Ground-based searches for interstellar H$_2$D$^+$

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Abstract. We present ground-based searches for the $1_{10} - 1_{11}$ line of interstellar H$_2$D$^+$ at 372 GHz which are more sensitive than those obtained from the Kuiper Airborne Observatory (KAO) by factors of 3-4 for extended sources and by more than two orders of magnitude for compact sources. The line was not detected in a variety of interstellar clouds, including NGC 2264 toward which a possible detection had been suggested previously. The inferred H$_2$D$^+$ abundance limits of $10^{-10} - 10^{-11}$ are still consistent with, but approach the abundances predicted by chemical models. Simultaneous observations of the DCO$^+$ 3-2 and N$_2$H$^+$ 4-3 lines have been used to place additional limits on the H$_2$O$^+$ abundance, and suggest $10^{-11} < x$(H$_2$O$^+$) $< 10^{-9}$. The N$_2$H$^+$ data also indicate that for NGC 2264, but perhaps not for the other sources, gas-phase N$_2$ contains a substantial fraction of the available nitrogen in the cloud.

Key words: Interstellar molecules: H$_2$D$^+$; Molecular Clouds

1. Introduction

The H$_2$O$^+$ ion is thought to play a central role in the ion–molecule reaction scheme which dominates gas–phase interstellar chemistry (Herbst & Klemperer 1973; Watson 1976). The ubiquitous observations of protonated molecules such as HCO$^+$ and N$_2$H$^+$ testify to its presence. However, the H$_2$O$^+$ ion has not yet been detected in interstellar clouds, despite sensitive searches for its infrared vibration–rotation lines in absorption against bright background sources (Geballe & Oka 1989; Black et al. 1990). In principal, the H$_2$O$^+$ isotopomer can more easily be observed by rotational spectroscopy owing to its permanent dipole moment. Moreover, at the low temperatures in interstellar clouds the reaction H$_2$O$^+$ + HD $\rightarrow$ H$_2$D$^+$ + H$_2$ (1) leads to significant fractionation, so that the H$_2$O$^+$/H$_2$O$^+$ ratio is much larger than the cosmic deuterium abundance of about 2 x $10^{-5}$. Indirect evidence for the presence of H$_2$O$^+$ comes from the large observed abundances of deuterated molecules like DCO$^+$, DCN and N$_2$D$^+$ (e.g. Güellín, Langer & Wilson 1982; Wootten 1987).

H$_2$D$^+$ has ortho and para modifications, with the lowest $1_{11}$ ortho state lying 86 K above the true ground state. The ground–state $1_{01} - 0_{00}$ para–H$_2$D$^+$ line lies at 1370 GHz, and can only be observed from airborne platforms. The ground–state $1_{10} - 1_{11}$ ortho–H$_2$D$^+$ transition occurs at the lower frequency of 372.421 GHz (Bogey et al. 1984), but lies in an unfavorable part of the spectrum since it is close to the strong 380 GHz atmospheric water line. Observations of this transition have therefore previously been attempted only from the KAO (Phillips et al. 1985; Pagani et al. 1992a). However, under exceptional conditions, the line is also accessible from high ground sites. With the availability of the new large submillimeter telescopes and improved high–frequency receivers, the ground–based searches can be more sensitive than those from the KAO because of longer possible integration times, much smaller beams and fewer restrictions on the choice of sources.

Additional impetus for the H$_2$D$^+$ search stems from the uncertainty regarding the detection of the ion in interstellar clouds. Phillips et al. (1985) reported a possible line at the expected H$_2$D$^+$ frequency in the dense cloud NGC 2264, and found upper limits for the cold cloud TMC–1. Black et al. (1990) subsequently searched for the H$_2$O$^+$ infrared lines in absorption against NGC 2264 IRS, but failed to detect the ion. More recently, Pagani et al. (1992a) obtained upper limits for the H$_2$D$^+$ 372 GHz line from the KAO in NGC 2264 and several other sources, which are comparable to the strength of the line reported by Phillips et al. We report here the results of ground–based searches for the 372 GHz line which are factors of 3-4 more sensitive than those obtained from the KAO for extended sources, and more than a factor 100 for small sources (<200$''$). We do not confirm the possible feature in NGC 2264, and obtain significant upper limits for other sources.

2. Observations

The H$_2$D$^+$ observations at 372 GHz were performed with the Caltech Submillimeter Observatory (CSO) on December 9, 1991 during a night of exceptional submillimeter transparency. The optical depth at 225 GHz was 0.02–0.03, corresponding to a transmission at 372 GHz of 50–70%. The lead alloy SIS junction receiver built by Ellison et al. (1989) was used in conjunction with a 1024 channel, 500 MHz bandwidth acousto-optical spectrometer (AOS) as the backend. The H$_2$D$^+$ line was centered in the upper sideband, and typical system temperatures including atmospheric losses were 2000 K. The calibration was performed using the ambient chopper method. A correction

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for unequal sideband atmospheric transmission of <10% was applied by means of an atmospheric model which has been adjusted over a two year period to best fit the Mauna Kea atmosphere. The CSO beam size at 372 GHz is about 18", significantly smaller than the KAO beam of 3.7. The main beam efficiency is about 55%, whereas the efficiency for extended sources is about 70%. The latter value has been used in the analysis. The overall uncertainty in the calibration is estimated to be of order 30%. The observed sources are summarized in Table 1. The position in NGC 1333 labelled WLS corresponds to the peak in the oco+ 1-0 map of Wootten et al. (1982).

The observed spectra at 372 GHz, presented in Figure 1, are summarized numerically in Table 1. It is clear that none of the sources shows a significant feature at the frequency of the H2D+ line. The 2σ limit for NGC 2264 obtained after 45 min on-source integration is about 90 mK when corrected for beam efficiency, which is substantially below the possible feature of r~230 mK by Phillips et al. (1985). Similar 2σ limits are found for the other sources; they are typically a factor 3 lower than the limits obtained by Pagani et al. (1992a).

Since the KAO observations refer to a much larger beam over which the conditions necessary to excite the H2D+ line may not exist, the current ground-based limits are effectively even more sensitive by up to two orders of magnitude.

At the edge of the spectra, a strong line with r~1-3 K is seen for most of the sources. It can be identified with N2H+ 4-3, previously seen only by Pagani et al. (1992a) in NGC 6334. Because the effective resolution of the AOS was only 3 km s^-1 at the time of observations, not all lines are resolved and only integrated antenna temperatures are given in Table 1. The presence of the N2H+ line in the H2D+ search band is fortunate, since it provides important indirect constraints on the H2D+ abundance in the clouds, as well as the excitation conditions. For completeness, the DCO+ 3-2 line at 217 GHz was observed using the sensitive new SIS receiver built by Kooi et al. (1992). The telescope beam size at this frequency is about 34" and the efficiency for extended sources about 77%.

3. Analysis

3.1. Excitation model

The derivation of column densities from observed line strengths requires information about the excitation conditions. The upper levels of the H2D+ 110 - 111, N2H+ 4-3 and DCO+ 3-2 transitions lie at 104, 45 and 20 K, whereas the critical densities are about 2 x 10^5, 10^7 and 5 x 10^6 cm^-3, respectively. Thus, high densities (n > 10^5 cm^-3) and not-too-low temperatures are required to excite the lines, even though the abundance of the H2D+ ion is greatly enhanced at T <20 K. The physical conditions in W3 IRS5 and NGC 1333 IRAS 4A have been constrained from observations of high-excitation lines of other species such as H2CO, HCO+ and CS in a similar beam (Phillips et al. 1992; Blake et al. 1992). The temperature in the protostellar NGC 1333 IRAS 4A region is somewhat uncertain, but is unlikely to be much different from the dust temperature of 37 K throughout the source (Sandell et al. 1991). Because of the lack of lines at the NGC 1333 WLS position, it will not be considered any further. The conditions in NGC 2264 and NGC 2024 are based on literature data (Black et al. 1990;
Mauersberger et al. (1992), together with unpublished H2CO spectra.

The adopted H2D+ model has been described by Black et al. (1990). In brief, the excitation within each of the ortho- and para-ladders is controlled by radiative transitions and inelastic collisions with H2, whereas transitions between the two ladders can only occur through reactive collisions with H2. The latter collisions are rapid enough that the ortho ladder cannot be considered separately, but has the zero para level as its effective ground state. A constant de-excitation rate coefficient of \(5 \times 10^{-10} \text{ cm}^3 \text{s}^{-1}\) was used for all inter-ladder transitions. For sufficiently high densities, this model approaches the "thermal" model of Phillips et al. and the LTE model of Millar et al. with their standard parameters. However, the models usually refer to a cloud with a density of \(10^5 \text{ cm}^{-3}\) in which the CO abundance is normal, about \(10^{-4}\). Since the H2D+ abundance is inversely proportional to density, the model predictions for H2D+ could be as low as \(10^{-12}\) at \(T \approx 50 \text{ K}\) for densities of \(10^8 \text{ cm}^{-3}\) or larger. On the other hand, H2D+ is significantly enhanced if CO is depleted, since reaction with this species is the principal removal mechanism. The enhancement for H2D+ may be even stronger if other heavy species such as O2, N2, and O are depleted as well, because reaction (1) then becomes the main destruction path of H2D+. For regions such as NGC 1333 IRS 4A and NGC 2024 FIR5, the effects of high density and low CO abundance may therefore cancel, and the H2D+ abundance may still be of order \(10^{-11}\) or more.

A second method to infer \(x(H_2D^+)\) is to combine the H2D+ limits with the DCO+ data. The derived DCO+ column densities are similarly distributed, which may not be valid if the fractionation scheme of Pagani et al. is used with their standard parameters. However, the models usually refer to a cloud with a density of \(10^5 \text{ cm}^{-3}\) in which the CO abundance is normal, about \(10^{-4}\). Since the H2D+ abundance is inversely proportional to density, the model predictions for H2D+ could be as low as \(10^{-12}\) at \(T \approx 50 \text{ K}\) for densities of \(10^8 \text{ cm}^{-3}\) or larger. On the other hand, H2D+ is significantly enhanced if CO is depleted, since reaction with this species is the principal removal mechanism. The enhancement for H2D+ may be even stronger if other heavy species such as O2, N2, and O are depleted as well, because reaction (1) then becomes the main destruction path of H2D+. For regions such as NGC 1333 IRS 4A and NGC 2024 FIR5, the effects of high density and low CO abundance may therefore cancel, and the H2D+ abundance may still be of order \(10^{-11}\) or more.

Finally, information on the H2D+ abundance can be derived from the N2H+ lines. The inferred N2H+ column densities range from \(10^{12} \text{ to } 10^{14} \text{ cm}^{-2}\), and the abundances from \(10^{-11} \text{ to } 10^{-9}\). Thus, significant variations in the N2H+ abundance occur from cloud to cloud. N2H+ is formed mostly by the reaction of N2 with H2 and is destroyed by reactions with CO and electrons. If we assume that at least 50% of the gas-phase nitrogen is in the form of N2 with \(x(N_2) \approx 5 \times 10^{-5}\) and \(x(\text{CO}) \approx 10^{-8}\), then a simple chemical scheme suggests \(x(H_2D^+) \approx x(N_2H^+)\). For lower N2 abundances, the H2D+ abundances will be higher. For NGC 2264, this leads to lower limits on the H2D+ abundance of \(4 \times 10^{-10} \text{ to } 3 \times 10^{-9}\), which are barely consistent with the upper limits derived above.

The three methods used to derive the H2D+ abundances are summarized in the last few columns of Table 2. Each has its advantages and disadvantages. The first method assumes that the H2D+ fractionation is well understood, and depends mostly on the adopted temperature. The second method requires additional independent data, and assumes that HCO+ and H2D+ are similarly distributed, which may not be valid if CO is heterogeneously depleted. The last method involves the most assumptions, and is very sensitive to the density adopted in the N2H+ analysis. In all methods, a major uncertainty is the H2...
column density, especially for NGC 1333 and NGC 2024. For the best case, NGC 2264, it is seen that the three methods are only consistent if the density is higher than $5 \times 10^{6}$ cm$^{-3}$. For the other sources, a large range of values is still possible.

Alternatively, the $N_{2}H^{+}$ abundance can be used to infer the gas-phase $N_{2}$ abundance, if the CO and $H_{2}$ abundances are assumed to be standard. Chemical models give $N_{2}/N_{2}H^{+} \approx 4 \times 10^{-4} - 10^{5}$ (Herbst et al. 1977; Millar et al. 1991), independent of time but linearly dependent on density and inversely proportional to the cosmic ray ionization rate $\zeta_0$. The resulting $N_{2}$ abundances are included in Table 2 and range from $10^{-3}$ to $10^{-1}$ in W3 IRS5 to $>10^{-3}$ in NGC 2264. Although they are not more accurate than an order of magnitude, it appears that most of the available nitrogen is locked up in gas-phase $N_{2}$ in NGC 2264. $N_{2}$ may, however, contain only 10% or less of the nitrogen in W3 IRS5. The nitrogen could be either in the form of gas-phase atomic $N$ in this cloud, or be depleted onto grains in some solid form, presumably solid $N_{2}$.

### Table 2. Derived Column Densities and Abundances.

<table>
<thead>
<tr>
<th>Source</th>
<th>T (K)</th>
<th>n (cm$^{-3}$)</th>
<th>$N_{2}D^{+}$</th>
<th>DCO$^{+}$</th>
<th>$N_{2}H^{+}$</th>
<th>$H_{2}$</th>
<th>$H_{2}D^{+}$</th>
<th>DCO$^{+}$</th>
<th>$N_{2}H^{+}$</th>
<th>$H^{+}$</th>
<th>$H^{+}$</th>
<th>$H^{+}$</th>
<th>$N_{2}$</th>
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<tr>
<td>W3 IRSS</td>
<td>50</td>
<td>5(6)</td>
<td>&lt;7(12)</td>
<td>&lt;2(11)</td>
<td>2(12)</td>
<td>2(23)</td>
<td>&lt;4(-11)</td>
<td>&lt;1(-12)</td>
<td>1(-11)</td>
<td>&lt;2(-7)</td>
<td>&gt;1(-11)</td>
<td>1(-5)</td>
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<tr>
<td></td>
<td>100</td>
<td>(5)</td>
<td>&lt;5(12)</td>
<td>&lt;2(11)</td>
<td>1(12)</td>
<td></td>
<td>&lt;3(-11)</td>
<td>&lt;1(-12)</td>
<td>5(-12)</td>
<td>3(-7)</td>
<td>&gt;5(-12)</td>
<td>5(-6)</td>
<td></td>
</tr>
<tr>
<td>N 1333 4A</td>
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<td>&lt;4(12)</td>
<td>1(12)</td>
<td>1(13)</td>
<td>3(23)</td>
<td>&lt;1(-11)</td>
<td>3(-12)</td>
<td>3(-11)</td>
<td>&lt;3(-9)</td>
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<td>1(-11)</td>
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<td>&lt;2(-10)</td>
<td>&gt;1(-11)</td>
<td></td>
</tr>
<tr>
<td>N 2024 FIR5</td>
<td>50</td>
<td>5(5)</td>
<td>&lt;3(12)</td>
<td>&lt;3(11)</td>
<td>3(13)</td>
<td>2(23)</td>
<td>&lt;2(-11)</td>
<td>&lt;2(-12)</td>
<td>2(-10)</td>
<td>&lt;1(-7)</td>
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<td>4(-11)</td>
<td>&lt;4(-9)</td>
<td>&gt;4(-11)</td>
<td>4(-5)</td>
<td></td>
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<tr>
<td>N 2264 IRS</td>
<td>30</td>
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<td>2(12)</td>
<td>2(14)</td>
<td>8(22)</td>
<td>&lt;1(-10)</td>
<td>3(-11)</td>
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<td>&lt;1(-8)</td>
<td>&lt;3(-9)</td>
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<tr>
<td></td>
<td>30</td>
<td>5(6)</td>
<td>&lt;9(12)</td>
<td>8(11)</td>
<td>3(13)</td>
<td></td>
<td>&lt;1(-10)</td>
<td>1(-11)</td>
<td>4(-10)</td>
<td>&lt;1(-8)</td>
<td>&lt;7(-9)</td>
<td>&lt;4(-10)</td>
<td></td>
</tr>
</tbody>
</table>

* From $H_{2}D^{+}$ assuming the theoretical $H_{2}^{+}/H_{2}D^{+}$ ratio computed by Pagani et al. (1992b) at the appropriate $T$ for their standard model.

* From the DCO$^{+}/H_{2}^{13}CO^{+}$ analysis (see text).

* From the $N_{2}H^{+}$ analysis, assuming most gas-phase nitrogen is in the form of $N_{2}$.

* From $N_{2}H^{+}$ using model $N_{2}/N_{2}H^{+}$ ratios with $\zeta_0 = 5 \times 10^{-17}$ s$^{-1}$ at the appropriate density.

### 4. Conclusions

The observations presented in this letter show that sensitive ground-based searches for the $H_{2}D^{+}$ ion are possible under exceptional weather conditions. The derived limits are up to two orders of magnitude more sensitive than those obtained previously from the KAO. The inferred $H_{2}D^{+}$ and $H_{2}^{+}$ abundances are still consistent with chemical models; however, several indirect lines of argument based on DCO$^{+}$ and $N_{2}H^{+}$ observations suggest that at least for NGC 2264, only a factor of a few improvement in $S/N$ is required to detect the ion. Dense clouds with temperatures in the range 20–30 K remain the best sources to search for the $H_{2}D^{+}$ 372 GHz line, both in terms of abundance and excitation.

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### References