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Letter to the Editor

Detection of DCO^+ in a circumstellar disk

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Abstract. We report the first detection of DCO^+ in a circumstellar disk. The DCO^+ $J = 5-4$ line at 360.169 GHz is observed with the 15 m James Clerk Maxwell Telescope in the disk around the pre-main sequence star TW Hya. Together with measurements of the HCO^+ and $H^{13}CO^+$ $J = 4-3$ lines, this allows an accurate determination of the DCO^+/HCO^+ ratio in this disk. The inferred value of 0.035 ± 0.015 is close to that found in cold pre-stellar cores and is somewhat higher than that measured in the envelope around the low-mass protostar IRAS 16293–2422. It is also close to the DCN/HCN ratio obtained for pristine cometary material in the jet of comet Hale-Bopp. The observed DCO^+/HCO^+ ratio for TW Hya is consistent with theoretical models of disks which consider gas-phase fractionation processes within a realistic 2-D temperature distribution and which include the effects of freeze-out onto grains.

1. Introduction

Disks around pre-main sequence stars are the likely sites of the formation of planetary systems (e.g., Beckwith 1999). Part of the gas and dust from the collapsing protostellar envelope settles into this disk, where it may undergo a complex chemistry before incorporation into planets and icy bodies. Tracing this chemistry is a key goal of molecular astrophysics, not only to establish a chemical inventory prior to planet formation but also as a probe of the dynamical processes in disks such as radial and vertical mixing (e.g., Aikawa et al. 1999; Markwick et al. 2002). Moreover, the abundances and excitation of the molecules provide unique insight into the physical structure of disks such as their temperature and density profiles (Dutrey et al. 1997; van Zadelhoff et al. 2001).

Deuterated molecules are a particularly interesting probe of the temperature history of interstellar and circumstellar gas. It is well known that the abundances of deuterated molecules in cold pre-stellar cores and protostellar envelopes are enhanced by orders of magnitude over the elemental [D]/[H] abundance ratio of 1.5×10^{-5} through fractionation (e.g., Watson 1976; Millar et al. 1989). In particular, at temperatures below ~50 K, the reaction

$$H_3^+ \; + \; HD \rightleftarrows H_2D^+ \; + \; H_2 \; + \; 232\ \mathrm{K} \qquad (1)$$

is driven strongly in the forward direction (e.g., Pagani et al. 1992). H_2D^+ can subsequently transfer a deuteron to the abundant CO molecule

$$H_2D^+ \; + \; CO \rightarrow \; DCO^+ \; + \; H_2 \qquad (2)$$

leading to DCO^+/HCO^+ ratios of order 0.01. Such high ratios have indeed been observed in interstellar clouds (e.g., Guélin et al. 1977; Wootten et al. 1982; Butner et al. 1995; Williams et al. 1998) and in protostellar regions (van Dishoeck et al. 1995; Loinard et al. 2000; Shah & Wootten 2001; Parise et al. 2002). Deuterium fractionation can also occur through reactions of atomic deuterium on the surfaces of interstellar grains (Tielens 1983), but this is thought to affect primarily molecules which are formed on grains such as H_2CO and CH_3OH. The DCO^+/HCO^+ ratio can thus serve as a clear measure of the importance of low-temperature gas-phase deuterium fractionation processes. Moreover, this ratio is enhanced if the main destroyer of H_3^+, – i.e., CO –, is depleted onto grains, since reaction (1) then becomes an important H_3^+ removal route in addition to recombination with electrons, enhancing H_2D^+ even more (Brown & Millar 1989; Stark et al. 1999; Caselli et al. 1999). Thus, the DCO^+/HCO^+ ratio can also trace the level of depletion.

We present here the first detection of the DCO^+ ion in a circumstellar disk, using the James Clerk Maxwell Telescope (JCMT). Together with observations of the HCO^+ ion and its optically thin isotope $H^{13}CO^+$, an accurate DCO^+/HCO^+ ratio is derived. This ratio is subsequently compared with that found in the envelopes of deeply embedded protostars – the precursor material of disks –, and with those observed in solar system objects, in particular comets – the remnant material of disks.

2. Observations

The DCO^+ $J = 5-4$ rotational line at 360.169 GHz was observed with the JCMT[1] on Mauna Kea, Hawaii. The dual

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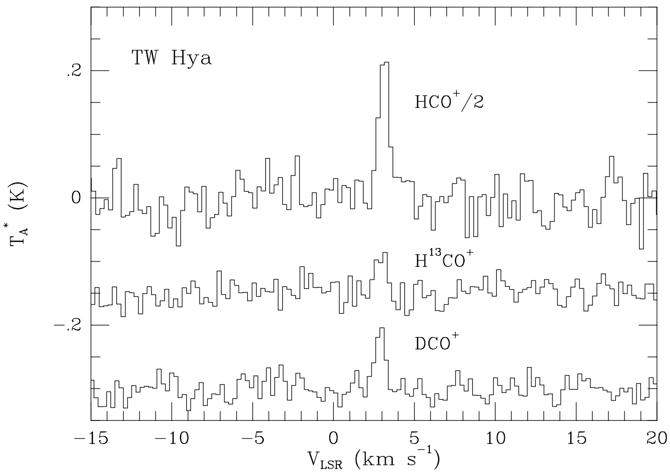

Fig. 1. JCMT observations of the HCO^+ $J = 4{-}3$, $H^{13}CO^+ J = 4{-}3$ and DCO^+ $J = 5{-}4$ lines toward TW Hya. The $H^{13}CO^+$ and DCO^+ spectra have been shifted by –0.15 and –0.3 K, respectively.

Table 1. Summary of observational data.

Species	Line	$\int T_{\rm MB} dV$ (K km s^{-1})	N^a_{200} (10^{12} cm^{-2})
HCO^+	$J = 4{-}3$	0.49	8.5^b
$H^{13}CO^+$	$J = 4{-}3$	0.07	0.14
DCO^+	$J = 5{-}4$	0.11	0.30

[a] Column density derived under the assumption of LTE excitation at 25 K for a 200 AU radius disk.
[b] The HCO^+ value is obtained from the optically thin $H^{13}CO^+$ column density assuming $[^{12}C]/[^{13}C] = 60$.

polarization receiver B3 was used in single-sideband mode. The backend was the Digital Autocorrelator Spectrometer (DAS) set at a resolution of ~0.15 km s^{-1}. The observations were taken in beam-switching mode with a throw of 180″. The same set-up was used to observe the HCO^+ and $H^{13}CO^+$ $J = 4{-}3$ lines at 356.734 and 346.998 GHz, respectively. The antenna temperatures were converted to main-beam temperatures using a beam efficiency of 62%, calibrated from observations of planets by the telescope staff. The flux calibration was checked against bright sources with well-determined fluxes for different lines and was generally found to agree within 10%. The data were reduced and analyzed in the SPECX and CLASS data reduction packages.

The DCO^+ search focussed on the disk around TW Hya, an isolated T Tauri star (K8Ve) which is part of a young group of stars at a distance of only ~56 pc (Webb et al. 1999). Its age is estimated to be ~7–15 Myr, somewhat older than most classical T Tauri stars, but its large lithium abundance and Hα equivalent width are indicative of continued active disk accretion at a rate of 10^{-8} $M_\odot$ yr^{-1} (Kastner et al. 2002). TW Hya is surrounded by a nearly face-on disk of $\sim 2 \times 10^{-2}$ $M_\odot$ (Wilner et al. 2000), which has been imaged recently in scattered light with the Hubble Space Telescope (Krist et al. 2000). The extent of the disk in the scattered light is ~200 AU, corresponding to a 3.6″ radius at 56 pc. Since this size is small compared with the ~13″ beam size of the JCMT at 360 GHz, the data suffer from beam dilution. Thus, long integration times of typically 2–4 hrs were needed to detect the weak lines reported here.

The DCO^+ and HCO^+ observations are part of a larger survey for molecular lines from disks, which will be reported in Thi et al. (2003).

3. Results

In Fig. 1, the HCO^+, $H^{13}CO^+$ and DCO^+ spectra toward TW Hya are presented. All three lines are clearly detected at the same velocity, $V_{\rm LSR} = 3.0 \pm 0.1$ km s^{-1}. The lines are very narrow, $\Delta V \approx 0.6$ km s^{-1}, and do not show the characteristic double-peak profile of a rotating disk, consistent with the nearly face-on orientation. The lack of detection of the ^{12}CO 3–2 line at 30″ offset positions demonstrates that the molecular emission is indeed associated with the disk and not due to any remnant cloud material in the vicinity (Thi et al. 2003). The critical densities of the observed HCO^+ and DCO^+ lines are at least 10^6 cm^{-3}, further assuring that only the dense gas in the disk is probed. The integrated line intensities are summarized in Table 1.

Molecular column densities and abundances can be derived from the observed line strengths under different assumptions. In general, the emerging lines from interstellar gas are a complex function of abundance, excitation and radiative transfer effects. In circumstellar disks, where strong chemical gradients can exist in both vertical and radial directions, the interpretation of spatially unresolved data is particularly uncertain. However, since the main interest of this study is in the DCO^+/HCO^+ ratio, the analysis can be considerably simplified if it is assumed that DCO^+ and HCO^+ occupy roughly the same regions of the disk. Moreover, since the densities in disks are generally high in the regions where these molecules exist ($>10^6$ cm^{-3}) (van Zadelhoff et al. 2001), the excitation can be assumed to be in local thermal equilibrium to first order. A single excitation temperature of 25 K is adopted in the following analysis. Finally, both the $H^{13}CO^+$ and DCO^+ lines are assumed to be optically thin. The observed line intensity ratio of $HCO^+/H^{13}CO^+$ of ~7 compared with the optically thin ratio of ~60 clearly indicates that the main isotope HCO^+ $J = 4{-}3$ line is optically thick.

The inferred column densities for a 200 AU radius disk are included in Table 1. For an assumed gas + dust disk mass of 2×10^{-2} $M_\odot$, the beam-averaged HCO^+ abundance is $\sim 2\times10^{-11}$, derived from the optically thin $H^{13}CO^+$ line assuming LTE excitation at 25 K (see Thi et al. 2003 for details). This is significantly lower than the typical HCO^+ abundance of $\sim 10^{-9}{-}10^{-8}$ in dark clouds (e.g., Ohishi et al. 1992) and some protostellar envelopes (e.g., Schöier et al. 2002). Most of the observed emission is thought to originate from the warm intermediate layer of the disk just below the surface where the HCO^+ abundance reaches a few $\times 10^{-10}$ (e.g., Aikawa et al. 2002; Willacy & Langer 2000). The molecules are significantly depleted in the cold midplane of the disk where the bulk of the mass resides. For the TW Hya disk, observations of CO and other

Table 2. Deuterium fractionation ratios in different environments.

Type of region	Object	Species	D/H	Reference
Dark cores	Various	DCO^+	0.02–0.07	Butner et al. (1995)
	Various	DCO^+	0.02–0.06	Williams et al. (1998)
	TMC-1 CP-peak	DCO^+	0.012	Turner (2001)
	L1544	DCO^+	0.04	Caselli et al. (2002)
	L1689N D-peak	DCO^+	0.08	Lis et al. (2002)
	L134N	DCO^+	0.18	Tiné et al. (2000)
Low-mass protostars	IRAS 16293-2422	DCO^+	0.009	Schöier et al. (2002)
		DCN	0.012	Schöier et al. (2002)
	NGC 1333 I4A	DCO^+	0.01	Stark et al. (1999)
	Various	DCO^+	0.005–0.035	Shah & Wootten (2001)
		DCN	0.01–0.02	Shah & Wootten (2001)
Disk	TW Hya	DCO^+	0.035	This work
Comet	Hale-Bopp jet	DCN	0.09	Blake et al. (1999)
	Hale-Bopp coma	DCN	0.002	Meier et al. (1998)
Disk model	Outer ≥200 AU	DCO^+	0.05	Aikawa et al. (2002)
		DCN	0.03	Aikawa et al. (2002)
	Inner 50 AU	DCO^+	0.002	Aikawa et al. (2002)
		DCN	0.001	Aikawa et al. (2002)

species indicate depletions up to a factor of 100 in the midplane (van Zadelhoff et al. 2001).

4. Discussion

The inferred column densities imply a beam-averaged DCO^+/HCO^+ abundance ratio of 0.035 ± 0.015, assuming a $[^{12}C]/[^{13}C]$ isotopic ratio of 60 (see Table 1). The error bar reflects the observational uncertainties. The DCO^+/HCO^+ value is more than three orders of magnitude higher than the elemental [D]/[H] ratio of 1.5×10^{-5}, illustrating that strong deuterium fractionation occurs in disks.

Models of the deuterium fractionation in disks have been calculated by Aikawa & Herbst (1999, 2001) and Aikawa et al. (2002), with the latter models using a realistic 2-dimensional (2D) temperature and density structure of a flaring disk. The models include a detailed gas-phase chemistry network with freeze-out onto grains, but do not contain an active grain-surface chemistry. The resulting DCO^+/HCO^+ abundance is found to decrease with decreasing radius from ~0.1 at 400 AU to <0.01 at <50 AU, owing to the increasing temperature in the inner disk. The DCO^+/HCO^+ ratio also decreases with height in the outer disk, because of the higher temperatures in the upper layers. Close to the midplane where strong CO freeze-out occurs, the DCO^+/HCO^+ ratio reaches high values, but this region contributes negligibly to the observed emission due to the much lower overall abundances. Time-dependent effects appear to play a minor role, although results for disks as old as 10 Myr have not been published. Overall, the observed DCO^+/HCO^+ ratio of 0.035 ± 0.015 averaged over the entire TW Hya disk appears consistent with these models.

Roberts et al. (2002) show that the model results for molecular clouds are lowered by a factor of a few if updated rate coefficients for reaction (1) are used. Since the main processes affecting the DCO^+/HCO^+ ratio in disks, namely low-temperature gas-phase reactions and freeze-out of CO on grains, are the same as those in clouds, similar effects are expected for disk models using updated rate coefficients.

Only few other measurements of deuterated molecules in disks have been reported. Qi (2001) and Kessler et al. (2003) searched for DCN and HDO in several disks using the Owens Valley Millimeter Array but obtained mostly upper limits. The inferred DCN/HCN ratio of <0.002 is much lower than that for DCO^+/HCO^+ found here.

Table 2 summarizes the observed DCO^+/HCO^+ and DCN/HCN ratios in different environments. It is seen that the DCO^+/HCO^+ ratio in the TW Hya disk is comparable to that found in cold dark cores where freeze-out has been observed (e.g., L1544), testifying to the low temperatures in disks. Indeed, DCO^+/HCO^+ ratios as high as 0.035 are difficult to produce in models which do not include CO depletion (Roberts et al. 2002). It is higher than that found in most protostellar envelopes, where heating has affected a larger fraction of the material resulting in higher temperatures and less CO freeze-out.

Because comets spend much of the time since their formation in the cold outer region of the Solar System, they are likely to contain the most primitive record of solar nebula material. No DCO^+ is observed in comets, but DCN/HCN has been measured. In cold clouds and protostellar envelopes, the observed DCN/HCN ratios are often comparable to the DCO^+/HCO^+ ratios (see Table 2), even though they involve different fractionation reactions. The most pristine material originating from below the comet surface and emanating in jets shows very high DCN/HCN ratios comparable to those seen in cold dark clouds and in the TW Hya disk. The upper surface layers which evaporate to produce the coma have significantly lower ratios, indicative of processing in the solar nebula.

The similarity of the deuterium fractionation ratios in cold clouds, disks and pristine cometary material suggests that the gas spends most of its lifetime at low temperatures and is incorporated into the disks before the envelope is heated, i.e., before the Class I stage. Alternatively, the DCO^+/HCO^+ ratio may be reset in disks by low-temperature gas-phase chemistry. Comparison of D/H ratios of molecules which enter the disk in the gas phase (such as HCO^+) and those which are likely incorporated as ices (e.g., H_2CO, CH_3OH) can distinguish between these scenarios. Also, spatially resolved data can further test the models, since the high ratios observed here probe largely the outer disk.

The data presented in this paper are at the limit of the capabilities of current observational facilities. The Atacama Large Millimeter Array (ALMA) will be essential to provide high-resolution measurements of D/H ratios in disks down to comet- and planet-forming regions.

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