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First detection of ND in the solar-mass protostar IRAS16293-2422*


(Affiliations are available on page 5 of the online edition)

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ABSTRACT

Context. In the past decade, much progress has been made in characterising the processes leading to the enhanced deuterium fractionation observed in the ISM and in particular in the cold, dense parts of star forming regions such as protostellar envelopes. Very high molecular D/H ratios have been found for saturated molecules and ions. However, little is known about the deuterium fractionation in radicals, even though simple radicals often represent an intermediate stage in the formation of more complex, saturated molecules. The imidogen radical NH is such an intermediate species for the ammonia synthesis in the gas phase. Many of these light molecules however have their fundamental transitions in the submillimetre domain and their detection is hampered by the opacity of the atmosphere at these wavelengths. Herschel/HIFI represents a unique opportunity to study the deuteration and formation mechanisms of species not observable from the ground.

Aims. We searched here for the deuterated radical ND in order to determine the deuterium fractionation of imidogen and constrain the deuteration mechanism of this species.

Methods. We observed the solar-mass Class 0 protostar IRAS16293-2422 with the heterodyne instrument HIFI in Bands 1a (480–560 GHz), 3b (858–961 GHz), and 4a (949–1061 GHz) as part of the Herschel key programme CHESS (Chemical Herschel Survey of Star forming regions).

Results. The deuterated form of the imidogen radical ND was detected and securely identified with 2 hyperfine component groups of its fundamental transition (N = 0–1) at 522.1 and 546.2 GHz, in absorption against the continuum background emitted from the nascent protostar. The 3 groups of hyperfine components of its hydrogenated counterpart NH were also detected in absorption. The absorption arises from the cold envelope, where many deuterated species have been shown to be abundant. The estimated column densities are ~2 × 10^{14} cm^{-2} for NH and ~1.3 × 10^{13} cm^{-2} for ND. We derive a very high deuterium fractionation with [ND]/[NH] ratio of between 30 and 100%.

Conclusions: The deuterium fractionation of imidogen is of the same order of magnitude as that in other molecules, which suggests that an efficient deuteration mechanism is at play. We discuss two possible formation pathways for ND, by means of either the reaction of N^+ with HD, or deuteron/proton exchange with NH.

Key words. ISM: molecules – stars: formation

1. Introduction

The envelopes of low-mass Class 0 protostars have been known to be characterised by high levels of molecular deuteration, as shown e.g., by Loinard et al. (2002), Roberts et al. (2007, 2002), and the detection of multiply deuterated species (Ceccarelli et al. 1998 for D_2CO, Parise et al. 2002 for CHD_2OH, Parise et al. 2004 for CD_2OH, van der Tak et al. 2002 for ND). The high abundance of deuterated molecules is believed to originate in the pre-stellar phase (Bacmann et al. 2003): at the low temperatures (<20 K) and high densities (n > 10^{4} cm^{-3}) prevailing in pre-stellar cores (and similarly in protostellar envelopes), heavy molecules such as CO are depleted on the dust grains, so that species such as H_2D^+, D_2H^+, or D_3^+ reach high abundances. The increase in the [H_2D^+]/[H^+] ratio (and similar ratios involving multiply deuterated counterparts) enhances both the molecular deuterium fractionation by means of gas-phase reactions and the atomic D/H ratio, therefore also increasing the deuteration of species forming on grain surfaces (e.g. Roberts et al. 2003).

Most deuterated molecules detected to date are either saturated molecules or ions. The deuteration of radicals, which are important intermediate pieces leading to the formation of saturated molecules, has so far not been thoroughly investigated. Their observation could however provide an important clue to the formation process of the major deuterated species. For example, it is not yet completely understood if saturated deuterated molecules are formed directly (from deuterated ion intermediates, whose dissociative recombination may lead to deuterated radicals) like their hydrogenated counterparts, or if...
they are formed by proton-deuteron exchange starting from the saturated hydrogenated molecule. The observation of the D/H ratio in the radical may help us to disentangle these two processes. With this in mind, we study the deuterium ratio in the NH radical, which is formed from the dissociative recombination of NH$_2^+$ and NH$_2^+$, two precursors of ammonia in the gas-phase. Roueff et al. (2005) argued that highly-deuterated ammonia can form from pure gas phase reactions. These models however require highly deuterated radicals, and we propose to observationally test this model.

Light hydrides such as NH have fundamental transitions in the submillimetre domain. NH possesses 3 groups of hyperfine transitions around 950 GHz–1 THz and its deuterated counterpart ND has its 3 groups of fundamental hyperfine structure transitions around 490–550 GHz. At all of these frequencies apart from 490 GHz, the atmosphere is opaque and precludes observations from the ground. However, these transitions can all be observed with the HIFI instrument on board the Herschel Space Observatory. Since hydrides generally have high Einstein A$_{ul}$ coefficients, only the ground state is expected to be significantly populated. As a consequence, it is possible to detect these species in absorption against the continuum background originating from the heating of the nascent protostar. Moreover, as already mentioned above, deuterated molecules are very abundant in cold, dense medium, so that the envelopes of young protostars represent ideal targets to study the deuteration of the NH radical.

In the course of the CHESS key programme (Ceccarelli et al. 2010), we carried out a spectral survey of the frequencies covered by HIFI in the young low-mass protostar IRAS 16293-2422 (hereafter IRAS16293). The frequency bands contain the fundamental hyperfine transitions of NH and ND. In this Letter, we report the first detection by HIFI of ND, as well as the detection of the hyperfine transitions of NH. Section 2 describes the observations and the determination of the radicals' column densities, and Sect. 3 discusses the implications of the derived deuterium fractionation on our understanding of deuteration processes in N-bearing species.

2. Observations and results

The solar-mass protostar IRAS16293 was observed with the HIFI instrument (de Graauw et al. 2010; Roelfsema et al. 2010) on board the Herschel Space Observatory (Pilbratt et al., 2010), as part of the HIFI guaranteed time key programme CHESS (Ceccarelli et al. 2010). A full spectral coverage of bands 1a (480–560 GHz), 3b (858–961 GHz), and 4a (949–1061 GHz) was performed on 2010 March 1, 19, and 3, respectively, using the HIFI spectral scan double beam switch (DBS) mode with optimisation of the continuum. In this mode, the HIFI acousto-optic wide band spectrometer (WBS) was used, providing a spectral resolution of 1.1 MHz ($\approx 0.6$ km s$^{-1}$ at 520 GHz and 0.3 km s$^{-1}$ at 1 THz) over an instantaneous bandwidth of 4 x 1 GHz. The targeted coordinates were $\alpha_{2000} = 16^h32^m22^s75$, $\delta_{2000} = -24^\circ28'34''.2$. The DBS reference positions were situated approximately 3 east and west of the source. The beam sizes at the frequencies of the ND and NH transitions are about 41'' and 22'', respectively, and the theoretical main beam and forward efficiencies are about 0.72 and 0.96, respectively. Calibration uncertainties are $\leq 16\%$ for band 1 and $\leq 32\%$ for bands 3 and 4 (June 2010 estimates).

The data were processed using the standard HIFI pipeline up to frequency and amplitude calibrations (level 2) with the ESA-supported package HIPE 2.8 (Ott et al. 2010). A single local oscillator tuning spectrum consists, for each polarisation, of 4 sub-bands of $\approx 1$ GHz for the SIS bands (1 to 5). The 1 GHz scans are then exported as FITS files into CLASS/GILDAS format$^1$ prior to data reduction and analysis using generic spectral survey tools developed in CLASS by our group. Spurious features in the spectra were first removed in each 1 GHz scan, and a low order (typically 3) polynomial baseline was then fitted over line-free regions to correct for residual bandpass effects. These polynomials were subtracted and used to determine an accurate continuum level by calculating their medians. Higher order oscillations in the baseline are possible, but their amplitudes remain low in the spectra considered here. The continuum values obtained in this way are well fitted by a degree 1 polynomial over the frequency range $500–1200$ GHz. Sideband deconvolution is computed with the minimisation algorithm of Comito & Schilke (2002) implemented into CLASS90 using the baseline-subtracted spectra. The single side-band continuum derived from the polynomial fit at the considered frequency (Table 1) was eventually added to the spectra. The temperatures were converted to the $T_{\text{mb}}$ scale, using the theoretical values of the main beam and forward efficiencies given above.

We detect for the first time the 3 groups of hyperfine transitions of ND at 491.9, 522.1, and 546.2 GHz of the $N = 0$–1 transition as well as the 3 groups of hyperfine components of the NH fundamental transitions at 946.5, 974.5 GHz, and 1 THz (see Klaas et al. 1997 for an energy diagram of the $N = 0$–1 transition of NH). The transitions are seen in absorption against the continuum from the protostar and the hyperfine structure is partially resolved. The transitions of ND at 522.1 and at 546.2 GHz are presented in Fig. 1. From Fig. 1, the lines can be unambiguously attributed to ND (but see Olofsson et al. 2007, who tentatively assign an unidentified line to ND). The transition of ND at 491.9 GHz is not shown here because some of its components are strongly blended with a bright H$_2$CO line at 491.9683 GHz, with an SO$_2$ line at 491.9347 GHz and with an HDCHO line at 491.9370 GHz. This transition was not used in our analysis and will not be discussed further. Figure 2 presents the 3 detected hyperfine groups of the fundamental transition for NH.

The analysis was carried out by fitting the hyperfine structure using the HFS method in the CLASS software$^2$. The line parameters (frequencies, Einstein A$_{ul}$ coefficients, and level degeneracies), originally from spectrophotometric studies of Klaus et al. (1997) and Saito & Goto (1993) for NH and ND, respectively, were taken from the Cologne Database for Molecular Spectroscopy (Müller et al., 2001, 2005). The routine assumes a zero-baseline spectrum (i.e., from which the continuum emission has been subtracted) and therefore fits a line profile of the form $1 - e^{-\tau}(J(T_{\text{ex}}) - J(T_{\text{bg}}) = J_{\text{ex}})$, where $\tau$ is the optical depth, $T_{\text{ex}}$ the intensity of the continuum, and $J_{\text{ex}}(T_{\text{ex}})$ and $J(T_{\text{bg}})$ the radiation temperature for the excitation temperature $T_{\text{ex}}$ and the radiation temperature of the cosmological background, respectively. The parameters given by the HFS fitting procedure are reported in Table 2, Cols. (2) to (4). From the total optical depth $\tau$ given by the fit, we can infer the opacities of single hyperfine components by multiplying $\tau$ by the relative intensities of these components. The total column density of the considered species is given by

$$N = \frac{8\pi\nu^3}{c^3} \frac{Q(T_{\text{ex}})}{g_{\text{up}} A_{\text{ul}}} \cdot \left( e^{\frac{h\nu}{kT}} - 1 \right) \int \tau d\nu$$

$^1$ http://www.iram.fr/IRAMFR/GILDAS

$^2$ see the CLASS manual at http://www.iram.es/IRAMES/otherDocuments/manuals/index.html for more details.
Table 1. Measured rms (at a frequency resolution of 1.1 MHz) and assumed continuum values for the different transitions (in $T_{mb}$ scale).

<table>
<thead>
<tr>
<th>HIFI band</th>
<th>Transition $(N_{i}−N_{f})$</th>
<th>Frequency (GHz)</th>
<th>rms (mK)</th>
<th>Continuum (mK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>ND $(0_{1}−1_{1})$</td>
<td>522.1</td>
<td>12</td>
<td>205 ± 22</td>
</tr>
<tr>
<td>1a</td>
<td>ND $(0_{1}−1_{1})$</td>
<td>546.2</td>
<td>15</td>
<td>230 ± 24</td>
</tr>
<tr>
<td>3b</td>
<td>NH $(0_{1}−1_{1})$</td>
<td>946.5</td>
<td>58</td>
<td>832 ± 80</td>
</tr>
<tr>
<td>4a</td>
<td>NH $(0_{1}−1_{1})$</td>
<td>974.5</td>
<td>49</td>
<td>892 ± 143</td>
</tr>
<tr>
<td>4a</td>
<td>NH $(0_{1}−1_{1})$</td>
<td>1000.0</td>
<td>50</td>
<td>942 ± 146</td>
</tr>
</tbody>
</table>

where $v$ is the frequency of the transition, $c$ the velocity of light, $g_{ap}$ the upper level degeneracy, $A_{ej}$ the spontaneous emission Einstein coefficient, $T_{ex}$ the excitation temperature, $Q(T_{ex})$ the partition function at $T_{ex}$, and $E_{up}$ the upper level energy. For the values of the excitation temperature and the frequencies considered here, the factor with the exponentials is nearly equal to 1. The velocity integrated optical depth of component $i$ is given by $\tau_{i} = \frac{A_{ej} \nu^{2}}{2 \sqrt{2 \pi} \sigma_{i}}$ with $\tau_{i}$ the optical depth of component $i$ and $\Delta \nu$ the linewidth determined by the HFS method (full width at half maximum). The obtained values of the column density are given for each group of hyperfine components in Col. (6) of Table 2. In our derivation of the excitation temperature, it was assumed that the zone where the absorption arises completely fills the emission zone of the continuum. In the HFS fitting method, the determination of the depth comes only from the measured values of the hyperfine components and is independent of any assumption about the filling factor. Overall, since the exponential factor is close to 1 in Eq. (1), and the partition function depends only mildly on $T_{ex}$ (in the case of NH for example, it increases by 10% when $T_{ex}$ increases from 10 to 15 K), the inferred value of the column density depends very little on the assumptions about the value of the continuum, beam efficiency values, or absolute calibration uncertainties.

The column density found for NH is $N$(NH) = $(2.0 \pm 0.8) \times 10^{14}$ cm$^{-2}$. For ND, the column density values found from the 2 observed transitions differ slightly but are consistent within the error bars. A reasonable estimate for the ND column density is therefore: $N$(ND) = $(1.3 \pm 0.8) \times 10^{14}$ cm$^{-2}$.

With these values, we find an imidogen deuterium fraction of $[ND]/[NH] \sim 30–100\%$ in the envelope of IRAS16293. We note however that because of the differences in beam sizes, the region sampled by the ND observations is larger and on average characterised by lower densities and temperatures than the region sampled by the NH observations for which the contribution of the warmer inner regions is larger. To take these effects into account, a more detailed radiative transfer modelling – taking into account the source structure and the exact coupling between the source and the instrument – would be necessary. The similarity of the determined linewidths (around 0.5 km s$^{-1}$ in both lines, when deconvolved from the resolution of the spectrometer) is consistent with the bulk of the signal from both molecules arising from the same (cold) region.

3. Discussion and conclusions

The very high deuterium fractionation observed in IRAS16293 is of the same order of magnitude as the molecular D/H ratio previously measured in other species in the envelope of IRAS16293, i.e., $[HDCCO]/[H_{2}CO] = 15\%$, $[NH_{2}D]/[NH_{3}] = 10\%$ (van Dishoeck et al. 1995) $[CH_{2}DOH]/[CH_{3}OH] = 30\%$ (Parise et al. 2004). The $[ND]/[NH]$ ratio even appears to be the highest measured deuterium fractionation in this source, though this result needs to be confirmed with a more detailed modelling.
are needed to constrain the deuteration and formation of NH and this will be the subject of a future study.

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References
