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DETECTION OF D_2H^+ IN THE DENSE INTERSTELLAR MEDIUM

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ABSTRACT

The 692 GHz para ground-state line of D_2H^+ has been detected at the Caltech Submillimeter Observatory toward the prestellar core 16293E. The derived D_2H^+ abundance is comparable to that of H_2D^+, as determined by observations of the 372 GHz line of ortho-H_2D^+. This is an observational verification of recent theoretical predictions, developed to explain the large deuteration ratios observed in cold, high-density regions of the interstellar medium associated with low-mass prestellar cores and protostars. This detection confirms expectations that the multiply deuterated forms of H_3^+ were missing factors of earlier models. The inclusion of D_2H^+ and D_3^+ in the models leads to predictions of higher values of the D/H ratio in the gas phase.

Subject headings: ISM: abundances — ISM: clouds — ISM: molecules — molecular data — molecular processes — radio lines: ISM

1. INTRODUCTION

Recently, millimeter and submillimeter spectroscopy of the dense interstellar medium has shown that, in cold dense regions, deuterated molecular species are highly abundant, sometimes more than 10^{-1} of the H version. Amazingly, doubly and triply deuterated species can be observed, e.g., D_2CO (Ceccarelli et al. 1998), NHD_2 (Roueff et al. 2000), CHD_2OH (Parise et al. 2002), D_2S (Vastel et al. 2003), ND_3 (Lis et al. 2002; van der Tak et al. 2002), and CD_3OH (Parise et al. 2004). Several models have been developed to account for such high levels of deuteration (Tielens 1983; Roberts & Millar 2000a, 2000b). Phillips & Vastel (2003) have pointed out that the deuteration of H_3^+ will be extended beyond H_2D^+, to D_2H^+ and D_3^+, and that detection of D_2H^+ might be possible. A calculation taking a high degree of deuteration into account has been carried out by Roberts, Herbst, & Millar (2003) and Walmsley, Flower, & Pineau des Fôrets (2004), confirming the expectation that, in dense depleted regions, the abundance of D_2H^+ will be similar to that of H_2D^+, and that D_3^+ will be abundant.

The key enabling work in the astronomical search for D_2H^+ is the laboratory measurement of the para ground-state transition (1_{10}–1_{01}) by Hirao & Amano (2003). We report here the first astronomical detection of that transition.

Chemical reactions go in the direction to minimize energy. The chemical fractionation process favors the production of the heavier more deuterated species, because of the mass dependence of the zero-point vibration energies of the isotopic variants. Gas-phase species are expected to be depleted at the centers of cold, dark clouds, since they accrete on the dust grains (see, e.g., Charnley 1997). A series of observations has shown that the abundances of molecules like CO decrease in many prestellar cores (Bacmann et al. 2002). The removal of these reactive species affects the gas-phase chemistry and particularly the deuterium fractionation within the cloud. Indeed, the removal of species that would normally destroy H_3^+ (e.g., CO; Roberts & Millar 2000a) means that H_3^+ is more likely to react with HD and produce H_2D^+. For example, if $[CO/H_2] \sim 5 \times 10^{-6}$ (Bacmann et al. 2002), this leaves HD at $[HD/H_2] \sim 5 \times 10^{-5}$ as the most abundant molecule available for reaction with H_3^+ and H_2D^+ and favors the production of high deuterium content molecules:

$$H_3^+ + HD \leftrightarrow H_2D^+ + H_2 + \Delta E_a, \tag{1}$$

$$H_2D^+ + HD \leftrightarrow D_2H^+ + H_2 + \Delta E_b, \tag{2}$$

$$D_2H^+ + HD \leftrightarrow D_3^+ + H_2 + \Delta E_c, \tag{3}$$

where ΔE_a, ΔE_b, and ΔE_c are the released energies of the exothermic reactions. Using the zero-point energies computed by Ramanlal, Polyansky, & Tennyson (2003), and the energy of the first allowed rotational state of the H_3^+ molecule permitted by the Pauli exclusion principle (~92 K), these values are $\Delta E_a \simeq 230$ K, $\Delta E_b \simeq 180$ K, and $\Delta E_c \simeq 230$ K.

After a long frustrating search (Phillips et al. 1985; Pagani et al. 1992; van Dishoeck et al. 1992; Boreiko & Betz 1993), and with the advent of new submillimeter receivers, H_2D^+ was detected toward two young stellar objects, NGC 1333 IRAS 4A (Stark, van der Tak, & van Dishoeck 1999) and IRAS 16293−2422A (Stark et al. 2004), although with relatively low signal strength. The H_2D^+ search has now been extended to prestellar cores, and it has been detected with relatively strong emission (Caselli et al. 2003; P. Caselli et al. 2004, in preparation; C. Vastel et al. 2004, in preparation), confirming that H_2D^+ is dramatically enhanced in a gas depleted of most molecules.

The ammonia and DCO^+ emission around the proto-binary system IRAS 16293−2422 (Wootten & Loren 1987; Mizuno et al. 1990; Lis et al. 2002) does not only peak on IRAS 16293−2422 itself but shows a second peak, about 90″ to the southeast, in a condensation called 16293E. Lis et al. (2002) found that CO in this region is depleted by a factor of 7. It is known to be a region where deuterium fractionation is strong and was chosen to be searched for D_2H^+.

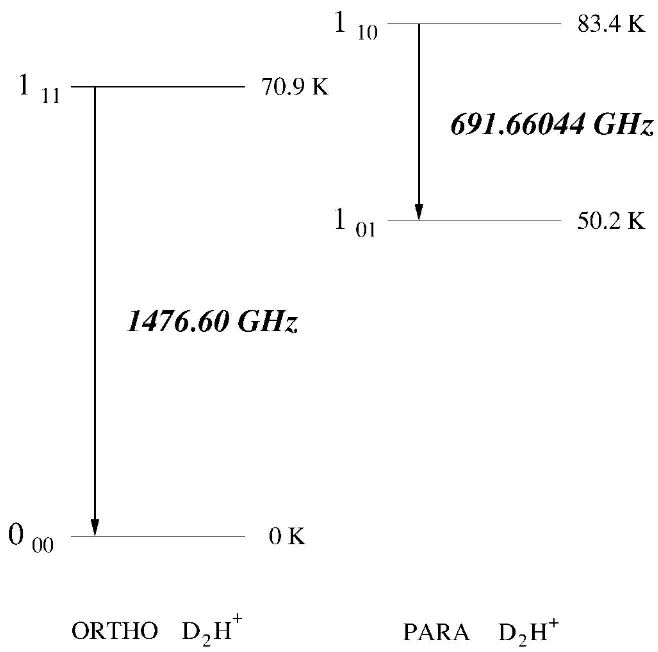

FIG. 1.—Diagram of the lowest energy levels of the D_2H^+ molecule

2. OBSERVATIONS AND RESULTS

The pure rotational transition (1_{10}–1_{01}) of D_2H^+ has been measured in the laboratory by Hirao & Amano (2003). Spectroscopic observations of 16293E, presented here, were carried out in 2004 February using the facility receivers and spectrometers of the Caltech Submillimeter Observatory (CSO) on Mauna Kea, Hawaii. The position chosen was the DCO^+ peak emission ($\alpha_{J2000.0} = 16^h32^m29\overset{s}{.}4$, $\delta_{J2000.0} = -24°28'52\overset{''}{.}6$; Lis et al. 2002). We observed both the 1_{10}–1_{11} transition of ortho-H_2D^+ [ν = 372.42134(20) GHz; Bogey et al. 1984] and the 1_{10}–1_{01} transition of para-D_2H^+ [ν = 691.660440(19) GHz; Hirao & Amano 2003] (see Figs. 1 and 2), which are the only lines currently available for these species. The data were taken under good weather conditions (225 GHz zenith opacity between 0.03 and 0.05). The CSO main-beam efficiencies are ∼60% for the 345 GHz receiver and ∼40% for the 650 GHz receiver, determined from total power observations of Mars and Saturn. If the emission is extended compared to the beam size of CSO, as appears to be the case for DCO^+ (Lis et al. 2002), then the efficiency is about 70% at 372 GHz and 60% at 692 GHz. The FWHM beam size at 372 GHz is about 20″, compared to ∼11″ at 692 GHz. Typical calibration uncertainties are ∼24%. The pointing of the telescope was determined from observations of Jupiter and was stable about ∼2″ (rms). We used both the 50 and 500 MHz bandwidth acousto-optical facility spectrometers. The 500 MHz system was used to check system performance and calibration with the CO (6 → 5) line, which is offset by ∼82 km s^{-1} from D_2H^+. There are no known lines of other interstellar molecules within 50 MHz likely to emit from such a cold region. In Table 1, we report the frequency, the antenna temperature, the line width, and the velocity relative to the local standard of rest, for the two lines. In Figure 3, we present 8.2 σ and 4.4 σ detections of H_2D^+ and D_2H^+, respectively, obtained in 23 and 103 minutes on-source integration time, respectively.

Since the para ground-state transition for D_2H^+ is the only line available to existing telescope facilities, it is not possible

TABLE 1
RESULTS OF GAUSSIAN FITS TO THE H_2D^+ AND D_2H^+ SPECTRA

Line (1)	ν (GHz) (2)	T_a^* (K) (3)	Δv (km s^{-1}) (4)	V_{LSR} (km s^{-1}) (5)
H_2D^+ (1_{10}–1_{11})	372.42134(20)[a]	1.31	0.36 ± 0.04	3.55 ± 0.02
D_2H^+ (1_{10}–1_{01})	691.660440(19)[b]	0.34	0.29 ± 0.07	3.76 ± 0.03

[a] Measured frequency by Bogey et al. (1984).
[b] Measured frequency by Hirao &Amano (2003).

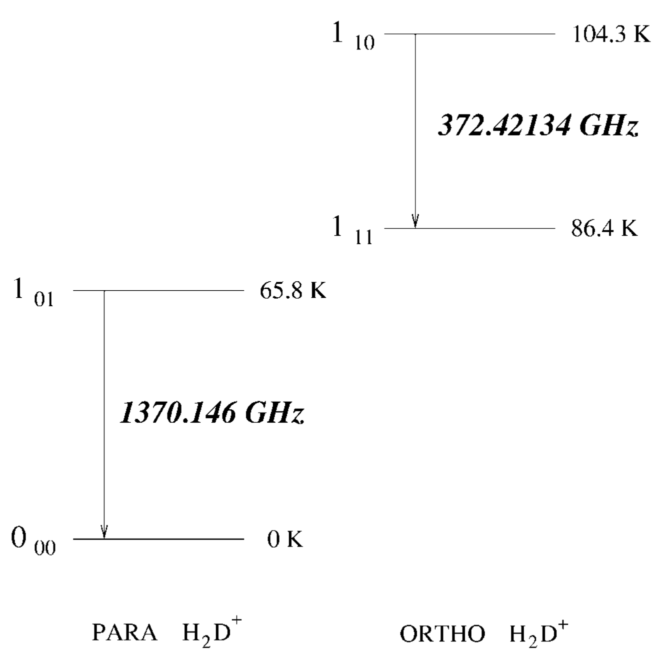

FIG. 2.—Diagram of the lowest energy levels of the H_2D^+ molecule

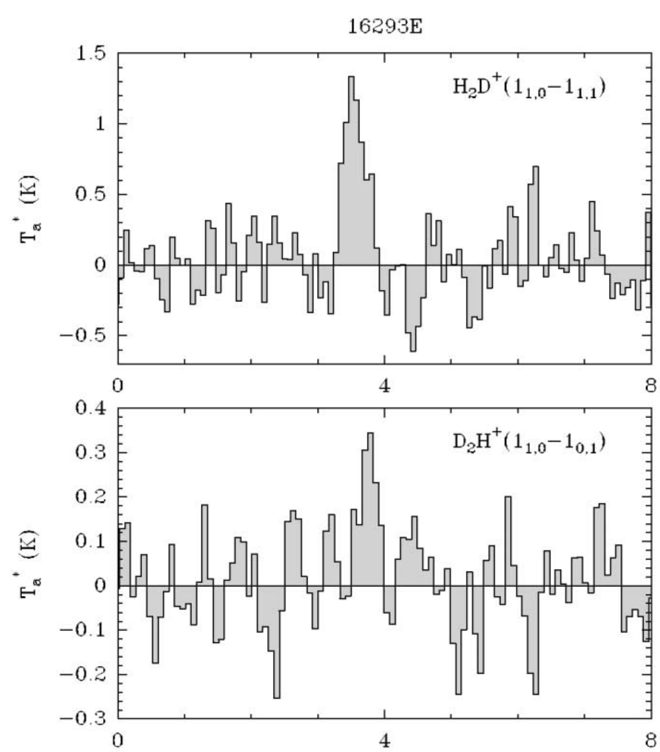

FIG. 3.—Spectra of the ortho-H_2D^+ 1_{10}–1_{11} and para-D_2H^+ 1_{10}–1_{01} transitions toward 16293E.

TABLE 2
Ortho-H_2D^+ and Para-D_2H^+ Column Densities at $T_{ex} = 10$ K[a]

Line	τ	N (10^{13} cm^{-2})
Ortho-H_2D^+	0.74	1.73 ± 0.43
Para-D_2H^+	0.61	1.29 ± 0.32
Para-D_2H^+/ortho-H_2D^+		0.75 ± 0.37

[a] In the case where the source emission is extended compared to the beam size (see text).

to obtain confirmation of the identification. However, the situation is very different from molecule detection in hot core regions, such as OMC-1, where line confusion is rampant. At the 692 GHz transition frequency, any heavy molecule would need to be in a high J state, but the 10 K excitation temperature means that any such state cannot be occupied. Of course, CO ($6 \rightarrow 5$) is observable, but only at $T_a^* = 2.3$ K. No U-lines have been observed in this source. The identification rests on the comparison of the deduced V_{LSR} for D_2H^+ with that for other deuterated molecules, and also the line width and line strength. Note that the quoted uncertainty for the line frequency is about 0.16 km s^{-1} for H_2D^+ and 0.008 km s^{-1} for D_2H^+. The very slight difference in the observed V_{LSR} for these two lines (~0.2 km s^{-1}) could be due, in part, to the uncertainty in the line frequencies, particularly H_2D^+. Also, the accuracy of the astronomical measurement is limited by the resolution of the acousto-optic spectrometer at about 0.1 km s^{-1}.

3. DISCUSSION

From the observed line strengths, given in column (3) of Table 1, we estimate the H_2D^+ and D_2H^+ column densities (see Table 2) for an excitation temperature T_{ex} of 10 K, assuming a 25% calibration uncertainty (3 σ). The column density is given by

$$N_{tot} = \frac{8\pi\nu^3}{c^3}\frac{Q(T_{ex})}{g_u A_{ul}}\frac{e^{E_u/T_{ex}}}{e^{h\nu/kT_{ex}}-1}\int \tau\, dv, \quad (4)$$

where $Q(T_{ex})$ is the partition function. Assuming LTE conditions, we can estimate the optical depth from the observed line intensity:

$$T_{mb} = [J_\nu(T_{ex}) - J_\nu(T_{bg})](1 - e^{-\tau}), \quad (5)$$

where $J_\nu(T) = (h\nu/k)/(e^{h\nu/kT} - 1)$ is the radiation temperature of a blackbody at a temperature T, and T_{bg} is the cosmic background temperature of 2.7 K. In the case of the H_2D^+ transition, $g_u = 9$, $A_{ul} = 1.04 \times 10^{-4}$ s^{-1}, and $E_{ul} = 17.9$ K; in the case of the D_2H^+ transition, $g_u = 9$, $A_{ul} = 4.55 \times 10^{-4}$ s^{-1}, and $E_{ul} = 33.2$ K. The derived column densities depend on the assumed value of the excitation temperature. Using NH_3, Mizuno et al. (1990) estimate the gas temperature to be 12 K. Using D_2CO line ratios, Loinard et al. (2001) obtained a rotational temperature of 8–10 K. Thus, we quote, in Table 2, the values obtained for an excitation temperature of 10 K. Figure 4 presents the evolution of the ortho-H_2D^+ and para-D_2H^+ column densities as well as the para-D_2H^+/ortho-H_2D^+ ratio, as a function of temperature between 9 and 15 K. Figure 4 and Table 2 represent the case where the source emission is extended compared to the beam size. If the source emission is comparable to or smaller than the CSO beam size, the para-D_2H^+/ortho-H_2D^+ ratio is then increased by a factor of ~1.5

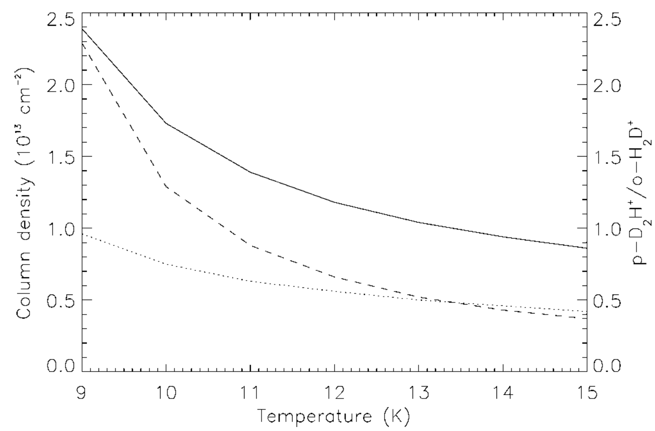

Fig. 4.—Column densities of the ortho-H_2D^+ 1_{10}–1_{11} (*solid line*) and para-D_2H^+ 1_{10}–1_{01} (*dashed line*) on the left side of the graph and the para-D_2H^+/ortho-H_2D^+ ratio (*dotted line*) on the right side, in the case where the source emission is extended compared to the beam size (see text).

at the average excitation temperature of 10 K. At thermal equilibrium, the ortho-to-para (respectively, para-to-ortho) concentration ratio for H_2D^+ (respectively, D_2H^+) is equal to 9 × exp $(-86.4/T)$ [respectively, 9/6 × exp $(-50.2/T)$], so that at 10 K, this ratio would be ~2 × 10^{-3} (respectively, ~10^{-2}). However, taking into account the limited rates of the spin allowed collisions with H_2, it is found that at these low temperatures, the ortho-to-para H_2D^+ concentration ratio is close to unity (Gerlich, Herbst, & Roueff 2002). The para-to-ortho D_2H^+ ratio is estimated by Walmsley et al. (2004) to be about 1, for the same conditions. The para-D_2H^+/ortho-H_2D^+ ratio presented in Figure 4 should then approximately represent the actual D_2H^+/H_2D^+ ratio.

The 1.3 mm dust continuum strength (see Lis et al. 2002) is ~0.3 Jy in an 11″ beam and ~1.3 Jy in a 20″ beam, corresponding to the angular resolution of the H_2D^+ and D_2H^+ data. Assuming a dust temperature of 12 K and a mass opacity coefficient of 0.005 cm^2 g^{-1} (appropriate for prestellar cores), we derive an H_2 column density of ~5 × 10^{23} cm^{-2}. We then derive the H_2D^+ and D_2H^+ abundances to range between ~10^{-10} (at 10 K) and ~10^{-11} (at 15 K), compatible with abundances found by Roberts et al. (2003) for a cloud at 10 K and $n(H_2) = 3 \times 10^6$ cm^{-3}.

The main result of this work is *the detection of* D_2H^+, *with an abundance comparable to that of* H_2D^+. This is a remarkable verification of recent theoretical predictions, aimed at explaining the large deuteration ratios observed in low-mass prestellar cores and protostars. Two models, Roberts et al. (2003) and Walmsley et al. (2004), have recently considered the effect of including all possible deuterated isotopomers of H_3^+ in the chemical networks, as suggested by Phillips & Vastel (2003). Roberts et al. (2003) studied the temporal evolution of a cold and dense cloud and found that at late times (~10^4 yr), when CO is severely depleted in the gas phase (more than a factor of 1000), the D_2H^+/H_2D^+ ratio reaches unity. Walmsley et al. (2004) studied the evolution of gas, depleted in CO, as a function of gas density and grain size distribution. For densities larger than 10^6 cm^{-3}, they also found that D_3^+ can be the most abundant ion and that the D_2H^+/H_2D^+ ratio reaches unity (see their Fig. 2). Both models need an extreme CO depletion to account for such a ratio. As discussed in § 1, the measured CO depletion in 16293E is a factor of 7 (Lis et al. 2002), rather than the extreme CO depletion needed by the models. However, the CO was measured in a large region (31″) compared with that probed by the present observations: 20″ for the H_2D^+ and 11″ for the D_2H^+ observations. Also, regions containing CO will not contain much H_2D^+ and D_2H^+ and vice versa, so the inevitable inhomogeneities in the region inhibit a clear result.

In summary, after some years of inconclusive results for theoretical models in understanding the observed high deuteration ratios of doubly and triply deuterated molecules, the present observation seems to suggest that the basic process is now almost completely understood: the large deuteration is due to extreme CO depletion, and the factor that was previously missing in the models is the multiply deuterated forms of H_3^+. This is quite an achievement, and one remaining step will be to verify that the last prediction, a significant abundance of D_3^+, is also fulfilled. At present, the lines detected here are the only ones available for H_2D^+ and D_2H^+. Knowledge of the ortho-to-para ratios and abundances of H_2D^+ and D_2H^+ would be considerably improved if the ground-state transitions of para-H_2D^+ (at 1370.15 GHz) and ortho-D_2H^+ (at 1476.60 GHz) were available. These lines could be detected from space telescopes such as *Herschel* with the Heterodyne Instrument for the Far-Infrared and also possibly from the stratospheric observatory SOFIA. However, D_3^+, like H_3^+, has no permanent dipole moment. Therefore, this molecule probably can only be detected in absorption in the near-infrared.

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