 and 2 mm to fix the angular resolution of the detector at 0.3°, 0.6°, 1.2° and 2.4° fwhm, respectively. The discs are fixed in identical positions on the axis of a small step motor (7).

The detector is coupled to a multi-channel analyzer, each channel corresponding to a defined angular position of the detector. The detector is rotated by the stepmotor, the smallest step of the detector being 0.07°. A special-purpose computer drives the detector over the desired range with the required angular resolution, rotation step and integration time. An electrostatic 127° energy analyzer (8) has been used at the present measurements only to separate the scattered sodium ions with an energy in the eV range from the large number of thermal ions emitted by the oven.

The ions produced in the chemi-ionization process are detected using a channel electron multiplier (12). The lens system (11) focuses the ions into the detector (12). The ion signal does not contain any background and is measured by pulse counting.

The iridium band (13) and a second channeltron (14) give the possibility to detect scattered neutral alkali atoms passing the energy analyzer by a slit. The relative intensity of the primary sodium beam is measured by a surface-ionization detector (3) [General details of this apparatus are given in a mesoscopic module [link type: 'detailed in/focused on in/clarified in/generalised in/segregated in/wider range/project'; target: MESO-m3a-Lr].

With respect to the reliability of the analysis and detection, we remark the following. Angular-dependent detection of eV-ions requires much attention in order to avoid electromagnetic deflection. As much as possible the whole region of the collision center up to the shieldplating plate (9) has been coated by a thin layer of graphite to avoid contact potentials and stray charges. Distortion of the oven current has been avoided by heating the oven with a current which is pulsed synchronously with the already chopped detection. However, there still exists a drift in time resulting in a smoothing of the fine structure of the differential cross section if scans are added over too long a time. It is suspected that evaporation from the oven causes contamination of the graphite layer and again gives rise to electric charges, and therefore the measurements have been done with a total integration time as short as possible with respect to the statistical noise.

Generally the measurements consist of four scans added in the multi-channel analyzer, each

![Figure A08-m3a-F1](image_url) Schematic drawing on scale of the apparatus showing the charge-exchange source, the dissociation oven and the rotating detector.
scan consisting of two corresponding angular ranges on both sides of the zero axis to check for symmetry, while each measuring point has an integration time of four seconds per scan.

[Next step on the essay-path: Experimental treated results (link type: ‘essay-next/used for’; target: A08-m4b1)]
[Next step on the complete sequential path: Theoretical methods (link type: ‘seq-next’; target: A08-m3c)]
[Step back on the essay-path: Central problem (link type: ‘essay-back/summarised in/context in’; target: A08-m2b)]
[Step back on the complete sequential path: Methods (link type: ‘sq-back/part of/aggregates in/summarised in/context in’; target: A08-m2a)]

Comments on Experimental methods=A08-m3a:

- The set-up is an aggregate of distinct components. In the original article, subsections are distinguished for some of these components. In the modular version, these components are not represented in separate modules at the microscopic level, although they are presented in different paragraphs of the elementary Experimental methods module. We have mentioned in this module every component sketched in the schematic drawing of the apparatus.

At the mesoscopic level the Experimental methods are represented in a compound module consisting of constituent modules about the various components. In this appendix, we have not provided all of these modules. We have indicated which modules can be created and we have provided, as examples, two particular mesoscopic modules Experimental methods. Firstly, the details on the iodine oven that are given in the original article are recast in MESO-m3a-I. Secondly, the information about the Ir-wire surface ionisation detector that is dispersed over several original articles is cast into the module MESO-m3a-Ir.

- This module corresponds quite closely to the section 2.Experimental. The difference is that we have recast the description of the iodine source into a mesoscopic module, as it is a complex set-up that can be used again, even though it turned out to be used only for this article. We have included the use of interstitial points, as described in subsection 2.5 Data, in the module A08-m4b Treated results. Also, the sequence of the account of the components has been changed with respect to the original version.

- Information with respect to the restrictions of the set-up, i.e. the precision, has been made explicit in this module.

- The size of the collimation slits seems to change between articles. Therefore it is microscopic information and therefore it is mentioned in this module.

- In the original article, the authors state that the charge-exchange source is “described elsewhere”, namely is $R_{f_{A08}}$. In the modular version, this reference is recast in a link to a mesoscopic account of that source.
Theoretical methods = A08-m3c

Characterisation

<table>
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<tr>
<td>Physics</td>
<td>Atom-atom model, Landau-Zener-Stueckelberg, Rotational coupling, Semi-classical, impact-parameter approximation, lowest-order stationary-phase approximation, uniform rainbow approximation, JWKB phase shifts</td>
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<td>Bibliographic</td>
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<tr>
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The atom-atom model for ion-pair formation [More on the model in a mesoscopic Theoretical methods module [link type: ‘detailed in/generalised in/wider range/project’; target: Meso-m3c-mod]] explains chemi-ionization in collisions via crossing of the diabatic potential energy surfaces of the system, or in other words, via a transition between two states of the system. A transition between two states can take place when the states are electronically coupled. [Particulars on the transition [link type: ‘contains/segregated in/focused in’; target: A08-m3c].]

The atom-atom model for ion-pair formation takes into account the Landau-Zener transition probability between electronically coupled states of the same species [Focus on the LZ transition [link type: ‘contains/segregated in/specialised in/detailed in/focused in/essay-next’; target: A08-m3c]]. The model can be further refined by also taking into account rotational coupling [Focus on the rotational coupling [link type: ‘contains/segregated in/specialised in/detailed in/focused in’; target: A08-m3c]].

The differential cross section of chemi-ionization in sodium iodine collisions can be calculated via the potential curves of the system and the deflection function [More about the deflection function in a mesoscopic Theoretical methods module [link type: ‘detailed in/focused in/generalised in/wider range/project’; target: Meso-m3c-def]]. For the semi-classical treatment of the cross section, the different contributions to the differential cross section are to be approximated. Here the stationary phase approximation, uniform approximation and JWKB phase shifts are used [Particulars on these approximations in the Theoretical methods [link type: ‘contains/segregated in/detailed in/focused in’; target: A08-m3c]].]
Comments on Theoretical methods=A08-m3c:

- This module *Theoretical method* is a compound module, containing two components: firstly the theoretical methods used to determine the states of the system and the transition probabilities between them, and secondly the methods for the calculation of the semiclassical differential cross section starting from those states and probabilities.

- The different theoretical methods presented in this complex module are used at different stages of the problem-solving process. Therefore they were presented in different sections in the original article (3. *Potential curves*, the first half of 4. *Calculations, Rotational coupling*), and therefore they are visited at different stages by the essay-type sequential path. A result of the complexity of this module is that we have included this complex module in the essay-type path, in order to enhance the reader’s understanding of the scientific discourse.

- The ‘standard coupling’ (associated to the Landau-Zener probability) is called the Landau-Zener coupling. That is an electronic coupling. In the original article the rotational coupling was presented as a refinement, when the model without rotational coupling turned out to be inadequate.

- This complex module is included in the essay-type sequential path for the sake of clarity, because the essay-type path through its constituent elementary modules is interrupted when the path first leads through part of the *Interpretation* module (see the *Map of contents*). Also, the module contains constituent modules at different levels.
Theoretical methods: transition probabilities = A08-m3ci

The atom-atom model for ion-pair formation [Particular on the model in a mesoscopic module [link type: 'detailed in/wider range/project'; target: MESO-m3c-mod]] explains chemi-ionization in collisions via crossing of the diabatic potential energy surfaces of the system, or in other words, via a transition between two states of the system. A transition between two states can take place when the states are coupled.

The atom-atom model for ion-pair formation takes into account the Landau-Zener transition probability between electronically coupled states [Focus on LZ transition [link type: 'contains specialised in/detailed in/focused in'; target: A08-m3ci] . The model can be further refined by also taking into account rotational coupling [Focus on rotational coupling [link type: 'contains specialised in/detailed in/focused in'; target: A08-m3ci2] .

[Next step on the complete sequential path: Theoretical methods [link type: 'seq-next/contains specialised in'; target: A08-m3c1]]

[Step back on the complete sequential path: Theoretical Methods [link type: 'sq-back/part of segregated in/summarised in/context in'; target: A08-m3c]]

Comments on Theoretical methods=A08-m3ci:

- This is a cluster module containing two constituent modules about specific types of transition probabilities.
- The text of this module is a copy of the first part of the module summary of the complex module Theoretical methods A08-m3c
C.3. THE MODULARISED VERSION OF A08

Theoretical methods: LZ coupling=A08-m3ci1

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According to the atom-atom model for ion-pair formation in molecular collisions, chemi-ionization in two-body collisions takes place via pseudo-crossing of the potential energy surfaces of the interacting atoms. [More on the model in a mesoscopic module (link type: 'elaborated in/elucidated in/project/wider range'; target: MESO-m3c-mod]}

Potential curves

Fig. MESO-m3c-mod-F1 shows the lowest ionic and covalent potential curves of sodium iodide. The general shape of the curves is explained in [[link type: 'explained in/To cause/detailed in/project/wider range'; target: MESO-m3c-mod#crossing curves', and the precise shape is determined in another module [The exact figure is generated in the Interpretation] (link type: 'detailed in'; target: Interpretation A08-m5b)]]. The species of the ionic electronic state, indicating the symmetry and multiplicity properties, is given by $^1\Sigma^+$. By building up the molecule from the two separate neutral particles $\text{Na}^+$(2$^3S_1/2$) and Cl$^-$($^2P_3/2$), the LS-coupling gives rise to eight molecular states. One of them has the same

![Image](image_url)
species $^1\Sigma^+$ as the ionic state, which can according to the Neumann–Wigner rule give rise to transitions. We assume that we can ignore the excited covalent state, only taking into account the lowest states of the system, thus reducing the case to a two-state problem. [unfold explanation / justification]

For the lowest states the important parameter $H_{12}$ has been estimated experimentally by Moutinho et al. [The value is input from a previous article [link type: 'input from/project'; target: A04-m4b] from total cross section measurements for chem-ionization of Na + Cl, giving a value $H_{12} = 0.05$ eV. Two different types of theoretical calculations by Herschbach and Grice [These values are input from other articles [link type: 'input from/external'; target: RF05-10-m*]) result in the values of 0.06 and 0.09 eV. These values of $H_{12}$ all give, in our energy range from 10 up to 100 eV, a transition probability $P_0$ of the order of 1/2 for the pseudo-crossing of the ionic and lowest covalent state.

An estimation of the internuclear crossing distance of the ionic and excited covalent state leads to a value of the relevant $H_{12}$ [This value is input from another article [link type: 'input from/external'; target: RF05-10-m*] much smaller than for the former pseudo-crossing. Then the diabatic transition probability for the outer pseudo-crossing hardly differs from unity, so the excited covalent state is an unimportant outgoing channel.

The first excited covalent state with species $^1\Sigma^+$ does have an avoided crossing with the ionic state at large internuclear distance, but this covalent state is not an incoming channel in the collisions considered, because all the thermal dissociated iodine atoms are in the $^2\Sigma_1^+$ state. Therefore we shall ignore the excited covalent state in our considerations.

Then, for our collision process, one of the eight collisions has the probability $P_0$ for a diabatic transition at a single passage of the pseudo-crossing at $R_c$ given by the Landau–Zener formula [The formula is given in a mesoscopic module [link type: 'input from/project/wider range'; target: MESO-m3c-mod#Pb].

Summarising, the following approximations have been used:

1. The Landau–Zener transition-probability formula.

2. The use of the Landau-Zener formula to collisions where the distance of closest approach $R_0$ and the distance of pseudo-crossing $R_c$ are not well separated [Arguments against the applicability [link type: 'arguments/external'; target: RF05-25].

3. The use of the diabatic potentials [These potentials are given in a mesoscopic module [link type: 'input from/project/wider range'; target: MESO-m3c-mod#U[R]] in the classical deflection function in spite of small deformation of the curves at the pseudo-crossing.

4. The use of a transition point in spite of a transition region around the pseudo-crossing predicted by the Landau–Zener theory.

5. The neglect of rotational coupling so far [Compare this to the module about the rotation coupling [link type: 'compare/sq-next'; target: A08-m3ci2]]

[Next step on the essay-path: Theoretical methods [link type: 'essay-next/used for'; target: A08-m3ci]]
[Next step on the complete sequential path: Theoretical methods [link type: 'seq-next/compared to'; target: A08-m3ci2]]
[Step back on the essay-path: Theoretical methods [link type: 'essay-back/part of/aggregated in/generalised in/summarised in/context in'; target: A08-m3c]]
[Step back on the complete sequential path: Theoretical Methods [link type: 'sq-back/part of/generalised in/summarised in/context in'; target: A08-m3ci]]
Comments on Theoretical methods: LZ coupling=A08-m3e11:

- This constituent module contains (in the beginning) a brief summary of the mesoscopic account of the atom-atom model, tailored to the specific situation: what are the coupled states.

- The ionic potential of NaI is said to be well-known; the covalent potential is determined in the Interpretation module m5. However, the general features of the potential are part of the theoretical toolbox, because they do not depend on the new measurements.

- In the original article, the approximations are listed in the 7. Discussion section. We also summarised them as the restrictions of the Theoretical methods in this module.

- The original Introduction contained some discussion about the applicability of the semiclassical LZ model to the differential cross section of chemi-ionization of Na+I. The rest was presented in section 3. Potential curves. The last part of that section, however, describes and discusses the specific potential curve that has been determined in this work. In the modular version, we give an account of how the potential parameters have been determined in the Quantitative interpretation module A08-m5bi and also provide the resulting potential in the Treated results module A08-m4bi1.

- It has been assumed that the species of the relevant states are known or can be determined independently of the experimental results. If this is not the case, the information about the species would belong in the Interpretation.

- The LS-coupling is the spin-orbit coupling in the lowest states of the NaI molecule, which is explained in textbooks on molecular spectroscopy.

- The terms radial coupling, translational coupling, electronic coupling and Landau-Zener coupling are used as synonyms.
Theoretical methods: Rotational coupling = A08-m3ci2

Chemical ionization in collisions between Na and I can be explained via crossing of the two lowest $^1\Sigma^+$ diabatic potential energy surfaces of the NaI molecule [Particulars on the model] in a mesoscopic

Theoretical methods module (link type: 'detailed in/external in/wider range/project'; target: MESO-m3c-mod) . A transition between two states can take place when the states are coupled. The LZ model gives the probability of a diabatic transition between two states of the same species due to electronic coupling. In collisions between Na and I, only the lowest states play a role and are therefore taken into account [Arguments why we did this, involving an explanation why only those states play a role, are given in another Theoretical methods module (link type: 'detailed in/external in/argued in/sq-back'; target: A08-m3ci1) .

A transition can also [Compare with the LZ transition in another Theoretical methods module (link type: 'compare/sq-back'; target: A08-m3ci1) be caused by rotational coupling. Referring to the detailed description by Russek [[link type: 'detailed in/external'; target: [RA08-5-m*]] we only give the main features of rotational coupling as far as it is of interest for the present collision process.

Rotational coupling couples two states with different $z$ components of angular momentum. The coupling takes place in the region of the crossing point of the potential curves. In case of LS coupling, the covalent ground state of NaI is split up into the $^1\Pi$, $^3\Pi$, $^1\Sigma$ and $^3\Sigma$ state while the ionic ground state of Na$^+$Cl$^-$ only consists of the $^1\Sigma$ state. Because rotational coupling acts only on the angular momentum and does not influence the spin, only the $^1\Pi$ covalent state couples to the ionic $^1\Sigma$ state. As with the Landau-Zener coupling, only one of the eight covalent entrance channels at the collisional coupling states will produce significant spin-contraction properties at a weight factor of 1/8. The probability for the $^1\Pi$-$^1\Sigma$ transition is given by:

$$R_{b, \text{rot}} = 1 - \exp\left(\frac{-2\pi H_{\text{rot}}^2 \omega^2}{\hbar v_f \frac{d}{dt}(H_{11} - H_{22})|_{R_c}}\right),$$

where $H_{\text{rot}}$ is the coupling parameter, $\omega$ and $v_f$ are the angular and radial relative velocities of the colliding particles at the level crossing $R_c$.

The most striking contrast to the Landau-Zener transition probability $R_{b, LZ}$ given by [The formula input from a mesoscopic Theoretical methods module (link type: 'input from/project/wider range'; target: MESO-]
is the linear variation of the exponent with the relative velocity while the exponent of \( P_{b,LZ} \) varies inversely with the velocity. It is obvious that \( P_{b,rot} \) is large for high relative kinetic energies and for large impact parameters. Of course the probability to go from the covalent entrance channel to the ionic final state equals \( P_{b,rot}(1 - P_{b,rot}) \), but also this product easily leads to larger probabilities in case of large values of \( E \) and \( b \).
Comments on Theoretical methods: Rotational coupling = A08-m3ci2:

- What happens is that the electron jump not only can occur via the ‘normal’ LZ transition, involving the $\Sigma^1_+$ covalent state, but also via rotational coupling, involving another covalent state, the $\Pi$ state (which is also a low lying state, agreeing with the previous assumption that only low lying states are considered).

- The atom-atom model for ion-pair formation in molecular collisions takes into account the Landau-Zener coupling, but not the rotational coupling. The introduction of rotational coupling actually introduces a third state, so that this case then is a three-state problem. However, this three state problem is dealt with as if the cross section is a sum of two two-state problems.

In this module, however, we do not go into detail, as this issue is not explored very thoroughly in the original article either. The necessary background knowledge and computer facilities were not available at that time.

An important theoretical article published a year later by Levine and Bernstein showed that the experimental results could be reproduced by simply applying a radial coupling and an adiabatic representation, such that rotational coupling is not required to explain the results.

- This is the module that readers can consult when they want to know how to take the rotational coupling into account in the explanation of chemi-ionisation. This module does not argue that rotational coupling is indeed necessary in the explanation, because that part of the Interpretation, where the measurements are compared with the calculations.

- The first part of the original section 8.Rotational coupling is recast in this Theoretical methods module. The rest of the section is recast in the Quantitative interpretation module A08-m5bi2.

- This module appears late in the essay-type sequential path: after the Interpretation module A08-m5biil and before A08-m5bi2, where the rotational coupling is taken into account (see the Map of contents). The same sequence was apparent in the original version of the article: the results were first discussed using the Landau-Zener coupling, before a section was devoted to the idea of rotational coupling.
C.3. THE MODULARISED VERSION OF A08

Theoretical methods: Semiclassical differential cross section=\text{A08-m3cii}

<table>
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<th>Characterisation</th>
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<td>Range: Microscopic</td>
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<tr>
<td>Physics: Atom-storm model, Semiclassical differential cross section, impact-parameter approximation, lowest-order stationary-phase approximation, uniform rainbow approximation, JWKB phase shifts</td>
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<td>Bibliographic: Delvigne,Los [AMOLF]; Physica [1973]</td>
</tr>
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<td>Identification: A08-m3cii</td>
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</table>

Based on the potential curves, the deflection function [The definition of deflection function is given in a mesoscopic module [link type: defined in/wider range/project; target Meso-m3c-defl#1(b)]] of the system can be calculated [To details on the method to calculate the deflection function [link type: 'detailed in/proj ect'; target: A06-m*] (assuming the impact-parameter approximation) [The notion of a deflection function is clarified in [link type: 'elaborated in/clarified in/wider range/project'; target: Meso-m3c-defl]]. Starting with the deflection function, the classical differential cross section for chemi-ionization is given by [The formula is copied from a mesoscopic module [link type: 'input from/wider range/project'; target: Meso-m3c-defl#2] (C.3)]:

\[
I(\theta) = \frac{1}{\sin(\theta)} \sum_{i=1,2, \cdots} P_b_i (1 - P_b_i) h_i \left| \frac{db_i}{d\theta} \right|
\]

where \( \theta = |\Theta| \). Figure Meso-m3c-defl-F1 of the deflection function [The figure is copied from a mesoscopic module [link type: 'input from/project/wider range'; target: Meso-m3c-defl#1(b)]] shows that up to the rainbow angle [The notion of a rainbow angle is clarified by Bernstein [link type: 'detailed in/clarified in/wider range/external'; target: Bernstein] the summation is over four impact parameters and over two impact parameters for larger scattering angles.

The same impact parameters are important in the semiclassical treatment extended with the stationary phase approximation [The semi-classical treatment is elucidated by Ford and Wheeler [link type: 'elucidated in/detailed in/external'; target: Ra0821-*]]. Then the scattering amplitude \( f(\theta) \) is built up
again either by four or by two contributions:

\[ f(\theta) = \sum_{i=1,2} f_i(\theta), \quad (C.4) \]

leading to the differential cross section

\[ I(\theta) = |f(\theta)|^2. \quad (C.5) \]

The contributions to the differential cross section are to be approximated. We use the lowest order stationary-phase approximation and the uniform approximation, which in their turn both require the JWKB approximation.

**Lowest-order stationary-phase approximation**

In the lowest-order stationary-phase approximation [This approximation has to be elucidated elsewhere, in some macroscopic module Theoretical methods [link type: 'detailed in/elucidated in/wider range'; target: MACRO-m3c]] the possible contributions \( f_i(\theta) \) to \( f(\theta) \) are then given by

\[ f_a(\theta) = \left[ \left| \frac{db_a}{d\theta} \right| b_a P_b (1 - P_{ba}) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_{ba} + kb_a \theta - \pi) \right] \equiv A e^{i\alpha}, \quad (C.6) \]

\[ f_b(\theta) = \left[ \left| \frac{db_b}{d\theta} \right| b_b P_b (1 - P_{ba}) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_{ba} + kb_b \theta - \frac{1}{2} \pi) \right] \equiv B e^{i\beta}, \quad (C.7) \]

\[ f_c(\theta) = \left[ \left| \frac{db_c}{d\theta} \right| b_c P_b (1 - P_{bc}) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_{bc} + kb_c \theta - \pi) \right] \equiv C e^{i\gamma}, \quad (C.8) \]

\[ f_d(\theta) = \left[ \left| \frac{db_d}{d\theta} \right| b_d P_b (1 - P_{bd}) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_{bd} + kb_d \theta - \frac{1}{2} \pi) \right] \equiv D e^{i\delta}, \quad (C.9) \]

Figure MESO-m3c-defl-F1. Typical deflection curves for chemi-ionization scattering (CM system). The two curves due to ionic and covalent scattering are connected \( b \approx R_c \). Because of the several interference features, the ionic curve is split up into b, c and e branches, the covalent curve into a and d branches. [copy from MESO-m3c-defl].
\[ f_\theta(\theta) = \left[ \frac{\partial^2}{\partial \sigma^2} b_\sigma P_{\sigma} (1 - P_{\sigma}) / \sin \theta \right]^{1/2} \]
\[ \times \exp \left[ i \left( 2n_b + \frac{k_b \theta - 1}{2} \right) \right] \equiv E e^{i \varepsilon}, \] (C.10)

where \( n_b \) indicates the phase shift and \( k \) is given by \( k = (2\mu E_\beta)^{1/2} \). For a certain scattering angle \( \theta \) where four contributions form the cross section (for instance the contributions from the branches a, c, d and e), the differential cross section is given by:

\[ I(\theta) = \left| A e^{i \alpha} + C e^{i \gamma} + D e^{i \delta} + E e^{i \varepsilon} \right|^2 \]
\[ = A^2 + C^2 + D^2 + E^2 + 2AC \cos(\alpha - \gamma) \]
\[ + 2AD \cos(\alpha - \delta) + 2AE \cos(\alpha - \varepsilon) \]
\[ + 2CD \cos(\gamma - \delta) + 2CE \cos(\gamma - \varepsilon) \]
\[ + 2DE \cos(\delta - \varepsilon). \] (C.7)

The lowest-order stationary-phase approximation is not applicable to the entire range, as it fails in giving a good description of the rainbow. Also the usual Airy description [This description is elucidated by Airy [link type: 'elicited in/ is detailed in/external': target: RfA0822-m*] is not very suitable because the shape of the deflection curve in the rainbow-angle region deviates too much from the supposed parabolic behaviour.

**JWKB approximation**

The phase shift \( n_b \) in equations C.41 and C.9 is given in the JWKB approximation [This approximation is elucidated by Bernstein link type: 'detailied in/elicited in/wider range/external; target: Bernstein] by

\[ \eta_b = \frac{1}{2} k \int_9^\infty \Theta \, db \] (C.8)

so making necessary an integration over the deflection curve.

However, the first problem in applying this approximation is that in the present case there does not exist a deflection curve for collision parameters from infinity down to the largest value of \( b \) that gives rise to chemi-ionization \( (b_{\text{max}} \approx R_c) \). Fortunately, Eq. (C.38) shows that for the calculation of the differential cross section we only need the phase-shift differences of the relevant contributions. In our calculations therefore we have taken arbitrarily \( n_{b_{\text{max}}} = 0 \).

A second point is that due to the coulombic nature of the outgoing channel, the argument of the sine of the wave function contains a term with \( \ln(2kR) \), and therefore the validity of the semiclassical approximation is questionable. However, as in the asymptotic wave functions the phase shifts contain for all deflection branches this \( \ln(2kR) \) term; this term cancels out for phase-shift differences and the problem is circumvented. Thus, the JWKB approximation can be applied in the present case.

**Uniform approximation**

The approximation that can be applied to the area of the rainbow angle is the uniform approximation of rainbow scattering [The uniform approximation is elucidated and its applicability argued by Berry [link type: 'elicited in/argued in/detailed in/external'; target: RfA0823-*], in which the actual shape of the deflection function is used. In our case it turns out that the uniform approximation is only necessary to describe the primary rainbow because the supernumerary rainbows calculated in this way completely coincide with the ones calculated by the stationary-phase method. [These rainbows are calculated in the Interpretation [link type: 'depends on'; target A08-m5bi]].
In the uniform approximation of rainbow scattering the resulting formula to calculate the rainbow structure for $\theta < \theta_{\text{class.rainbow}}$, being the interference of the $b$ and $c$ branches, reads:

$$I(\theta) \sin(\theta) = \pi \left[ \left( b_b \times P_{b_b} (1 - P_{b_b}) \times \left| \frac{db_b}{d\theta} \right| \right)^{1/2} \right.$$  

$$+ \left( b_c \times P_{b_c} (1 - P_{b_c}) \times \left| \frac{db_c}{d\theta} \right| \right) \right]^{1/2} |\xi|^{1/2} \text{Ai}(\xi)^2$$  

$$+ \pi \left[ \left( b_b \times P_{b_b} (1 - P_{b_b}) \times \left| \frac{db_b}{d\theta} \right| \right)^{1/2} \right.$$  

$$- \left( b_c \times P_{b_c} (1 - P_{b_c}) \times \left| \frac{db_c}{d\theta} \right| \right) \right]^{1/2} |\xi|^{1/2} \text{Ai}'(\xi)^2,$$

where

$$\xi = -\left( \frac{3}{4} \right) \{2\eta_c - 2\eta_b + k[b_c - b_b]\theta\}^{2/3}.$$  

The Airy functions $\text{Ai}$ and $\text{Ai}'$ have been replaced by their asymptotic approximations.

**Applicability of this theoretical method**

The semiclassical differential cross section can be calculated using the stationary phase approximation, the uniform approximation of rainbow scattering and JWKB phase shifts.

The application of the semiclassical approximation on two-state collisional processes and the Landau-Zener theory have been discussed recently in a series of papers by Delos and Thorsen [link type: 'argued in/external'; target: Rf086-m*]. As far as the applicability of the semiclassical approximation is concerned, they conclude with four statements about kinetic energy and potential states of the collision partners [To these statements link type: 'external/clarified in'; target: Rf086-m*]. The collisional process discussed now does not fulfill completely those statements.
Comments on Theoretical methods: Differential cross section—A08-m3cii:

- In the original article, the calculation methods were given in the first part of the section 4. Calculations. The rest of that section was devoted to the result of the calculations.

- The figure with the general shape of the deflection function (and related expressions) has been copied from the mesoscopic module MESO-m3c-defl. Such a copy can be implemented via a hyperlink that puts the existing figure on the screen, for example in a separate window, instead of being ‘hard wired’ as a new copy into the text of the new module.

- We have tried to split the description and discussion of the complete set of theoretical tools for the calculation of the cross section into separate constituent modules, because of the size and complexity of the module: the model with the general expression would then be separated from the different approximations used to calculate actual results using the model.

However, these parts are too closely entangled, because all components refer to the expression for the semiclassical cross section and to the branches of the deflection function, both approximations use the JWKB approximation for the phase shift, and the theoretical results are calculated using both approximations (for different angles, but in the same figure).

A full account of the approximations could still warrant separate modules, but they are applied to the specific case of NaI presupposing that the reader knows about the general idea - which is explicit in links to that general info. For full accounts of the JWKB phase shift, stationary phase, and uniform approximation, we refer the reader elsewhere. In this appendix, we have not provided any higher-level modules providing that information.
The differential cross sections of charge-transfer collisions between Na atoms and I atoms have been measured in the eV range, using an atomic beam set-up [Particulars on the set-up in the Experimental methods [link type: 'depends on/detailed in'; target: A08-m3a] . The differential cross section have also been calculated semi-classically [Particulars on the calculation methods in the Theoretical methods [link type: 'depends on/detailed in'; target: A08-m3c] .

This module contains two main components: raw data [Raw data [link type: 'contains/segregated in/sq-next'; target: A08-m4a] and graphically presented, treated results [Treated results [link type: 'contains/segregated in'; target: A08-m4b] ] that have been generated in experiments [Experimental raw data [link type: 'contains/segregated in/specialised in'; target: A08-m4a] [Experimental treated results [link type: 'contains/segregated in/specialised in'; target: A08-m4b] and calculations [Experimental raw data [link type: 'contains/segregated in/specialised in'; target: A08-m4a] [Experimental treated results [link type: 'contains/segregated in/specialised in'; target: A08-m4b] . In particular we have results for:

- measured differential cross sections of Na + I → Na⁺ + I⁻, 13.85 eV [Raw data [link type: 'detailed in/focused on in/contains/segregated in/specialised in'; target: A08-m4a]] [Treated results [link type: 'detailed in/focused on in/contains/segregated in/specialised in'; target: A08-m4b]]

- measured rainbow structures 13-63 eV [Raw data [link type: 'detailed in/focused on in/contains/segregated in/specialised in'; target: dataA08-m4a]] [Treated results [link type: 'detailed in/focused on in/contains/segregated in/specialised in'; target: dataA08-m4b]]

This module also contains a copy of 'theoretical data and results' obtained as intermediary results in the course of the interpretation [link type: 'input'; target: interpretation A08-m5b]
C.3. THE MODULARISED VERSION OF A08

- raw data and treated results of the calculated differential cross section Na + I, 13.1 eV
  [Raw data (link type: ‘detailed in/focused on in/contains/segregated in/specialised in’; target: A08-m4ai2)] [Treated results (link type: ‘detailed in/focused on in/contains/segregated in/specialised in’; target: A08-m4bi2)].

- theoretical rainbow structure 13-63 eV [Raw data (link type: ‘detailed in/focused on in/contains/segregated in/specialised in’; target: A08-m4ai3)] [Treated results (link type: ‘detailed in/focused on in/contains/segregated in/specialised in’; target: A08-m4bi3)]

[Next step on the complete sequential path: Raw data (link type: ‘seq-next’; target: A08-m4a)]
[Step back on the complete sequential path: Theoretical Methods (link type: ‘seq-back’; target: A08-m3ci)]

Comments on Results=A08-m4:

- This is a complex module containing three different levels of constituent modules. In the first place, in this module two components are aggregated: Raw data and Treated results. In the second place, these components focus on the general case of two specific cases: experimental and theoretical results. In the third place, the experimental results are represented in a compound module with two components: an elementary module with the measurements of the differential cross sections, and an elementary module about the measured the rainbow structure. The theoretically oriented module Treated results is a compound of three components: an elementary module about the potential and deflection function, one about the calculated differential cross section, and one about the theoretical rainbow structure.

- We have followed the guidelines specified in appendix A and considered the Treated results to be primary. We have results of only one ‘level of treatment’, so we present them in the Treated results. However, we have provided empty Raw data modules in the structure, as an indication of the role that raw data could play in a scientific article. Assuming that relevant raw data are available for both the experimental and the theoretical cross sections, and for the rainbow structure, we have reflected the internal structure of the module Treated results in the internal structure of the module Raw data, except for the elementary module in which the potential and the deflection function are represented, which assumed not to have a counterpart in Raw data.
Treated results= A08-m4b

The differential cross sections of charge-transfer collisions between Na atoms and I atoms have been measured in the eV range, using an atomic beam set-up [Particulars on the set-up in the Experimental methods][link type: 'depends on/detailed in'; target: A08-m3a]. The differential cross section have also been calculated semiclassically [Particulars on the calculation methods in the Theoretical methods][link type: 'depends on/detailed in'; target: A08-m3c].

We graphically present treated results that have been generated in experiments [Experimental treated results][link type: 'contains/segmented in/specialised in'; target: A08-m4b] and calculations [Experimental treated results][link type: 'contains/segmented in/specialised in'; target: A08-m4b]. In particular we have results for:

- measured differential cross sections of Na + I → Na⁺ + I⁻, 13-85 eV [Treated results][link type: 'detailed in/focused on in/contains/segmented in/specialised in'; target: A08-m4b]
- measured rainbow structures 13-63 eV [Treated results][link type: 'detailed in/focused on in/contains/segmented in/specialised in'; target: A08-m4b]

This module also contains a copy of ‘theoretical data and results’ obtained as intermediary results in the course of the interpretation [link type: 'input'; target: interpretation A08-m5b]

- Treated results potential, deflection function Na + I, 13.1 eV [Treated results][link type: 'detailed in/focused on in/contains/segmented in/specialised in'; target: A08-m4b]
- treated results of the calculated differential cross section Na + I, 13.1 eV [Treated results][link type: 'detailed in/focused on in/contains/segmented in/specialised in'; target: A08-m4b]
- theoretical rainbow structure 13-63 eV [Treated results][link type: 'detailed in/focused on in/contains/segmented in/specialised in'; target: A08-m4b]

[Next step on the complete sequential path: Treated results][link type: 'seq-next'; target: A08-m4b]
[Step back on the complete sequential path: Raw data][link type: 'seq-back/part of/summarised in/context in'; target: A08-m4b]
Comments on Treated results=A08-m4b:

- This is a complex module containing two different levels of constituent modules. In the first place, two specific cases are brought together in this module: experimental and theoretical results. In the second place, these specific types of results are each represented in a compound module in which various elementary modules are aggregated.
Treated results: measurements = A08-m4bi

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The differential cross sections of charge-transfer collisions between Na atoms and I atoms have been measured in the eV range, using an atomic beam set-up [Particulars on the set-up in the Experimental methods (link type: ‘depends on/detailed in’; target: A08-m3a)].

We have treated results for:

- measured differential cross sections of Na + I → Na⁺ + I⁻, 13-85 eV ([link type: ‘detailed in/focused in/contains/specialised in’; target: A08-m4bi1])

- experimental rainbow structure 13-63 eV ([link type: ‘detailed in/focused in/contains/specialised in’; target: results A08-m4bi2])

[Next step on the complete sequential path: Treated results (link type: ‘seq-next/contains/specialised in’; target: A08-m4bi1)]

[Step back on the complete sequential path: Treated results (link type: ‘seq-back/part of/generalised in’; target: A08-m4b)]

**Comments on Treated results** = A08-m4bi:

- This is a compound module with experimental results, which contains two components: an elementary module with the measurements of the differential cross sections, and one about the measured the rainbow structure.
Treated results: Experimental differential cross section = A08-m4bi1

Characterisation

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On the chemi-ionization collisional process of sodium atoms on iodine atoms measurements have been done [particularly on the measurements in the Experimental methods module [link type: 'depends on/essay-back'; target: A08-m3a]] in the kinetic-energy range from 13 up to 85 eV. Fig. A08-m4bi1-F1 shows relative polar differential cross sections of collisions with initial relative kinetic energies $E_i$ of 13.1 and 18.2 eV.

The general shape of the differential cross section has been measured at collision energies of 13.1, 20.7, 29.7, 38.7 and 55.0 eV, as shown in Figs. A08-m4bi1-F1 a, b, c, d, e. [Compare these results to the theoretical results [link type: 'compare'; target: A08-m4bi2].]

Data analysis and presentation

The transformation of the raw data of the detector signal [[link type: 'depends on'; target: A08-m4a1] into the differential cross section needs the effective size of the collision region as a function of the scattering angle [This effective size is determined by the Experimental methods [link type: 'depends on'; target: A08-m4b2]].

![Figure A08-m4bi1-F1. Relative polar differential cross section for chemi-ionization (CM system). The cross sections, measured at a colliding energy of 13.1 and 18.2 eV, have been set in scales with shifted zero points.](image-url)
A priori there are doubts on the normalization of the detector signal to an angular-independent scattering volume viewed by the detector. The calculated angular-dependent normalization factor seems to be reliable by observing the result that the total cross section due to covalent scattering is about equal to the total cross section due to ionic scattering, independent of the kinetic energy and thus independent of the different angular ranges. This requirement is postulated by the equal Landau–Zener probability $P_0(1 - P_0)$ for both chemi-ionization trajectories and means about equal areas enclosed by the relevant parts of the differential cross section [Why these cross sections are equal is explained in a mesoscopic Theoretical methods module [link type: 'explained in/To cause/wider range/project'; target: MESO-m3c-deb]].

Actually the iodine oven [Particulars on the oven are given in a mesoscopic Experimental methods module [link type: 'depends on/detailed in/wider range/project'; target: MESO-m3a-l]] is a hybrid between a collision chamber and a secondary beam with a collision region neither large nor small as compared to the field of view of the detector. The effective size simply has been calculated geometrically for all angular resolutions and angular positions of the detector supposing that there is no gas density gradient inside the inner tantalum cylinder of the oven and a zero density outside.

This calculation leads to correct normalization curves since the measurements given in Fig. A08-m4bil-F2 indeed result in a general shape of the differential cross section independent of the relative collision energy, as expected.

The polar cross section is plotted against $\tau$. [The mesoscopic Data treatment module argues why that should be done [link type: 'elaborated in/argued in/wider range/project'; target: MESO-m3c-treat]]. The measurements are only relative and have been given for the different energies on arbitrary, non-related scales. Because of the large differences in intensity, the curves in figure A08-m4bil-F1 have been divided into three parts ('with small overlaps') and have been multiplied by the factors 1/3, 1 and 5. The reproducible interference structure due mainly to net-attractive scattering, has been indicated by full lines. The reproducible maxima of the interference structure due to net-repulsive scattering have been indicated by arrows.

The angular resolution of the detector used for the several angular ranges is shown at the top of figure A08-m4bil-F1. The bar above the angular-resolution number means that on the relevant range the measured points have been substituted by an equal number interstitial points to reduce the statistical noise in order to show the fine structure more clearly.

![Figure A08-m4bil-F2. Smoothed differential cross sections for five different collision energies: (a), (b), (c), (d), (e): Full curves show the measured relative differential cross section, averaged over the interference structures.](image-url)
C.3. **THE MODULARISED VERSION OF A08**

Reliability

Figure A08-m4bi1-F1 shows the applied angular resolution for the various stages. Going up in scattering angle the sharply decreased detector signal requires a decreasing angular resolution.

Determination of complete and resolved differential cross sections at lower kinetic energies is prevented by the quickly decreasing intensity of the sodium beam while the apparatus is not suitable to resolve the structure at small scattering angles at kinetic energies above 20 eV. [The restrictions of the set-up are given in the module Experimental methods](link:Experimental methods) [target: A08-m3a].

[Next step on the essay-path: Treated results](link:Treated results) [target: A08-m4bi2]
[Next step on the complete sequential path: Treated results](link:Treated results) [target: A08-m4bi2]
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[Step back on the complete sequential path: Treated results](link:Treated results) [target: A08-m4bi2]

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<td>• The cross sections have been measured in the range of 13-85 eV at about 12 different kinetic energies. The number of energies and their precise value are not explicitly stated in the article; they can be derived from figure of the rainbow structure versus the initial colliding energy.</td>
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<td>• In the original article, the results of the experimental cross sections at 13.1 and 18.2 eV are presented in full in a figure. The results for 13.1 are the ones that are used throughout the article: the deflection function and the calculated differential cross sections presented in the figures are determined for 13.1 eV. Furthermore, the detector signal versus the scattering angle is given in a figure for 18.2 eV, 38.7 eV, 55.0 eV, 83.5 eV. For 13.1 eV, 20.7 eV, 29.7 eV, 38.7 eV and 55.0 eV the general shape of the differential cross section is given.</td>
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<td>• The modular model allows for the distinction of elementary modules each with the differential cross section at one particular energy. However, this would lead to the creation of tens of strongly overlapping modules. It is not only unpractical to distinguish such modules, but also unnecessary, as the reaction at different energies are not considered to be different concepts of interest by any reader.</td>
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<td>• In the modularisation process, we have derived the information represented in this module from various sections. In the original article, the core of the experimental results was given in the 5 Measurements section, the information about the data analysis in the section 2.5 Data, and the smoothed curves were given in 6.4 General shape.</td>
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Treated results: Experimental rainbow structure = A08-m4bi2

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Fig. A08-m4bi2-F1 shows the rainbow structures at collisional energies from 13.1 eV up to 55 eV [Compare to the theoretical results [link type: compare; target: results A08-m4bi3]]. From twelve measured rainbow structures the relative positions of the maxima of primary rainbow and supernumeraries have been given while, arbitrary, always the third supernumerary rainbow has been chosen as a zero point and has been placed on a straight line. [The results are identified in the plots of the differential cross section [link type: depend on; target: A08-m4bi1]]. In the figure the outer curves indicate the boundaries of the rainbow structure. At the left side the curve connects the maxima of the primary rainbows, at the right-hand side the curve connects the measured maxima in the polar differential cross section curve at \( \tau \approx 65 \), indicating scattering with maximal collision parameter \( b \approx R_c \). The other full lines connect the measured maxima of the corresponding supernumeraries.

The wavelength of the repulsive interference as a function of the kinetic energy has been given in Fig. A08-m4bi2-F2 [Compare to the theoretical results [link type: compare; target: results A08-m4bi3]]. In the energy range from 13 to 84 eV these values concern the wavelength of the oscillations directly beyond the primary rainbows. Because a varying value of the wavelength as a function of the scattering angle could not be observed, the values given in Fig. A08-m4bi2-F2 ?? form the

Figure A08-m4bi2-F1. Rainbow structure versus initial colliding energy (CM system).
averaged values of ten oscillations just beyond the rainbow angle. The error bars only indicate the error in the relative position of first and tenth oscillation.

**Reliability**

Figure A08-m4bil-F1 shows the applied angular resolution for the various stages. Going up in scattering angle the sharply decreased detector signal requires a decreasing angular resolution. Fortunately the wavelength of the oscillations increases with increasing scattering angle.

Determination of complete and resolved differential cross sections at lower kinetic energies is prevented by the quickly decreasing intensity of the sodium beam while the apparatus is not suitable to resolve the structure at small scattering angles at kinetic energies above 20 eV [The restrictions on the experimental methods [link type: ‘depends on’; target: A08-m3a]]. The large-angle part of the rainbow structure and the repulsive scattering oscillations beyond the rainbow angle are easier to detect over a wide energy range.

The data of Fig. A08-m4bi2-F1 and Fig. A08-m4bi2-F2 have been taken directly from the detector signal without normalization on the scattering volume and without multiplying by sin(θ) to form the polar differential cross section.

Fig. A08-m4bi2-F3 shows the detector signals in the rainbow region of collisions with kinetic energies of 38.7 and 55 eV. The statistical noise of the 38.7 eV curve has been reduced by substitution of interstitial points for the real measured points; the 55.0 eV curve shows the real measurements. The intensity sharply decreases with increasing scattering angle.

The detector signals from repulsive scattering beyond the rainbow angle have been given in Fig. A08-m4bi2-F4 for kinetic energies of 18 and 84 eV.

![Graph](image)

Figure A08-m4bi2-F2. Wavelength of the oscillatory differential cross section (CM system) due to net-repulsive scattering, versus the colliding energy.
Figure A08-m4b2-F3. Detector signal versus laboratory scattering angle at relative colliding energies of 38.7 and 55.0 eV. The arrows indicate the maxima of the structure due to primary and supernumerary rainbows of the differential cross section. The ordinate scales differ by a factor of ten and have been shifted at the zero points.

Figure A08-m4b2-F4. Detector signal versus laboratory scattering angle measured at colliding energies of 18.2 and 84 eV in the angular range just beyond the primary rainbows. The abscissas of the corresponding curves have been shifted in such a way that the maxima of the primary rainbows, indicated by $\theta_{1b}$, coincide.
Comments on Treated results: Experimental rainbow structure=A08-m4bi2:

- We have assumed that the experimental rainbow structure is an experimental result, which should be presented in the module Results. Given the results of the experimental differential cross section, the rainbows can be pinpointed directly in the figures.

- In the original version the experimental and the theoretical rainbow structure were plotted in the same figure. There are many methods of comparing theoretical and experimental results. As in this case 1) the experimental results were used to fit some theoretical parameters, and 2) the theoretical results came close to the experimental ones, the authors chose in most cases to plot them in the same figure.

  We have separated these two types of (intermediary) results, because they have been obtained in different procedures. However, the reader can plot them in the same picture. The explicit ‘comparison’ link between this module A08-m4bii and its theoretical counterpart A08-m4bii3.

- A graphical presentation is given of the experimentally and theoretically determined rainbow angles at 12 (not explicitly specified) initial energies. The initial energies for the rainbow angles lie in the range of the energies of 13-55 eV according to the text, but 13-63 eV according to the figure. All energies can be obtained from the figure.

- We are not entirely sure why the authors included the figures with the detector signals in the original article. In the text, the only reference to the figures deal with the sharp decrease of the signal. In the arrows that are added to the figures indicate the theoretical rainbow structure. So, probably these figures serve some purpose in the interpretation. However, as we don’t know what purpose, we merely consider them as results.

- The figures with the detector signals represent rawer results than the figures with the rainbow structure. However, the difference in the degree of treatment is not large, as some treatment has already taken place, with respect to the interstitial points as is mentioned explicitly. Therefore, these have included these figures in the same complex module as the figures with the differential cross section, i.e. the module Treated results rather than the Raw data.

- From this module, the complete sequential path leads to the theoretical results. In the essay-type path, the theoretical results do not appear at all. Following that path the reader is led to the Theoretical methods.
Treated results: calculations = A08-m4bii

The differential cross sections of charge-transfer collisions between Na atoms and I atoms have been calculated semiclassically. [Particulars on the calculation methods in the Theoretical methods [link type: 'depends on/detailed in'; target: A08-m3c]].

This module contains a copy of 'theoretical results' obtained as intermediary results in the course of the interpretation [[link type: 'input'; target: interpretation A08-m5b]].

1. Potential and deflection function Na + I, at 13.1 eV [link type: 'detailed in/focused in/contains/specialised in/sq-next'; target: results A05-m4bii1].

2. Calculated differential cross section Na + I, 13.1 eV [Treated results [link type: 'detailed in/focused in/contains/specialised in'; target: A08-m4bii2].

3. Theoretical rainbow structure 13-63 eV [Treated results [link type: 'detailed in/focused in/contains/specialised in'; target: A08-m4bii3].

[Next step on the complete sequential path: Treated results [link type: 'see-next/contains/specialised in'; target: A08-m4bii]].

[Step back on the complete sequential path: Treated results [link type: 'sq-back'; target: A08-m4bii]].
C.3. THE MODULARISED VERSION OF A08

Treated results: Potential and deflection function=A08-m4biil

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- meta mlc
- Treated results
- [ME-m3c-mod]

The sodium-iodine potential curves are given by the following expressions. The ionic ground state is usually described by the Rittner potential [The formulae are given in the microscopic Theoretical methods module [link type: project/wider range/input from; target: MESO-m3c-mod#Potential curves]:

\[
U_{\text{ion}}(R) = -\frac{e^2}{R} - \frac{\alpha_{\text{Na}^+} + \alpha_{\text{Cl}^-}}{2R^4} - \frac{2e^2 \alpha_{\text{Na}^+} \alpha_{\text{Cl}^-}}{R^6} - \frac{C_{\text{ion}}}{R^6} + A_{\text{ion}} e^{-\frac{R}{\rho_{\text{ion}}}} + \Delta E. \tag{C.10}
\]

and we describe the covalent potential only by two terms:

\[
U_{\text{cov}}(R) = -\frac{C_{\text{cov}}}{R^6} + A_{\text{cov}} e^{-\frac{R}{\rho_{\text{cov}}}}, \tag{C.11}
\]

where the potential parameters are given in table A08-m4biil-T1 [The values are input from the Interpretation [link type: input from; target: A08-m3bi]].

Starting from these potential curves, the deflection function for chemi-ionisation in collisions between Na and I is given by figure A08-m5bi-F2. The two curves due to ionic and covalent

![Figure A08-m5bi-F1. Na-Cl, adiabatic potential curves. The pseudo-crossing potentials are all of the same species $^1\Sigma^\text{r}$. [Copied from the Quantitative interpretation [link type: input from; target: A08-m5bi]}.](image)
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<td>$C_{\text{ion}} = 11.3$ eV $^b$</td>
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<td>$\rho_{\text{ion}} = 0.3489$ $^d$</td>
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<td>$\varepsilon = 3.11 + \Delta E$ eV $^e$</td>
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<tr>
<td>$r_e = 2.71143(2.664^1)$ $^f$</td>
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<td>$\Delta E = 2.075$ eV $^r$</td>
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**Notes:**

$^a$ Dipole polarizability, from Rf$_{\text{A08}}$14.

$^b$ Van der Waals coefficient, from the London formula: $C_{\text{ion}} = 3\alpha_{\text{Na}}^+\alpha_{\text{Cl}^-} - I_2 A / 2(I_2 + A)$, where $I_2$ is the second ionization potential of Na and A is the electron affinity of I.

$^c$ Value are input from another article [link type: 'input from/external'; target: Rf$_{\text{A08}}$15-m*].

$^d$ [Value are input from another article [link type: 'input from/external'; target: Rf$_{\text{A08}}$16-m*]].

$^e$ Potential well depth, [Value are input from another article [link type: 'input from/external'; target: Rf$_{\text{A08}}$17-m*]].

$^f$ Intermolecular equilibrium distance, [Value are input from another article [link type: 'input from/external'; target: Rf$_{\text{A08}}$18-m*]].

$^g$ From $I_{\text{Na}} - A_{\text{Cl}}$.

$^h$ From Rf$_{\text{A08}}$19.

$^i$ Arbitrary value.

$^j$ From the London formula: $C_{\text{cov}} = 3\alpha_{\text{Na}}\alpha_{\text{Cl}}^+ I_{\text{Na}} I_{\text{Cl}} / 2(I_{\text{Na}} + I_{\text{Cl}})$, where I is the first ionization potential.

$^k$ Present work.

$^1$ Alternative value due to overdefinition of the potential curve.

---

**Figure A08-m5bi-F2.** Deflection curves for chemi-ionization scattering (CM system) at $E_i = 13.1$ eV. [Copied from the Quantitative interpretation (link type: 'input from'; target: A08-m5bi)].

scattering are connected $b \approx R_e$. Because of the several interference features, the ionic curve is split up into b, c and e branches, the covalent curve into a and d branches.
C.3. THE MODULARISED VERSION OF A08

[Next step on the complete sequential path: Treated results [link type: ‘seq-next’; target: A08-m4bi12]]
[Step back on the complete sequential path: Treated results [link type: ‘seq-back/part of/summarised in/context in’; target: A08-m4bi1]]

**Comments on Treated results: Potential and deflection function = A08-m4bi1:**

- The potential parameters and the deflection function have been obtained as intermediary results in the Quantitative interpretation A08-m5bi, in the course of the interpretation of the experimental results. They are presented in a table and in figures. These results are copied from the Quantitative interpretation to this module. Some additional text is supplied, in order to make the module self-contained.
Treated results: Theoretical differential cross section = A08-m4bii2

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Fig. A08-m5bii1-F1 a shows the polar differential cross section, defined by $I(\theta)\sin(\theta)$, plotted against $\tau$ [why this plot is preferred is argued in a microscopic module Data treatment [link type: ‘elaborated/argued in/sider range/project’; target: MESO-m3c-treat] for the chemi-ionization process of sodium on iodine and calculated by the lowest-order stationary-phase approximation. [Particulars on the calculation methods in Theoretical methods [link type: ‘depend on’; target: A08-m3ci1, The calculation itself is performed in the Interpretation [link type: ‘input from’; target: A08-m5]. The region of the classical rainbow angle has been omitted because the lowest-order approximation leads to a wrong result.

Fig. A08-m5bii1-F1 b shows the differential cross section with simplified interference structure. An additional simplification in Fig. A08-m5bii1-F1 b is the separate reproduction of the attractive and repulsive scattering contribution as though they could be distinguished.

The general shape of the differential cross section has been calculated at collision energies of 13.1, 20.7, 29.7, 38.7 and 55.0 eV, as shown in Figs. A08-m5bii-F4a, b, c, d, e. The calculated values have been given on absolute scales. [Compare to the experimental results [link type: ‘compare’; target: A08-m4bii1].]
Figure A08-m5bil1-F1. Polar differential cross section for chemi-ionization (CM system) at $E_i = 13.1$ eV, calculated in semi-classical approximation with the potential parameters of Table C.5 and the coupling parameters $H_{12} = 0.065$ eV and $H_{rot} = 0$ eV s. (a) Differential cross section with complete interference structure, calculated with the lowest-order stationary-phase approximation. The region of the classical rainbow angle $(\theta_{cl,eb})$ has been omitted. (b) Differential cross section calculated with the stationary-phase approximation and uniform rainbow approximation showing separated the long-wavelength interference structures due to $a + c$ ($\tau = 0 \rightarrow 65$, full curve), $b + c$ ($\tau = 65 \rightarrow 250$, full curve) and $d + e$ ($\tau = 0 \rightarrow 2500$, dashed curve) interferences. (c) Full bars indicate the measured maxima of the interference structure on the differential cross section due to net-attractive scattering. Dashed bars indicate the maxima due to net-repulsive scattering. The complete measured cross section curve at $E_i = 13.1$ eV is given in Fig. A08-m4bil1-F1. [Copied from the Quantitative interpretation (link type: ‘input from’; target: A08-m5bil1)].

Figure A08-m5bil1-F4. Smoothed differential cross sections for five different collision energies. (a), (b), (c), (d), (e): Absolute differential cross sections, calculated semi-classically and also averaged over the interference structure, have been given by the dashed curves. Use has been made of $H_{12} = 0.05$ eV. (f): At $E_i = 29.7$ eV the curves show the calculated differential cross section for $H_{12} = 0.04, 0.05$ and $0.07$ eV. [Compare to the experimental results (link type: ‘compare’; target: A08-m4bil1)].
Figure A08-m5bi2-F1. Smoothed differential cross section for five different collision energies. (a), (b), (c), (d), (e): calculated absolute cross sections using the coupling elements \( H_{12} = 0.0024 \) a.u. (0.065 eV) and \( H_{\text{rot}} = 0.04 \) a.u. (f): Effect of rotational coupling on the minimum of the differential cross section due to collisions with large collision parameters. Abscissa and ordinate scales have been extended by a factor of two with respect to the corresponding figure (e). [Compare to the experimental results [link type: 'compare'; target: A08-m4bi1] [Copied from the Quantitative interpretation [link type: 'input from'; target A08-m5bi2]].

[Next step on the complete sequential path: Treated results [link type: 'seq-next'; target: A08-m4bi3]]
[Step back on the complete sequential path: Treated results [link type: 'seq-back'; target: A08-m4bi1]]

**Comments on Treated results: Theoretical differential cross section=A08-m4bi2:**

- The theoretical differential cross sections have been calculated in the Quantitative interpretation A08-m5bi1, in the course of the interpretation of the experimental results. They are presented in figures, which are copied from the Quantitative interpretation to this module.
C.3. THE MODULARISED VERSION OF A08

Treated results: Theoretical rainbow structure = A08-m4bi3

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The calculated relative positions of the rainbow maxima at collisional energies from 13.1 eV up to 55 eV have been given in figure A08-m4bi3-F1. [Compare to the experimental results [link type: ‘compare’; target: results A08-m4bi2i] [These are intermediary results copied from the Interpretation [link type: ‘input from’; target: A08-m5bi]] To particular on the calculation methods [link type: ‘depends on’; target: A08-m3cii] |

The wavelength of the repulsive interference as a function of the kinetic energy has been given in Fig. A08-m5bi1-F3. In the energy range from 13 to 84 eV, the curve in this figure represents the calculated wavelengths after a fitting procedure that delivered the missing parameters of the covalent repulsive potential. [Compare to the experimental results [link type: ‘compare’; target: results A08-m4bi2i] |

[Next step on the complete sequential path: Interpretation [link type: ‘seq-next’; target: A08-m5]]

[Step back on the complete sequential path: Treated results [link type: ‘seq-back’; target: A08-m4bi2i]]

![Figure A08-m5bi1-F2. Rainbow structure versus initial colliding energy (CM system). The dashed curves show the calculated positions of the maxima of rainbow and supernumeraries.](image-url)
Comments on Treated results: Theoretical rainbow structure=A08-m4bi3:

- The theoretical rainbow structure is determined for the differential cross sections, which have been calculated in the Quantitative interpretation A08-m5bi2, in the course of the interpretation of the experimental results. They are presented in figures, which are copied from the Quantitative interpretation to this module.

Figure A08-m5bi1-F3. Fig.: Wavelength of the oscillatory differential cross section (CM system) due to net-repulsive scattering, versus the colliding energy. The curve gives the calculated wavelengths.
Interpretation=A08-m5

Characterisation

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**Physics:**
Differential cross section [chemi-ionization; Na⁺:4.85 eV],
Semi-classical atom-atom model for ion-pair formation in
molecular collisions, Landau-Zener, Rotation

**Bibliographic:**
Delvigne.Los [AMOLF]; Physica [1973]

**Identification:**
A08-m5

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The differential cross sections [experimental results given in *Treated results* module [link type: ‘depends on’; to: A08-m4bi]] for chemi-ionization in Na + I → Na⁺ + I⁻ collisions are explained qualitatively [details qualitative interpretation in constituent module *Qualitative interpretation* [link type: ‘contains/specialised in/detailed in/focused in’; to: A08-m5a]] via the general shape of the deflection function [calculation method via deflection given in *Theoretical methods* link type: ‘depends on’; to: A08-m3ci]] with a semi-classical atom-atom model for ion pair formation in molecular collisions [model given in *Theoretical methods* module [link type: ‘depends on’; to: A08-m3ci]].

In order to interpret the results quantitatively [quantitative interpretation in constituent module *Quantitative interpretation* [link type: ‘contains/specialised in’; to: A08-m5b]], the potential parameters and the classical deflection function of the system are determined by fitting the results calculated according to the model with the experimental results [determining the potential and the deflection function in constituent module *Quantitative interpretation* [link type: ‘contains/specialised in/segmented in/detailed in/focused in’; to: A08-m5bi]]. Based on the potential parameters and the deflection function thus determined, the absolute values of the differential cross section of the collision are calculated and compared to the measurements [determining the theoretical cross section in constituent module *Quantitative interpretation* [link type: ‘contains/specialised in/segmented in’; to: A08-m5bi]] . The comparison between the experimental and the theoretical cross sections in the fitting procedure is facilitated by the rainbow and the Stueckelberg structure.

Because of a serious disagreement between theory and experiment [details quantitative interpretation in constituent module *Quantitative interpretation* [link type: ‘contains/specialised in/segmented in/detailed in/focused in’; to: A08-m5bi1]], a new quantitative interpretation is given, based on an extension of the model: not only the Landau-Zener coupling, but also the rotational coupling is taken into account [details second quantitative interpretation in constituent module *Quantitative interpretation* [link type: ‘contains/specialised in/segmented in/detailed in/focused in’; to: A08-m5bi2]] extension of the model given in *Theoretical methods* [link type: ‘depends on’; to: A08-m3ci2]].

[Next step on the complete sequential path: Interpretation [link type: ‘see-next/contains/generalised in’; target: A08-m5a]]
Comments on Interpretation = A08-m5:

- The theory or theories and technique(s) used for the interpretation are described and discussed (with respect to their reliability and applicability) in the theoretical methods module m3c. The description and discussion of the interpretation(s) of the experimental results in terms of physical phenomena is put in this module.

- In this article, a quantitative interpretation is aimed for, because an adequate qualitative explanation has already been established in the previous article A05. Nevertheless, we have distinguished in this article a separate module with a qualitative explanation, in which the tripartition of the cross section curve is discussed and the rainbow and Stueckelberg oscillations are pointed out.

- The qualitative and the quantitative interpretations are special cases of a general interpretation, such that, on this level, this is a cluster module. As the module is very complex, the module summary plays an important role in ensuring its clarity.
Qualitative interpretation—A08-m5a

In the measured differential cross sections of the process Na + Cl → Na⁺ + Cl⁻, as shown in Fig. A08-m4bil-F1 [figure copied from Treated results module [link type: 'input from'; target: A08-m4bil]] , three parts can be distinguished: the cross sections at scattering angles between 0 and 65 eV degree, at angles between 65 and 250 eV degree, and at larger angles. Also, oscillation is visible in all three domains. Both the tripartition and the oscillations can be explained with the semi-classical atom-atom model for ion-pair formation in molecular collisions [Model given in Theoretical methods [link type: 'depends on'; target: A08-m3c]] .

Figure A08-m4bil-F1. Fig. A08-m4bil-F1: Relative polar differential cross section for chemi-ionization (CM system). The cross sections, measured at a colliding energy of 13.1 and 18.2 eV, have been set in scales with shifted zero points [Copied from the experimental Treated results A08-m4bil.}
Figure A08-m4bii-F1. Polar differential cross section for chemi-ionization (CM system) at \( E_i = 13.1 \) eV, calculated in semi-classical approximation with the potential parameters of Table C.5 and the coupling parameters \( H_{12} = 0.065 \) eV and \( H_{\text{rot}} = 0 \) eV s. (a) Differential cross section with complete interference structure, calculated with the lowest-order stationary-phase approximation. The region of the classical rainbow angle \( \theta_{\text{cl},1} \) has been omitted. (b) Differential cross section calculated with the stationary-phase approximation and uniform rainbow approximation showing separated the long-wavelength interference structures due to \( a+c \) (\( \tau = 0 \rightarrow 65 \), full curve), \( b+c \) (\( \tau = 65 \rightarrow 250 \), full curve) and \( d+e \) (\( \tau = 0 \rightarrow 2300 \), dashed curve) interferences. (c) Full bars indicate the measured maxima of the interference structure on the differential cross section due to net-attractive scattering. Dashed bars indicate the maxima due to net-repulsive scattering [Copied from the Quantitative interpretation A08-m5bii].

Figure A08-m5a-F3. Deflection curves for chemi-ionization scattering (CM system) at \( E_i = 13.1 \) eV.

We have calculated [Calculation methods given in the module Theoretical methods [link type] 'depends on/detailed in'; to: A08-m3ci and A08-m3ci] the theoretical differential cross sections via the deflection curve. The general shape of the deflection curve is given in the mesoscopic module Theoretical methods [link type] 'input from/detailed in/wider range/project'; to: MESO-m3c-def#fig]. The absolute value of the theoretical cross sections, which is shown in figure A08-m5bi-F1 [figure of the theoretical cross sections copied from the Quantitative interpretation [link type] 'input from'; to: A08-m5bi#fig], is determined in the Quantitative interpretation, with the necessary potential parameters [parameters copied from the Quantitative interpretation [link type] 'input from'; to: A08-m5bi#table]]. Here we consider the qualitative features of the calculated curve.

Fig. ?? demonstrates very clearly the tripartition of the theoretical cross section curve. The covalent scattering causes the narrow but high peak between 0 and 65 eV degree while the separated broader and lower part between 65 and 250 eV degree is due to ionic scattering. Both types of scattering supply small contributions to the very small differential cross section beyond
the classical rainbow angle, due to net-repulsive scattering.

For covalent as well as ionic net-attractive scattering the contributions to the cross section go to zero at \( \tau \approx 65 \) because the deflection function \( \frac{\mathrm{d}b}{\mathrm{d}\theta} \to 0 \) for \( b \to b_{\text{max}} \). In addition there is a sharp decreasing value of the transition probability \( P_b \) for \( b \to b_{\text{max}} \) caused by the decreasing value of the radial velocity of the colliding particles at the pseudo-crossing \( R_c \).

Eq. (C.38) [Equation given in Theoretical methods [link type 'input from'; to: A08-m3di]]

\[
I(\theta) = |Ae^{i\alpha} + Ce^{i\gamma} + De^{i\delta} + Ee^{i\xi}|^2
= A^2 + C^2 + D^2 + E^2 + 2AC \cos(\alpha - \gamma)
+ 2AD \cos(\alpha - \delta) + 2AE \cos(\alpha - \varepsilon)
+ 2CD \cos(\gamma - \delta) + 2CE \cos(\gamma - \varepsilon)
+ 2DE \cos(\delta - \varepsilon).
\] (C.12)

shows that the differential cross section contains six superposed or only one interference oscillation depending whether four or two scattering trajectories contribute to the cross section.

An estimation of the wavelengths of the different oscillations gives the result that only the interferences of a+c, b+c and the d+c branches have a wavelength of a few eV degrees or more on the \( \tau \)-scale and only that kind of structure could be detected in our measurements [methods for the measurements given in Experimental methods [link type: 'depends on'; to: A08-m3a]].

[unfold details: estimation of the wavelength]

Because in our case a+c and b+c interferences never occur together, the differential cross section contains only one or two superposed interesting oscillations. In the case of two oscillations one occurs from net-attractive scattering, the other one from net-repulsive scattering. Then, for our purpose, Eq. (C.38) can be changed into:

\[
I(\theta < 0) = A^2 + C^2 + 2AC \cos(\alpha - \gamma)
\] (C.13)

or

\[
I(\theta < 0) = B^2 + C^2 + 2BC \cos(\beta - \gamma)
\] (C.14)

and

\[
I(\theta > 0) = D^2 + E^2 + 2DE \cos(\delta - \varepsilon).
\] (C.15)

Actually Eqs. (11a) and (11c) for the theoretical differential cross section describe the Stueckelberg oscillations, that is the interference due to trajectories from different potentials. Those oscillations are shown in Fig. ?? b on the covalent scattering cross section peak and on the net-repulsive scattering differential cross section.

Eq. (11b) describes the interference of two contributions of ionic scattering, normally called rainbow scattering. The differential cross section shows the rainbow structure between \( \tau \approx 65 \) and \( \tau \approx 250 \) eV degree.

For the experimental differential cross sections, Fig. A08-m5a-F1 shows over a wide angular range all main features of the cross section of interest. The longwavelength Stueckelberg and rainbow oscillations due to net-attractive scattering interference have been resolved completely while the repulsive (Stueckelberg) interference can be seen clearly beyond 250 eV degrees. In the \( \tau \)-range between 25 and 55 eV degrees there is some evidence of a double structure. Particularly on the 13.1 eV curve heavy and small maxima succeed each other and indicate a repulsive oscillation on that range with half the frequency of the attractive oscillation.

Thus the experimental and the theoretical differential cross sections of chemi-ionization in collisions between Na and Cl agree qualitatively.
Comments on Qualitative interpretation=A08-m5a:

- In the original article, the (tripartition of the) shape of the calculated cross sections is discussed in section 4. Calculations, separately from the comparison to the experimental cross sections.

- Based on an estimation of the wavelength, the author decides to focus on particular branches of the deflection function, neglecting the others. More details could be given about this. This estimation is rather qualitative in nature and therefore a part of this module.

- The experimental figure is copied from the (experimental) results A08-m4bi, and the theoretical figure is copied from the quantitative interpretation A08-m5bi2, so that they can be compared qualitatively.

- Equation C.38 for \( I(\theta) \) is copied from the Theoretical Methods A08-m3c, in order to make this module self-contained following our definition 3.1.1 Copying equations and figures to the location where they are used makes reading more efficient. In the original versions, the reader sometimes has to turn quite a few pages in order to locate the required object.

- The precise theoretical cross section can only be obtained from the potential parameters and the coupling parameters, which are determined in a Quantitative interpretation module A08-m5b. In this module the general shape of the curve is used qualitatively.

- \( H_{\text{rot}} = 0 \) eV s in the theoretical figure means that the rotational coupling has not been taken into account yet.
C.3. THE MODULARISED VERSION OF A08

Quantitative interpretation = A08-m5b

Characterisation

<table>
<thead>
<tr>
<th>Conceptual function:</th>
<th>Interpretation, quantitative</th>
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<td>Range:</td>
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<td>Physics:</td>
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<tr>
<td>qnt.m5bi1</td>
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<tr>
<td>qnt.m5bi2</td>
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</table>

For a quantitative explanation of the measured differential cross sections for the chemi-ionization process in collisions between Na and Cl [experimental results given in Treated results [link type: 'depends on'; to: A08-m4b]], we calculate the theoretical cross sections using a semi-classical atom-atom model for ion-pair formation in molecular collisions [model given in Theoretical methods [link type: 'depends on'; to: A08-m3c]].

In order to calculate the differential cross section [differential cross section determined in Quantitative interpretation [link type: 'contains/segregated in'; to: A08-m5bi]], the deflection function of the collision process has to be determined as a first step, which in its turn depends on the potential of the system. The potential parameters and the deflection function are determined by fitting the theoretical cross sections on the experimental ones in the Quantitative interpretation A08-m5bi [potential and deflection function determined in Quantitative interpretation [link type: 'contains/segregated in/detailed in/focused in/essay-next/sq-next'; to: A08-m5bi]].

In the first specific calculation of the differential cross section, we only take into account the Landau-Zener coupling between the potential curves of the system when we determine the theoretical differential cross section. Comparison between the experimental and the theoretical curves shows some persisting discrepancies [interpretation of cross sections with LZ in Quantitative interpretation [link type: 'contains/segregated in /specialised in/detailed in/focused in'; to: A08-m5bi1]]. Therefore we take into account rotational coupling as well, which explains the discrepancies. Interpretation of cross sections with LZ and rotation given in Quantitative interpretation [link type: 'contains/segregated in/specialised in/detailed in/focused in'; to: A08-m5bi2]].
Comments on Quantitative interpretation=A08-m5b:

- The quantitative interpretation takes place in different steps: the Quantitative interpretation is an aggregation of the determination of the potential and the deflection function in A08-m5bi, and the calculation of the differential cross section in A08-m5bi (which in its turn is a generalisation of two specific calculations, with and without taking into account the rotational coupling).

- The essay-type path does not lead the reader consecutively through the constituent modules of the Quantitative interpretation. After consulting the module A08-m5bi1, in which the Landau-Zener coupling is taken into account, the reader is expected to consult the Theoretical methods module A08-m3ci2 pertaining to the rotational coupling, before consulting A08-m5bi2 for an interpretation in which the rotational coupling is taken into account as well.
Quantitative interpretation: potential and deflection function =A08-m5bi

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<td>- Differential cross section [chemi-ionization; NaI; 15-85 eV]</td>
<td>- meta mlc → - meta mlc</td>
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<td>- Semi-classical atom-atom model for ion-pair formation in molecular collisions, Landau-Zener, Rittner potential [V(r) Na+I], Endothermicity ΔE, Electron affinity E[Br2], Polarizability αBr&lt;sup&gt;−&lt;/sup&gt;&lt;sub&gt;−&lt;/sub&gt;, Crossing distance R&lt;sub&gt;c&lt;/sub&gt;, Resonance energy H&lt;sub&gt;12&lt;/sub&gt;, Ionic-well depth ε, Repulsive steepness coefficient ρ, Deflection function.</td>
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<td>Delville, Los (AMOLF); Physica (1973)</td>
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</table>

We determine the potential parameters that govern the chemi-ionization reaction Na + Cl → Na<sup>+</sup> + Cl<sup>−</sup> according to the atom-atom model for ion-pair formation in molecular collisions [The model is given in Theoretical methods [link type: ‘depends on/detailed in’; to: A08-m3ci]], [More details in the mesoscopic Theoretical methods [link type: ‘project/wider range/depends on/detailed in’; to: MES0-m3c-mod]]. From the potential parameters, the theoretical cross section of the chemi-ionization reaction can be calculated via the deflection function. We determine the potential parameters, and simultaneously the deflection curve, by fitting the calculated cross section (that is based on assumed potential parameters) with the experimental cross sections.

We now restrict ourselves as much as possible to the determination of some potential parameters and to the comparison of measurements and calculations used for that purpose. The calculated differential cross section and its discrepancies with the measurements will be treated in module Quantitative interpretation A08-m5bi [theoretical cross section given and discussed in Quantitative interpretation [link type: ‘detailed in/used in’; to: A09-m5bi1]].

Fig. A08-m5bi-F1 b [figure given in Quantitative interpretation [link type: ‘input from’; to: A08-m5bi1]] shows the differential cross section with simplified interference structure. An additional simplification in Fig. A08-m5bi-F1b is the separate reproduction of the attractive and repulsive scattering contributions as though they could be distinguished. Because the origin of the oscillatory features of the calculated cross sections can be seen easily from Fig. A08-m5bi-F1b and the latter figure is more easily related to the deflection function and the potential curves, Fig. A08-m5bi-F1b is more suitable to fit the interference structure of the calculated and measured differential cross section by adjustment of the potential parameters. Moreover, convolution of the differential cross section of the complete calculated cross section, which is given in Fig. A08-m5bi-F1a [figure given in Quantitative interpretation [link type: ‘input from’; to: A08-m5bi1]], and Fig. A08-m5bi-F1b even with the smallest angular resolution of the detector of 0.3° fwhm will lead to equal results.
Figure A08-m5bi-F1. Polar differential cross section for chemi-ionization (CM system) at $E_i = 13.1$ eV. (b) Differential cross section calculated with the stationary-phase approximation and uniform rainbow approximation showing separated the long-wavelength interference structures due to $a + c$ ($\tau = 0 \rightarrow 65$, full curve), $b + c$ ($\tau = 65 \rightarrow 250$, full curve) and $d + e$ ($\tau = 0 \rightarrow 2300$, dashed curve) interferences. (c) Full bars indicate the measured maxima of the interference structure on the differential cross section due to net-attractive scattering. Dashed bars indicate the maxima due to net-repulsive scattering.

Figure A08-m5bi-F2. Deflection curves for chemi-ionization scattering (CM system) at $E_i = 13.1$ eV. [Copied to the Treated results (link type: 'output to'; target: A08-m4bi1)].
C.3. THE MODULARISED VERSION OF A08

By comparison of measurements and calculations, the missing parameters of the covalent potential curve and the value of $H_{12}$ can be estimated. For that purpose are very important particularly the wavelengths of the rainbow and Stueckelberg oscillations [oscillations are identified in Qualitative interpretation [link type: ‘detailed in’; to A08-m5a] , which result from the semi-classical interference of different contributions to the scattering angle [semi-classical model given in Theoretical methods [link type: ‘depends on’/‘detailed in’; to A08-m3ai] ].

For a fitting procedure of the potential curves to the measurements, it is very helpful that the interference wavelengths can be estimated directly from the deflection curves. The oscillations are generated by the cosine of the Eqs. (11) [equation given in Qualitative interpretation [link type: ‘input from’; to A08-m5a]]

\[ I(\Theta < 0) = A^2 + C^2 + 2AC \cos(\alpha - \gamma) \]  
(C.14)

or

\[ I(\Theta < 0) = B^2 + C^2 + 2BC \cos(\beta - \gamma) \]  
(C.15)

and

\[ I(\Theta > 0) = D^2 + E^2 + 2DE \cos(\delta - \varepsilon). \]  
(C.16)

The difference in the cosine argument for two neighbouring scattering angles $\theta_1$ and $\theta_2$ can be shown easily, with the help of Fig. MESO-m3c-defl-F1 and Eqs. (A08-m5bii1-F2) for the contributions to the scattering angle in lowest-order stationary-phase approximation .

[unfold equation]

\[ f_a(\theta) = \left[ \frac{db}{d\Theta} \right] b_A P_{b_a}(1 - P_{b_a}) \sin \theta \]  
\[ \times \exp \left[ i(2\eta_b + k b_A \theta - \pi) \right] \equiv Ae^{i\alpha}, \]  
(C.15)

\[ f_b(\theta) = \left[ \frac{db}{d\Theta} \right] b_B P_{b_b}(1 - P_{b_b}) \sin \theta \]  
\[ \times \exp \left[ i(2\eta_b + k b_B \theta - \frac{1}{2}\pi) \right] \equiv Be^{i\beta}, \]  
(C.16)

\[ f_c(\theta) = \left[ \frac{db}{d\Theta} \right] b_C P_{b_c}(1 - P_{b_c}) \sin \theta \]  
\[ \times \exp \left[ i(2\eta_b + k b_C \theta - \pi) \right] \equiv Ce^{i\gamma}, \]  
(C.17)

\[ f_d(\theta) = \left[ \frac{db}{d\Theta} \right] b_D P_{b_d}(1 - P_{b_d}) \sin \theta \]  
\[ \times \exp \left[ i(2\eta_b + k b_D \theta - \frac{1}{2}\pi) \right] \equiv De^{i\delta}, \]  
(C.18)

\[ f_e(\theta) = \left[ \frac{db}{d\Theta} \right] b_E P_{b_e}(1 - P_{b_e}) \sin \theta \]  
\[ \times \exp \left[ i(2\eta_b + k b_E \theta - \frac{1}{2}\pi) \right] \equiv Ee^{i\epsilon}, \]  
(C.19)

where $\eta_b$ indicates the phase shift and $k$ is given by $k = (2\mu E_0)^{1/2}$.

For interferences as indicated in Eqs. (11) this difference is exactly the part of the deflection curve enclosed by $\theta_1$ and $\theta_2$ and multiplied by a factor of $k/2\pi$. Then the local oscillation frequency is linearly proportional to the distance along the $b$-scale of the relevant branches of the deflection curve. For net-attractive and net-repulsive scattering Fig. MESO-m3c-defl-F1 shows two slices with equal areas. It is clearly shown that in the chosen angular ranges the repulsive-scattering wavelength is much larger compared to the attractive one.
Figure A08-m5bi-F3. Wavelength of the oscillatory differential cross section (CM system) due to net-repulsive scattering, versus the colliding energy. The measurement gives the wavelength averaged over ten oscillations just beyond the rainbow angle. The error bars only indicate the error in the relative position of first and tenth oscillation. The curve gives the corresponding calculated wavelengths.

**Repulsive scattering oscillation** $A_{\text{cov}}$ and $\rho_{\text{cov}}$

By fitting the repulsive scattering oscillations of the experimental and the theoretical cross section curves, we found $A_{\text{cov}} = 3150$ eV and the repulsive steepness to be $\rho_{\text{cov}} = 0.435$. Then the calculated repulsive oscillation is in perfect agreement with the experimental one.

[unfold details] A08-m5bi-F3 [experimental part copied from the Results [link type: 'input from'; to: A08-m4bi2] shows the measured oscillation wavelength due to interference of the ionic and covalent repulsive-scattering contributions just beyond the rainbow angle. The corresponding branches of the deflection curve are d and e, where the e-branch is calculated from the known ionic potential. Because the attractive Van der Waals term of the covalent potential is not important at our kinetic-energy range, the repulsive oscillation wavelength leads to a determination of the repulsive part of the covalent potential: $A_{\text{cov}} = 3150$ eV and $\rho_{\text{cov}} = 0.435$.

**Reliability**

With the repulsive-potential parameters $A_{\text{cov}} = 3150$ eV and $\rho_{\text{cov}} = 0.435$ the measured wavelength as a function of the kinetic energy can be fitted perfectly with the calculations.

Although in first-order approximation the $\tau = \text{constant}$ rule predicts the wavelength being proportional to $E^{-1/2}$, the measured as well as the calculated wavelengths increase more rapidly at decreasing kinetic energy. Another date from the measurements is the fact that no angular-dependent wavelength beyond the rainbow angle could be detected. The values of $A$ and $\rho$ have been chosen in such a way that the calculated wavelength too is rather angular independent. However, it is difficult to separate the effects of varying $A$ or $\rho$. Consequently the given set of values of $A_{\text{cov}}$ and $\rho_{\text{cov}}$ is more reliable then the separate values. Moreover, it should be noted that the steepness of the covalent repulsive potential has been determined relative to the steepness of the ionic repulsive potential that is supposed to be known.

**Inelastic energy** $\Delta E$

The general shape of the polar differential cross section is the cross section averaged over the quantal oscillations. The angular positions of special features at different collision energies agree very well: namely the maximum of the peak at $\tau \approx 35$ due to covalent scattering, the minimum at $\tau \approx 65$ due to scattering with maximal impact parameter and the maximum of the primary rainbow. These agreements determine that $\Delta E$, the potential-energy difference of the ionic and covalent state at infinite internuclear separation, is $\Delta E = 2.075$ eV.

[unfold details] Due to the flat long-range character of the covalent potential curve the chemi-ionization collision with maximal collision parameters $b \approx R_e$ is affected only by the
coulombic outgoing potential branch. Therefore the correct position of the minimum in the
differential cross section establishes the inelastic energy \( \Delta E \) (see Fig. A08-m5b1-F4 ).

**Potential well-depth \( \varepsilon \)**

The agreement of the angular positions of the special features of the general shape also establishes
the well-depth of the ionic potential curve: \( \varepsilon = -3.1 \pm 0.2 \) eV.

[unfold details] The collision process with a distance of closest approach at the inflection
point of the ionic potential curve causes the classical rainbow angle where \( |dI/d\Theta| \to \infty \).
The inflection point is related to the minimum of the potential well when the shape of the
potential curve is qualitatively known. Moreover, the classical rainbow angle is related to
the position of the maximum of the rainbow by Eq. (C.9) and is situated on the “dark side”
slope of the rainbow. Then the measured positions of the primary rainbows lead to the
position of the minimum of the ionic potential well at \(-3.1 \pm 0.2 \) eV, enclosing the values of
3.0, 3.07, 3.11 and 3.16 as tabulated by Herzberg[Value are input from another article (link type:
‘input from/external’; target: R\textsubscript{A08}24-m\textsuperscript{a})].

**Coupling \( H_{12} \)**

The relative intensities of several parts of the general shape of the cross section lead to an
estimation of \( H_{12} \) of 0.05 eV for energies in the range of 30-55 eV. However, for the 13.1 eV
curve the estimation is \( H_{12} = 0.065 \).

[unfold details reliability] **Reliability**

Using \( H_{12} = 0.05 \) eV in the calculations, the relative intensities of several parts of the
calculated and measured differential cross sections are in good agreement only for the curves of
29.7, 38.7 and 55.0 eV shown in Figs. A08-m5b1-F3c, d, e. This is in agreement with the equal value of \( H_{12} \) being 0.05 eV estimated from total cross section measurements on the
energy range 2-20 eV [Value are input from another article (link type: ‘input from/external’; target: R\textsubscript{A08}9-m\textsuperscript{a})].

The sensitivity of the relative and absolute differential cross sections to the value of
\( H_{12} \) has been indicated by three curves in Fig. A08-m5b1-F3, using \( H_{12} = 0.04, 0.05 \) and
0.07 eV. Because an obvious disagreement occurs for the curves of 13.1 and 20.7 eV shown
in Figs. A08-m5b1-F3a, b, it is not possible to give only one value of \( H_{12} \) resulting in
an overall good fit. A consideration of the 13.1 eV curve only should lead to a value of
0.065 eV for \( H_{12} \) (see Fig. A08-m5b1-F1) while the 20.7 eV curve needs a coupling constant
of 0.060 eV.

The determination of \( H_{12} \) especially requires the proper transformation of detector signal
to differential cross section. \textit{A priori} there are doubts on the normalization of the detector
signal to an angular-independent scattering volume viewed by the detector. The calculated
angular-dependent normalization factor seems to be reliable by observing the result that the
total cross section due to covalent scattering is about equal to the total cross section due
to ionic scattering, independent of the kinetic energy and thus independent of the different
angular ranges. This requirement is postulated by the equal Landau-Zener probability
\( P_b(1-P_b) \) for both chemi-ionization trajectories and means about equal areas enclosed by
the relevant parts of the differential cross section.

[Table copied to the Treated results (link type: ‘output to’; target: A08-m4b1i)]

Now we have determined the potential parameters of the ionic and the covalent system
Na \(-\) I. The parameters are summarized in Table C.5.

The ionic ground state is well known. It is described by the Rittner potential [The formulae are
input from elsewhere (link type: ‘input/external’) R\textsubscript{A08}13-m\textsuperscript{a})]:

\[
U_{\text{ion}}(R) = -\frac{e^2}{R} - \frac{e^2(\alpha_{\text{Na}^+} + \alpha_{\text{Cl}^-})}{2R^4}
\]
Table C.5  

<table>
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<tr>
<th>Ionic-potential parameters</th>
<th>Covalent-potential parameters</th>
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<tbody>
<tr>
<td>$\alpha_{\text{Na}^+} = 0.408 , 3^a$</td>
<td>$\alpha_{\text{Na}} = 27 , 3^b$</td>
</tr>
<tr>
<td>$\alpha_{\text{Cl}^-} = 6.431 , 3^a$</td>
<td>$\alpha_{\text{Cl}} = 7 , 3^i$</td>
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<td>$C_{\text{ion}} = 11.3 , \text{eV} , 6^b$</td>
<td>$C_{\text{cov}} = 1000 , \text{eV} , 6^i$</td>
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<tr>
<td>$A_{\text{ion}} = 1913.6(2760^1) , \text{eV} , c$</td>
<td>$A_{\text{cov}} = 3150 , \text{eV}$</td>
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<tr>
<td>$\rho_{\text{ion}} = 0.3489 , d$</td>
<td>$\rho_{\text{cov}} = 0.435$</td>
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<tr>
<td>$\varepsilon = 3.11 + \Delta E , \text{eV} , e$</td>
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<td>$r_e = 2.71143 (2.664^1) , f$</td>
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<td>$\Delta E = 2.075 , \text{eV} , r$</td>
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$^a$ Dipole polarizability; [Value are input from another article (link type: ‘input from/external’; target: Rf$_{\text{A0814-m*}}$)]. $^b$ Van der Waals coefficient, from the London formula: $C_{\text{ion}} = 3\alpha_{\text{Na}} + \alpha_{\text{Cl}} - I_2A/2(I_2 + A)$, where $I_2$ is the second ionization potential of Na and $A$ is the electron affinity of I. $^c$ [Value are input from another article (link type: ‘input from/external’; target: Rf$_{\text{A0815-m*}}$)]. $^d$ [Value are input from another article (link type: ‘input from/external’; target: Rf$_{\text{A0815-m*}}$)]. $^e$ Potential well depth; [Value are input from another article (link type: ‘input from/external’; target: Rf$_{\text{A0815-m*}}$)]. $^f$ Interatomic equilibrium distance; [Value are input from another article (link type: ‘input from/external’; target: Rf$_{\text{A0815-m*}}$)]. $^g$ From $I_{\text{Na}} - A_{\text{Cl}}$. $^h$ [Value are input from another article (link type: ‘input from/external’; target: Rf$_{\text{A0818-m*}}$)]. $^i$ Arbitrary value. $^j$ From the London formula: $C_{\text{cov}} = 3\alpha_{\text{Na}}\alpha_{\text{Cl}}/I_{\text{Na}}I_{\text{Cl}}/2(I_{\text{Na}} + I_{\text{Cl}})$, where $I$ is the first ionization potential. $^k$ Present work. $^l$ Alternative value due to overdefinition of the potential curve.

Figure A08-m5bi-F4. Na-Cl, adiabatic potential curves. The pseudo-crossing potential are all of the same species $^1\Sigma^+$. [Copied to the Treated results (link type: ‘output to’; target: A08-m5bi1)].

$$\frac{-2e^2\alpha_{\text{Na}^+}\alpha_{\text{Cl}^-}}{R^2} - \frac{C_{\text{ion}}}{R^6} + A_{\text{ion}} e^{-R/\rho_{\text{ion}}} + \Delta E. \tag{C.16}$$

We describe the covalent potential only by two terms:

$$U_{\text{cov}}(R) = -\frac{C_{\text{cov}}}{R^6} + A_{\text{cov}} e^{-R/\rho_{\text{cov}}}. \tag{C.17}$$

We have determined for the covalent Na - I system most of the potential parameters; the missing parameters have been chosen to construct the potential curves in Fig. A08-m5bi-F1 and the deflection functions in Fig. A08-m5bi-F1.

The ionic potential curve is overdefined by the given parameters. That is why the values for $A$ and $r_e$ have not been used but the other parameters give rise to the values given in parentheses.
For small values of the internuclear distance $R$ the ionic and covalent potential curves bend over to negative values, leading to $\lim_{R \to 0} U(R) = -\infty$. This is due only to the mathematical form of the potential-energy expressions [Eqs. (C.16) and (C.17)]. Using the parameters of Table C.5, the maxima of the potential curves are $U_{\text{ion}} = 29.7$ eV and $U_{\text{cov}} = 21.4$ eV for $R = 1.16$ and $R = 1.70$, respectively. However, this effect does not handicap the calculations. Even for the smallest impact parameter considered, the distances of closest approach are $R_0 = 2.02$ and $R_0 = 2.84$ corresponding to the potential energies $U_{\text{ion}} = -0.3$ eV and $U_{\text{cov}} = 2.7$ eV, respectively.
Comments on Quantitative interpretation: potential and deflection function = A08-m5bi:

- Before the theoretical differential cross section can be calculated, the covalent potential of NaI has to be determined first. The ionic potential is said to be well-known. The actual covalent potential is a result, generated in the interpretation of the experimental results. In the original text, the potential parameters have been summarized in a table as well, and $A_{\text{core}}$, $\rho_{\text{core}}$, $H_{12}$ and $H_{\text{rot}}$ are said to be derived from the present work. So the covalent potential is determined using the experimental results, the deflection function is determined using the potential and the theoretical differential cross section is determined using the deflection function.

- In this module we aim for an exact expression of the potential and the deflection function, not yet for the differential cross section. Especially the potential may be of interest separately. The results of this module will also be used as input in A08-m5bii, where the theoretical differential cross section will be calculated.

- The potential curves (including the parameters) and deflection functions that are determined here can be seen as ‘theoretical results’. As such, they are copied to the Results module A08-m4bii1. They could also be provided in some other way with an extra label that permits interested readers to locate them.

- In this module we concentrate on determining the potential parameters and $H_{12}$. We have separated the determination of these parameters from the calculation of the differential cross section for two reasons:
  1) In theory, the potential has to be known in order to calculate the cross section;
  2) In practice, the interpretation module is large and complicated, so that it is important to provide it with an explicit structure, for the sake of clarity.

Therefore we try to enhance the information network by making explicit additional modular structure.

- Separating the determination of the potential parameters and the cross section nevertheless poses a problem. The calculation did not take place linearly (following the steps of the determination of the potential, the subsequent deflection function and the subsequent calculation of the cross section), but in an entangled fitting process. In the original version of the article, a section was dedicated to the comparison of the calculations and the measurements. During this comparison some potential parameters were obtained. The discrepancies identified in this section were summarized and then discussed in the next section called 7.Discussion.

- The distinction of a module about the parameters, separate from the module about the cross section, implies that the comparison between the calculations and measurements that does not directly lead to the determination of a parameter takes place in module A08-m5bii about the cross section.
Quantitative interpretation: differential cross section = A08-m5bii

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[Next step on the complete sequential path: Results [link type: 'sq-next/contains/is specialised in'; target: A08-m5bii1]]

[Step back on the complete sequential path: Quantitative interpretation [link type: 'sq-back'; target: A08-m5bi]]

**Comments on Quantitative interpretation: differential cross sections = A08-m5bii:**

- We have grouped in this complex module the two Quantitative interpretation modules with the two specific cases of the calculation of the differential cross section: with the LZ coupling only, and with the LZ and the rotational coupling.
### Quantitative interpretation: theoretical differential cross section with LZ =A08-m5bii1

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By comparison of measurements and calculations the missing parameters of the covalent potential curve and the value of $H_{12}$ can be estimated. Moreover, the suitability of the applied stationary-phase approximation and Landau-Zener theory can be rated at its true value because the ionic potential curve is well known.

Fig. A08-m5bii1-F1 shows the polar differential cross section, defined by $I(\theta) \sin(\theta)$, for the chemi-ionization process of sodium on iodine and calculated by the lowest-order stationary-phase approximation [More on the approximation in the Theoretical methods [link type: 'depends on/clarified in/detailed in'; target: A08-m3ci)].

[unfold details] Use has been made of the Landau-Zener formula [details on Landau-Zener in the Theoretical methods [link type: 'detailed in/input from'; target: A08-m3ciii]] Eqs. (C.7)

$$R_b = \exp \left( \frac{-2\pi H_{12}^2}{\hbar^2} \right)_{\frac{H_{11} - H_{22}}{h_c}},$$

(C.18)

The scattering amplitude (C.35) and the semi-classical differential cross section (C.41)

$$f(\theta) = \sum_{\omega=1/2,\ldots} f_{\omega}(\theta),$$

(C.19)

leading to the differential cross section [details on the cross section in the Theoretical methods [link type: 'detailed in/input from'; target: A08-m3ci]]

$$I(\theta) |f(\theta)|^2,$$

(C.20)

the JWKB approximation (C.21)

$$\eta_b = \frac{1}{2} k \int_{b}^{\infty} \Theta db$$

(C.21)
and the classical deflection function. The region of the classical rainbow angle has been omitted because the lowest-order approximation leads to a wrong result. [discussion on the applicability of the approximation in the Theoretical methods (link type: 'reasons in'; target: A08-m3ii)]

With the potential parameters and $H_{12}$ of Table C.5 and taking into account a weight factor 1/8, the calculation leads to absolute values of the differential cross section [The potential parameters and the deflection function are determined in another Quantitative interpretation module (link type: 'input from'; target: A08-m5bi)].

Fig. A08-m5bi1-F1 b shows the differential cross section with simplified interference structure. The major part has been calculated by the lowest-order stationary-phase approximation in the form of Eq. (7) and Eq. (11). The rainbow region has been calculated by Eq. (C.9). An additional simplification in Fig. A08-m5bi1-F1 b is the separate reproduction of the attractive and repulsive scattering contribution as though they could be distinguished.

Because the origin of the oscillatory features of Fig. A08-m5bi1-F1 a can be seen easily from Fig. A08-m5bi1-F1 b and the latter figure is more easily related to the deflection function and the potential curves, Fig. A08-m5bi-F1 b is more suitable to fit the interference structure of the calculated and measured differential cross section by adjustment of the potential parameters. Moreover, convolution of the differential cross section of Fig. A08-m5bi1-F1 a and Fig. A08-m5bi1-F1 b even with the smallest angular resolution of the detector of 0.3° fwhm will lead to equal results.

Reliability & applicability of the interpretation with LZ

Rainbow oscillation

The rainbow structure of the experimental cross sections is explained nearly perfectly by the theoretical description.

[unfold details]
The ionic potential curve of Na\(^+\)Cl\(^-\) is well known. Moreover, the energy difference \(\Delta E\) of ionic and covalent ground state at infinite separation is known and the covalent potential must be about zero for \(R \geq R_c\). So the ionic scattering takes place via well-known potential curves leading to a complete knowledge of the relevant deflection curve (branches b, c and e of Fig. Meso-m3c-deff-F1).

By applying the stationary-phase approximation and the uniform rainbow approximation, the positions of primary and supernumerary rainbows from interference of the b and c contributions are calculated. Fig. A08-m5bi1l-F3 compares the measured and calculated relative positions of the rainbow maxima, where the measured as well as the calculated third supernumeraries have been placed on the same straight line.

**Reliability**

From the primary rainbows up to the third supernumeraries the agreement is nearly perfect. Further up an increasing deviation is observed of measured and calculated spacings of the successive supernumeraries. Moreover, the deviation increases with increasing collision energy. For 13.1 eV the deviation increases from 5 up to 20 percent while for the rainbow structure at 38.7 eV the corresponding quantities are 5 and 40 percent. A look at the
potential and deflection curves shows that even for the 13.1 eV deviation, a reasonable adjustment of the potential parameters is not able to decrease the distance between the b and c branches of the deflection curve enough to fit the measured and calculated rainbow structures. Moreover, an energy-dependent deviation cannot be eliminated in this way.

Small-angle oscillations

The cross sections exhibit Stueckelberg oscillations due to interference of the ionic and covalent repulsive-scattering contributions just beyond the rainbow angle. The corresponding branches of the deflection curve are d and e, where the e-branch is calculated from the known ionic potential.

The Stueckelberg oscillations in the experimental cross sections shown in Fig. A08-m4bi-F1 for \( \tau < 65 \) eV degree are due to the interference of the differential cross-section contributions related to the a and c branches of the deflection curves. The measured maxima of the 13.1 eV curve have been indicated in Fig. A08-m5biil-F1 c together with the calculated structure in Fig. b.

Reliability

For Stueckelberg oscillations just beyond the rainbow angle, the measured wavelength as a function of the kinetic energy can be fitted perfectly with the calculations.

However, on the range \( \tau = 40 \to 65 \) obviously the distances between the calculated maxima are too small. The relative wavelength discrepancy is the largest at \( \tau \approx 60 \).

For decreasing scattering angles the measured and calculated oscillation wavelengths increase while the deviation decreases from twenty percent at \( \tau \approx 60 \) to zero percent at \( \tau \approx 40 \) and ends up in an opposite deviation meaning a calculated wavelength too large compared to the measurements. However, the latter deviation is not precarious because it can be improved by a careful adjustment of the onset of the covalent repulsive potential as can be seen from Fig. A08-m5bi-F1 and Fig. MESO-m3c-defl-F1.

More serious is the deviation on the \( \tau = 40 \to 65 \) range because this part of the differential cross section deals only with scattering from the known ionic potential and the flat part of the covalent potential curve. It is very remarkable that the deviation on this range is the same as the deviation of measured and calculated maxima just on the other side of the minimum in the differential cross section (the range of the high-number supernumeraries). The completely resolved differential cross section curve with \( E_i = 18.2 \) eV gives the same trend with equal deviations of measured and calculated wavelengths around \( \tau = 65 \) eV degree.

Some evidence of repulsive interference at small scattering angles has been indicated also in Fig. A08-m5biil-F1 c. This structure gives a check on the estimated repulsive part of the covalent potential. Because Fig. A08-m5biil-F1 b clearly shows that at small angles the repulsive oscillation is the straight continuation of the attractive oscillation it is not very surprising that the calculated wavelength is somewhat too large compared to the measurements. The same applies to the 18.2 eV curve.

General shape

The general shape of the polar differential cross section is the cross section averaged over the quantal oscillations. This shape will nearly correspond to the classical differential cross section except at the classical rainbow angle, and thus is given by the relevant values of \( b, |db/d\theta| \) and the Landau–Zener transition probability \( R_b \) [see Eq. (C.3)].

The general shape of the differential cross section has been measured and calculated at collision energies of 13.1, 20.7, 29.7, 38.7 and 55.0 eV, as shown in Figs. A08-m5bi-F1a, b, c, d, e. The calculated values have been given on absolute scales, the measurements are only relative and have been given for the different energies on arbitrary, non-related scales.
The angular positions of special features agree very well: namely the maximum of the peak at \( \tau \approx 35 \) due to covalent scattering, the minimum at \( \tau \approx 65 \) due to scattering with maximal impact parameter and the maximum of the primary rainbow.

A permanent local disagreement is observed at the minimum of the differential cross section at \( \tau \approx 65 \), showing that the calculated cross section is too small continuously. The deviation increases at increasing energy. At least the major part cannot be caused by convolution effects on the measurements.

It has been shown that scattering from well-known parts of the internuclear potentials gives rise sometimes to a discrepancy of the calculated and measured interference structure. In spite of that, we have determined the repulsive parameters of the covalent potential curve from the repulsive interference structure.

However, the reliability is enlarged by the very good agreement of the kinetic-energy behaviour of the wavelength (see Fig. A08-m5bi-F3), while the disagreement of the interference wavelength on the range \( \tau = 40 \rightarrow 150 \) shows an energy-dependent discrepancy. Perhaps the collisions with large impact parameters cause this discrepancy. The comparable calculated and measured interference structures due to collisions with smaller impact parameters consist of the primary rainbows and low-number supernumeraries that are in very good agreement.

**Serious discrepancies**

In the preceding we have seen that there are only a few serious deviations of measurements and calculations that cannot be ascribed to measuring faults or doubts as to the correctness of the potentials used. Summarizing, these discrepancies are:

a) disagreement of the oscillation wavelength around \( \tau = 65 \). This discrepancy increases for increasing collision energy;

b1) large intensity deviation at the very minimum of the cross section at \( \tau \approx 65 \). Also this discrepancy increases for increasing energy;

b2) rather small intensity deviation separated from \( \tau = 65 \) somewhat more and preventing an estimation of \( H_{12} \) that gives an overall good fit. This discrepancy is dependent on the energy.
(A priori it is not obvious whether the deviations $b_1$ and $b_2$ have the same origin.)

The deviations must be viewed in the light of the used approximations, i.e. in the light of the restrictions of the theoretical methods we used [these restrictions are given in the module Theoretical methods [link type: ‘depends on/detailed in’; target: A08-m3c]], the most important of which are:

A. The stationary-phase approximation.

B. The uniform rainbow approximation.

C. The Landau–Zener transition-probability formula.

D. The use of the Landau–Zener formula to collisions where the distance of closest approach $R_0$ and the distance of pseudo-crossing $R_c$ are not well separated [arguments against the applicability of LZ in such a case given in Dkitin [link type: ‘external/argument’; to: RfA0825-m*]] .

E. The use of the diabatic potentials [as given in Eqs. (C.16), (C.17)] in the classical deflection function in spite of small deformation of the curves at the pseudo-crossing.

F. The use of a transition point in spite of a transition region around the pseudo-crossing predicted by the Landau–Zener theory.

G. The neglect of rotational coupling so far.

Comparing figures A08-m4bil-F1 and A08-m5bil-F2, we see that the deviations between measurements and calculations occur only near $\tau = 65$ eV degree, for covalent as well as ionic scattering. The deviations are energy dependent and deal with the oscillation wavelengths and relative intensities. It is very remarkable that the approximations C, D, E, F and G mostly violate the real differential cross sections at the region around $\tau = 65$. Those approximations don’t change the oscillatory structure but only the relative intensities. Some estimates of corrections to the approximations have been made, especially in view of the influence on the differential cross section at $\tau \approx 65$.

A correction to approximation D

[unfold approximation]

The use of the Landau–Zener formula to collisions where the distance of closest approach $R_0$ and the distance of pseudo-crossing $R_c$ are not well separated.

reduces $R_0$ by passing an incomplete transition region. Because then in our energy range the product $R_0(1 - R_0)$ decreases too, the differential cross section even decreases in the region of interest.

However, a correction to $E$

[unfold approximation]

The use of the diabatic potentials [as given in Eqs. (C.16), (C.17)] in the classical deflection function in spite of small deformation of the curves at the pseudo-crossing.

indeed predicts a somewhat larger value of the differential cross section close to $\tau = 65$, but there still exists the feature of $db/db_\theta \to 0$ for $b \to b_{max}$.

It is very difficult to introduce a correction to approximation $F$

[unfold approximation]

The use of a transition point in spite of a transition region around the pseudo-crossing predicted by the Landau–Zener theory.

in the impact-parameter method. It will lead to a collection of deflection curves with the greatest differences of the relative shapes near $\theta_{max}$. Indeed, a summation over the deflection curves never gives a zero value of the differential cross section due to collisions with large impact
parameters. However, this averaging effect does not cause an important rise of the cross section on the whole region around $\tau = 65$.

The remaining corrections to the intensity at $\tau \approx 65$ are C and G dealing with the Landau–Zener coupling and rotation coupling. It is not expected [arguments for the applicability of the LZ formula given in Child (link type: ‘external/argument/detailed in’; to: RfA0825-m*)] that the Landau–Zener transition formula gives such wrong results, although this formula has been derived using the approximations that $U_{\text{ion}}(R)$ and $U_{\text{cov}}(R)$ are linear in the region of the crossing and $H_{12}$ is an essentially constant coupling element.

We have greater expectations for the rotation coupling to explain the intensity deviation. Rotational coupling will be treated in more detail in module A08-m5bi2 Quantitative interpretation [(link type: ‘used in’; target: A08-m5bi2)].

If the rotation coupling is taken into account as well, the only one of the approximations A–G that can give a wrong result for the oscillatory wavelength of the differential cross section at $\tau \approx 65$ is the lowest-order stationary-phase approximation. Delos and Thorson [an argument for the application of the approximation is given in Delos (link type: ‘external/input from/argument’; to: RfA086-m*)] have given four statements that justify the application of this approximation on two-state collisions. One of them should not be satisfied in our case, namely the requirement of a collisional energy large compared to the potential-energy differences of the two states. This statement requires about equal classical trajectories along the two states. The deflection curves of Fig. MESO-m3e-defl-F1 show that this requirement is not fulfilled.

Comments on Quantitative interpretation: differential cross section with LZ coupling = A08-m5bi1:

- The list of discrepancies repeats information that has already been given in module A08-m5bi, in the fitting procedure leading to the potential. The original, linear version of the article has the same repetition.
Quantitative interpretation: Landau-Zener and rotational coupling

Chemio-ionization in collisions between Na and I can be explained via crossing of the potential energy surfaces of the collisions [The model is given in a mesoscopic Theoretical methods module [link type: \( ^{\text{depend}} \text{ on/detailed in/wider range/project} \); target: Meso-m3c-mod]]. The Landau-Zener formula gives the transition probability between translationally coupled states. However, the Landau-Zener transition probability does not give an adequate quantitative explanation [This inadequacy is shown in another Interpretation module [link type: \( ^{\text{detail}} \text{ in/clarified in} \); target: A08-m5bi2]] of the experimentally determined differential cross sections of the chemio-ionization process. It is likely that rotationally induced transitions could explain the discrepancy of measured and calculated differential cross section.

The discrepancy that the rotational coupling could explain is where the calculated cross section is too small for collisions with large impact parameters [This discrepancy is shown in another Interpretation module [link type: \( ^{\text{detail}} \text{ in} \); target: A08-m5bi2]]. Fig. A08-m5bi2-F1 clearly shows for increasing kinetic energy an increasing deviation of the relative differential cross section at \( \tau \approx 65 \, \text{eV} \) degree without rotational coupling. Even the relative cross sections more separated from the minimum would lead for a fitting procedure to an unphysical energy dependence of the Landau-Zener coupling parameter \( H_{12} \).

We have calculated [particularly on the calculation method in the module Theoretical methods [link type: \( ^{\text{depend}} \text{ on/detailed in/ev-back} \); target: Theoretical methods A08-m3c2]].

[unfold details of the calculation]

Fig. A08-m5bi2-F1 gives again the measured general shapes of the differential cross sections at kinetic colliding energies of 13.1, 20.7, 29.7, 38.7 and 55.0 eV. A comparison has been made with calculated cross sections taking into account some rotational coupling.

Indeed, the minimum in the differential cross section has been increased to a degree dependent on the kinetic energy.

Moreover, it is very obvious that now it is possible to find one set of coupling constants giving a good fit of measured and calculated cross sections for all energies. This set consists of
the values $H_{12} = 0.065 \text{ eV}$ and $H_{\text{rot}} = 3 \times 10^{-17} \text{ eV s}$ corresponding to the values of 0.0024 a.u. and 0.04 a.u., respectively.

A comparison of the corresponding cross section curves of Fig. A08-m5bi2-F1 and Fig. A08-m5bi2-F2 shows that rotational coupling at low kinetic energies increases the differential cross section only at the very minimum but for higher kinetic energies there is a rise over a larger $\tau$-range. This feature makes it possible to use only one value of $H_{12}$.

On the range $\tau = 50 \rightarrow 200 \text{ eV degree}$ Fig. A08-m5bi2-F1 gives the dependence of the cross section on some values of $H_{\text{rot}}$ at $E_i = 55 \text{ eV}$. For increasing coupling constant, the maximum contribution of rotational coupling to chemi-ionization moves to collisions with smaller impact parameters.

It must be noted that for impact parameters $b \approx R_c$ Eq. (C.1) does not hold any more because a sufficient separation is supposed between the classical turning point and the crossing
point $R_c$. [A similar remark to the Landau-Zener coupling has been made the Theoretical methods [link type: compare'; target: A08-m3c###point 2]]. For an incomplete passage of the transition region around $R_c$ Eq. (C.1) gives too large a value of $P_{b,rot}$. In the present case with the parameters used the resulting effect is the product $P_{b,rot}(1 - P_{b,rot})$, too small for collisions with $E_i = 55$ eV and $b \approx R_c$ and too large for the corresponding collisions at $E_i = 13.1$ eV. Indeed, a correction to this effect should improve the agreement of measured and calculated curves of Fig. A08-m5bii2-F1a and Fig. A08-m5bii2-F1c. It is suspected that the remaining apparent discrepancy of the relative intensities at $\tau \approx 65$ eV degree is due to convolution effects, measuring faults and the improper use of Eq. (C.1) for $b \approx R_c$.

Reliability

The estimated value $H_{12} = 0.065$ eV differs rather much from the value of 0.05 eV, estimated from total cross-section measurements [The value is input from a previous article [link type: 'input from/project'; target: A04-m4(b)] on the collision energy range 2–20 eV. The effect of these two values on the absolute differential cross section can be observed from Fig. A08-m5bii1-F3 ($H_{12} = 0.05$ eV) and Fig. A08-m5bii2-F1 ($H_{12} = 0.065$ eV). At $E_i = 55$ eV the cross sections of Fig. A08-m5bii1-F3 and Fig. A08-m5bii2-F1 have hardly different values, while at $E_i = 13.1$ eV the cross sections differ by a factor of two. Of course, relative measurements on the differential cross section versus the kinetic energy should give a hint to the correct value of $H_{12}$. However, at the present measurements it is impossible to distinguish in this way these values of $H_{12}$. It is expected that the surface-ionization detector as well as the scattered-ion detector have large and unknown energy-dependent efficiencies.

[Next step on the essay-path: Findings [link type: 'essay-next/used in'; target: A08-m6a]]
[Next step on the complete sequential path: Outcome [link type: 'sq-next'; target: A08-m6]]
[Step back on the essay-path: Theoretical methods [link type: 'essay-back/depends on'; target: A08-m3c2]]
[Step back on the complete sequential path: Quantitative interpretation [link type: 'sq-back'; target: A08-m5bii1]]

Comments on Interpretation with both Landau-Zener and rotational coupling=A08-m5bii2:

- In this module, all details of the calculation of the differential cross section, taking into account the rotational transition, could have been included. However, these details were not available.
- The figures with the general shapes of the differential cross section are copied to the Results module, to allow readers to locate them as results.
Outcome=A08-m6

Characterisation

**Conceptual function:** Outcome

**Range:** Microscopic

**Physics:** Atom-atom model, Chemi-ionisation, Landau-Zener, Rotation

**Bibliographic:** Dévigne, Los [AMOLF]; Physica [1973]

**Identification:** A08-m6

The process of chemi-ionization in alkali atom-halogen atom collisions in the eV range can be explained with an atom-atom model for ion-pair formation [An account of the model is given in a mesoscopic Theoretical methods module [link type: `detailed in/clarified in/wider range/project`; target: MESO-m3c-mod], via potential curve crossing by means of the Landau-Zener coupling and rotational coupling [Why this explanation is reliable is argued in the Findings [link type: `contains/segmented in/argued in`; target: A08-m6a]]. Therefore we will in the future be able to address the case of atom molecule collisions [Leads for further research [link type: `contains/segmented in/detailed in`; target: A08-m6b]].

[Next step on the complete sequential path: Findings [link type: `seq-next/contains/segmented in`; target: A08-m6a]]
[Step back on the complete sequential path: Quantitative interpretation [link type: `seq-back`; target: A08-m5bii2]]

Comments on Outcome=A08-m6:

- The Outcome is a compound module that is an aggregate of the Findings and the Leads for further research,
C.3. THE MODULARISED VERSION OF A08

Findings=A08-m6a

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The differential cross sections of the process Na + Cl \( \rightarrow \) Na⁺ + Cl⁻ on the energy range from 13 to 85 eV have been measured using hybrid crossed beam/gas target atomic beam setup [particulars on the experimental methods (link type: ‘detailed in/depends on’; target: A08-m3a)]. They have also been calculated using a semi-classical LZ model with the lowest-order stationary-phase approximation, uniform rainbow approximation and JWKB phase shifts [particulars on the theoretical methods (link type: ‘detailed in/depends on’; target: A08-m3c)]. We conclude that for these cross sections:

a) the Landau-Zener theory can be applied by the simple use of the transition probability [The theory is clarified in a mesoscopic Theoretical methods module [clarified in/wider range/project’; target: MESO-m3c-LZ]] [The applicability of the theory is justified in the Interpretation [link type: ‘detailed in/argued in/depends on’; target: A08-m5bii]] in order to calculate the energy-dependent and impact-parameter dependent differential cross section contributions A value of the parameter \( H_{12} \) can be estimated from the measurements. [This estimation is performed in the Interpretation [link type: ‘detailed in/clarified in/depends on’; target: A08-m5bii#H12]];  

b) the rotational coupling makes clear the large contribution to the differential cross section for collisions with large impact parameters [The Interpretation justifies the statement (link type: ‘detailed in/argued in/depends on’; target: A08-m5bii2)], leading to an experimental estimation of \( H_{101} \). [This estimation is performed in the Interpretation (link type: ‘detailed in/clarified in/depends on’; target: A08-m5bii2#Hrot)];  

c) impact-parameter method and classical deflection function [These methods are clarified in a Theoretical methods module [clarified in/depends on’; target: A08-m3cii]] give the correct angular positions of special features of the differential cross section due to scattering from the known ionic potential curve and from the known part of the covalent potential. [The applicability of the methods is justified in the Interpretation (link type: is detailed in/argued in/depends on’; target: A08-m5bii)];  

d) lowest-order stationary-phase approximation, uniform rainbow approximation and JWKB phase shifts [These approximations methods are clarified in a Theoretical methods module [clarified in/depends on’; target: A08-m3cii]] give a perfect description of the primary rainbow and some low-number supernumeraries, but a rather serious discrepancy arises with the interference
structure when collisions with large impact parameters contribute to the differential cross section. The discrepancy is dependent on the kinetic energy. [The discrepancies are shown in the Interpretation (link type: 'detailed in/clarified/depends on'; target: A08-m5bi11)];

e) interference structure of the contributions due to scattering with small impact parameters leads to an estimation of the covalent repulsive potential relative to the known ionic repulsive potential. It is expected that the objection of conclusion d) to the interference structure does not hold because of the very good agreement of calculated and measured energy dependence of the repulsive interference structure. [agreement shown in the Interpretation (link type: 'detailed in/clarified in/depends on'; target: A08-m5bi11)].

**Comments on Findings=A08-m6a:**

- The findings were explicitly listed in the original 9.Conclusions section, so that we could copy most of the text. In the introductory paragraph, we have added some information on the methods, for the completeness of the recapitulation that is prescribed by the rules for writing modular articles given in appendix A. We have also added links to the modules that support the statements made in this Findings module.
The process of chemi-ionization in alkali atom-halogen atom collisions in the eV range can be explained with an atom-atom model for ion-pair formation [particular in the model in a mesoscopic Theoretical methods module [link type: `detailed in/wider range/project`; target: MESO-m3c-mod]], via potential curve crossing by means of the Landau-Zener coupling and rotational coupling [This is concluded in the Findings [link type: `detailed in/clarified in/depends on/nq-back/es-back`; target: A08-m6a]].

The question now is how to explain the process of charge transfer in more complicated, molecular, collisions, e.g., between alkali atoms and halogen molecules. This process cannot be described quantitatively with the atom-atom model.

In a molecular charge transfer reaction, there may not only be a correlation between the transfer of the electron and the intermolecular motions of the nuclei, but also between the electron transfer and the intramolecular motions:

\[ M + XY \rightarrow M^+ + (X...Y)^-. \]  \hspace{1cm} \text{(C.22)}

The electron transfer itself can be considered instantaneous, compared to the other velocities involved. However, the time between the two passages of the crossing between the atom M and the molecule XY may be large enough for the bond of the XY$^-$ molecule (which is formed at the first crossing) to stretch.

Therefore the influence of vibration on the electron transfer, i.e. the vibronic coupling at intersections of covalent and ionic states, has to be studied systematically.

Comments on Leads for further research=A08-m6b:

- In the original version of this article, no suggestions were done for further research. We have created this entire module by hand, with the help of prof. Los.
- The information we have represented here was available to the authors at the time they wrote this article. Therefore the authors could have written this module directly themselves. At a later stage, the module could have been updated with references to later articles by Hubers, Aten; Faist & Levine, in which they lines set out in this module are explored.
C.4 Related mesoscopic and macroscopic modules

As an indication, we sketch in this appendix some mesoscopic and macroscopic modules that are cited in the microscopic modules of A06 and A08 that we have presented in the above. In these mesoscopic and macroscopic modules, we have recast information derived from the corpus articles, the review papers and the theses in the corpus, and we have added some information by hand.

Situation, mesoscopic = Meso-m2a

The research domain of molecular dynamics is being developed from a few experimental and theoretical investigations to a fully grown discipline. The rise of the discipline is strongly related to the discovery of a very powerful tool used in this study: molecular beam techniques. However, elementary chemical processes were already investigated decades before the development of the molecular beam method.

Already in 1932 Polanyi observed in sodium flame experiments that the cross section of the reaction between Na and Br2 or Cl2 is about 150 Å². It means that the reaction takes place when the particles are at a distance of about 7 Å. This is an order of magnitude larger than the range of the Van der Waals forces (1-2 Å).

Polanyi [The description of the model in Polanyi’s article [link type: ‘detailed in/external’; target: Polanyi]] suggested the basic features of a model, the harpoon model, which could explain the large cross sections for the formation of sodium halides, which he deduced from his flame experiments. This model was later developed by Magee [The details are given in Magee’s article [link type: ‘detailed in/external’; target: Magee]] in a theoretical study, explaining the mechanism of the electron jump from the alkali atom towards the reactant molecule, which jump initiates the reaction. A very lucid and clear discussion on the harpooning mechanism has been given by Hershbach in connection with reactive scattering in molecular beams [link type: ‘clarified in/detailed in/external’; target: Hershbach]].

Briefly, what this harpoon model comes to is that in the collision between an alkali atom and an electronegative molecule at some distance $R_c$, an electron will jump over from the approaching alkali atom towards the molecule. The negative molecular ion in most cases is formed in a highly excited vibrational state, close to the dissociation limit or even in a dissociative state. The Coulomb force exerted by the alkali ion during the remainder of the trajectory completes
the dissociation, and an alkali halide molecule is formed. The vibrational and rotational energy of the molecule will be high

\[ M + XY \to M^+ + (X^- ... Y) \to (MX)^+ + Y \]  

(C.1)

The name harpooning is reflecting the role the electron plays in the rearrangement of the heavy particles.

Crucial in this harpoon model is the transfer of the alkali valence electron at the crossing point, which initiates the reaction. The electron jump is due to the configuration interaction between the purely ionic and the purely covalent state at the point where these states cross at some cross distance \( R_c \). [The model is further clarified in a mesoscopic Theoretical methods module [link type: 'elaborated in/clarified in/project'; target: Meso-m3o-mod]]. This initial step now can be investigated by applying the molecular beam method in the electronvolt energy range [More about the molecular beam technique in the mesoscopic Experimental methods module [link type: 'elaborated in/clarified in/project'; target: Meso-m3a]. In that case the transfer of the electron would not lead to MX formed in a chemical reaction, but to an ion-pair \( M^+ + XY^- \). These experiments might indicate in how far a generalised Landau-Zener formula could be formulated.

About a decade ago the investigation of reactive collisions by means of molecular beams became a well established method for measuring cross sections and investigating reaction dynamics. In the early experiments mainly alkali beams were used for the obvious reason of detection feasibility. As a consequence much attention has been paid to charge transfer reactions. Especially the alkali atom-halogen-molecule reactions, including the methyl halides and hydride halides as reactants have been subject of detailed experimental investigations.

With the development of the cathode sputtering method [The details can be presented in a mesoscopic Experimental methods module [link type: 'elaborated in/clarified in/project'; target: Meso-m3a-sput]] and the charge exchange method [The details can be presented in a mesoscopic Experimental methods module [link type: 'elaborated in/clarified in/project'; target: Meso-m3a-charge]], it became possible to investigate these chemi-ionisation scattering processes in the electronvolt range, allowing for the analysis of the ‘pure’ first step of the harpoon reaction, namely the ion pair formation.

The research project initiated at the Institute for Atomic and Molecular Physics in Amsterdam is concerned with this charge transfer process in atom-atom and atom-molecule collisions [The central problem given this situation is detailed in the mesoscopic Central problem module [link type: 'used for/detailed in/project'; target: Meso-m2b]]. We use atomic and molecular beam techniques in the electronvolt range to study the scattering process, including total and differential cross sections, the electronic transfer probability and the theoretical description and interpretation.

Comments on Situation=MESO-m2a:

- This module provides background information concerning entire research project. In a modular environment, each article issuing from that project can be connected to this introductory module.

- In principle, the full meta-information concerning the mesoscopic modules has to be provided. Here, we do not present Meta-information modules at the mesoscopic or macroscopic level.

- The body of this module is extracted from review R1, which summarises the first part of the corpus, but the sequence of the text has been changed.
Central problem, mesoscopic = MESO-m2b

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In this project, charge transfer is studied in atom-atom and atom-molecule collisions between alkali atoms and electronegative atoms and molecules (especially halogen compounds). Total and differential cross sections of these chemi-ionisation reactions are measured in beam experiments in the eV range [The experimental methods are elaborate in a mesoscopic module [link type: ‘elaborated in/clarified in/project’; target MESO-m3a]]. In these experiments the transfer of an electron in this type of collisions, i.e., the initiation of the harpoon mechanism [The background against which this problem is set is sketched in a mesoscopic module [link type: ‘elaborated in/project’; target MESO-m2a]] is considered. A model [The model is clarified in a mesoscopic Theoretical methods module [link type: ‘elaborated in/clarified in/project’ target: MESO-m3c-mod]] is tested qualitatively in atom-molecule collisions, reducing the problem to an atom-atom interaction by neglecting the vibrational and rotational coordinates of the molecule; for the motion of the heavy particles the impact parameter approximation is used, while the electron transfer is described by the Landau-Zener model. In the atom-atom case, a semi-quantal description is used for a description of the interference effects with the Landau-Zener approximation for the electron transfer.
The atom-atom model for ion-pair formation in molecular collisions = MESO-m3c-mod

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<tr>
<td><strong>Bibliographic:</strong></td>
<td>Delvigne, Los (AMOLF); Physica [1972]</td>
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<tr>
<td><strong>Identification:</strong></td>
<td>MESO-m3c-mod</td>
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In this module we give an account of an atom-atom model for ion-pair formation in molecular collisions. In short, this simple classical model describes the electronic states of the system as coupled covalent or ionic states. Because the states are coupled, the potential energy curves cross and a non-adiabatic transition between the states is possible [The transition is explained in a macroscopic Theoretical methods module [link type: 'elaborated in/project/wider range'; target: MACRO-m3c-diab] • diabatic]. Thus the ion pair formation is induced by the crossing of the potential curves or (hyper)surfaces, i.e., ionisation takes place via surface hopping. In collisions between alkali atoms and halogen molecules, this electron jump is the first step of the harpoon reaction [The harpoon reaction is described in Henschbach [link type: 'detailed in/context/external'; target: Henschbach], [The context is sketched in the mesoscopic Situation module [link type: 'context/project'; target: MESO-m3a] •].

**Crossing potentials**

Let us consider the ion-pair formation process

$$A + B \rightarrow A^+ + B^-,$$  

where A is an electropositive particle (such as an alkali atom) and B an electronegative one (such as a halogen atom or molecule). In the diabatic representation [The diabatic representation is elaborated in a macroscopic module [link type: 'elaborated in/project/wider range'; target: MACRO-m3c-diab] • diabatic], the states of the system are described as either purely ionic (A$^+$ + B$^-$) or purely covalent (A + B). According to the model, the electron transfer is due to the configuration interaction between the purely ionic and the purely covalent state at the point where these states cross, e.g., at the point where the energies of these states are equal. The crossing of the two potentials is caused by the fact that the energy of the ionic state at infinite separation is of the order of one eV higher than the energy of the covalent state, whereas the ionic potential at smaller distances will be lower than the covalent one because of the attractive Coulomb potential.

The typical shape of the A-B intermolecular potential is shown in Fig. MESO-m3c-mod-F1. From A05 The chemi-ionization process is seen to be endothermic with an energy

$$\Delta E = I(A) - EA(B),$$  

(\text{C.3})
where \( I(A) \) represents the ionization potential of the electropositive particle and \( E_A \) (B) the electron affinity of the electronegative particle. The ionic and covalent ground-state potential curves cross at the intermolecular distance \( R_c \).

The crossing distance \( R_c \) is approximately given by

\[
R_c \approx \frac{e^2}{I(A) - E_A(B)}
\]  

(C.4)

This approximation is quite good for large crossing distances \( R_c \) of about 5 \( \text{Å} \) as in that case the induction and dispersion forces can be neglected; At large distances the two potentials can be represented by \( V = 0 \) for the covalent state and \( V(R) = \Delta E - \frac{e^2}{R} \) for the ionic state.

From A05

The groundstates of the system are described by two curves. There exist many analytical expressions to describe the ionic alkali-halide potential curve. [Recently, a review has been given by Patel and Gehel [link type: 'elaborated in/external'; target: Patel-m1].]

From A05

For the ionic-potential curve we have chosen a Rittner potential [The formula for the potential is input from Rittner’s publication [link type: 'input/external'; target: Rittner]] of the form:

\[
U_{\text{ion}}(R) = -\frac{e^2}{R} - \frac{e^2(\alpha_{M^+} + \alpha_{X^-})}{2(R^4 + a^4)} - \frac{2e^2\alpha_M\alpha_{X^-}}{R^4} - \frac{C_{\text{ion}}}{R^6} + A_{\text{ion}}e^{-R/\rho_{\text{ion}}} + \Delta E.
\]  

(C.5)

The covalent potential is given by:

\[
U_{\text{cov}}(R) = -(C_{\text{cov}}/R^6) + A_{\text{cov}}e^{-R/\rho_{\text{cov}}}.
\]  

(C.6)

The covalent potential consists of a Van der Waals term and the repulsive term, for the ionic potential we add a coulombic term, a screened polarization term, dipole–dipole interaction and at last the endothermicity \( \Delta E \).

From A05

The species and the multiplicity of the ionic and covalent ground states are the same. At the crossing point the transitions between the covalent and the ionic configurations are induced by a strong coupling between the state [The coupling is explained in a macroscopic module [link type: 'elaborated in/explained in/project/wider range'; target: MACRO-m3o-diab#diabatic]]. The Landau-Zener theory provides a simple expression for this transition as a function of the radial velocity at the crossing point. At a collision, ionization of the neutral particles takes place via such a non-adiabatic transition by electron transfer.

![Figure Meso-m3o-mod-F1](Image)

Figure Meso-m3o-mod-F1. The typical shape of the A-B intermolecular potential.
C.4. RELATED MESOSCOPIC AND MACROSCOPIC MODULES

Trajectories

From A08 The potential curves of Fig. MESO-m3c-mod-F1 clearly show the two collision trajectories leading to chem-ionization. Incoming on the covalent curve and outgoing on the ionic one, the particles follow either the ionic potential curve inside the crossing distance with a covalent-ionic transition at the first passing of $R_c$ followed by a covalent-covalent crossing, or the covalent potential curve inside the crossing distance $R_c$ (with a covalent-covalent transition followed by a covalent-ionic one). The former process will be indicated by “ionic” scattering, the latter one by “covalent” scattering. In terms of an electron jump between the two interactants, ionic scattering means that the electron has jumped from A to B when these first approached to the crossing distance $R_c$ of each other and that it remains there during the transition that takes place the second time the particles are at $R_c$. In covalent scattering there is no charge transfer in a diabatic transition at the first passing of the crossing distance, but the electron jumps when the separating interactants are again at $R_c$.

Landau-Zener theory

In the two-dimensional case the transition probability between different configurations has been given firstly by Landau, Zener and Stueckelberg (commonly called the Landau-Zener theory and abbreviated here as L–Z theory). This theory has been criticized and extended by different authors [Nikitin’s survey of the LZ theory [link type: detailed in/external target: E.E. Nikitin, Chemische Elementar Prozesse (Springer, Berlin, 1968) p. 43]]. Transitions between multi-dimensional surfaces have been treated by Teller [To the details on Teller’s work [link type: detailed in/external target: Teller]]. Further work has been done during the last decade by Nikitin [To the details on Nikitin’s work [link type: detailed in/external target: Nikitin]].

The probability $P_b$ for a covalent-ionic transition at a single passage of the crossing at $R_c$ is given by the Landau-Zener formula:

$$P_b = \exp \left( \frac{-2\pi H_{12}^2}{\hbar v_b \left| \frac{dH_{11}}{dR} - \frac{dH_{22}}{dR} \right| R_c} \right),$$  \hspace{1cm} (C.7)

where $dH_{11}/dR$ and $dH_{22}/dR$ are the slopes of the diabatic potentials at $R_c$ and $H_{12}$ is half the energy difference of the adiabatic potential curves at $R_c$. For a given collision energy, the radial velocity at the crossing point $v_b$ depends on the collision parameter $b$. The probability of a covalent-covalent or ionic-ionic transition is $(1 - P_b)$. Thus both the ionic and the covalent scattering trajectories leading to ionization have the equal probability $P_b(1 - P_b)$.

At thermal energies the probability of the electron jump will be close to unity, except for the largest $R_c$ values. At higher energies, however, the probability for a transition from covalent to ionic at the crossing point decreases, while the covalent-covalent transition probability increases: at centre of mass energies larger than $\Delta E$ the probability that only one electron jump takes place is non-negligible, such that ion pair formation can occur due to an electron jump at the first crossing while passing the second time no change occurs or vice versa. The context is sketched in the mesoscopic Situation module [link: ‘context/project’; target: MESO-m2a]]

From the potential-energy curves and the transition probability, the total and differential [The details on the calculation method are given in a mesoscopic Theoretical methods module [link type: ‘detailed in/focused on in/project’; target: MESO-m3c-def]] cross sections for ion-pair formation via the different trajectories can be calculated via the deflection function.
Restrictions of the model

In the simplified atom-atom model, it is assumed that the system has an isotropic, static two-body potential; vibrational and rotational degrees of freedom are neglected. The potential associated to harpoon reaction

$$M + XY \rightarrow M^+ + (X\ldots Y)^- \rightarrow MX + Y$$ (C.8)

for example should be described using hypersurfaces.

Calculations on three-atomic systems are very difficult because they require a knowledge of the complete energy surfaces involved. Moreover, the situation is complicated very much because multiple passing of the crossing region is possible in contrast with the two-atom case, where the crossing region is passed only twice during the collision. An attempt has been made by Bjerre and Nikitin [Details on this attempt in their article (link type: detailed in/external; target: Bjerre-n*)] to calculate cross sections for quenching of Na* by N2. This quenching is also supposed to take place via crossings of potential surfaces. They made trajectory calculations on three-dimensional crossing surfaces, determining the transition probabilities at the crossings by an extended L–Z theory. Such calculations are very computer-time consuming and, because the knowledge of the potential energy surfaces is very poor, one may not expect results with more than only qualitative meaning.

It is known now that the quantitative validity of the L–Z theory is very limited. Moreover, this theory in its simple form is applicable neither to three-particle collisions nor to endothermic processes. Indeed it is found to be impossible to fit the energy dependence of the measured cross section with that predicted by the L–Z theory. However, one can try to use the results of the theory as a kind of “adiabatic criterion” to determine the position and also the order of magnitude of the maximum cross section of this type of inelastic processes.

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<td>• The atom-atom model for ion-pair formation described and discussed in this module plays a central role in the articles in the first part of the corpus. In the various original articles, the model is given partially. We have grouped all information concerning the model in this mesoscopic module, so that in the modularised version, each article only has to contain a brief indication of the model, in addition to a link to this module.</td>
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<td>• In this module the restrictions of the atom-atom model are discussed. This entire discussion is lifted from A03 [Baede and Los; 1971]</td>
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<td>• In the original article A05, the terms adiabatic and diabatic states, and adiabatic and diabatic transitions were used. This terminology, is rather common in the domain of chemical physics, leads to confusion. The confusion is, for example, apparent in the term ‘pseudo-crossing’: the crossing of the potential curves in the diabatic representation of the electronic states that is forbidden in the adiabatic representation; [O’Malley, 1971] cautions that this term is “nonsensical”. In this mesoscopic module, we prefer to describe the configurations as covalent and ionic and the transitions are covalent-ionic, covalent-covalent or ionic-ionic.</td>
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Adiabatic and diabatic states in the Born-Oppenheimer approximation = MACRO-m3c-diab

The motion of a diatomic system is described by the Schrödinger equation. This yields the formal set of exact coupled equations for the nuclear wave functions $\chi_i(R)$ given in equation C.12. From O’Malley

\begin{equation}
H = T_R + H_e
\end{equation}

where $M$ is the reduced mass of the nuclei $M = M_A M_B / (M_A + M_B)$ and $R$ the internuclear radius vector, and of the electronic Hamiltonian $H_e$ defined as the remainder of the Hamiltonian:

\begin{equation}
H_e = \sum_{i=1}^{N} \left( -\hbar^2 / 2m \right) \nabla_i^2 - \frac{Z_A e^2}{r_{iA}} - \frac{Z_B e^2}{r_{iB}} + \sum_{j=i+1}^{N} \frac{\epsilon^2}{r_{ij}} + \frac{Z^2 A Z_B}{R},
\end{equation}

where the sum is over all $N$ electron, $m$ is the electron mass, $r_{ij}$ the distances of electron $i$ from nucleus $A$, $B$ or electron $J$ and $Z$ is the nuclear charge. The full wave function for the diatomic system is given by

\begin{equation}
\Psi(r, R) = \sum_{i} \phi_i(r, R) \chi_i(R)
\end{equation}

for some chosen set of electronic functions $\{\phi_i(r, R)\}$ (adiabatic or diabatic) where $r$ is all electronic co-ordinate and where $\chi_i(R)$ are nuclear wave functions.

Substituting $\Psi$ into the Schrödinger equation, multiplying on the left by $\phi_j^\dagger$ and integrating over all electronic functions gives the equations for the nuclear wave functions:

\begin{equation}
[T_R + T''_{ii} + V_{ii}(R) - E] \chi_i(R) = -\sum_{j \neq i} \left( V_{ij} + T'_{ij} + T''_{ij} \right) \chi_j(R),
\end{equation}

where $T_R$ is the nuclear kinetic energy operator in the Hamiltonian $H = T_R + H_e$ and where

\begin{equation}
V_{jk}(R) = \langle \phi_j | H_e | \phi_k \rangle
\end{equation}

are the electronic matrix elements of $H_e$, and

\begin{equation}
T_{ij} = -2(\hbar^2 / 2M) < \phi_i | \nabla_R | \phi_j > \cdot \nabla_R
\end{equation}

\begin{equation}
T''_{ij} = -2(\hbar^2 / 2M) < \phi_i | \nabla_R^2 | \phi_j >.
\end{equation}
The Born-Oppenheimer approximation allows for a substantial simplification of the equations of motion of a molecular system. The Born-Oppenheimer approximation is probably the most powerful tool to describe forces acting between two atoms. This approximation, which is also known as the adiabatic approximation, is based on the enormous mass difference between light and therefore very mobile, electrons, and the heavy slow nuclei. The ratio \( M/m \) of nuclear to electronic mass runs from a minimum value of 2000 for H to 30,000 for atmospheric gases and over 400,000 for the heaviest atoms.

The physical consequence of that large mass ratio, is that, to first order, the motion of the nuclei does not influence the highly quantized motion of the electrons. In other words, the interactions between the atoms are described by potentials, which actually are the expectation values of the energy of electronic states. The potentials, as well as the wave functions of the electrons, depend parametrically upon the internuclear separation of the two atoms.

The Born-Oppenheimer approximation can be expected to be valid in the region of nuclear velocity below \( v \ll e^2/h \), if the following assumptions hold: firstly the rotational velocity is not much larger than the radial, such that we can concentrate on the radial component of \( \nabla_R \), and secondly the electronic states do no vary greatly over distance much smaller than the atomic unit of distance \( a_0 \), i.e.

\[
|\nabla \phi_i | < a_0^{-1} |\phi_i|. \tag{C.16}
\]

[Arguments for the validity of the approximation in this region are given by O’Malley (link type: ‘detailed in/argued in/external’; target: O’Malley)]

The mathematical counterpart of the qualitative difference between the electronic motion \( (\phi_i) \) and the nuclear motion \( (\chi_i) \) is the recognition that under all reasonable conditions the \( T' \) and \( T'' \) terms in equation C.12 are totally negligible compared with the other terms in the equation. If one accordingly makes the Born-Oppenheimer approximation to neglect \( T' \) and \( T'' \), equation C.12 becomes

\[
[T_R + V_{ii}(R) - E] \chi_i(R) = -\Sigma_{i\neq j}(V_{ij}\chi_j(R)). \tag{C.17}
\]

**Adiabatic representation**

In the adiabatic representation, or more precisely the stationary adiabatic representation, of the electronic states, the electronic functions \( \phi_i^{ad} \) of the system are defined as the stationary eigenvalues of the electronic Hamiltonian \( H_e \):

\[
H_e \phi_i^{ad} = V^{ad}_{ii}(R)\phi_i^{ad} \tag{C.18}
\]

or equivalently in matrix form

\[
V_{ij}^{ad} = <\phi_i^{ad}|H_e|\phi_j^{ad}> = V^{ad}_{ii}\delta_{ij}. \tag{C.19}
\]

This is the diagonal representation of \( H_e \) in stationary states, called adiabatic states. With this representation in the adiabatic states, equation C.12 for the nuclear motion reduces to

\[
[T_R + V_{ii}^{ad}(R) - E] \chi_i(R) = 0. \tag{C.20}
\]

The essential element of equation C.20 is that the nuclear functions \( \chi_i \) are totally uncoupled, so that the states, \( i \), are permanent. In other words, the equation describes a one-state problem.

A further interesting property of the stationary adiabatic representation is the famous non-crossing rule of von Neumann and Wigner [details on this rule in their article (link type: ‘detailed in/external’ target: Neumann)], which states that two potential curves, \( V_{ii}^{ad}(R) \) and \( V_{jj}^{ad}(R) \) may not cross if they have the same symmetry (spin, parity, angular momentum).
Diabatic representation

The diabatic representation is used to describe two-state and many-state problems: the electronic state is described as either covalent or ionic, with the corresponding electronic wave functions $\phi_{\text{cov}}$ and $\phi_{\text{ion}}$. In this diabatic representation, electronic states of the same symmetry can violate the non-crossing rule, because they are not the stationary eigenvalues which diagonalise $H_e$

$$V_{ij} = \langle \phi^a_{i} | H_e | \phi^a_{j} \rangle = \begin{bmatrix} V_{\text{cov}} & V_{\text{cov,ion}} \\ V_{\text{ion,cov}} & V_{\text{ion}} \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix}. \quad (C.21)$$

Let us choose the wave functions $\phi_{\text{cov}}$ and $\phi_{\text{ion}}$ as the electronic basis for expanding the full molecular function $\Psi$ in the fashion of equation C.11

$$\Psi(r, R) = \phi_{\text{cov}} \chi_{\text{cov}}(R) + \phi_{\text{ion}} \chi_{\text{ion}}(R). \quad (C.22)$$

For these $\phi$’s the Born-Oppenheimer approximation is accurate, so that the two relevant nuclear wave functions $\chi_{\text{cov}}$ and $\chi_{\text{ion}}$ satisfy the equation of motion C.12 in the simple form

$$[T_R + V_{\text{cov}}(R) - E] \chi_{\text{cov}}(R) = -V_{\text{cov,ion}} \chi_{\text{ion}}(R)$$

$$[T_R + V_{\text{ion}}(R) - E] \chi_{\text{ion}}(R) = -V_{\text{ion,cov}} \chi_{\text{cov}}(R). \quad (C.23)$$

The diagonal $V_{\text{ion}}$ and $V_{\text{cov}}$ are the potential energies for elastic motion in that particular state $\phi_{\text{ion}}$ and $\phi_{\text{cov}}$, while the non-diagonal elements of $V_{\text{ion,cov}}$ and $V_{\text{cov,ion}}$ provide the coupling between the two states.

The probability of the transition from one state to the other is given by the Landau-Zener formula [More about the Landau-Zener formula in Zener’s publication [link type: ‘elaborated in/external’; target: Zener]]. The probability is only appreciable in the neighbourhood of the point where the potential energy curves $V_{\text{cov}}$ and $V_{\text{ion}}$ cross and for larger velocities.

Comments on Theoretical methods, diabatic and adiabatic = MACRO-mSc-diab:

- The purpose of this module is to provide a ‘textbook background’ for the atom-atom model for ion-pair formation in molecular collisions. Thus the module simulates some part of a presupposed textbook available in the same network as the articles. The diabatic representation in particular, as opposed to the adiabatic one, plays an important role in the theoretical methods used in the corpus. Therefore an elaboration on these representations has to be accessible to the reader.

- The body of this module is based on the Physics Report R4 and [O’Malley, 1971].
Deflection function and differential cross section = MESO-m3c-defl

The deflection function expresses the deflection angle of a scattered particle as a function of the collision parameter. In the study of differential cross sections, the deflection function can be used for three purposes: The value of the classical differential cross section is proportional to the derivative of the deflection curve $|dB/d\theta|$ at the relevant angle, while the semiclassical interference structure needs the calculation of phase shifts by integrating over the deflection cube. Moreover, the deflection curve is a handy visual link at the adjustment of the potential parameters to fit the measured and calculated differential cross sections.

Consider two colliding particles interacting via a spherically symmetric potential function $V(r)$ and suppose that the relative motion of the particles can be described by classical mechanics. Fig. MESO-m3c-defl-F1 shows the scattering trajectory in the centre of mass system near the scattering centre $M$ in the case of a central-force field, consisting of attractive forces at large distances and short-range repulsive forces. The particles approach each other with an impact parameter $b$ and a relative kinetic energy at infinity $E$.

Using polar coordinates $r, \varphi$ with the origin at $M$, the scattering angle $\Theta$ can be deduced by applying the conservation theorems for energy and angular momentum. [click to unfold details]

In a centre of mass system and polar coordinates energy conservation is given by

$$E = \frac{1}{2}m_1r^2 + \frac{1}{2}m_2(r_0^2) + V(r), \quad (C.24)$$

with $\mu$ the relative mass and $v_0$ the initial relative velocity, and the conservation of angular momentum by

$$L = \mu v_0 \hat{\theta} = \mu r^2 \hat{\phi}. \quad (C.25)$$

![Figure MESO-m3c-defl-F1. Scattering of a particle by a symmetric central-force field with centre at $M$.](image)
Therefore
\[ \phi = \frac{v_0 b}{r^2} \]  \hspace{1cm} (C.26)
and eliminating \( \dot{\phi} \) from \( E \) we get
\[ \dot{r} = \pm \sqrt{1 - \frac{b^2}{r^2} - \frac{2V(r)}{\mu_0^2}}, \]  \hspace{1cm} (C.27)
such that
\[ \frac{d\phi}{dr} = -\frac{b}{r^2\sqrt{1 - \frac{b^2}{r^2} - \frac{V(r)}{E}}}, \]  \hspace{1cm} (C.28)
as \( \phi \) decreases for increasing \( r \). Integrating from \( \phi = 0 \) \((\text{for } \lim_{r \to \infty})\) to \( \phi(r) \) we get
\[ \phi(R) = -\int_{\infty}^{R} \frac{b\,dr}{r^2\sqrt{1 - \frac{b^2}{r^2} - \frac{V(r)}{E}}}, \]  \hspace{1cm} (C.29)
The deflection angle is given by
\[ \Theta = \pi - 2\phi|_{R=R_0} \]  \hspace{1cm} (C.30)
(see figure MESO-m3c-defl-F1)
This leads to the classical deflection-angle formula:
\[ \Theta = \pi - 2b \int_{R_0}^{\infty} \frac{dr}{r^2[1 - V(r)/E - b^2/r^2]^{1/2}}, \]  \hspace{1cm} (C.31)
where the distance of closest approach \( R_0 \) is the outermost zero point of the square root term:
\[ 1 - \frac{V(R_0)}{E} - \frac{b^2}{R_0^2} = 0. \]  \hspace{1cm} (C.32)
By substituting the potential functions in the classical scattering function, the deflection curve can be calculated numerically. For small angle scattering, the impact parameter approximation is often used, in which it is assumed that \( V(r)/E \ll 1 \)
We consider the deflection functions for ion-pair formation (in a centre of mass system), which can be described via the crossing of ionic and covalent potential surfaces [The crossing of potential surfaces is clarified in a segment of a mesoscopic Theoretical methods module (link type: ‘detailed in/clarified in/project’; target: MESO-m3c-mod#crossing potentials)].
An asymmetric collision process needs a summation over the different contributions to the total scattering angle. Incoming on the covalent curve and outgoing on the ionic one, the scattering angle is given by:
\[ \Theta = \pi - b \int_{R_0}^{\infty} \frac{dR}{R^2(1 - U_{\text{cov}}(R)/E_i - b^2/R^2)^{1/2}} \]
\[ - b \int_{R_0}^{\infty} \frac{dR}{R^2(1 - U_{\text{ion}}(R)/E_i - b^2/R^2)^{1/2}} \]
\[ - 2b \int_{R_0}^{R_c} \frac{dR}{R^2(1 - U(R)/E_i - b^2/R^2)^{1/2}} \]  \hspace{1cm} (C.33)
where \( U_{\text{cov}}(R) \) is the covalent potential function, \( U_{\text{ion}}(R) \) the ionic potential function and \( U(R) \) in the third term is the ionic or covalent potential function, depending on the scattering path considered inside the crossing radius \( R_c \) \([\text{Why the third term depends on the path is explained in the mesoscopic module on the model (link type: ‘elaborated in/explained in/project’) target: MESO-m3c-mod#trajectories)\.}] \) \( R_0 \) means the distance of closest approach. The exclusive use of the initial parameters \( b \) and \( E_i \) is permitted
by an appropriate choice of the zero point of the potential energy at the entrance channel of the collision.

Experimentally, only the absolute value of the classical deflection function \( \theta = |\Theta| \) is meaningful, because the deflection angles \( \Theta \) and \(-\Theta\) resulting from repulsive resp. attractive scattering on different sides of the target cannot be distinguished.

Typical shape of the deflection function

Fig. MESO-m3c-defl-F2 shows the typical shape of the deflection function for ion-pair formation. The deflection function shows several peculiar features. Because there are two trajectories leading to ionization, the deflection functions consist of two parts connected at \( b \approx R_c \), resulting in a closed deflection function. Of course there is no large-\( b \) deflection curve because the classical turning point has to be smaller than or equal to \( R_c \) to have the possibility of ionization. In the case in which the classical turning point is equal to \( R_c \), both trajectories merge leading to the connection point of the two branches of the deflection function.

Differential cross section

Due to this composite character of the deflection function there are up to four impact parameters leading to scattering over the same angle for small-angle scattering. Even at large-angle scattering there are always two impact parameters for one angle. By simple addition of the contributions of both trajectories, the classical chemi-ionization differential cross section is given by [The derivation of this formula is given in a macroscopic module (link type: 'explained in/elaborated in/project/wider range'; target: MACRO-m3c-diff]

\[
I(\theta) = \frac{1}{\sin \theta} \sum_{i=1,2} P_{b_i} (1 - P_{b_i}) b_i \left| \frac{\text{d} b_i}{\text{d} \theta} \right| ,
\]

(C.34)

The same impact parameters are important in the semiclassical treatment [More on the semiclassical treatment in Ford (link type: 'elaborated in/external'; target: Ford) extended with the stationary-phase approximation [Somewhere, more details and more context concerning this approximation should be given (link type: 'elaborated in'; target: stationary phase)]. Then the scattering amplitude \( f(\theta) \) is built up again either

![Figure MESO-m3c-defl-F2. Typical deflection curves for chemi-ionization scattering (CM system). The two curves due to ionic and covalent scattering are connected \( b \approx R_c \). Because of the several interference features, the ionic curve is split up into b, c and e branches, the covalent curve into a and d branches.](image-url)
by four or by two contributions:
\[ f(\theta) = \sum_{i=1,2,\ldots} f_i(\theta), \]  
(C.35)
leading to the differential cross section
\[ I(\theta) = |f(\theta)|^2. \]  
(C.36)

For simplicity we shall split up the deflection curve into five branches a, b, c, d and e, where a refers to that part of the deflection curve corresponding to attractive covalent scattering, b to the outer attractive ionic branch, c to the inner attractive ionic branch, d to the repulsive covalent branch and e to the repulsive ionic branch as indicated in Fig. MESO-m3c-defl-F2. Then the possible contributions \( f_i(\theta) \) to \( f(\theta) \) are given in lowest-order stationary-phase approximation by

\[ f_a(\theta) = \left[ \left| \frac{db_a}{d\theta} \right| b_a P_a (1 - P_a) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_a + k b_a \theta - \pi) \right] \equiv A e^{i\alpha}, \]  
(C.37)

\[ f_b(\theta) = \left[ \left| \frac{db_b}{d\theta} \right| b_b P_b (1 - P_b) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_b + k b_b \theta - \frac{1}{2} \pi) \right] \equiv B e^{i\beta}, \]  
(C.38)

\[ f_c(\theta) = \left[ \left| \frac{db_c}{d\theta} \right| b_c P_c (1 - P_c) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_c + k b_c \theta - \pi) \right] \equiv C e^{i\gamma}, \]  
(C.39)

\[ f_d(\theta) = \left[ \left| \frac{db_d}{d\theta} \right| b_d P_d (1 - P_d) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_d + k b_d \theta - \frac{1}{2} \pi) \right] \equiv D e^{i\delta}, \]  
(C.40)

\[ f_e(\theta) = \left[ \left| \frac{db_e}{d\theta} \right| b_e P_e (1 - P_e) / \sin \theta \right]^{1/2} \times \exp \left[ i(2\eta_e + k b_e \theta - \frac{1}{2} \pi) \right] \equiv E e^{i\varepsilon}, \]  
(C.41)

where \( \eta_b \) indicates the phase shift and \( k \) is given by \( k = (2\mu E_1)^{1/2} \). For a certain scattering angle \( \theta \) where four contributions form the cross section (for instance the contributions from the branches a, c, d and e), the differential cross section is given by:

\[ I(\theta) = \left| A e^{i\alpha} + C e^{i\gamma} + D e^{i\delta} + E e^{i\varepsilon} \right|^2 \]
\[ = A^2 + C^2 + D^2 + E^2 + 2AC \cos(\alpha - \gamma) \]
\[ + 2AD \cos(\alpha - \delta) + 2AE \cos(\alpha - \varepsilon) \]
\[ + 2CD \cos(\gamma - \delta) + 2CE \cos(\gamma - \varepsilon) \]
\[ + 2DE \cos(\delta - \varepsilon). \]  
(C.38)
Comments on Theoretical methods, deflection function= MESO-m3c-defl:

- This is a mesoscopic module that provides background information that less-informed reader needs to understand the calculation and discussion of the differential cross section: both the classical and the semiclassical differential cross section are ‘derived’ from the deflection function, which in its turn depends on the potential.

- The account on the deflection function is extracted from A08 (default) and A05. A general description of the idea and formula of the deflection function is derived from A06. The details of the derivation are included for completeness but hidden from first view, in order to preserve the flow of discourse in the module.
C.4. RELATED MESOSCOPIC AND MACROSCOPIC MODULES

Classical differential cross section = MACRO-m3c-diff

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Scattering events can be described in terms of total cross sections [Compare with the total cross section described elsewhere (link type: ‘compare’; target: a macroscopic module)], differential cross sections or double differential cross sections [Compare with the double differential cross section described elsewhere (link type: ‘compare’; target: a macroscopic module)]. Cross sections contain all information about momentum, energy (electronic, vibrational and rotational) and angular momentum transfer.

The differential cross section $d\sigma$ is defined as the number of events of a particular type per unit of time, divided by the total flux $F$, where $F$ is the number of particles crossing a unit of transverse area per unit of time.

For the process of elastic scattering sketched in figure MACRO-m3c-diff-F1, the differential cross section per unit solid angle is given by

\[
\frac{d\sigma}{d\Omega} = \frac{b}{\sin \theta} \frac{db}{d\theta},
\]

where $\theta$ is the angle over which the particle incoming with an impact parameter $b$ is scattered.

Thus the differential cross section can be calculated if the deflection function $\theta(b)$ is known.

### Comments on Theoretical methods, differential cross sections MACRO-m3c-diff:

- The target audience is already sufficiently aware of the basics of scattering theory, which are ‘textbook material’. Less informed readers can consult this ‘background module’, which simulates the relevant part of a textbook made accessible in the network of information.

- This module is based on A06
Treatment of raw data = MESCO-m3c-treat

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In order to obtain an insightful presentation of results for differential cross sections, we treat the raw data generated in scattering experiments or calculations and present the results in the following way.

All values of the initial kinetic energy $E_i$, and expressions for the scattering angle $\Theta, \theta$ and $\tau$ are in the center of mass system. Because in inelastic-collision processes the centre of mass transformation formulas require a value of the inelasticity $\Delta E$, the most probable value of this quantity has been used.

Normally we shall plot the polar differential cross section defined by $2\pi I(\theta) \sin \theta$ in arbitrary units against the quantity $\tau$ defined by $\tau = E_i \theta$, the latter by analogy with the significant reduced scattering angle for elastic-collision processes.

Experimentally, only the absolute value of the classical deflection function $\theta = |\Theta|$ is meaningful, because the deflection angles $\Theta$ and $-\Theta$ resulting from repulsive resp. attractive scattering on different sides of the target cannot be distinguished [Why different sides cannot be distinguished is argued and explained in a mesoscopic module (link type: ‘argued in/explained in/elaborated in/project; target: MESCO-m3c-defl)]

The reason we prefer to show deflection curves and differential cross sections on a $\tau$-scale, is that for elastic scattering $E\theta$ is in first approximation dependent only on the impact parameter $b$ and not on the kinetic energy, and because in the collision process considered the inelastic energy $\Delta E$ is small compared to $E_i$.

Comments on Theoretical methods, data analysis = MESCO-m3c-treat:

- This module provides some techniques to treat raw data, concerning the deflection function and the differential cross section, in such a way that an insightful presentation of the results is obtained. We consider these techniques as part of the 'theoretical toolbox'. They are used within the context of an article in microscopic Results modules (that have a sub-problem-solution pattern dealing with the problem how to present the results).

- Here, also details could be provided about this transformation of the raw data to the center of mass system.

- The body of this module is based on A05
C.4. RELATED MESOSCOPIC AND MACROSCOPIC MODULES

Molecular beam set-up = MESO-m3a

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Molecular beam techniques provide a well established method for measuring cross sections of collision processes and investigating reaction dynamics in the electronvolt range [The context is sketched in the mesoscopic Situation module [link type: 'context in/project'; target: Meso-m2a].]

A typical set-up for a molecular beam experiment consists of the following components. The first collision partner is prepared in a primary beam, which is generated in a source and filtered with respect to the state of the particles in a (velocity) selector. The second collision partner is prepared in a secondary beam, a static target, or a hybrid. These collision partners collide in an interaction region. The reaction products are analysed (i.e., the different types of products are separated) and the products relevant to the research at hand are measured in a detector.
Comments on Experimental methods = Meso-m3a:

- The complete experimental set-up is an aggregate of the components indicated in the text. In the course of the research project, several components have been replaced, while the other components were reused. For example, the sputtering source was replace by a charge-exchange source, but the same surface-ionisation detector was used to measure the intensity of the beam. Therefore we have collected all mesoscopic modules on experimental methods used in the corpus in this complex module.

- In this appendix, we do not provide complete mesoscopic Experimental methods modules. Instead, we indicate here what kind of modules can be created:

  - *Source of electronvolt beams.* This a cluster modules with constituent modules on the various sources used in the corpus, including:
    * Sputtering source. The information to be represented in this module can be derived from the theses by Političek (T1) and Moutinho (T2)
    * Charge exchange source. The information on this source has originally been published by Aten and Los in the journal *Journal of Physics E: Scientific instruments*

  - *Selection.* The detailed information about the velocity selector presented in T1 and T2, including a discussion of the precision, can be grouped in this module.

  - *Interaction.* A cluster module, including:
    * Iodine oven. In A08, detailed information is given on the apparatus in which, firstly, the iodine atoms are created and, secondly, sodium atoms collide with them.

  - *Analysis.*

  - *Detection* A cluster module, including:
    * Surface ionisation detector. Different aspects of this detector are presented in subsequent articles in the corpus. The complete description and discussion can be given in this mesoscopic module.
### C.4. RELATED MESOSCOPIC AND MACROSCOPIC MODULES

**Experimental methods, interaction: iodine oven = MESSO-m3a-I**

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In order to study the charge transfer in harpoon reactions [The context of this study is sketched in the mesoscopic module Situation (link type ‘context/project’; target: MESSO-m2a)] we measure the differential cross section of Na + Cl → Na⁺ + Cl⁻, using a molecular beam set-up [The set-up as a whole is given in a mesoscopic Experimental methods module (link type: ‘part of/generalised in/aggregated in/summarised in/project’; target: MESSO-m3a)]. We have build an an oven to create iodine atoms, to serve as target for the sodium atoms in the collision.

Dissociated iodine target gas is formed in the oven drawn in detail in Fig, MESSO-m3a-I-F1.

#### Source of the I atoms

Each of the tantalum cylinders A and B is formed by a double winding of 0.01 mm sheet, closed by spotwelding while the two cylinders are connected at the bottom by a tantalum ring. The electrical resistance of the two-cylinder system is about 0.15 Ω at high temperature. The cylinders are heated directly by applying a voltage difference of a few volts. The tantalum gas supply C is thus heated indirectly, while the heat contact with the iodine gas is enlarged by a platinum multi-channel array at the end of the pipe. The tantalum heat shield D and the stainless steel heat shield E restrict the heat loss while the upper side of the outer shield is cooled by water. By supplying a power of 300 Watt, the temperature of the inner tantalum

![Figure MESSO-m3a-F1. Schematic drawing on scale of the dissociation oven.](image-url)
cylinder near the collision center can be about 1900°C. This temperature is high enough to form an intense beam of dissociated iodine or bromine atoms.

**Selection / interaction conditions I atoms**

The iodine flow through the oven is restricted because of the limited pumping capacity of the liquid-air cooling trap [The oven is put in context in the figure of the entire set-up as used in the particular experiment reported in A08; the cooling trap is [15] [link type: 'context/used in/project/nr'; target: A08-m3a#F1]], placed close to the oven. Moreover, a very low pressure of recombinant iodine molecules in the vacuum chamber is required to avoid serious distortion of the atom–atom collision measurement, especially because the total cross section for chemi-ionization of Na + Cl is only 20 percent of the cross section of Na + Cl₂ [This percentage has been determined by Rittner [link type: 'input from/external'; target: RIT08]]. At a limited iodine flow through C, the iodine pressure in the collision region is maximal in this closed-type oven. Actually, the iodine oven is a hybrid between a collision chamber and a secondary beam.

At working conditions the iodine pressure in the collision region is estimated to be about 3 × 10⁻⁴ torr, while the temperature of the oven was about 1200°C to ensure complete dissociation.

**Configuration of the interaction chamber**

By closing the inner cylinder with an end cap F and by restricting other leakages, the pressure of dissociated iodine is enlarged by a factor of four as compared to the pressure in the beam of an open source. Because the oven rotates simultaneously with the detector, the slots in the tantalum cylinders and heat shields to the detector are only 7 × 2.5 mm². The entrance slots of the sodium beam are 7 × 8 mm², which enables the measurements of scattered particles up to a laboratory angle of 22 degrees. Other apertures in the heat shields raise the pumping speed for recombinant halogen gas between the cylinders.

**Comments on Experimental methods=MESO-m3a-I:**

- Making neutral iodine atoms was very difficult and the construction and operation of the iodine oven was quite an accomplishment. Assuming that, once the iodine oven had been designed, it would be used for more research in the project, we have recast the information in a mesoscopic module, to facilitate multiple usage of the module in the context of subsequent articles.

- In the original version of A08, this detailed description is given in subsection 2.2 Iodine beam of section 2.Experimental. The introductory remarks, embedding this description in its context of the set-up, have been supplied by hand.
Experimental methods, detection: surface ionisation = MESOM3a-Ir

<table>
<thead>
<tr>
<th>Characterisation</th>
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<td>Conceptual function:</td>
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<td>Range:</td>
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<td>Physics:</td>
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<td>Identification:</td>
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We have a molecular beam set-up for collisions between alkali atoms and halogen molecules or atoms [The set-up as a whole is subject of the complex Experimental methods module [link type: 'aggregated in/generalised in/project'; target: MESO-m3a1] The primary beam of the alkali atoms is monitored by two A04 surface-ionization detectors, before and after crossing the secondary beam.

The surface ionization detector consists of a 0.1 mm hot iridium wire. The iridium wires were kept at 1325 K and periodically flashed in oxygen at $10^{-5}$ torr.

The work function of Ir

We use Ir wire, because the work function of this element is quite high; about 5.4 eV [Lacmann A04, A03 and Henschbach have determined this work function [link type: 'input from/external'; target: RA943 = Chem. Phys. Lett. 6 (1970) 106].

Nevertheless, we sometimes had problems detecting Na and Li, especially in the low-energy range. We found that we could overcome these problems by a procedure, similar to that used by Touw and Trischka. We treated the wire at a working temperature of 1325 K in an oxygen bath of $1 \times 10^{-5}$ torr for 5 minutes. This treatment guarantees a stable high work function of the detecting wire for at least one day, which is essential for the detection of sodium and lithium.

Restrictions: Energy dependence of the efficiency

It was checked that the efficiency of the detector was insensitive for small temperature changes around 1325 K. For that purpose, the relative detection efficiency was measured as a function of the wire temperature and the incident energy for the three different alkali beams. This was done by keeping one of the detectors at constant temperature and varying the temperature of the other one. The temperatures at which the detection efficiency is no longer dependent on temperature was determined to be 875 K for potassium, 945 K for sodium and 1095 K for lithium. The setting of the temperature was well above these values, in order to ensure reproducible detection. The temperature of the wire was measured by a pyrometer and corrected for the emissivity [Husmann provides details on this correction for the emissivity [link type: 'detailed in/depends on/external'; target: RA9G18 = J. Appl. Phys. 37 (1966) 4621]].

This, however, does not guarantee an energy-independent efficiency. Reflection of atoms on the surface is possible at high energies [Arguments supporting the standpoint that reflection is possible are given by Politiek and Los [link type: 'argued in/detailed in/project'; target: RA9]] and hence the detection efficiency may be lower. Such an energy dependence was found by different authors for potassium atoms above 3 eV. [The energy dependence found by Holstein and Pasy serving as an argument in favour of the reasoning provided here [link type: 'argued in/detailed in/external'; target: RA9G20 = Z. Phys. 196 (1966) 353]]; [Hulpke and Schier (link type: 'argued in/detailed in/external'; target: RA9G21 = Z. Phys. 207 (1967) 294)]; [Politiek and Los [link type: 'argued in/detailed in/external'; target: RA9G7]]

All the measurements presented here should be corrected by a factor $\beta(E)$ taking this effect
into account. But, as the detection efficiency varies smoothly with the energy and because the energy range is not very large, it does not substantially affect the measurements.

The beam monitor placed before the interaction region intercepts 1/5 of the beam.

**Comments on Experimental methods=MESO-m3a-Ir:**

- In the original versions of A05 and A08, this detector is used but mentioned only briefly. In A05, a reference about the detector efficiency is given, and in A08 no reference concerning the detector is provided at all. The reader was probably supposed to be already sufficiently informed about the workings of this detector.

- In various earlier corpus articles, details were provided about the surface ionisation detector. However, in no article the account was complete. For example, in A04 it is not mentioned that 1) the Ir wire is 0.1 mm and that 2) the flashing treatment has been developed by Touw and Trischka. However, it is the only article in which 1) it is justified that the working temperature is well above the temperatures at which the detection efficiency is no longer dependent on temperature, and 2) the influence of this detector on the beam it is monitoring is mentioned.

- In order to make the entire description and discussion available to the reader, we have created this mesoscopic module MESO-m3a-Ir and linked it explicitly to the microscopic Experimental methods modules of the articles in which this detector is used.
Appendix D

Appendix: modularisation in other domains

We have developed a modular model for experimental sciences, in conjunction with an analysis of articles on experimental molecular dynamics. In the following sections, we shall consider four examples of linear publications of other types, to see if these might also be recast in modular form.

D.1 Generating experimental results: high temperature superconductors

As an example of a predominantly experimental publication, we consider [Ihara et al, 1997]. This short publication is one of hundreds of contributions to the proceedings of the International Conference on Materials and Mechanisms of Superconductivity, which are published as six special volumes of the journal Physica C. These contributions may not exceed two pages, which often leads to very cramped publications. A telling example is that, to save room, authors in many cases even abbreviate the list of references by only mentioning the first author of cited articles. In an electronic environment, there is no need for this draconian page limit.

The subject of research in this domain is superconductivity. In 1911, it was discovered that at very low temperatures certain materials do not have any electrical resistance, which implies that an electrical current can run through them unimpeded. The main purpose of research in this domain is to find a material that is superconducting at temperatures that can easily be reached outside a laboratory, so that the material can be applied in everyday life. The temperature below which the material is superconducting is called the critical temperature $T_c$. A good superconductor not only has a high critical temperature, but it also satisfies some other requirements, e.g. it should remain in the superconducting state in high magnetic fields and be easy to make. There are no theoretical rules for determining what type of material will be a good superconductor. Therefore, the search is predominantly experimental: based on intuition, trial and error, samples of materials are prepared and studied. The accumulated results of work in this area could be presented in the format of a 'catalogue' of superconducting materials.

[Ihara et al, 1997] consists of the sections 1.Introduction, 2.Experimental and Results and discussion, which may be recast into the following modules.

Positioning

The central question addressed in this publication is whether the critical temperature of the compound CuBa$_2$Ca$_3$Cu$_4$O$_{12-y}$, which is abbreviated as Cu-1234, can be increased by doping it
with Tl, Hg, Pb, Bi, Au, Ag, C, N, S or another element (i.e. by replacing some of the Cu atoms in the sample with atoms of another type). In addition, the authors search for a preparation method at lower pressures. This information may be presented in a module Central problem.

The reason why the authors consider this compound can be presented in a Situation module: they have found in previous work that Cu-1234 will be a promising superconductor if its critical temperature can be increased and if it can be synthesised at low pressure.

Methods
Roughly speaking, the experimental methods concern the preparation and the characterisation of the sample. The sample preparation is described very briefly in section 2. Experimental. In section 3. Results and discussion, additional details are given. In a modular, electronic environment, the editors could instruct authors to provide all information necessary for others to repeat the sample preparation in a module Experimental methods.

The characterisation of the sample, firstly, involves the determination of the structure of the sample by an x-ray diffraction analysis and of its composition by an energy dispense x-ray analysis. The characterisation, secondly, involves the determination of the critical temperature $T_c$, by electrical resistivity and magnetisation measurements left unspecified, and the determination of the anisotropy based on the measurement of the magnetic susceptibility of a powder sample and a straightforward calculation. No details are given about these analyses or the apparatus used to perform the measurements. In a modular environment, these details could be made available by means of a link to a mesoscopic or macroscopic module published elsewhere, for instance by the manufacturers of the apparatus.

Results
Measurements have been performed for samples with various types of doping. Only the results with Tl are given in the original publication, because only the sample 
$\text{Cu}_{1-x}\text{Ti}_x\text{Ba}_2\text{Ca}_3\text{Cu}_4\text{O}_{12-y}$ allows for an improvement. If that would be of interest to specific readers, the complete results could in a modular, electronic environment be given in a cluster module Results consisting of constituent modules, each concentrating on a different type of sample.

The x-ray diffraction patterns of the samples form raw data. The data sets can be given in a module Raw data, accompanied by the visualisation in the figure shown in the original publication. By comparing these patterns with patterns stored in a database, using existing software, the structure of the sample can be determined; that structure can be represented in a module Treated results. The techniques for this data treatment are not mentioned in the original publication. In a modular version, they may be made explicit by means of a link to a mesoscopic Numerical methods module. Other raw data are generated in, for example, the measurement of the resistivity at different temperatures. The treated results derived from those data are the values for the critical temperature and anisotropy for the samples.

In a modular environment, the Results module would be the core module of this publication, rather than a module Interpretation. Although there is some discussion about the results (for example, the structure of the sample Cu$_{0.5}$Tl$_{0.5}$-1234 is briefly compared with that of the ‘parent materials’ Cu-1234 and Tl-1234), this discussion does not warrant the creation of a separate Interpretation module.

Outcome
The main result presented in this publication is the fact that the samples Cu$_{1-x}$Tl$_x$-1234 (with $x=0.4$ to 0.5) show a superconducting anisotropy of $\gamma = 4$ and a critical temperature of 126 K, which is higher than that of the ‘parent’ materials Cu-1234 and Tl-1234. In a modular environment, it may be summarised in a module Findings.
D.2 The development of new methods: bioorganic and medicinal chemistry

Hutchison and Brouillette, 1998 is an example of a straightforward report on a new method: an article published in the journal Bioorganic & Medicinal Chemistry about the synthesis of a particular compound. It contains only three main sections: an Introduction, a section Results and discussion, which is specified as chemistry¹, and a section Experimental, which has a subsection general and nine subsections about specific compounds.

**Positioning**

The central problem addressed in the article is the synthesis of 2-[6-(2,4-Dinitrophenoyl)hexyl]-oxiranecarboxylic Acid. In the abstract and the introduction, it is told that this compound is of interest, because it has been reported that it is a selective inhibitor for a particular isoform² of carnitine Palmitoyltransferase-1, also called CPT-1. And the inhibition of CPT-1 may help in the treatment a particular type of diabetes. In a modular publication environment, this information can be summarised in a Situation module, which is linked to a more detailed account elsewhere.

**Results**

A textual overview of the synthesis process is given in the section Results and discussion. This summary refers to the procedures reported elsewhere that were used in various steps of the process, namely the synthesis of subsequent ‘intermediary compounds’. The clearest overview of the subsequent steps in the process is provided in schematic form, in terms of chemical structure formulae.

For each step represented in the scheme, a self-contained description of the synthesis of the intermediary compound is given in a subsection of the section Experimental, as a ‘cookbook’ written in past tense and a telegraphic style. In the subsection general, the (commercial) equipment used for specified tasks is listed, as well as the companies where solvents were obtained. It is also specified how the non-commercial reagents were prepared. The instructions to authors of this journal specify that the experimental section must contain all the information necessary to guarantee reproducibility. These subsections can, even automatically, be recast in constituent modules. The schematic overview of the process can serve as an excellent module summary, supplemented with the text summarising the subsequent steps.

This article can be modularised very easily and successfully. In a modular environment, the authors could have restricted their introductory text to a statement of their goal in the module Central problem and a link to a previous discussion of the relevance of the compound they aimed to synthesise. The core of the article is the structured description of the result of their work: the synthesis procedure, which is imminently suited to multiple use. Later authors who employ this procedure in their work merely have to provide in their Methods module a link to the Results module of this article.

In a modular version of this article, the modules Positioning and Results would be supplemented with a module Meta-information, but not necessarily with any others. Little information is required about how the authors came up with the synthesis procedure, so that there is no

¹If the article had reported and discussed biological or medicinal results, the section Results and discussion would have included subsections about those types of results as well.

²CPT-1 exists in at least two isoforms with different physical and kinetic properties. Liver and skeletal muscle each contain a different isoform, and the heart contains both of them. The compound that the authors have synthesised inhibits the liver isoform.
need for a Methods module. In addition, this type of result does not lend itself to interpretation. For retrieval purposes, the main finding, namely the synthesis procedure, might be stated (redundantly) in a module Findings. Alternatively, the instructions to authors of modular articles of this domain might specify that a new method should be labelled as a finding, rather than as a result, and presented accordingly in a module Findings.

D.3 Empirical research in the humanities: argumentation theory

[Van Eemeren et al., 1995] is an example of empirical work in the domain of argumentation theory. In this article, the authors report about experimental investigations on the performance of Dutch secondary education students in identifying unexpressed premises and argumentation schemes as defined in the theoretical framework of pragma-dialectics.

In argumentation, arguers aim to justify a standpoint by means of premises that they think are accepted by their interlocutors. Not all premises have to be made explicit. An example given in the article is: “Amos is pig-headed, because he is a teacher.”; the premise that teachers are pig-headed is unexpressed. The unexpressed premise serves as a connecting principle between the explicit premise and the standpoint. There are different ways to connect a standpoint to premises. In other words, arguers can use different argumentation schemes. In pragma-dialectics, three main categories of argumentation schemes are distinguished. Following these argumentation schemes, arguers point out that there is a relation of concomitance, analogy or causality between standpoint and premise. In the example, there is a concomitance relation between the standpoint that Amos is pig-headed and the premise that he is a teacher; Amos’s pig-headedness is ‘symptomatic’ of him as a teacher. In the pragma-dialectical analysis of argumentative discourse, two of the analytical tasks are to make unexpressed premises explicit and to identify the argumentation scheme that is being employed. The question addressed in this article is whether or not ordinary language users can also identify them in practice.

The article consists of the following main sections: 1. Introduction, 2. Theoretical background, 3. Hypotheses, 4. Design, 5. Results and 6. Discussion. The information presented in this linear article may be recast in the following modules.

Positioning

This work is embedded in the research programme of pragma-dialectics, regarding argumentative discourse. This embedding does not have to be made explicit in the text of the article, because it is published in a book providing a collection of articles, by various authors, on the pragma-dialectical approach to argumentation. In particular, these investigations are part of a project aimed at establishing a sustained connection between argumentation theory and argumentative practice. This project is only implicitly mentioned in the very short introduction.\(^3\)

In a modular version of this article, the Situation module could be linked to mesoscopic or macroscopic modules about the research programme and the project.

The central problem is formulated in terms of the testing of precise hypotheses concerning the ability of students to identify unexpressed premises and argumentation schemes. The hypotheses, that are given in the section 3. Hypotheses, can be represented in a module Central problem.

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\(^3\)This project is mentioned in a later version of this article [Van Eemeren et al., 1995], which has been published in a scholarly journal. In that version, the research is not reported explicitly in terms of the testing of hypotheses. Its main sections are titled 1. Introduction, 2. Theoretical background, 3. Research questions, 4. Design, 5. Results, 6. Discussion.
Methods
The authors have asked groups of students to identify, in two separate tests, unexpressed premises and argumentation schemes in multiple choice items. In the original article, the tests are described in section 4. Design, which includes subsections about the test format in general, about the two tests and about the test subjects.

In the domain of empirical discourse studies, a module Empirical methods could be defined as a counterpart of the module Experimental methods in science. This module could be defined as a compound module containing the constituent modules Test format, Test samples and Test conditions. In the module Test format, the general design of the empirical test could be described — in this case, a paper-and-pencil test with multiple choice items constructed following a specified design method. This module may be linked to mesoscopic or macroscopic modules about test methods (e.g., multiple choice items, other questionnaires, or interviews). In a modular version of this article, the module Test samples could in its turn consist of two constituent modules, distinguished by the domain-oriented characterisation of the information as ‘unexpressed premises’ and ‘argumentation schemes’, each providing the series of multiple choice items that had been submitted to the test subjects. This would allow others to use the samples of multiple choice items in other experiments pertaining to these issues. The description of the test subjects and the situation of this particular experiment can be given in a constituent module Test conditions.

With respect to the theoretical framework, a full account of the pragma-dialectical model, including the idea of unexpressed premises and argumentation schemes, can be given in mesoscopic or macroscopic Theoretical methods modules and linked to this article.

Results
The results can easily be represented in a complex Results, with separate constituent modules about unexpressed premises and about argumentation schemes. The finished test-papers of the test subjects form the most basic raw data of the experiment. The proportions of correct responses in the test subjects’ output are calculated and presented in tables. These results are then used as input in an analysis of the variance of these results with particular fixed factors (e.g. the type of argumentation scheme, and the type of school of the test subjects). For this purpose, statistical methods (i.e. numerical methods) are used. In the linear article, these methods are referred to in section Results. In a modular version, a link can be made explicit to a mesoscopic or macroscopic module Statistical methods. In the analysis of variance, the significance, i.e. reliability, of the results is explicitly taken into account. The statistical methods are also used to determine the reliability of the test, which is given in section 4. Design.

Interpretation and Outcome
In the section Discussion, it is discussed to what degree the results confirm the hypotheses. Because these hypotheses have already been formulated in detail, the discussion is relatively short. This tallies with the observation in [Buxton and Meadows, 1978, p.177] that the Discussion sections in social sciences in which explicitly formulated hypotheses are tested are shorter than the Discussions in natural sciences. The interpretation of the empirical results in the light of the hypotheses could be represented in a short Interpretation module.

Outcome
The findings of this article are that the hypotheses are indeed confirmed. In the printed article, these conclusions are drawn in the section Discussion. In a modular version, they could be summarised in a module Findings. Since this work is relevant both in the academic context of the development of argumentation theory and in the practical context of teaching, some
implications for the educational system are suggested. For this type of publication, the module
Outcome could be defined as a compound of constituent modules Findings, Leads for further
research and Practical implications.

D.4 Abstract research: logic for artificial intelligence

As an example of a publication in an abstract domain, we consider a contribution to a book
published in consequence of a conference about game theory and epistemic logic, in the domain
of logic for artificial intelligence [Van der Hoek and Meyer, 1997].

The objects of study in this domain are ‘logics’. In the broad definition of the word, a logic
consists of: 1) a language (determining what are well-formed formulas), 2) a model (a slice of a
‘universe’ in which formulas are interpreted (as true or false), and 3) a deductive or axiomatic
system (for proving formulas). The main goal of the research in this area is to find a combination
of a deductive system and a class of models for which all formulas that can be proven in the
deductive system are true in the models (this is called ‘soundness’) and for which all formulas
true in the models can be proven by the deductive system (‘completeness’). The soundness and
completeness of a deductive system with respect to a class of models must be proven. Conse-
quently, [Van der Hoek and Meyer, 1997] might be modularised as follows.

Positioning

In [Van der Hoek and Meyer, 1997], the main goal was to prove the soundness and completeness
of an epistemic logic called $S5_m(CDE)$, with respect to a particular class of models. This logic
forms (according to the abstract) “one overall system for describing the knowledge in a group of
$m$ agents, in which distributed knowledge, everybody’s knowledge and common knowledge can
be dealt with at the same time.”

The situation was as follows: separate logics already existed for individual distributed knowl-
edge, and for common knowledge and everybody’s knowledge. For the combination of these types
of knowledge, however, only conjectures about completeness of this logic with respect to some
intended class of models had been found. Applying standard techniques to obtain complete-
ness, the obtained class of models was too general, and a justification was needed to specialise
this class to the desired class. This information, that was presented in the 1.Introduction, can
be recast in a module Positioning, consisting of the constituent modules Situation and Central
problem, in a straightforward way.

Description of the logic

In section 2.A system for knowledge of $M$ agents, the deductive system and the language are
defined. The class of models is described in section 3.Semantics. The desired class of models for
this deductive system and language could be formulated intuitively and was already conjectured
to be the ‘proper’ class in the literature. The problem was to prove that the deductive system
was sound and complete with respect to that class of models.

The logic under consideration, i.e. the deductive system, the language and the model, is a
key element in the publications. In a modular environment, the logic could therefore be given in
a module Description of the logic, with constituent modules Description of the deductive system
and Description of the model. The definition of the language is very brief here, but it could be
presented in a third constituent module.

In the original publication, it is explicitly stated that the definition of the general logic for
knowledge of a group of $m$ agents is part of the background. In a modular environment, the
information could be presented in a separate module for multiple use, and then it could be linked
to this publication.
Proving
In section 4. Transferring truth, the soundness and completeness of the deductive system with respect to the desired class of models are proven. The method consists, in essence, of the application of two standard techniques and a more novel one, which has been developed by the authors in a previous publication. In experimental science, the main activities are measuring, using experimental methods, and calculating, using numerical and theoretical methods. In the domain of logic, the main activity is proving, and the techniques that are used are proof techniques.

A modular version of this article might, therefore, contain a module Proving, consisting of two constituent modules. In the constituent module, Proof techniques, a brief summary might be given of the techniques, in addition to a link to three separate, wide-range Proof techniques modules that are designed for multiple use. In the second constituent module, Proofs, the actual proofs are given. The fact that the proofs can be isolated from the rest of the discourse is indicated by the fact that, in linear articles, the proofs are often presented in an appendix. This constituent module could be a compound module, with the proofs of key theorems, which form the main steps in the procedure. The summary of the subsequent steps of the proof given in section 3, could serve as the module summary of the module Proof.

Theorems
The 'results' are several proven theorems. The difference between a lemma and a theorem is that a theorem is an important result that is likely to be used by others, whereas a lemma is only used within the context of the proof of a theorem (as an intermediary result). In order to allow receivers to locate and consult a theorem separately, the theorems could be presented in a separate module.

Outcome
The following findings are summarised in the section 5. Conclusions. It is proven that the overall logic is sound and complete with respect to the desired class of models, the standard techniques can indeed be applied to this proof, and, in passing, another relevant property of the epistemic system has been proven. At the end of section 4, some open problems are stated. It is would be easy to create a module Outcome for this publication, consisting of Findings and Leads for further research.

Thus, the following modules might be distinguished by the conceptual function in the domain of logic for artificial intelligence:

1. Meta-information, as in our modular model, including the standard constituent modules;

2. Positioning, as in our modular model:
   (a) Situation;
   (b) Central problem;

3. Description of the logic, a domain-specific module in which the main objects of the research can be grouped:
   (a) Description of the deductive system;
   (b) Description of the model;
   (c) Description of the language.
Because the same deductive system, model or language can be examined in more than one publication, these modules are suitable for multiple use;

4. **Proving**, a domain-specific module in which the ‘action’ takes place:

   (a) *Proof techniques*, with a description of the techniques. These techniques can be standard, so that this module is suitable for multiple use.

   (b) *Proofs* in these techniques are used to give the actual proofs.

5. **Theorems**, a domain-specific module providing the result of the research in terms of proven theorems in the module.

6. **Outcome**, as in our model

   (a) *Findings*

   (b) *Leads for further research*. In this domain, this module is optional, as the research can be considered to be complete if the theorems are proven.
Appendix E

Glossary

In this glossary, we summarise our definitions. We also clarify how we use some terms that may give rise to misunderstanding.

Article: A scientific article is a document in which scientific information is presented, in particular a refereed original account of an original piece of research dealing with a particular topic, addressed to (relative) peers, published in a scientific journal.

Comment: In a broader sense of the word, a scientific article is a document in which information obtained from research is presented. We concentrate on scientific articles in the narrow sense of the word, which have the following distinguishing characteristics: the core of the information represents original research, the article is aimed at a target audience of fellow experts or at least other scientists, the article has been subjected to some form of peer review and the article has been published in a scientific journal of some form. This definition is given in section 2.1.3

Article, linear: An article is called linear if it consists of a single unit in which the information is presented in a single narrative, i.e. in the form of a traditional essay.

Comment: The linearity of an article is a property determined by the author. See also ‘sequential consulting’.

Article, modular: A modular article is an article with a modular structure, i.e. an article which consists of modules and links between modules that constitute a coherent unit for the purpose of communication.

Comment: A modular article represents a network of information within the total network of information in which the information presented in the article is embedded. The general definitions given in section 3.3, guidelines for writing a modular article in appendix A and examples in the electronic version of appendix C.

Characterisation space: A characterisation space is a space spanned by the dimensions of the typology, in which an entity is characterised by its location.

Comment: Our characterisation spaces are based on Gärdenfors’s idea of conceptual spaces. See section 3.2.

Communication: By communication we mean the transfer of information from a human sender to a human receiver, for the purpose of increasing the receiver’s knowledge, enabling him to carry out tasks, or influencing his attitudes and behaviour.
Comment: We consider a human-oriented, rather than a machine-oriented, notion of communication. See section 2.1.1.

**Communication criteria:** Communication criteria are the criteria which the presentation of scientific information, and in particular the structure of scientific articles, has to satisfy in order to be adequate in the light of the interactants profile.

Comment: The discussion of the characteristics of the process scientific communication via articles and the requirements of the interactants in that process lead to the formulation of communication criteria for electronic articles in section 2.4.

**Communicative function:** Apart from its (propositional) content, a text has a communicative function.

We concentrate on the communicative functions 'informing' and 'justifying'. We have used the communicative function in the analysis of articles (see section 4.1.2). We also use the communicative function of the text (or other representation forms) in one module with respect to that in another module, i.e. the relation based on the communicative function, in the characterisation of the link between these modules. See section 4.3.3.

**Conceptual function:** The conceptual function of information is its function in the problem-solving process of the research.

A module distinguished by the conceptual function of the information is thus characterised by its function in the problem-solution patterns reflected in the article. We have called it the 'conceptual function' to emphasise the fact that it works at the conceptual level, rather than the grammatical level for example (where we consider a concept as a largely learned open mental representation of some aspect of some universe of discourse. See [Thagard, 1992] for an overview of different interpretations of the notion of concept.)

**Discourse:** By discourse we mean a formal, orderly and usually extended expression of thought on a subject.

Comment: (Definition from WWWebster Dictionary) The discourse in a scientific article is the 'story' that the authors are telling, reporting their work and justifying its reliability and relevance.

**Document:** A document is a representation of a 'portion' of information (in some language, in some medium) that can be stored and retrieved separately.

Comment: Articles and books are examples of documents, as are modules. Thus a document may consist of 'subdocuments'. Traditionally documents are written on paper. However, in our broad definition a document may for example consist of an electronically stored non-verbal representation of information.

**Documentbase:** A documentbase is a structured collection regularly structured documents which can be accessed by more than one person and/or used for more than one purpose.

Comment: An example of a documentbase is a journal. This definition is phrased like the definition of a database given in [Frost, 1986]: a structured collection of regularly formatted data which can be accessed by more than one person and/or used for more than one purpose. That collection is arranged for ease and speed of retrieval, mostly by a computer. A knowledge base is then a collection of simple facts and general rules (i.e. complex facts) representing some universe of discourse.
**Effectiveness:** Having an intended or expected effect.

Comment: Communication is effective if the information needs of each interactant are satisfied, for example. We do not use the terms effectiveness and efficiency as synonymous, but as complementary.

**Efficiency:** The ratio of the effective output to the total input in a system.

Comment: Communication is efficient if no effort is wasted in the process, for example in the transmission of unneeded information.

**Information, scientific:** Scientific information is a conceptual representation of aspects of a universe (in particular ‘the real world’), based on scientific research.

Comment: We use a mental interpretation of the term information which allows for information to exist without successful communication. It has to be represented in terms of a language and then encoded in a signal for communication. In the term ‘information’, we do not restrict ourselves to with simple facts: information can be complex, consisting of smaller ‘chunks’ of information and various relations between them, which is sometimes called knowledge. Data are simple, factual information. See section 2.1.1

**Interactants profile:** A model in which the presumed characteristics are given of the prototypical interactants in the process of scientific communication via articles, as well as their requirements for effective and efficient communication.

Comment: A profile of the interactants in communication via scientific articles is sketched in section 2.2.2 and specified for the domain of experimental molecular dynamics in section 5.1.2.

**Journal, scientific:** A scientific journal is a documentbase in which certified documents of a particular type on a specified subject in science aimed at a specific target audience are published.

Comment: A journal thus is defined by its functions of certification and registration of articles, of (allowing for) archiving and of making the audience aware of it. In our broad definition of the word journal, we do not specify the medium or that is has to be a periodical. See section 2.1.3.

**Library:** A library is an information managing institution with tasks including acquisition and storage of published information with the purpose of making it available to and accessible for the target public.

Comment: The functions of libraries are changing. See [Scovill, 1995].

**Link:** A link is a uniquely characterised, explicit, directed connection between (parts of) modules that represents one or more different kinds of relevant relations between (parts of) modules or (parts of) the information units underlying those modules.

Comment: See section 3.1.2 for the abstract definition. Types of relations that can be represented in links in articles on experimental sciences are given in section 4.3, and on experimental molecular dynamics in general in section A.3.

**Meta-information:** Meta-information is information about the article.
Comment: Likewise, metadata are simple data about the article. Examples of metadata are: the names of the authors, the date of publication and the abstract. We define the module *Meta-information* representing the meta-information of a modular article in section 4.2.7.

**Modular model:** A modular model is a model for structuring the representation of information in a distributed storage environment, in a particular domain and genre. The modular model gives the definitions of the types of 1) modules and 2) links that can constitute a modular structure, and 3) the rules for the composition of a modular structure.

Comment: See section 3.3 for the abstract definition, and chapter 4 for a domain specific modular model for articles on experimental sciences. In section 6.2.1 we indicate how our model can be adapted to other domains.

**Modular structure:** A modular structure is a pattern of modules and explicit links between modules.

Comment: See section 3.1.1 for the abstract definition. The structure is determined by the definition of the modules, the definition of the links and the rules for putting these together. A domain and genre specific definition of the ingredients of the modular structure is given in chapter 4 for articles on experimental sciences and in section A.1 for experimental molecular dynamics in particular. See appendix C for concrete examples of articles with a modular structure.

**Module:** A module is a uniquely characterised self-contained representation of a conceptual information unit, which is aimed at communicating that information.

Comment: Depending on the language in which the information is represented, a segment of a module can consist of, for example, a phrase, a paragraph, a mathematical formula, a figure, or a movie. See section 3.1.1 for the abstract definition. A domain and genre specific definition of modules is given in chapter 4 for articles on experimental sciences and in section A.1 for experimental molecular dynamics in particular. See appendix C for concrete examples. There are different kinds of modules: elementary modules and complex modules, including compound and cluster modules.

**Module, cluster:** A cluster module is a complex module in which the central concept is a generalisation of the specific concepts focused on in each (elementary or complex) constituent module.

Comment: A cluster module does not change in nature when a particular constituent is added or removed. See section 4.2.2, and appendix A for domain specific definitions of cluster modules.

**Module, complex:** A complex module consists of a coherent collection of (elementary or complex) constituent modules and the links between them.

Comment: A complex module can contain elementary modules, as well as smaller complex modules. The relation between the constituent modules is a necessary ingredient, such that a set of unrelated modules does not form a complex module. See section 3.1.3 for the abstract definition. We distinguish two special kinds of complex modules: compound modules and cluster modules.

**Module, compound:** A compound module is a complex module that is an aggregate of (elementary or complex) constituent modules.
Comment: A compound module has to consist of a necessary minimum (and maximum) of constituent modules. See section 3.1.3 for the abstract definition, and section 4.2.2 and appendix A for domain specific definitions of compound modules.

**Module, elementary:** An elementary module contains information that cannot be represented in more than one separate module

Comment: See section 3.1.3 for the abstract definition.

**Peer review:** Peer review is the process of judging the quality of the information in and the presentation of an article by experts on the subject the article deals with, where the judgement is explicitized in the form of a recommendation.

Comment: The demarcation between the duties of the editor and the referee depend on the strategy of the journal or the publisher. In some journals, the editor is solely responsible for the rejection of the article, or the acceptance, possibly after modification. In other journals, the editor's work is of a more administrative nature, and the article is always judged by at least two referees. Peer review is part of the process of scientific communication via articles. It can also take place after publication of the article, in the form of comments or ratings in some form attached to the published article. See section 2.1.3.

**Publication:** 1. The act or process of publishing or making public information represented in some language, in some medium.
2. A published document, representing information in some language, in some medium.

Comment: The act of making public primary scientific information is part of the process of scientific communication via articles described in section 2.1.1. Publication can take place in two ways: by disseminating the work to be published directly to the target audience, or by archiving it and making it available to the audience.

A publisher is an information managing person or institution whose tasks include the acquisition of unpublished information, the organisation of refereeing and certification, and the actual publication. Thus, the term ‘publisher’ covers a lot more than ‘company selling paper journals’.

**Relata:** A relatum (plural relata) is one end of a relation: relations are between relata.

Comment: In section 4.3, we explain how the relata correspond to the source and the target of the link expressing the relation, and which types of relata can be distinguished in different cases.

**Review paper:** A review paper is a non-trivial compilation of articles.

Comment: In a review paper the information of existing articles is not only presented but also improved upon, made more explicit, detailed, precise, complete. It may be a review of the author's your own work or an overview of the current state of affairs in a certain area of science, in which the different approaches and developments are compared. Review papers are often used as the ‘tutorials of the researcher’, who cannot find information advanced enough in existing books

**Sequential reading:** An article is consulted sequentially when it is consulted in a predefined order.
Comment: Contrary to linearity, 'sequentiality' is not a property of the article but of the way to consult it. The natural way to consult linear articles is sequentially. Modular articles can also be consulted sequentially. The author of a modular article has to indicate a preferred route which the reader can follow.

**Typology** A typology is a multidimensional classification, in which the categories are distinguished from a conceptual rather than an empirical perspective.

Comment: We use a typology to identify and characterise the modules and the links in the modular structure. In section 3.2 the general features of the required typologies are discussed.
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*Something is rotten in the state of scientific communication.* Wetenschappers publiceren hun werk, maar omdat de communicatiewegen overbelast raken is het helemaal niet zeker dat ze daarmee de beoogde lezers bereiken. Voor een wetenschapper die op zoek is naar informatie is het soms eenvoudiger om een experiment te herhalen dan om uit te vinden dat er al een publicatie over bestaat. De opkomst van de nieuwe, elektronische communicatietermologie, en met name Internet, wordt gezien als een miraculeuze oplossing. Zodra iets op het Internet openbaar gemaakt wordt, kan in principe iedereen, overal ter wereld, het meteen opzoeken en raadplegen. In praktijk kan de communicatie juist slechter worden, als de geïnteresseerde lezer in een wereldwijde rijstbrij van beschikbare informatie de gewenste krenten eruit moet zien te pikken. Filevorming en vertraging op de ‘elektronische snelweg’ maken het er ook niet gemakkelijker op.

De centrale vraag in dit proefschrift is hoe wetenschappelijke informatie in elektronische artikelen zo gestructureerd kan worden dat de communicatie verbetert. De structuur die wij voorstellen is modular: wetenschappelijke artikelen kunnen worden gestructureerd als netwerken van expliciet gëëktetteerde modules en eveneens gëëktetteerde verbindingen daartussen. Hieronder wordt eerst de inhoud van het proefschrift samengevat – voor een breder publiek dan de Engelse samenvatting – en daarna de indeling in hoofdstukken toegelicht.

**De stroomlijning van wetenschappelijke artikelen op de elektronische snelweg**

We denken dat wetenschappelijke artikelen op het Internet inderdaad aan een efficiëntere en effectievere communicatie kunnen bijdragen, *mits* de techniek op de juiste manier wordt toegepast en de traditionele vorm van het artikel zelf ook wordt aangepast aan de nieuwe techniek. Als we werkelijk gebruik willen te maken van de voordelen van een nieuwe technologie zijn de bestaande vormen immers niet automatisch optimaal. De eerste auto’s leken bijvoorbeeld sprekend op koetsen, behalve dat het paard voor de wagen vervangen was door een motor erin. Het duurde een tijdje voordat auto’s passend gestroomlijnd werden. Net zo lijken de eerste elektronische tijdschriften zo nauwkeurig mogelijk op de oorspronkelijke papieren tijdschriften; dat wordt zelfs expliciet voorgeschreven door sommige redacties. Zo’n tijdschrift wordt verspreid via het Internet, in plaats van door de postbode, maar de lezer wordt geacht het meteen uit te printen, zodat het Internet alleen als een soort lange-afstandskopieermachine wordt gebruikt.

Het ‘traditionele’ natuwwetenschappelijke artikel vormt een lopend verhaal dat begint met “de laatste jaren wordt er veel onderzoek verricht naar...” en eindigt met suggesties voor verder onderzoek. Het verhaal is wel verdeeld in een aantal standaardparagrafen, maar het wordt als één geheel beschouwd. Van deze structuur, die ontstaan is voor publicatie op papier, is het de vraag of het voor een elektronische omgeving de meest geschikte vorm is. In dit proefschrift hebben we een model ontwikkeld om artikelen zo te stroomlijnen dat communicatie via de elektronische snelweg effectiever en efficiënter kan verlopen.

We gaan er van uit dat lezers betrouwbare en duidelijk gepresenteerde informatie willen hebben die bovendien relevant is voor de beantwoording van hun vragen, en dat ze niet willen
worden lastig gevallen met informatie waar ze in dat onderzoeks- fase niets aan hebben. Uit onderzoek is gebleken dat de lezers van wetenschappelijke artikelen zeker niet in ieder stadium geïnteresseerd zijn in alles wat er in het artikel staat. Ze raadplegen bijvoorbeeld selectief eerst de conclusies en dan de figuren met de resultaten. Wat en hoe onderzoekers lezen, hangt af van hun achtergrond, als expert of als nieuweling in het onderzoeksgebied, en van hun behoeften op dat moment – willen ze een bepaald meetresultaat opzoeken, of de ontwikkelingen in het gebied volgen? Verder gaan we er van uit dat belangrijkste drijfveer van auteurs is dat ze willen dat lezers hun werk leren kennen, het aanvaarden en het zelfs gebruiken in hun eigen onderzoek. Ze willen hun werk ook kunnen presenteren zonder tijd en energie te verspillen.

Een modulaire structuur

Om tegemoet te komen aan de wensen van de verschillende gebruikers en tegelijkertijd gebruik te maken van de voordelen van de nieuwe media stellen we voor om elektronische artikelen *modulair* te structureren. Een modulaire artikel is niet georganiseerd als een lineaïr verhaal, maar als een verzameling samenhangende eenheden – *modules* – die aan elkaar geknoopt zijn door middel van expliciete verbindingen. We duiden verbindingen aan met het Engelse woord *link*. Lekers kunnen dan zowel één enkele module als een verzameling modules opzoeken en raadplegen, in de volgorde die op dat moment het beste tegemoet komt aan hun informatiebehoeften. Aangezien die links zowel modules binnen een en hetzelfde artikel als modules in verschillende publicaties aan elkaar koppelen, vormt een artikel als het ware een informatie netwerk binnen het grotere netwerk van alle gepubliceerde informatie.

De modulaire structuur is mogelijk dankzij de opkomst van ‘hypertext’. Hypertext wordt wel gedefinieerd als niet-lineaire tekst. Strikt genomen is een tekst op papier met voet- en eindnoten dus ook een hypertext. De tekst wordt echter meestal gebruikt voor elektronische niet-lineaire tekst waarin de verwijzingen ‘hyperlinks’ zijn: in plaats van te bladeren kunnen we met één druk op de knop een ‘hyperlink’ volgen en zo naar een andere tekst of naar een andere plaats in dezelfde tekst springen. Overigens hoeven het beginpunt en het eindpunt van zo’n link geen tekst te zijn; het kan bijvoorbeeld ook een figuur of een filmpje zijn. De term ‘hypermedia’ benadrukt dit aspect. In de hypertexten die we nu op het Internet tegenkomen, is het alleen niet altijd even duidelijk wat de aan elkaar geknoopte onderdelen precies inhouden, en wat er gebeurt er als we op die knop drukken: wordt de betekenis van een vreemd woord verklaard, of komen we terecht bij het bestelformulier van een *pizza*-koerier in New York? Het is erg gemakkelijk om te verdwalen in ‘hyperspace’.

In de modulaire structuur die wij ontwikkeld hebben, worden systematisch verschillende typen informatie ondergebracht in verschillende typen modules. De modules worden voorzien van een etiket dat lezers in staat moet stellen ze te vinden. Voorts worden modules die met elkaar verband houden systematisch aan elkaar gekoppeld met links waarin de verschillende soorten relevante relaties tussen de modules worden weergegeven. Die links worden ook voorzien van een etiket, zodat ze een rol kunnen spelen in het zoekproces en de lezers in staat stellen te besluiten of ze een link volgen of niet.

De samenhang van de informatie drukken we niet alleen uit in links, maar ook in de samen- stelling van modules. De kleinste bouwstenen zijn elementaire modules. Hiermee kunnen we een samengestelde module maken: een module die op zichzelf als een eenheid kan worden beschouwd en die tevens ‘lagere orde’ modules bevat die zelfstandig raadpleegbaar zijn. Zo kan van een verzameling elementaire modules over mussen, merels, meeuwen en pinguïns een samengestelde module worden gemaakt over vogels in het algemeen. En elementaire modules over kop, lijf, vleugels en poten kunnen worden gegroepeerd in een samengestelde module over de vogel als geheel. Voor het overzicht over de onderdelen en de verbanden daartussen bevat de samengestelde module een ‘modulesamenvatting’, net zoals het artikel als geheel een ‘abstract’
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heeft. Aangezien een modulair artikel bestaat uit een verzameling modules en links is het eigenlijk een speciaal geval van een samengestelde module.

We hebben een model uitgewerkt voor het schrijven van wetenschappelijke artikelen in modulaire vorm. Om bij het ontwikkelen van de nieuwe structuur met beide benen op de grond van de praktijk van wetenschappelijke communicatie te blijven, zijn we in ons onderzoek uitgegaan van bestaande publicaties. We hebben een analyse gemaakt van op papier gepubliceerde artikelen over experimentele moleculaire dynamica, de studie van onderlinge bewegingen van atomen en moleculen in elementaire fysische en chemische processen. Daarbij hebben we gekozen wat voor soorten informatie en wat voor relaties we in die artikelen konden identificeren, en vervolgens hoe we die informatie anders konden organiseren. Met andere woorden, we hebben bestaande, lineaire artikelen gemodulariseerd. We hebben daarbij ervaren dat die modularisering bepaald niet triviaal is, zodat er vooral nog geen zicht is op automatische modularisering en auteurs dus zelf in modulaire vorm zouden moeten schrijven.

De soorten informatie uitgedrukt in modules

De vraag is nu wat we soortgelijke informatie noemen, welke typen informatie we dan onderscheiden, en wat de relevante relaties zijn die we in hyperlinks willen weergeven. We zijn gekomen tot een typologie op basis waarvan we de informatie in modules groeperen vanuit vier elkaar aanvullende gezichtspunten. Twee daarvan sluiten aan bij de standaardkarakterisering van wetenschappelijke informatie. De eerste is de bibliografische informatie, zoals de namen van de auteurs en de publicatiemoment. Vanuit het tweede gezichtspunt hanteren we een vakinhoudelijke karakterisering, die meestal wordt uitgedrukt in trefwoorden. Daarmee kan bijvoorbeeld worden aangegeven wat voor soort metingen in een artikel gerapporteerd worden en welke stoffen daarbij bestudeerd zijn – bijvoorbeeld zuurstof, of juist chloor. Omdat de bibliografische en de vakinhoudelijke karakterisering al onderwerp zijn van veel onderzoek heeft er aangenomen dat hiervoor geschiktte classificatie-onderdelen beschikbaar zullen zijn, die in ons model kunnen worden geplukt.

We hebben in ons model deze twee standaardkarakteriserings aangevuld met twee andere:

• een karakterisering van de informatie op basis van haar bereik en één op basis van de rol die zij speelt in het probleem-oplossingsproces van het onderzoek, die we de conceptuele functie van de informatie noemen. We onderscheiden de volgende soorten informatie op basis van het bereik:
  - microscopische informatie, die alleen een rol speelt in een individueel artikel. Een artikel bevat dus microscopische modules;
  - mesoscopische informatie, die een rol speelt binnen het onderzoeksproject als geheel;
  - macroscopische informatie, die zelfs het project overstijgt en een rol speelt binnen het hele onderzoeksgebied. Dit is het soort informatie dat in standaardwerken wordt gepresenteerd;

Veel natuurwetenschappelijk onderzoek wordt verricht in projecten of grotere programma's. Daarin werken verscheidene onderzoekers in de loop van een langere periode aan een centraal probleem, en ze publiceren verscheidene artikelen over dat onderzoek. De gepubliceerde artikelen die we hebben geanalyseerd komen voort uit één onderzoeksproject. In die reeks artikelen werden bijvoorbeeld de experimentele opstelling en het theoretische model in opeenvolgende artikelen telkens weer kort beschreven, zonder dat die beschrijving in enig artikel compleet was. We hebben die verspreide informatie gegroepeerd in mesoscopische modules, die we gekoppeld hebben aan de microscopische modules van onze modulaire versies van de artikelen. Zo beschikken lezers van elk modulair artikel over de complete beschrijving van de methoden, zonder dat de auteurs hem hoeven te herhalen.
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Net als de traditionele structuur van wetenschappelijke artikelen is de modulaire structuur een weerspiegeling van het onderzoek als probleem-oplossingsproces. De hoofdmodulen die we onderscheiden op basis van de conceptuele functie zijn daardoor verwant aan de geijkte paragrafen in traditionele artikelen: Inleiding, Methoden, Resultaten, Discussie en Conclusies. Het verschil is dat de modules zelfstandige eenheden zijn en de paragrafen niet. Modules zijn bovendien expliciet geëtiketteerd, waardoor ze opgezocht kunnen worden in een digitale bibliotheek, en ze kunnen apart geraadpleegd worden. We onderscheiden de volgende (samengestelde) modules op basis van de conceptuele functie van de informatie:

- **De Positionering-module** bevat een elementaire module met een schets van de context van het artikel, en een module met een korte beschrijving van het centrale probleem. De inhoud van deze module correspondeert met de inhoud van de traditionele Inleiding. Een groot deel van de informatie over de context kan worden gegeven in een mesoscoopische module. Experts op het vakgebied kunnen die zo overslaan, terwijl nieuwkomers hem juist goed lezen.

- **De Methoden-module** bevat modules over de experimentele, numerieke en theoretische methoden die gebruikt zijn. De experimentele methoden werden in de oorspronkelijke artikelen besproken in een afgeronde paragraaf en ze zijn daardoor het eenvoudigst in een zelfstandige module te representeren. De informatie over de theorie was meer verweven met de rest van het wetenschappelijke betoog.

- **De Resultaten-module** bevat bewerkte resultaten, zoals de grafieken van metingen, en ook de ruwe meetgegevens, als die zo bewerkt zijn dat ze niet meer herkenbaar zijn in de uiteindelijke resultaten. De ruwe meetgegevens nemen te veel ruimte in beslag om in aanmerking te komen voor publicatie op papier, maar in een elektronische omgeving hoeven geen drastische ruimtebeperkingen te worden opgelegd. De module met de bewerkte resultaten is vaak zelf ook een samengestelde module. Vakinhoudelijk verschillende soorten resultaten, bijvoorbeeld van metingen aan verschillende stoffen, worden in verschillende elementaire modules ondergebracht.

- **In de Interpretatie-module** worden de resultaten kwalitatief en/of kwantitatief geïnterpreteerd aan de hand van een theorethisch model en bijvoorbeeld de resultaten van anderen. Zoals de Discussie paragraaf waarvan deze module verwant is, is deze module het lastigste onderdeel van het artikel. Er komen diverse overwegingen aan bod en een groot deel van de interpretatie is verweven met de resultaten die geïnterpreteerd worden en met de theoretische methoden die gebruikt zijn om ze te interpreteren. Daarom is het extra belangrijk om de lezer houvast te geven in de vorm van expliciete structuur en van modulesamenvattingen.

- **De Uitkomst-module** bevat de belangrijkste bevindingen van het onderzoek en een module met suggesties voor verder onderzoek.

We hebben aan deze ‘inhoudelijke’ modules een ‘administratieve’ module toegevoegd:

- **De samengestelde module Meta-informatie** bevat informatie over het artikel bevat. Hierin zit, onder andere, een opsomming van de bibliografische gegevens van het artikel als geheel; welke gegevens dat precies zijn hangt af van de keuze van de bibliografische karakterisering. Daarnaast bevat de module zowel een (tekstuele) samenvatting als een (visuele) plattegrond van het artikel als geheel. Deze module helpt te voorkomen dat de lezer verdwaalt in het niet-lineaire netwerk van modules.
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Door de informatie vanuit deze vier gezichtspunten te karakteriseren en in geëtiketteerde modules onder te brengen maken we het zoeken naar en het raadplegen van specifieke soorten informatie mogelijk. Iemand die een bepaald getal nodig heeft om verder te kunnen rekenen, kan naar een microscopische Resultaten met meetresultaten zoeken. En iemand die bezig is met het bouwen van een opstelling kan de mesoscoopische Methoden module opzoeken en raadplegen, waarin bepaalde autoriteiten op het gebied beschrijven hoe hun opstelling in elkaar zit.

De soorten relaties uitgedrukt in links

We verbinden modules of onderdelen van modules met expliciet geëtiketteerde links. Een enkele link kan daarbij verschillende soorten relaties uitdrukken. We onderscheiden twee hoofdsoorten. Organisatorische relaties hebben betrekking op de modules als ‘informatievaten’, ongeacht de specifieke inhoud. De tweede hoofdsoort gaat juist wel over de inhoud; we noemen dat wetenschappelijke ‘discourse’ relaties.

Binnen de hoofdsoort van organisatorische relaties onderscheiden we de volgende relaties:
1) Hierarchische relaties identificeren we tussen samengestelde modules en hun onderdelen.
2) Relaties gebaseerd op de ‘nabijheid’ van twee gekoppelde modules expliciteren we om te voorkomen dat de lezer onverwacht in een heel andere artikel belandt. 3) Relaties gebaseerd op het bereik drukken we uit opdat de lezers meteen weten dat, bijvoorbeeld, de module waarnaar ze vanuit een microscopische module verwzen worden meso- of macroscopisch is. 4) Administratieve relaties worden expliciet gemaakt tussen alle ‘inhoudelijke’ modules en de modules in de Meta-informatie, zodat de lezer altijd beschiwt over de informatie over de module. 5) Representatienamele relaties kunnen worden geïdentificeerd als dezelfde informatie op verschillende manieren is geregistreerd, bijvoorbeeld in tekst, in een figuur en in een filmje; dan verbinden we die verschillende representaties. 6) Ten slotte leggen we sequentiële relaties neer in sequentiële leespaden voor lezers die het artikel als geheel willen lezen. (Op pagina 189 staat een figuur met de organisatorische relaties en de bijbehorende etiketten voor links.)

De meeste organisatorische relaties kunnen in principe automatisch worden geïdentificeerd, als daar de benodigde technische hulpmiddelen voor ontwikkeld worden. Bij de wetenschappelijke ‘discourse’ relaties ligt dat niet zo eenvoudig. De links die dit soort relaties uitdrukken zijn meer dan een ondersteuning van het leesproces. Ze maken deel uit van de wetenschappelijke rapportage en het wetenschappelijke betoog, zodat eigenlijk alleen de auteur ze kan aanbrengen.

De hoofdkategorie van relaties met betrekking tot het wetenschappelijke ‘discourse’ splitsen we op in twee deelcategorieën: relaties gebaseerd op de communicatieve functie en inhoudsrelaties. Als auteurs verwachten dat sommige lezers een module anders meten begrijpen of aanvaarden, kunnen ze een link aanleggen waarin de communicatieve functie expliciet wordt gemaakt. Een module kan fungeren als een opheffering van een andere module, bijvoorbeeld als een toelichting bij wat er staat of een verklaring van waarom iets het geval is. Of hij kan als argumentatie fungeren voor wat er in een andere module beweerd wordt.

We onderscheiden ook verschillende soorten inhoudsrelaties. De auteur kan bijvoorbeeld zijn standpunt dat zijn meetresultaten betrouwbaar zijn beargumenteren via een vergelijking met de resultaten van een andere onderzoeksgrup. Hij kan ook iets verklaren of beargumenteren door te wijzen op een oorzaakelijk verband, en gebruik maken van generalisatie of aggregatie. Verder kan de module waarmee verwzen wordt meer informatie bevatten: gedetailleerde, beter ingebed in de context, of allebei.

Een belangrijke ‘inhoudsrelatie’ is de afhankelijkheid in het probleem-oplossingsproces: resultaten hangen bijvoorbeeld af van de methoden die gebruikt zijn om ze te verkrijgen. Om de inhoud van een bepaalde module goed te kunnen begrijpen en aanvaarden moet de lezer weten waarvan die inhoud afhankelijk is. Een speciaal geval is de overdracht van gegevens. Als auteurs bijvoorbeeld in een berekening meetresultaten van iemand anders gebruikt, dan moeten ze een
link aanleggen naar de bron van die gegevens; in die link drukken ze zo’n afhankelijkheidsrelatie uit. (De wetenschappelijke ‘discourse’ relaties zijn samengevat in de figuur op pagina 200.)

**De hoofdstukken en appendices in dit proefschrift**

In hoofdstuk 1 wordt onze centrale vraag naar de structurering van elektronische wetenschappelijke artikelen geplaatst in de context van de ontwikkelingen van het artikel als wetenschappelijk communicatiemiddel en van de nieuwe, elektronische media. In hoofdstuk 2 gaan we na welke eigenschappen wetenschappelijke communicatie via artikelen heeft en wat voor eigen auteurs en lezers stellen. Dat leidt tot een lijst met criteria waaraan de structuur van artikelen moet voldoen.

In hoofdstuk 3 geven we de abstracte definitie van ‘modulaire structuur’. Voor de overzichtelijkheid zijn de definities uit dit hoofdstuk, samen met een aantal andere sleuteltermen, opgenomen in een glossarium (Appendix E). We maken het idee van modulaire structuur concreet in hoofdstuk 4, in termen van een modulair model voor natuurwetenschappelijke artikelen. Daarin geven we de definities van de typen modules en links waaruit een modulair artikel kan bestaan en de regels voor het samenstellen daarvan. Meer specifieke schrijfregels voor modulaire artikelen over moleculaire dynamica worden gegeven in Appendix A. De lijst van de publicaties waarover we daarvoor beschikken is gegeven in Appendix B. Om aan te geven hoe modulaire elektronische artikelen er uit zouden kunnen zien geven we in Appendix C van de elektronische versie van dit proefschrift modulaire versies van twee artikelen uit de verzameling gepubliceerde artikelen die we geanalyseerd hebben.

In hoofdstuk 5 evalueren we het modulaire model. Aan de hand van de voorbeelden laten we zien dat het haalbaar is om een modulair artikel te schrijven op basis van het model en dat dat ons ook nuttig lijkt. In hoofdstuk 6 concluderen we dat het modulaire model wetenschappelijke communicatie inderdaad efficiënter en effectiever kan maken, mits zowel de auteur als de lezer beschikt over de juiste hulpmiddelen. De modulaire structuur maakt het voor de lezer namelijk mogelijk om selectief de gewenste versameling modules te vinden en te raadplegen, gebruikmakend van de etiketten van de modules en de links. Omdat de modulaire structuur systematisch en expliciet is, zijn modulaire artikelen ook duidelijker dan lineaire artikelen nu veelal zijn. En de modulaire structuur maakt het voor de auteur gemakkelijk om modules opnieuw te gebruiken.

We hebben het model ontwikkeld voor natuurwetenschappelijke artikelen, aan de hand van een analyse van artikelen over experimentele moleculaire dynamica. Het model echter ook bruikbaar als uitgangspunt voor andersoortige publicaties. In Appendix D schetsen we, aan de hand van een paar voorbeelden, hoe we de modularisering van een paar andere soorten publicaties zouden aanpakken.
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Ik heb mijn promotie-onderzoek gedaan aan het Van der Waals-Zeeman Instituut in het kader van het project ‘Communicatie in de Natuurkunde’. Dit is een samenwerkingsverband van de Faculteit der Wiskunde, Informatica, Natuurkunde en Sterrenkunde en de Faculteit der Geesteswetenschappen onder auspiciën van de Stichting Physica.

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Ik wil de andere leden van de leerstoelgroep Taalbeheersing Argumentatietheorie en Retorica en met name prof. Frans van Eemeren, prof. Rob Grootendorst, Francisca Snoeck Henke-
DANKWOORD

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Élévation

Au-dessus des étangs, au-dessus des vallées,
Des montagnes, des bois, des nuages, des mers,
Par delà le soleil, par delà les ethers,
Par delà les confins des sphères étoilées,

Mon esprit tu te meus avec agilité,
Et, comme un bon nageur qui se pâme dans l’onde,
Tu sillones gaïement l’immensité profonde
Avec une indicible et mâle volupté.

Envole-toi bien loin de ces miasmes morbides;
Va te purifier dans l’air supérieur,
Et bois, comme une pure et divine liqueur,
Le feu clair qui remplit les espaces limpides.

Derrière les ennuis et les vastes chagrins
Qui chargent de leur poids l’existence brumeuse,
Heureux celui qui peut d’une aile vigoureuse
S’élançon vers les champs lumineux et sereins;

Celui dont les pensers, comme des alouettes,
Vers les cieux le matin prennent un libre essor,
– Qui plane sur la vie, et comprend sans effort
Le langage des fleurs et des choses muettes!

–Charles Baudelaire, *Les fleurs du mal*