DETECTION OF INTERSTELLAR H$_2$D$^+$ EMISSION

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ABSTRACT

We report the detection of the $^{1}l_0-^{1}l_1$ ground-state transition of ortho-H$_2$D$^+$ at 372.421 GHz in emission from the young stellar object NGC 1333 IRAS 4A. Detailed excitation models with a power-law temperature and density structure yield a beam-averaged H$_2$D$^+$ abundance of $3 \times 10^{-12}$ with an uncertainty of a factor of 2. The line was not detected toward W33A, GL 2591, and NGC 2264 IRS (in the latter source at a level that is 3–8 times lower than previous observations). The H$_2$D$^+$ data provide direct evidence in support of low-temperature chemical models in which H$_2$D$^+$ is enhanced by the reaction of H$_3^+$ and HD. The H$_2$D$^+$ enhancement toward NGC 1333 IRAS 4A is also reflected in the high DCO$^-$/HCO$^+$ abundance ratio. Simultaneous observations of the N$_2$H$^+$ 4–3 line show that its abundance is about 50–100 times lower in NGC 1333 IRAS 4A than in the other sources, suggesting significant depletion of N$_2$. The N$_2$H$^+$ data provide independent lower limits on the H$_3^+$ abundance that are consistent with the abundances derived from H$_2$D$^+$. The corresponding limits on the H$_3^+$ column density agree with recent near-infrared absorption measurements of H$_3^+$ toward W33A and GL 2591.

Subject headings: ISM: abundances — ISM: molecules — molecular processes — radio lines: ISM — submillimeter

1. INTRODUCTION

The recent detection of the H$_3^+$ ion in interstellar clouds through its infrared vibration-rotation lines (Geballe & Oka 1996; McCall et al. 1998) is an important confirmation of the gas-phase chemical networks (Herbst & Klemperer 1973; Watson 1973b). Because of its symmetry, H$_3^+$ has no allowed rotational transitions contrary to its deuterated isotopomer H$_2$D$^+$, which has a large permanent dipole moment (Dalgarno et al. 1983). This makes it possible to initiate a vibrational transition in the interstellar ion-molecule chemistry at low temperatures where significant enhancement of deuterated molecules occurs as a result of fractionation (e.g., Watson 1973a; Herbst 1982; Millar, Bennett, & Herbst 1989). This process is initiated by the isotope exchange equilibrium reaction

$$\text{H}_3^+ + \text{HD} \rightleftharpoons \text{H}_2\text{D}^+ + \text{H}_2,$$

which is shifted in the forward direction at low temperatures (Smith, Adams, & Alge 1982; Herbst 1982). The formation of H$_2$D$^+$ is followed by deuteron transfer reactions with, e.g., CO to form DCO$^+$, and the H$_2$D$^+$ enhancement is reflected in the observed large abundance ratios of, e.g., DCO$^+$/HCO$^+$, NH$_3$/NH$_2$, and DCN/HCN in cold clouds (e.g., Wootten 1987; Butner, Lada, & Loren 1995; Williams et al. 1998).

Over the last 20 years, numerous attempts have been made to detect the $^{1}l_0-^{1}l_1$ ortho-H$_2$D$^+$ and $^{1}l_0-^{0}l_0$ para-H$_2$D$^+$ ground-state lines at 372 and 1370 GHz, respectively. These searches have mainly been done with the Kuiper Airborne Observatory (KAO) (Phillips et al. 1985; Pagani et al. 1992b; Boreiko & Betz 1993), and a possible absorption feature at 1370 GHz has been reported by Boreiko & Betz (1993) toward Orion. Observations from the ground are very difficult since the 372 GHz line is at the edge of a strong atmospheric water absorption line, while the atmosphere at 1370 GHz is almost completely opaque. With the advent of new submillimeter receivers equipped with sensitive niobium SIS mixers, it has become possible to search for weak ortho-H$_2$D$^+$ lines from high, dry sites such as Mauna Kea. Indeed, a ground-based search for this line from the Caltech Submillimeter Observatory by van Dishoeck et al. (1992) yielded limits that are up to a factor of 100 more sensitive than those obtained with the KAO. Comparison with chemical models suggested that only a factor of a few improvement would be needed to detect the line. With the new facility receiver RxB3 at the James Clerk Maxwell Telescope (JCMT), an improvement in sensitivity is now achievable. Here we report the detection of the H$_2$D$^+$ 372.421 GHz line toward NGC 1333 IRAS 4A and significant upper limits toward W33A, GL 2591, and NGC 2264 IRS. Simultaneous observations of the N$_2$H$^+$ 4–3 line at 372.672 GHz toward these young stellar objects (YSOs) are used to place additional constraints on the H$_3^+$ abundance.

2. OBSERVATIONS

The observations of the $^{1}l_0-^{1}l_1$ ground-state transition of ortho-H$_2$D$^+$ at 372.42134 GHz (Boge et al. 1984) were done with the JCMT in 1998 August 31 and September 15 and 18 during three nights of very good submillimeter transparency with a zenith opacity at 225 GHz below 0.05. The dual-polarization heterodyne receiver RxB3 was used. Both mixers were tuned to 372.5469 GHz in the upper sideband. The big advantage of RxB3 is that it has a dual-beam interferometer that allows single-sideband (SSB) operation, enhancing the sensitivity and calibration at 372 GHz considerably. The digital autocorrelator spectrometer was split into four parts of

1. The JCMT is operated by the Joint Astronomy Centre (JAC) in Hilo, Hawaii, on behalf of the Particle Physics and Astronomy Research Council in the UK, the Netherlands Organisation for Scientific Research, and the National Research Council of Canada.

2. The junctions for the RxB3 mixers were fabricated by SRON/DIMES.
125 MHz. This setup allows observations of both lines in two orthogonal polarizations simultaneously, with a spectral resolution of 376 kHz (≈0.3 km s⁻¹ at 372 GHz). Typical SSB system temperatures, including atmospheric losses, were about 1200 K. The effective total integration time was 7 hr on NGC 1333 observed over two nights, 2.7 hr on W 33A, 4.3 hr on GL 2591, and 4 hr on NGC 2264. The absolute calibration uncertainty is estimated at 30%, and the relative calibration between the H₂D⁺ and N₂H⁺ lines is much better. The JCMT beam size at 372 GHz is 13″ FWHM; the main-beam efficiency is 70%. JCMT data on HCO⁺ and DCO⁺ were taken from the literature (see below), except for DCO⁺ toward W 33A and GL 2591, for which the 3–2 transition at 216.113 GHz was observed with receiver RxA3. The beam size at this frequency is 21″ FWHM, and the main-beam efficiency is 70%.

The observed H₂D⁺ and N₂H⁺ spectra are presented in Figure 1. The source and line parameters are listed in Table 1. The H₂D⁺ line is clearly detected with T_a = 0.08 ± 0.03 K toward NGC 1333 IRAS 4A and is seen in spectra of both nights. The velocity width shows good agreement with the N₂H⁺ line width, while the velocities are offset by about 0.5 km s⁻¹. Comparison with the line survey of Blake et al. (1995) shows that such an offset is small and common for this region.

No H₂D⁺ emission was detected toward NGC 2264 IRS, W 33A, and GL 2591. Assuming the same width as the N₂H⁺ line, 2σ upper limits of T_a ≤ 0.02–0.04 K are obtained. For NGC 2264, this limit is about a factor of 8 below the possible feature of Phillips et al. (1985) and a factor of 3 below the limit reached by van Dishoeck et al. (1992). Note that the N₂H⁺ emission toward NGC 1333 is much weaker than that toward the other sources. No other lines were detected in the 125 MHz bands.

### Table 1

| Source  | Molecule  | Transition | T_a (K) | ΔV (km s⁻¹) | V_{lsr} (km s⁻¹) |
|---------|-----------|------------|---------|-------------|-----------------|
| N1333   | H₂D⁺      | 1_0–1_11   | 0.08 (0.03) | 1.2 ± 0.3 | 7.4 ± 0.2 |
|         | N₂H⁺      | 4–3        | 2.57 (0.03) | 1.35  | 6.94  |
| N2264   | H₂D⁺      | 1_0–1_11   | ≤0.02     | ...    | ...    |
|         | N₂H⁺      | 4–3        | 4.51 (0.03) | 2.67  | 8.01  |
| W33A    | H₂D⁺      | 1_0–1_11   | ≤0.04     | ...    | ...    |
|         | N₂H⁺      | 4–3        | 3.06 (0.06) | 4.62  | 37.40 |
| GL 2591 | H₂D⁺      | 1_0–1_11   | ≤0.02     | ...    | ...    |
|         | N₂H⁺      | 4–3        | 1.41 (0.04) | 2.89  | −5.82 |

* The values in parentheses represent 1σ statistical uncertainties. The absolute uncertainty of the intensity is 30%; ΔV and V_{lsr} are accurate to better than 0.1 km s⁻¹.
* Position (B1950): NGC 1333 IRAS 4A (α = 03°26′29″, δ = +31°03′14″); NGC 2264 IRS (α = 06°38′25″, δ = +09°32′29″); W 33A (α = 18°11′44″, δ = −17°52′56″); and GL 2591 (α = 20°27′35″, δ = −40°01′14″).

3. Analysis

Model calculations were performed to determine the abundances of H₂D⁺, N₂H⁺, HCO⁺, and DCO⁺ using a power-law density structure n = n_0 (r/R₀)^α, as described in van der Tak et al. (1999a). In these models, the radial dust temperature profile is calculated from the observed luminosity, and n_0 is determined from submillimeter photometry, which probes the total dust mass. The grain heating and cooling are solved self-consistently as a function of radius, r, using grain properties from Ossenkopf & Henning (1994). The outer radius (R₀) is determined from high-resolution submillimeter line and continuum maps. The exponent α is constrained by modeling the relative strength of emission lines of CS and H₂CO at the central position over a large range of critical densities with a Monte Carlo radiative transfer program, assuming T_k = T_{dust}. Data were taken from Blake et al. (1995) (NGC 1333 IRAS 4A), de Boisanger, Helmich, & van Dishoeck (1996) and Schreyer et al. (1997) (NGC 2264 IRS), and van der Tak et al. (1999a, 1999b) (GL 2591 and W 33A). For NGC 1333 IRAS 4A, where CS is heavily depleted, α = 2 was taken based on the analysis of the continuum visibilities in interferometer data by Looney (1998).

Given the calculated temperature and density structure, the radiative transfer models were run in order to determine the abundances, assuming initially a constant abundance throughout the envelope. Both the ortho-H₂D⁺ and para-H₂D⁺ ladders have been considered since their spin states are coupled through reactive collisions with H₂; thus, the para 000 level is the true rotational ground state. A de-excitation rate coefficient of 1.0 × 10⁻¹⁰ cm³ s⁻¹ has been used for all inter-ladder transitions (see Herbst 1982 and Pagani, Salez, & Wannier 1992a for a detailed study of the ortho/para ratio). The lower level of the 1_0–1_1 transition lies at 86 K. The excitation energy of the 1₁₁ level is 18 K relative to the 1₁₁ level, and the critical density for this transition is about 2 × 10¹⁵ cm⁻³.

The calculated abundances are listed in Table 2. Toward NGC 1333, we infer a beam-averaged abundance x(H₂D⁺) = 3 × 10⁻¹². Upper limits on the abundance toward NGC 2264, W 33A, and GL 2591 are less than 1 × 10⁻¹¹. The N₂H⁺ abundance ranges between 10⁻¹¹ toward NGC 1333 and 10⁻⁹ toward...
W33A. All derived abundances have an absolute uncertainty of a factor of 2 because of the uncertainties in the dust opacities and CO abundances. The relatively high N$_2$H$^+$ abundance toward NGC 2264 was already found by van Dishoeck et al. (1992), who noted that nearly all of the gas-phase nitrogen must be in the form of N$_2$ in this cloud. Since N$_2$H$^+$ is formed mainly by the reaction of H$_3^+$ and N$_2$, the latter observations provide an independent lower limit on the H$_3^+$ abundance. Destruction occurs mainly via reactions with CO, O, and electrons. Considering CO destruction only,\[ n(H_3^+) \approx 0.5n(N_2H^+)x(CO)/x(N_2). \] (2)

Assuming 50% of the nitrogen is in N$_2$, x(N$_2$) = 5 × 10$^{-5}$δ(N$_2$), x(CO) = 2 × 10$^{-4}$δ(CO), and equal amounts of depletion δ for CO and N$_2$, this yields x(H$_3^+$) ≈ 2x(N$_2$H$^+$). These limits are listed in Table 2 and are consistent with the upper limits derived from the H$_2$D$^+$ observations using a theoretical H$_2$D$^+$/H$_3^+$ ratio (see § 4).  

### Table 2: Excitation Model Parameters and Deduced Abundances

| Source         | α | n$_0$ (cm$^{-3}$) | T (K) | H$_2$D$^+$ | N$_2$H$^+$ | H$_3$$^+$ | H$_3$$^+$ | H$_2$D$^+$/H$_3$$^+$ | DCO$^+$/HCO$^+$ | CO$^+$ | N$_2$ |
|----------------|---|------------------|------|------------|-------------|-----------|-----------|---------------------|----------------|--------|-------|
| N1333          | 2 | 1.7(6)           | 318  | 1 (11)     | 2 (10)      | 1 (11)    | 2 (4)     | 4 (11)              | 2 (10)         | 4 (11) |       |
| N2264          | 1.5| 1.5(4)           | 293  | 10 (11)    | 2 (10)      | 1 (11)    | 2 (4)     | 4 (11)              | 2 (10)         | 4 (11) |       |
| W33A           | 1 | 2 (1)            | 280  | 10 (11)    | 2 (10)      | 1 (11)    | 2 (4)     | 4 (11)              | 2 (10)         | 4 (11) |       |
| GL 2591        | 1.25| 3.5(4)           | 350  | 10 (11)    | 2 (10)      | 1 (11)    | 2 (4)     | 4 (11)              | 2 (10)         | 4 (11) |       |

*From statistical equilibrium calculations using the appropriate temperature and density structure as a function of distance r to the YSO, n(r) = n$_0$(r/R$_0$)$^{-a}$, where R$_0$ is the outer radius of the model envelope: NGC 1333 IRAS 4A [3.1(3) AU], NGC 2264 IRS 4.7(4) AU, W33A [2.4(5) AU], GL 2591 [3.1(4) AU], and R = R$_0$/300 is the inner radius. The notation a(b) indicates a × 10$^b$. The accuracy of the deduced abundances is a factor of 2.

* From H$_2$D$^+$ using a theoretical H$_3^+$/H$_2$D$^+$ ratio at the effective temperature from which most of the emission arises (see Fig. 2).

* From N$_2$H$^+$ analysis (see text).

* From H$^+$CO$^+$ assuming HCO$^+$/H$^+$CO$^+ = 60$.

* From C/O assuming CO/C$^{17}$O = 2500 and using the appropriate NH$_3$ from submillimeter dust emission in a 13° beam: NGC 1333 IRAS 4A [3.1(23) cm$^{-3}$], NGC 2264 IRS 1.2(23) cm$^{-3}$, W33A 5.2(23) cm$^{-3}$, and GL 2591 1.3(23) cm$^{-3}$.

### 4. H$_2$D$^+$/H$^+$ Chemistry

The above analysis assumes constant abundances throughout the YSO envelopes. In reality, the H$_2$D$^+$ abundance is a strong function of temperature and position. In chemical equilibrium, the H$_3^+$ abundance can be written as x(H$_3^+$) = γΣk$_x$n(X), with n(X) = n(H$_2$)x(X), X refers to any of O, C, CO, O$_2$, N$_2$, H$_2$O, etc., as are the principal removal agents of H$_3^+$ via the proton transfer reactions

\[ H_3^+ + X \rightarrow XH^+ + H_2, \] (3)

where k$_x$ are the rate coefficients (taken from the UMIST database; see, e.g., Millar, Farquhar, & Willacy 1997) and Σ is the cosmic-ray ionization rate (taken to be 5 × 10$^{-17}$ s$^{-1}$). A simple chemical model for the formation and destruction of H$_2$D$^+$ yields

\[ x(H_2D^+) = \frac{x(HD)k_1 + x(D)k_2}{x(e)k_3 + \sum k_x x(X) + k_4}, \] (4)

where k$_1$ and k$_2$ are the forward and backward rate coefficients of reaction (1), k$_3$ is the rate coefficient for the formation of H$_2$D$^+$ through the reaction H$_3^+$ + D, and k$_4$ is the rate coefficient of the electron recombination of H$_2$D$^+$ (see, e.g., Caselli et al. 1998 for a compilation of values). We assumed x(HD) = 10x(D) = 2.8 × 10$^{-17}$ throughout.

The above H$_3^+$ and H$_2$D$^+$ chemical equations were included in the power-law models, and abundances at each position were calculated for the appropriate temperature and density. We have fixed the expression for k$_3$ at T < 20 K to its value at 20 K, to ensure that x(H$_2$D$^+$) < x(H$_3^+$) throughout. For simplicity, only X = CO was considered. and the electron recombination was neglected. The CO depletions are inferred from C$^{17}$O observations using the method described by van der Tak et al. (1999a, 1999b) and are listed in Table 2. For a homogeneous temperature and density structure, our model agrees well with the models of Millar et al. (1989) and Pagani et al. (1992a).

The power-law model results for NGC 1333 IRAS 4A are presented in Figure 2. Using these abundances, the H$_2$D$^+$ emission has been calculated, most of which originates from gas at T = 25–35 K. The model intensity agrees within 30% with that measured toward NGC 1333 IRAS 4A and is consistent with the upper limit toward GL 2591. They are a factor of 2 and 4 larger than the upper limits toward NGC 2264 IRS and...
abundance will increase even stronger than that of since the statistical branching ratio of 1/3 within the uncertainties, since the latter species are directly formed by reactions served DCO.

column densities computed for W33A and GL 2591 agree and/or by an overestimate of the size of the cloud. The

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With the current sensitivity of heterodyne receivers, it is now possible to study the ortho-H₂D⁺ 1₁₀−1₁₁ 372.421 GHz line profile in emission in the early stages of star formation deep inside dense molecular clouds. Its importance lies in the fact that it is a tracer of H⁺ and that it provides information on the deuterium abundance and temperature history of a cloud and on the chemical evolution during star formation. Further observations of the H₂D⁺ and H⁺ lines in a sample of very young class 0 and class I YSOs will therefore be very valuable.

Since the ortho-H₂D⁺ ground state is at 86 K, the 1₁₀−₁₁₁ line traces both the warm and cold regions, although the H₂D⁺ enhancement will be strongest in the coldest regions. Observations of the 1₁₀−₀₀₀ para-H₂D⁺ ground-state line at 1.37 THz toward the continuum of embedded YSOs may reveal cold H₂D⁺ in absorption. The dual-channel German Receiver for Astronomy at Terahertz frequencies (GREAT), to be flown on the Stratospheric Observatory For Infrared Astronomy (SOFIA), would allow such observations. Combined with 372 GHz observations from the ground, the total abundance and the relative population of the ortho- and para-modifications may be determined, and this would provide information on the formation, destruction, and excitation processes. Simultaneous deep observations of the HD J = 1−0 (2.7 THz) and para-H₂D⁺ ground-state lines toward YSOs may yield a direct measure of the (variation in) H⁺ abundance over the cloud and thus of the cosmic-ray ionization rate.

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