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Abundant H_2D^+ in the pre–stellar core L1544

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Abstract. We have detected the 372 GHz line of *ortho*–H_2D^+ towards the pre–stellar core L1544. The strongest emission ($T_{\rm mb}$ ~1 K) occurs at the peak of the millimeter continuum emission, while measurements at offset positions indicate that H_2D^+ is confined within ~20″, where CO is highly depleted. The derived H_2D^+ abundance of ~10^{-9} is comparable with previous estimates of the electron abundance in the core, which suggests that H_2D^+ is the main molecular ion in the central 20″ (2800 AU) of L1544. This confirms the expectations that H_2D^+ is dramatically enhanced in gas depleted of molecules other than H_2. The measured abundance even exceeds the present model predictions by about a factor ten. One possibility is that all CNO–bearing neutral species, including atomic oxygen, are almost completely (≳98%) frozen within a radius of ~2800 AU.

Key words. ISM: individual: L1544 – ISM: molecules – radio lines: ISM

1. Introduction

The last few years have seen a boom of the studies of molecular deuteration in star forming regions, triggered by the discovery of a large fraction of doubly deuterated formaldehyde in the low mass protostar IRAS 16293-2422 (Ceccarelli et al. 1998; Loinard et al. 2000), where the measured D_2CO/H_2CO ratio is 25 times larger than in Orion (Turner 1990). It is now clear that IRAS 16293-2422 is not unusual, for all Class 0 protostars show similar or larger D_2CO/H_2CO ratios (Loinard et al. 2002). Formaldehyde is not unusual either, as other molecules present astonishing deuteration degrees. Notable examples are methanol, whose deuterated forms are as abundant as the main isotopomer (Parise et al. 2002), or ammonia, where not only the doubly deuterated form (Roueff et al. 2000; Loinard et al. 2001), but also the triply deuterated form (van der Tak et al. 2002; Lis et al. 2002) has been detected.

The picture emerging from those studies is that this extreme molecular deuteration starts during the pre-collapse phase, when the gas is cold and dense (Ceccarelli et al. 2001). Whether formed in the gas phase (e.g. Roberts & Millar 2000) or on the grain surfaces (Tielens 1983; Caselli et al. 2002a), deuterated isotopomers of neutral species are stored into the grain mantles, and released back into the gas phase during the collapse phase, as the dust is heated by the new born star. This picture has been substantially confirmed by the recent observations of Bacmann et al. (2003), who measured D_2CO/H_2CO ~ 10% in a sample of pre-stellar cores presenting large degrees of CO depletion (Bacmann et al. 2002). A decisive factor for the large observed deuteration seems in fact to be the CO depletion: the larger the CO depletion, the larger the molecular deuteration. This suggests that the enhanced molecular deuteration is the product of gas phase chemistry, given that CO depletion leads to an increase of the H_2D^+/H_3^+ abundance ratio (Dalgarno & Lepp 1984) and thus stimulates the formation of deuterated molecules, mainly produced in ion–neutral reactions with H_2D^+.

Evidently, the key molecule for fully understanding the molecular deuteration process is indeed H_2D^+. Unfortunately, the only H_2D^+ transition observable from ground based telescopes, the ortho-H_2D^+ 1_{10}–1_{11} transition, lies at 372 GHz, next to an atmospheric band which makes the observation rather difficult. As a result, the search of H_2D^+ has been a very frustrating business for about two decades (e.g. Phillips et al. 1985; Pagani et al. 1992; van Dishoeck et al. 1992; Boreiko & Betz 1993), and although several massive protostars have been targetted, H_2D^+ has been so far detected, with a relatively low signal (main beam temperature, $T_{\rm mb}$ ≤ 0.1 K), in only two low mass protostars: NGC 1333–IRAS 4 (Stark et al. 1999) and IRAS 16293-2422 (Stark et al., in preparation). We decided to re-start the H_2D^+

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search in sources with the largest expected H_2D^+/H_3^+ ratio, even where the excitation conditions of the 372 GHz line may not be the most favorable. And, since molecular deuteration is indeed dramatically enhanced during the pre-collapse phase of low mass protostars, we decided to search for H_2D^+ in the best studied pre-stellar core.

L1544 consists of a dense core surrounded by a low density envelope which is undergoing extended infall (Tafalla et al. 1998; Williams et al. 1999). From dust emission and absorption observations, we know that the core has a central density of about 10^6 cm^{-3} inside a radius $r_{\rm flat}$ = 2500 AU (the "flattened" region), followed by $1/r^2$ density fall–off until a radius of about 10 000 AU (Ward–Thompson et al. 1999; Bacmann et al. 2000). Molecular species such as CO, CS, and CCS are highly depleted at densities above $\sim 10^5$ cm^{-3}, or inside radii of ∼6000 AU (Caselli et al. 1999; Ohashi et al. 1999; Tafalla et al. 2002). On the other hand, molecules such as NH_3, N_2H^+ and N_2D^+ do not show signs of depletion, probably because of the volatility of their precursor N_2 (Bergin & Langer 1997; Caselli et al. 2002b, hereafter CWZ). Indeed, N_2H^+ and N_2D^+ have been used to study gas kinematics (Caselli et al. 2002c) and the ionization degree (CWZ) of the high density core nucleus. The $N(N_2D^+)/N(N_2H^+)$ column density ratio toward the dust peak was determined to be ∼0.2, in agreement with chemical models which take into account differential depletion of molecular species in centrally concentrated clouds (Aikawa et al. 2001; CWZ). These models predict fractional abundances of H_2D^+ to be $\lesssim 10^{-10}$, a value which can be tested by the present observations.

2. Observations and results

During two nights in October 2002, we observed the dense core L1544 in the 1_{10}–1_{11} transition of H_2D^+ (ν = 372.42134 GHz), using the Caltech Submillimeter Observatory on Mauna Kea. The spectra were taken in wobbler switching mode, with a chop throw of 300″. The central position (the peak of the 1.3 mm continuum dust emission map of Ward–Thompson et al. 1999), as well as the 4 positions offset by ±20″ in Right Ascension and Declination were observed. The rms reached were of the order of 110 mK for the central position and 60–90 mK for the others. We used as backend an acousto-optical spectrometer with 50 MHz bandwidth. The velocity resolution, as measured from a frequency comb scan, is 0.101 km s^{-1}. The beam efficiency at ν = 372 GHz was measured on Saturn during the observations, and found to be ≈0.65 for a 22″*FWHM* beam size. Pointing was monitored every couple of hours and found to be better than 3″.

In Table 1 we report the integrated intensity, $V_{\rm LSR}$ velocity, and line width of the five observed H_2D^+ spectra. In Fig. 1 the peak spectrum is shown together with the average spectrum obtained by summing the four off-peak spectra. First, the most striking feature of the H_2D^+ (1_{10}–1_{11}) line at the dust peak is its intensity (∼1 K), which is at least ten times stronger than any other previously detected H_2D^+ line (Stark et al. 1999), suggesting that pre–stellar core conditions favour the production of H_2D^+. The second important result is the detection of a strong signal (∼0.4 K) about 20″ from the center. Assuming that the H_2D^+ emission is constant within a certain radius $r(H_2D^+)$ and then drops to zero, one can estimate $r(H_2D^+)$ by convolving the predicted H_2D^+ integrated intensity profile with the CSO beam and comparing it with the data. This comparison, shown in Fig. 2 (thin and dashed curves), gives $r(H_2D^+) \sim$ 15″–20″, consistent with $r_{\rm flat}$ = 17″, the size of the "flattened" region observed in the millimeter continuum emission. In the case of a power law distribution of the H_2D^+ integrated intensity ($\int T_{\rm mb} {\rm d}v \propto r^{-1}$; dotted curve in Fig. 2), the estimated (convolved) size is $r(H_2D^+)$ = 17″. This result suggests that the bulk of the H_2D^+ emission is concentrated *within* the highly depleted high density core nucleus.

Table 1. Results of Gaussian fits to the five H_2D^+ spectra.

Offset (″, ″)	$\int T_{\rm mb} {\rm d}v$ (K km s^{-1})	$V_{\rm LSR}$ (km s^{-1})	Δv (km s^{-1})
(0,0)	0.46 ± 0.04	7.23 ± 0.02	0.47 ± 0.04
(0,20)	0.22 ± 0.03	7.17 ± 0.04	0.49 ± 0.08
(−20,0)	0.26 ± 0.04	7.11 ± 0.06	0.69 ± 0.15
(20,0)	0.25 ± 0.03	7.22 ± 0.03	0.59 ± 0.08
(0,−20)	0.26 ± 0.04	7.26 ± 0.05	0.68 ± 0.11

The central line profile shows a dip at the rest velocity which may be due to the kinematics of the emitting gas (in analogy with other molecular ion profiles; see Caselli et al. 2002c) or it may indicate that the line is optically thick. We will get back on this issue in a future paper where the velocity structure of the L1544 core will be included in a detailed radiative transfer code (van der Tak et al., in preparation).

3. Column density and abundance

As shown in Fig. 2, the H_2D^+ emission appears to be concentrated within a radius of ∼2800 AU. In this region, the gas temperature is predicted to be ∼7 K (Evans et al. 2001; Galli et al. 2002), although molecular data suggest larger temperatures (∼9–10 K; Tafalla et al. 2002; Bacmann et al. 2002). However, because of the large amount of gas phase depletion (see Sect. 4), it is likely that molecular tracers do not provide information on the gas temperature in the central 2800 AU. Assuming LTE conditions ($T_{\rm ex}$ = 7 K), we can immediately determine the optical depth (τ) of the $H_2D^+(1_{10}$–$1_{11})$ line:

$$\tau = -\ln\left[1 - \frac{T_{\rm mb}}{J_\nu(T_{\rm ex}) - J_\nu(T_{\rm cb})}\right] = 1.0 \pm 0.2, \quad (1)$$

where $T_{\rm mb}$ = 0.91 ± 0.11 K at the peak, $T_{\rm cb}$ = 2.7 K is the cosmic background temperature, and $J_\nu(T) = T_0/(\exp(T_0/T) - 1)$ with $T_0 = h\nu/k$ = 17.9 K. Assuming a spontaneous transition coefficient $A = 1.08 \times 10^{-4}$ s^{-1}, the total column density of ortho–H_2D^+ is:

$$N_{\rm ortho} \simeq 5.15 \times 10^{13}\, \Delta v ({\rm km\,s^{-1}})\ \tau\ {\rm cm^{-2}} \quad (2)$$

so that at the dust peak, where $\tau \sim 1$ and the linewidth is 0.47 km s^{-1} (Table 1), we obtain $N_{\rm ortho} = 2.4 \times 10^{13}$ cm^{-2}.

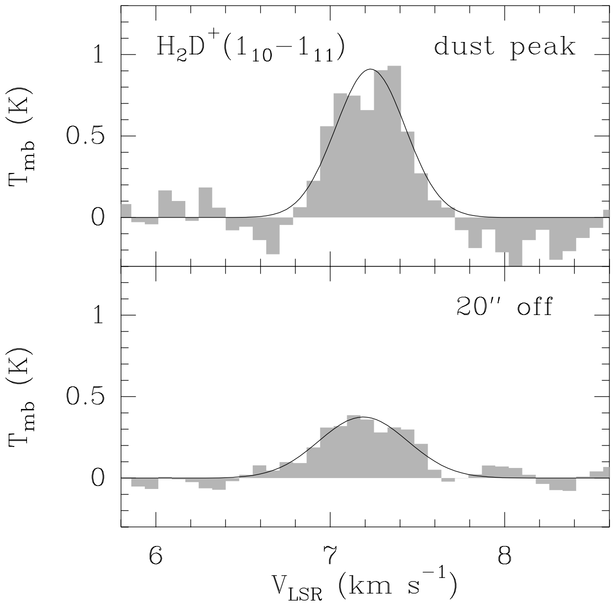

Fig. 1. (*Top*) The $H_2D^+(1_{10}–1_{11})$ line at the dust peak of L1544 (RA(1950) = 05:01:13.1, Dec(1950) = 25:06:35.0). The black curve is the Gaussian fit (see Table 1). (*Bottom*) The $H_2D^+(1_{10}–1_{11})$ spectrum averaged in the four positions 20″ off the dust peak.

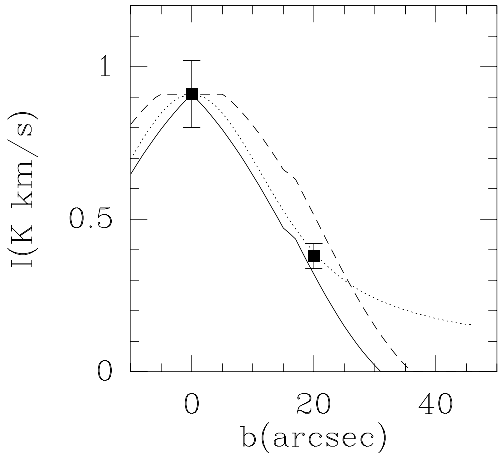

Fig. 2. Integrated intensity of the $H_2D^+(1_{10}–1_{11})$ line as a function of projected distance b from the core center. The solid and dashed curves show two "step" functions (null H_2D^+ integrated intensity at impact parameters larger than 15 (*solid*) and 20 (*dashed*) arcsec) convolved with the CSO beam. The dotted curve is a (convolved) power–law distribution in the H_2D^+ integrated intensity ($\propto r^{-1}$), and its size at half–maximum (*FWHM*) is 34″.

At the low assumed temperatures, where the ortho to para ratio is close to 1 (Gerlich et al. 2002), we deduce a total H_2D^+ column density of $\sim 4.8 \times 10^{13}$ cm^{-2}, about three times larger than $N(N_2H^+)$ (see CWZ).

To gauge the H_2D^+ abundance, the above estimate of the total H_2D^+ column density has been divided by the molecular hydrogen column density derived from the 1.3 mm continuum emission of Ward–Thompson et al. (1999), smoothed at a resolution of 22″ ($N(H_2) = 1.1 \times 10^{23}$ cm^{-2}): $x(H_2D^+) \equiv N(H_2D^+)/N(H_2) \sim 4.4 \times 10^{-10}$. This value is only four times lower than the estimated electron abundance $x(e)$ in the L1544 center ($\sim 2 \times 10^{-9}$, CWZ), suggesting that H_2D^+ is one of the major ions in the gas phase (see Sect. 4).

In case of subthermal emission, the line optical depth and the total column density increase. For example, if $T_{ex} = 6$ K, $\tau = 2.8$ and the total H_2D^+ column density becomes $\sim 1.2 \times 10^{14}$ cm^{-2}. This corresponds to $x(H_2D^+) \sim 1 \times 10^{-9}$, so that $x(H_2D^+) \simeq x(e)$. We note that $T_{ex} = 6$ K is the minimum excitation temperature possible to have a solution of Eq. (1) in the case of an optically thick ($\tau \gtrsim 0.5$) line with $T_{mb} = 0.9$ K. At the off–positions (20″ or 2800 AU from the dust peak), where $N(H_2) \sim 8 \times 10^{22}$ cm^{-2}, the derived H_2D^+ abundance is 2.3×10^{-10} (if $T_{ex} = 7$ K) and 4.0×10^{-10} (if $T_{ex} = 6$ K), a factor of about two lower than toward the dust peak.

We also carried out a radiative transfer analysis using the Monte Carlo program by Hogerheijde & van der Tak (2000)[1]. The H_2 density profile was taken from Tafalla et al. (2002), whereas dust temperatures are from Galli et al. (2002). Only thermal line broadening was included. Term energies, statistical weights and Einstein A coefficients were taken from the JPL catalog (Pickett et al. 1998). Besides collisional excitation, for which we used the scaled radiative rates proposed by Black et al. (1990), radiation from the cosmic microwave background and thermal radiation by local dust are taken into account, using grain opacities from Ossenkopf & Henning (1994). The abundance of H_2D^+ was assumed to be constant within a radius r_0 and zero at $r > r_0$. Model results are compared to line profiles at the center and offset positions to constrain the H_2D^+ abundance and r_0. The best-fit abundance is $H_2D^+/H_2 = 10^{-9}$, where calibration uncertainty allows a 50% decrease. Models with $r_0 = 20–25$ arcsec give good matches to the line fluxes at both the center and the offset positions. The optical depth at line center along the central pencil beam is 2.73. Here we limited our analysis to a static cloud. In a future paper (van der Tak et al., in prep.) we will explore the effects of including a velocity structure in the radiative transfer code.

[1] http://talisker.as.arizona.edu/~michiel/ratran.html

4. Chemistry

The main result of this study is that H_2D^+ has been detected for the first time in a pre–stellar core. The observed ($1_{10}–1_{11}$) line has a main beam temperature of ∼1 K, and the emission is concentrated in a region with radius of ∼2800 AU, roughly coincident with the so–called "flattened region" seen in the millimeter dust continuum emission, where the density is slowly changing with radius ($\sim r^{-1.4}$; see André et al. 2000) and/or the temperature is around 7 K (Evans et al. 2001; Galli et al. 2002).

The data have been analysed with a simple analytical model and with a Monte Carlo radiative transfer code. The derived H_2D^+ abundance ($x(H_2D^+) \sim 10^{-9}$) is consistent with the electron fraction estimated by CWZ in the center of L1544. This implies that H_2D^+ is the main molecular ion in the core center. The simple chemical code of CWZ, constrained by observations of several molecular ions, predicts $x(H_2D^+) \sim 7 \times 10^{-11}$ in the center of L1544, about one order of magnitude less than that deduced from the present data. A similar H_2D^+ abundance ($\sim 6 \times 10^{-11}$) at the cloud center was also predicted by the detailed chemical model of Aikawa et al. (2001), coupled with the Larson–Penston dynamical evolution which best reproduced the L1544 observational results.

CWZ found that to match the observed N_2D^+/N_2H^+ ($\sim$0.24) and DCO^+/HCO^+ ($\sim$0.06) column density ratios toward the L1544 center one needs to (i) allow differential depletion of molecular species onto dust grains (in particular, N_2 has to be more volatile than CO, to maintain a large fraction of N_2H^+ and N_2D^+ in the core center); and (ii) maintain a significant fraction of atomic oxygen in the gas phase, to limit the deuterium fractionation to the observed values ($\lesssim$0.2). As a by–product, H_3O^+ was predicted to be abundant ($x(H_3O^+) \sim 10^{-9}$) in the core center.

The results of the present paper apparently contradict the CWZ conclusions, because the large H_2D^+ abundance can only be produced if all neutral species, including O and N_2, are essentially frozen onto dust grains (see also Bergin et al. 2002). In fact, only in this case can the H_2D^+ abundance reach values close to the electron abundance. This can be seen with a simple chemical model, where the ingredients are H, H_2, HD, H_2D^+, H_3^+, CO, HCO^+, DCO^+ and electrons. We neglect recombination onto dust grains, which is likely not to be an important process for the above molecular ions in the high density core nucleus, where small grains and PAHs – significant carriers of negative charges (Lepp & Dalgarno 1988) – are expected to be deposited onto bigger grains (e.g. Ossenkopf & Henning 1994). Following Sect. 2 of Caselli (2002), assuming conditions appropriate for the central 2500 AU of L1544 (kinetic temperature = 7 K, $n(H_2) = 10^6$ cm^{-3}, see Galli et al. 2002), we have:

$$R_{\rm DEUT} \equiv \frac{x(H_2D^+)}{x(H_3^+)} = \frac{2 \times 10^{10}\, k_{\rm f}}{3 \times 10^2 / f_{\rm D} + x(e)/2 \times 10^{-9}} \quad (3)$$

where $k_{\rm f}$ is the forward rate coefficient of the proton–deuteron exchange reaction $H_3^+ + HD \rightleftharpoons H_2D^+ + H_2$ (see below), and $f_{\rm D}$ is defined as the ratio between the "canonical" CO abundance (9.5×10^{-5}; Frerking et al. 1982) and the observed $N({\rm CO})/N(H_2)$. The H_3^+ abundance can be estimated from the charge conservation equation, so that we obtain (with rate coefficients as in Caselli 2002):

$$x(H_3^+) = \frac{f_{\rm D}\, x(e)^2}{(f_{\rm D} x(e) + 4 \times 10^{-8})(R_{\rm DEUT} + 1) + 8 \times 10^{-8}}. \quad (4)$$

Equations (3) and (4) directly furnish the H_2D^+ and H_3^+ abundances as a function of $f_{\rm D}$, once $x(e)$ is known. Figure 3 shows the result of this simple chemical analysis, with $x(H_2D^+)$ (thin curves) and $R_{\rm DEUT}$ (dashed curves) as a function of $f_{\rm D}$, assuming $x(e) = 2 \times 10^{-9}$ (as roughly determined by CWZ in the L1544 center). We note that Eq. (3) breaks down at large values of $f_{\rm D}$ ($\gtrsim$100), when dissociative recombination starts to dominate over proton transfer reactions. In the figure, two different values for $k_{\rm f}$ have been used: (i) the "standard" value $k_{\rm f} = 1.5 \times 10^{-9}$ cm^3 s^{-1} (upper curves), and (ii) $k_{\rm f} = 3.5 \times 10^{-10}$ cm^3 s^{-1}, recently measured by Gerlich et al. (2002) (lower curves). The two data points in the figure are our present estimates of $x(H_2D^+)$, the arithmetic means of

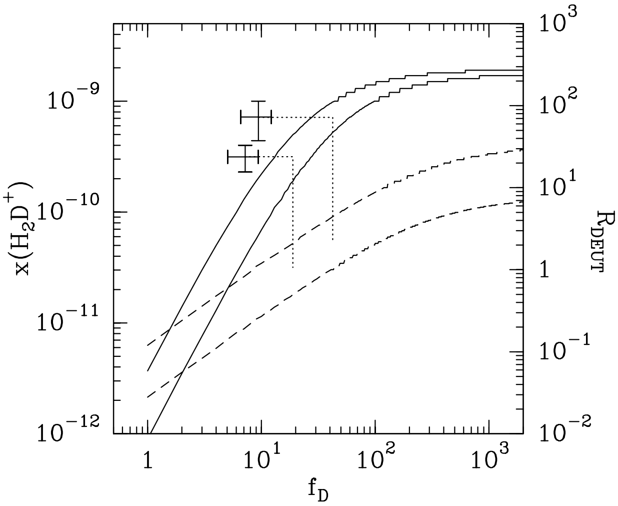

Fig. 3. (*thin curves*) $x(H_2D^+)$ vs. the depletion factor $f_{\rm D}$ in the high density core nucleus of L1544 (see text). (*dashed curves*) $R_{\rm DEUT}$ as a function of $f_{\rm D}$. Data points are the measured values at the peak and 20″ off–peak positions. Dotted lines indicate the $R_{\rm DEUT}$ and $f_{\rm D}$ values predicted by the simple chemical model applied to the L1544 central 2800 AU (see Sect. 4), at the observed $x(H_2D^+)$ values. Large H_2D^+ abundances ($\geq 10^{-9}$) are obtained only if $f_{\rm D} \geq 70$.

the abundances calculated with $T_{\rm ex}$ = 6 and 7 K (Sect. 3): 7.2×10^{-10} and 3.15×10^{-10} at the peak and off–peak positions, respectively. The corresponding $f_{\rm D}$ values are from CWZ. The error bars indicate the uncertainties in the excitation temperature ($\sim$1 K; Sect. 3) for estimating $x(H_2D^+)$, and calibration errors affecting the determination of $f_{\rm D}$ (about 30%; CWZ).

The observed H_2D^+ abundances cannot be reproduced unless the CO depletion factor is $\sim$20 in the off position and $\sim$40 at the peak (the "Monte Carlo abundance" indicates an even higher $f_{\rm D}$, $\simeq$70), whereas the observed $f_{\rm D}$ values are $\sim$7 and $\sim$9, at the same positions. Although our comprehension of the deuteration process in cold gas may be substantially incomplete, it is certain that measurements of $f_{\rm D}$ are contaminated by the CO emission along the line of sight coming from regions with marginal CO depletion, so that the resultant $f_{\rm D}$'s estimates are lower limits of the total amount of CO freeze out at the core center. Indeed, the chemical model of CWZ predicts an almost complete ($\gtrsim$99%) CO freeze out within the central 2800 AU of L1544. Following the model results in Fig. 3, the predicted $f_{\rm D}$ values at the observed H_2D^+ abundances correspond to $R_{\rm DEUT} \sim 1$ and 2 at the off and central positions, respectively.

If other neutrals reacting with H_2D^+ and H_3^+, such as O and N_2, are present in the gas phase, the predicted $x(H_2D^+)$ abundance will drop as in the case of a low $f_{\rm D}$ value (e.g. Caselli 2002). Thus, the present H_2D^+ observations also require a heavy depletion of O ($\gtrsim$99%) *and* N_2 ($\sim$97%). A way to overcome the apparent inconsistency with CWZ (who need significant fractions of molecular nitrogen and atomic oxygen in the gas phase at $r \sim 2800$ AU) and well reproduce both the moderate value ($\sim$0.2) of the $N(N_2D^+)/N(N_2H^+)$ column density ratio as well as the large H_2D^+ abundance (which implies $R_{\rm DEUT} \sim 2$) is to increase the depletion rate of O and N_2 *within* the "flattened" region. This case requires central core densities of about 10^7 cm^{-3} within a radius of 1000 AU, which is consistent with current mm continuum dust emission measurements if the central temperature drops to values of $\lesssim$7 K (e.g. Evans et al. 2001). The conclusion is that present observations are compatible with H_2D^+ *being the most abundant molecular ion and with a total depletion of elements heavier than helium in the central* $\lesssim$*2800 AU*. This can also explain the lower H_2D^+ abundance derived in the direction of NGC 1333–IRAS 4 ($x(H_2D^+) = 3 \times 10^{-12}$; Stark et al. 1999), where the young stellar object heats up the central zones, thus allowing the return of solid phase molecules back into the gas phase. A more comprehensive chemical model, coupled with a detailed radiative transfer code is however needed to better understand the whole data set available for L1544 and we are going to explore this in a future paper (van der Tak et al., in preparation).

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