Upper limit for the $D_2H^+$ ortho-to-para ratio in the prestellar core 16293E (CHESS)*

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ABSTRACT

The $H_2^+$ ion plays a key role in the chemistry of dense interstellar gas clouds where stars and planets are forming. The low temperatures and high excitations of such clouds make direct observations of $H_2^+$ impossible, but lead to large abundances of $H_2D^+$ and $D_2H^+$, which are very useful probes of the early stages of star and planet formation. The ground-state rotational ortho-$D_2H^+$ $1_{1,1} - 0_{0,0}$ transition at 1476.6 GHz in the prestellar core 16293E has been searched for with the Herschel** HIFI instrument, within the CHESS (Chemical Herschel Surveys of Star forming regions) Key Program. The line has not been detected at the 21 mK km s$^{-1}$ level (3σ integrated line intensity). We used the ortho-$H_2D^+$ $1_{1,1} - 0_{1,0}$ transition and para-$D_2H^+$ $1_{0,0} - 0_{1,0}$ transition detected in this source to determine an upper limit on the ortho-to-para $D_2H^+$ ratio as well as the para-/$D_2H^+$ ortho-/$D_2H^+$ ratio from a non-LTE analysis. The comparison between our chemical modeling and the observations suggests that the CO depletion must be high (larger than 100), with a density between 5 $\times$ 10$^3$ and 10$^6$ cm$^{-3}$. Also the upper limit on the ortho-$D_2H^+$ line is consistent with a low gas temperature ($\sim$ 11 K) with a ortho-to-para ratio of 6 to 9, i.e. 2 to 3 times higher than the value estimated from the chemical modeling, making it impossible to detect this high frequency transition with the present state of the art receivers.

Key words. astrochemistry – ISM: individual (16293E) – ISM: abundances – Line: identification – Radiative transfer

1. Introduction

In the recent years, the chemistry of dark clouds and star forming regions has constantly been revised with the discovery of multiply deuterated molecules: D$_2$CO (Turner 1990; Ceccarelli et al. 1998), ND$_3$H (Roueff et al. 2000), D$_2$S (Vastel et al. 2003), ND$_2$ (Lis et al. 2002; van der Tak et al. 2002), CHD$_3$OH, CD$_3$OH (Parise et al. 2002, 2004) and D$_2$H$^+$ (Vastel et al. 2004). Two main pathways can be invoked for understanding the observed large deuterium fractionation. The first is based on grain chemistry (Tielens 1983; Vastel et al. 2003) and Parsie et al. (2004) showed that grain chemistry models require a very high atomic D/H ratio accreting on the grains in order to explain their high deuterium fractionation ratio that could not be reproduced by gas-phase modeling at that time. New models can now reproduce the observed abundance of the multi-deuterated isotopologues of formaldehyde and methanol, both formed in the last stage of the prestellar phase (Faquet et al. 2012). The second pathway for forming deuterated molecules is based on gas-phase chemistry and results from the ion-molecule deuterium exchange reactions taking place at low temperatures. In this scenario, deuterated molecules are produced through successive reactions starting with H$_2D^+$, dominant at temperatures lower than 20 K, CH$_2D^+$ or C$_2$HD$^+$, dominant at higher temperatures (Roberts & Millar 2000; Gerlich et al. 2002). H$_2D^+$ has proven to be a very good probe of the dense cold cores, where CO disappears from the gas phase and is depleted onto the dust grains (Caselli et al. 2003, 2008). Phillips & Vastel (2003) pointed out that the deuteration should be extended beyond H$_2D^+$, to D$_2H^+$ and D$_3^+$ and suggested that the detection of the D$_2H^+$ ion might be possible. Calculations including all possible deuterated isotopomers of $H_2^+$ have confirmed that, in dense CO depleted regions, the abundance of D$_2H^+$ will be similar to that of H$_2D^+$, and the D/H ratio will be largely enhanced (Roberts et al. 2003, 2004; Walmsley et al. 2004; Ceccarelli & Dominik 2005).

D$_2H^+$ in its para form was detected for the first time in the prestellar core 16293E by Vastel et al. (2004), showing its importance, as well as that of D$_1^+$, in determining the total deuterium abundance in the gas phase. This dense core, revealed by amonia emission (Mizuno et al. 1990), is sheltered in the dense cloud L1689N (see Wootten & Loret 1987), and has been revealed by millimeter lines and continuum emission. This cloud, also harboring a young binary protostellar object (IRAS 16293-...
2422 A and B) and bipolar outflows (named Rho Oph East by Fukui et al. (1986)), has been extensively observed, revealing an extreme molecular deuteration in particular towards an extreme molecular deuteration in particular towards the cold dense core, named 16293E by Loinard et al. (2001) and Castets et al. (2001). Note that this core has been called p Oph E (as in Rho Oph East referring to the outflow emanating from IRAS 16293-2422) by Saito et al. (2000) and Gérin et al. (2001). However, we decided to use the name 16293E since p Oph E already refers to another condensation within the L1688 cloud in the Ophiuchi complex (Loren et al. 1990) and, therefore, is confusing. We present here recent Herschel/HIFI observations obtained within the Herschel guaranteed time Key Program CHESS, and modeling of both ground state transitions of para- and ortho–D$_2$H$^+$, as well as ortho–H$_2$D$^+$, using the recent collisional coefficients with ortho– and para–H$_2$ (Hugo et al. 2009).

Figure 1 shows the 1.3 mm continuum map as well as the DCO$^+$ contour map (blue) (Lis et al. 2002). Studies of the gas kinematics using CO, HCN, H$^13$CO$^+$, HCO$^+$ and DCO$^+$ tracers lead to the conclusion that the deuterium peak is a part of the ambient cloud that is pushed and compressed by the outflow. (Lis et al. 2002). Indeed this shock could have released deuterated species, that were condensed on the dust grains, into the gas phase with a subsequent cooling of the gas to lower temperatures. This effect, combined with the low temperature gas-phase chemistry in the high-density shock-compressed gas leads to a high molecular deuteration as observed in: DNC (9%; Hirota et al. 2001), D$_2$CO (40% ± 20% Loinard et al. 2001), Ceccarelli et al. 2002, N$_2$D$^+$ (Gérin et al. 2001), NH$_2$D (19% Mizuno et al. 1994; Loinard et al. 2001; Roueff et al. 2005), ND$_3$H (4%; Mizuno et al. 1996; Loinard et al. 2001; Lis et al. 2006), DCO$^+$ and DCN (HDS (Vastel et al. 2003), D$_2$H$^+$ (Vastel et al. 2004), HDO (Stark et al. 2005); ND$_3$ (0.1%: Roueff et al. 2005). Because no far-infrared or submillimeter point source has been found, the source can be classified as a prestellar core, the early phase of the formation of a protostellar object, before gravitational contraction occurs.

2. Observations and data reduction

The para–D$_2$H$^+$ ground state transition was observed towards the prestellar core 16293E with the HIFI instrument (de Graauw et al. 2010) on board the Herschel Space Observatory (Pilbratt et al. 2010), as part of the Herschel guaranteed time Key Program CHESS (Ceccarelli et al. 2010). A pointing at a frequency centered on the D$_2$H$^+$ line (~ 1476.6 GHz) with the band 6a HEB receiver was performed on February 16, 2011 using the pointed Double Beam Switch (DBS) mode with optimization of the continuum. In this mode, both the HIFI Wide Band Spectrometer (WBS) — providing a spectral resolution of 1.1 MHz (~ 0.2 km s$^{-1}$) over an instantaneous bandwidth of 2.4 GHz — and the HIFI High Resolution Spectrometer (HRS) — providing a spectral resolution of 125 kHz over an instantaneous bandwidth of 0.12 GHz — were used. The DBS reference positions were situated approximately 3’ East and West of the source. The HIFI beam size at the observed frequency is about 14”, and the main beam and forward efficiencies are about 0.72 and 0.96, respectively (Roelfsema et al. 2013). The data have been processed using the standard HIFI pipeline up to level 2 with the ESA-supported package HIPE 8.0 (Ott 2010). The on-source integration time for this observation was 18158 seconds. FITS files from level 2 data were created and translated into CLASS/GILDAS format for subsequent data reduction and analysis. For each scan, a low order polynomial baseline was fitted outside the line window. The antenna temperatures were finally converted to the T$_{mb}$ scale, using the theoretical values of the main beam and forward efficiencies given above. We present in Figure 2 this observation as well as the para ground state transition observed at the Caltech Submillimeter Observatory (CSO) (Vastel et al. 2004). Both observations were pointed towards the DCO$^+$ peak emission, at coordinates $\alpha_{2000} = 16^h 32^m 28.62^s$, $\delta_{2000} = -24^\circ 29' 27''$ (see for example Roueff et al. 2005, Figure 9). Note that the coordinates in Vastel et al. (2004) were not correctly...
The two nuclear-spin species of H$_2$D$^+$ and D$_2$H$^+$ (ortho and para) are considered separately. The parameters of the ortho- and para-D$_2$H$^+$ and ortho–H$_2$D$^+$ ground transitions are obtained using the CASSIS$^\text{1}$ software, which takes into account the ortho and para forms separately, with an independent computation of the partition function (cf. Formalism for the CASSIS software, http://cassis.irapomp.eu/), and are reported in Table 1. The Einstein coefficient for the ortho–D$_2$H$^+$ transition ($\sim 3 \times 10^{-3}$ s$^{-1}$) is much larger than for the para–D$_2$H$^+$ ($\sim 4.6 \times 10^{-4}$ s$^{-1}$) and ortho–H$_2$D$^+$ ($\sim 1.1 \times 10^{-4}$ s$^{-1}$) transition, since it varies as a function of $v^3$. Note that we adopt here the most recent measurement of Amano & Hirao (2005) of the para-D$_2$H$^+$ line frequency (691.660483 GHz), 372.421385 GHz for the ortho–H$_2$D$^+$ transition and 1476.605708 GHz for the ortho–D$_2$H$^+$ transition (Asvany et al. 2008). From a simple Gaussian fitting function, the inter-

tions (Loinard et al. 2001), with the ND$_2$H$^+$ $+$ transitions (Lis et al. 2002) and the N$_2$H$^+$ line width (0.32 km s$^{-1}$ for the 3–2 transition; Gérin et al. 2001) are systematically larger than the thermal line widths of 0.16, 0.12 and 0.16 km s$^{-1}$ respectively for a 10 K kinetic temperature. Considering the high critical densities for the (o-p) ND$_2$H and ND$_3$ transitions (larger than 10$^5$ cm$^{-3}$), it seems that systematic motions occur even in the dense part of the cloud. Also, at large enough densities/depletions, one expect to have the light ions left as the main tracers of the gas. This further confirms that H$_2$D$^+$ and D$_2$H$^+$ remain the only tracers of the cold, dense and CO/N$_2$ depleted central region where other molecular tracers are largely condensed onto the dust grains, rather than the lower density envelope when turbulence takes over.

3.2. H$_2$D$^+$ and D$_2$H$^+$ non-LTE modeling

The H$_2$ density is a critical parameter for the interpretation of our deuterated ions observations. CO observations of the 3–2, 4–3, 6–5 transitions give a lower limit for the molecular hydrogen density of 5 × 10$^3$ cm$^{-3}$ (Lis et al. 2002). In their analysis, Lis et al. 2002 used a kinetic temperature of 12 K (based on NH$_3$ observations of Menten et al. 1987) and a density of 5 × 10$^3$ cm$^{-3}$, consistent with their observed DCO$^+$ (5–4)/(3–2) and N$_2$D$^+$ (4–3)/(3–2) line ratios. From 450 and 850 $\mu$m continuum maps (Stark et al. 2004) inferred an isotothermal dust temperature $T = 16$ K and peak density of 1.6 × 10$^6$ cm$^{-3}$. Note however that their dust peak emission does not correspond to the peak of deuterated molecules (about 15” away) that we are studying in the present paper. This could be due to the release of the deuterated species that were condensed on the dust grains by the interaction between the outflow from IRAS 16293-2422 and the cold core 16293E. This compression is then likely to cool the

Fig. 3. Diagram of the lowest energy levels (in Kelvins) of the D$_2$H$^+$ molecule.

$^1$ CASSIS (http://cassis.irapomp.eu/) has been developed by IRAP-UPS/CNRS.
gas to lower temperatures. These observations possibly trace the parental cloud of the prestellar core 16293E. We will therefore consider in the following study densities between $10^5$ and $10^6$ cm$^{-3}$ and kinetic temperatures between 9 and 16 K (see section 3.1).

From the recent computations of the collision rates (Hugo et al. 2009), the critical densities for the ortho–H$_2$D$^+$, ortho–D$_2$H$^+$ and para–D$_2$H$^+$ transitions are $\sim 1.3 \times 10^5$ cm$^{-3}$, $\sim 7 \times 10^6$ cm$^{-3}$ and $\sim 5.6 \times 10^5$ cm$^{-3}$ respectively, using the Einstein coefficients from Ramal&n & Tennyson (2004). 1.2 $\times 10^{-4}$, 3.3 $\times 10^{-3}$ and 5.1 $\times 10^{-4}$ s$^{-1}$ respectively. From the large difference between the critical densities, the ortho–D$_2$H$^+$ transition will trace denser regions than the para transition. Since the typical density in the core seems to be less than these critical densities, a Local Thermodynamic Equilibrium approximation is not applicable. In Vastel et al. (2004), only LTE modeling could be performed because the collision rates were not available at that time. We produced collisional files, assuming a simple 2 level system, using the inelastic state-to-state rate coefficients for the ortho and para ground transitions of H$_2$D$^+$ and D$_2$H$^+$ in collision with para and ortho H$_2$, as a function of temperature. We used the non-LTE radiative transfer code RADEX (van der Tak et al. 2007) in the large velocity gradient (LVG) approximation with the collisional files that were created for these species. We could consider in the following non-LTE modeling two values for the H$_2$ ortho to para ratio of 3 (highest value at thermodynamic equilibrium) and 0 (only collisions with para H$_2$). However, the similarities of the collision coefficients with ortho and para H$_2$ for (o,p)H$_2$D$^+$ or (o,p)D$_2$H$^+$ will lead to a very small difference in the derived column densities.

The variation of the para–D$_2$H$^+$ to ortho–H$_2$D$^+$ ratio as a function of the gas temperature, for densities of $1 \times 10^5$ (green), $5 \times 10^5$ (blue) and $1 \times 10^6$ (red) cm$^{-3}$. The thick lines show the ratio derived from observations, using non-LTE modeling, whereas the thin lines show the chemical model results. Three depletion factors at steady-state are presented: complete depletion (CD: solid lines), depletion factor = 100 (dot-dashed lines) and depletion factor = 10 (dashed lines). The thin dashed vertical lines present the [9.5 – 12.4] K range.

The reduced Nahoon code has then been modified to include deuterium and deuterated species, with H$_2$, HD and D$_2$ forming on grain surfaces. Finally, the spin states of all isotopologues of H$_2$ and H$_2^+$ were included. The rate coefficients of the new reactions were taken from Sipilä et al. (2010), Hugo et al. (2009), Flower et al. (2004) and Walshney et al. (2004), choosing the most recent values in case of multiple choice. The reaction balancing routine within the Nahoon program (the one which checks the reaction list, to make sure that reactants and products have the same number of elements and charges) had to be modified after the inclusion of the different spin states, to avoid to balance spin states between reactants and products (as spin states are not conserved). For this purpose, different spin states were labelled adding an extra column in the element and species definition file. In this column we assigned -1 to the lower spin state and +1 to the higher spin state of all isotopologues of H$_2$ and H$_2^+$ (para–D$_2$H$^+$ has been assigned a value of +2 as it is the highest of three spin states). All other species have a zero in the corresponding column, indicating that no spin state is considered. The H$_2$ self shielding data has not been modified but new parameters for the self shielding of HD and D$_2$ have been introduced and have been each set to initially be equal to that of H$_2$. Coulomb focusing was taken into account for reactions invol-

Table 1. Derived parameters of the ortho–H$_2$D$^+$ transitions as well as the ortho and para D$_2$H$^+$ fundamental lines. DCO$^+$ 3–2 and 5–4 transitions used in Lis et al. (2002) are also quoted using the estimated frequencies from Caselli & Dore (2005). Note that a discussion on the V$_{LSR}$ can be found at the end of Section 2.

| Species | Transition | Frequency (GHz) | Telescope | beams| $T_{mb}$ dV (mK km s$^{-1}$) | rms (mK) | binsize (km s$^{-1}$) | $\Delta V$ (km s$^{-1}$) | V$_{LSR}$ (km s$^{-1}$) |
|---------|------------|----------------|-----------|------|--------------------------|---------|------------------|-----------------|----------------|
| ortho–H$_2$D$^+$ | 1_0$-1_1$ | 372.421385 | CSO | 20 | 720 | 80 | 0.080 | 0.36 ± 0.04 | 3.59 ± 0.02 |
| para–D$_2$H$^+$ | 1_0$-1_1$ | 691.660483 | CSO | 11 | 183 | 170 | 0.029 | 0.8 ± 0.05 | 3.78 ± 0.02 |
| ortho–D$_2$H$^+$ | 1_1$-0_0$ | 1476.605708 | HIFI/HRS | 14 | $\leq 30$ | 120 | 0.012 | 0.21 | 0.203 |
| ortho–D$_2$H$^+$ | 1_1$-0_0$ | 1476.605708 | HIFI/WBS | 14 | $\leq 21$ | 21 | 0.203 | 0.21 | 0.203 |
| DCO$^+$ | 3–2 | 321.1125822 | CSO | 35 | 323.5 | 94 | 0.134 | 0.67 ± 0.03 | 3.55 ± 0.01 |
| DCO$^+$ | 5–4 | 360.1697783 | CSO | 20 | 528 | 109 | 0.081 | 0.54 ± 0.03 | 3.65 ± 0.01 |

\[ \text{http://kida.obs.u-bordeaux1.fr/models} \]
A range of H$_2$ volume densities ($1 \times 10^5$, $5 \times 10^5$, $1 \times 10^6$ cm$^{-3}$), kinetic temperatures (9, 11, 13, 15, and 16 K), and depletion factors ($\equiv$ undepleted abundance / depleted abundance $= 10$, 100, infinity) of all the elements heavier than helium (C, N and O) have been explored and followed in time until the system reaches equilibrium. Since the CO molecule is the main destroyer of the H$_2^+$ ion (and its deuterated counterparts), we simulate three depletion values at steady-state: complete depletion, and elemental depletion factor of 10 and 100 corresponding to CO depletion factors of about 14 and 140, respectively, at equilibrium. From [Lis et al. 2002], C$^{18}$O observations at the deuterium peak of 16293E lead to a CO depletion factor (average along the line of sight) of $\sim 10$, representing a lower limit for the central core traced by D$_2$H$^+$. Considering the overall parameters in the chemical modeling we adopt the conservative values of $3 \times 10^{-17}$ s$^{-1}$ for the cosmic ionization rate, 0.01 for the dust to gas ratio, and 0.1 $\mu$m for the grain radius.

Figure 4–6 show the predictions (thin lines) of the model at equilibrium (reached in 2 $10^5$ years for the complete depletion case, 5 $10^5$ years for a depletion factor of 100 and 2 $10^5$ years for a depletion factor of 10) for temperatures between 9 and 16 K for three densities. The para–D$_2$H$^+$/ortho–D$_2$H$^+$ ratio increases with the depletion factor: indeed the disappearance of the CO molecule from the gas phase leads to the reactions of HD with H$_2^+$ with an increasing production of its deuterated counterparts [Phillips & Vastel 2003]. Also the increase of the ortho-to-para D$_2$H$^+$ ratio with the depletion factor can be explained by the fact that the reactions with HD, ortho–D$_2$ and para–D$_2$ converting para–D$_2$H$^+$ into ortho–D$_2$H$^+$ are dominant compared to the reverse reactions [Hugo et al. 2009]. From equations 4 and 5 we can say that a low ortho–H$_2$ value leads to a very high D$_2^+$ abundance for densities larger than $10^5$ cm$^{-3}$. Indeed the D$_2^+$ ion is likely to be the dominant ion in such high-density regions: e.g. Figure 3 from [Flower et al. 2006] and Figure 2 from [Sipilä et al. 2010]. The ortho-to-para D$_2$H$^+$ ratio consequently increases as the depletion factor increases, as seen in Figure 5.

Figure 5. Variation of the ortho-to-para D$_2$H$^+$ ratio as a function of the gas temperature, for densities of $1 \times 10^5$ (green), $5 \times 10^5$ (blue) and $1 \times 10^6$ (red) cm$^{-3}$. Three depletion factors at steady-state are presented: complete depletion (CD: solid lines), depletion factor = 100 (dot-dashed lines) and depletion factor = 10 (dashed lines). The thin dashed vertical lines present the [9.5 – 12.4] K range.

Figure 6. Prediction of the ortho-to-para H$_2$D$^+$ ratio as a function of the gas temperature, for densities of $1 \times 10^5$ (green), $5 \times 10^5$ (blue) and $1 \times 10^6$ (red) cm$^{-3}$. Three depletion factors at steady-state are presented: complete depletion (CD: solid lines), depletion factor = 100 (dot-dashed lines) and depletion factor = 10 (dashed lines). The thin dashed vertical lines present the [9.5 – 12.4] K range.

Figure 7. Variation of the ortho-to-para H$_2^+$ ratio as a function of the kinetic temperature, for densities of $1 \times 10^5$ (green), $5 \times 10^5$ (blue) and $1 \times 10^6$ (red) cm$^{-3}$. Three depletion factors at steady-state are presented: complete depletion (CD: solid lines), depletion factor = 100 (dot-dashed lines) and depletion factor = 10 (dashed lines). The thin dashed vertical lines present the [9.5 – 12.4] K range.

ing negatively charged ions on neutral grains [Draine & Sutin 1987]. Only neutral and negatively charged grains are present in the network. The final chemical network includes over 3,500 reactions involving nearly 130 different species. The full chemical network used in this work is available at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/cgi-bin/qcat?J/A+A/. Comparison with previous work and a parameter space exploration will be presented by Kong et al. (in prep.).

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overall chemistry, since it is critical for the degree of deuteration of \( \text{H}_2^+ \). Increasing the deuteration factor leads to a local decrease of the CO abundance. Therefore \( \text{H}^+ \) and \( \text{H}_2^+ \) will mainly react with ortho–\( \text{H}_2 \) (at the same temperature the backward reaction is negligible), and not \( \text{CO} \). This will lead to a high ortho-to-para \( \text{H}_2 \) conversion, consequently a lower ortho-to-para \( \text{H}_2 \) ratio as seen in Figure 7. Our chemical modeling also predicts a variation of the steady-state ortho-to-para \( \text{H}_2 \) ratio for the complete depletion case, a depletion factor of 100 and a depletion factor of 10, between 9 and 16 K (see Figure 7). Because of the large internal energy (\( \sim 170 \) K) of the lowest ortho–\( \text{H}_2 \) level (\( J = 1 \)) compared to the temperature range explored in this source, the ortho–\( \text{H}_2 \) form is a limiting factor for deuteration. It overcomes the energy barrier, leading to exothermic (i.e fast and temperature independent) reactions (e.g. Gerlich et al. 2002):

\[
o - \text{H}_2 \text{D}^+ + o - \text{H}_2 \rightarrow (o, p) - \text{H}_3^+ + \text{HD}
\]

(3)

\[
p - \text{D}_2 \text{H}^+ + o - \text{H}_2 \rightarrow p - \text{H}_2 \text{D}^+ + \text{HD}
\]

(4)

The excited nuclear spin state of the \( \text{D}_3^+ \) ion is removed preferentially by ortho–\( \text{H}_2 \) in the following endothermic (by only 18 K) reaction:

\[
m - \text{D}_3^+ + o - \text{H}_2 \rightarrow o - \text{D}_3 \text{H}^+ + \text{HD}
\]

(5)

Following Hugo et al. (2009) we have assigned meta–\( \text{D}_2^+ \) with the modification having the lowest ground state energy, corresponding to the A1 representation of the symmetry group S3. All forms should be taken into account in any chemical modeling involving deuterated ions.

Although Pagani et al. (2009) showed that the ratio is unlikely in steady-state in prestellar cores, this will not affect the computation of the column densities since, as mentioned in Section 2, the collisional rates for ortho–\( \text{H}_2 \text{D}^+ \) (as well as para– and ortho–\( \text{H}_2 \text{D}^+ \)) are similar for collisions with both para– and ortho–\( \text{H}_2 \). Note also that the difference between our modeling and Pagani et al. (2009) comes from the time-scale used. Our values are at equilibrium.

With a comparison between the chemical model predictions and the observations, three convergences can be found for the complete depletion case and \( f_{\odot} = 100 \). These domains are quoted in Table 2 for densities of \( 10^5 \), \( 5 \times 10^5 \) and \( 1 \times 10^6 \) cm\(^{-3} \). From the gas kinetic temperature range (9.5 – 12.4 K) found from the uncertainties on the para–\( \text{D}_2 \text{H}^+ \) and ortho–\( \text{D}_2 \text{H}^+ \) linewidths, the \( n_{\text{H}_2} = 10^3 \) cm\(^{-3} \) domain can be ruled out. Should we consider the highest gas kinetic temperature (12.4 K) the modeling results in a para–\( \text{D}_2 \text{H}^+ \)/ortho–\( \text{D}_2 \text{H}^+ \) abundance ratio 12% lower than the observations for a molecular density of \( 10^5 \) cm\(^{-3} \). This would reduce the upper limit on the ortho-to-para ratio to a value of \( \sim 6 \), \( \sim 40\% \) higher than the value modeled for the complete depletion case and with a depletion factor of 100 (see Figure 5). Also, the comparison between the chemical modeling and the ortho-to-para \( \text{D}_2 \text{H}^+ \) upper limit from the non detection of the ortho transition is consistent with a low gas temperature (\( \sim 11.7 \) K for a \( 10^6 \) cm\(^{-3} \) density). A proper model should consider the (unknown) physical structure and proper time-dependent freeze-out.

Note that no other molecular tracers like \( \text{DCO}^+ \) and \( \text{N}_2 \text{D}^+ \), observed by Lis et al. (2002) can be used as a comparison with the chemical modeling as it might prove difficult to disentangle their contribution from the more extended envelope to the central region.

Considering an average 11 K gas temperature the upper limit for the ortho-to-para \( \text{D}_2 \text{H}^+ \) ratio is 2 to 3 times larger than the value found from the modeling (around 3) for densities larger than \( 10^5 \) cm\(^{-3} \). We get, from the non-LTE radiative transfer modeling, \( N(\text{ortho–}\text{H}_2\text{D}^+) = (1.4 \pm 0.1) \times 10^{13} \) cm\(^{-2} \), \( N(\text{para–}\text{D}_2\text{H}^+) = (1.4 \pm 0.2) \times 10^{13} \) cm\(^{-2} \), and \( N(\text{ortho–}\text{D}_2\text{H}^+) \leq 1.4 \times 10^{14} \) cm\(^{-2} \). These values are reproduced by (or in the case of ortho–\( \text{D}_2 \text{H}^+ \) compatible with) our chemical modeling in the complete depletion case. The present state of the art instruments are clearly unable to detect the ortho–\( \text{D}_2 \text{H}^+ \) transition in this source. The CCAT (Cornell Caltech Atacama Telescope) project appears to be the most adequate to detect this ortho–\( \text{D}_2 \text{H}^+ \) transition in warmer regions.

From Figure 6 we can use the average 11 K gas temperature in the complete depletion case as well as with a depletion factor of 100 to estimate the radiation temperature of the para–\( \text{H}_2 \text{D}^+ \) transition at 1370.085 GHz for densities larger than \( 10^5 \) cm\(^{-3} \). Using a non LTE modeling described in Section 3.2, the resulting para–\( \text{H}_2 \text{D}^+ \) column density is \( (9.07 \pm 0.49) \times 10^{13} \) cm\(^{-2} \) (T\(_R\) = (60 ± 20) mK) for the complete depletion case, and (3.40 ± 0.19) \( \times 10^{13} \) cm\(^{-2} \) (T\(_R\) = (50 ± 10) mK) for a depletion factor of 100. This transition unfortunately falls in a frequency range not covered by the HIFI instrument, but could be a target for future instruments. Carbon monoxide in the LDN 1689N cloud is only moderately depleted in the single-dish beam (Lis et al. 2002) but it is possible that the angular resolution of the existing single-dish data is simply insufficient to show the spatial stratification predicted by our chemical model. The presence of completely depleted regions smaller than the CSO beam cannot be ruled out by our observations.

The deuterium peak in the LDN 1689N cloud has been argued in the literature to be a shock-compressed interaction region between a molecular outflow and an ambient cloud. Therefore high spatial resolution mapping observations of high density tracers, like \( \text{NH}_3 \) and its deuterated counterparts as well as \( \text{N}_2 \text{H}^+ \) and \( \text{N}_2 \text{D}^+ \) are necessary to allow investigating the kinematics of the high-density gas in this region. Both the Atacama Large Array Millimeter and Expanded Very Large Array are suitable for a follow-up of this source that reveals to be a non typical prestellar core.

4. Conclusions

1. The ground-state ortho–\( \text{D}_2 \text{H}^+ \) \( 1_{1,1} – 0_{0,0} \) transition at 1476.6 GHz in the prestellar core 16293E has been searched for with the Herschel/HIFI instrument.

2. The collision rates for the ortho and para \( \text{H}_2 \text{D}^+ \) and \( \text{D}_2 \text{H}^+ \) ions with molecular hydrogen have been used with a non-LTE radiative transfer code (RADEX) to derive the column densities of the detected ortho–\( \text{H}_2 \text{D}^+ \) and para–\( \text{D}_2 \text{H}^+ \) ground transitions as well as the upper limit on the ortho–\( \text{D}_2 \text{H}^+ \) observed with the HIFI instrument on board the Herschel observatory.

3. We used a gas-phase chemical model, in which deuterium chemistry and the spin states have been added and compared our modeling with the inferred para–\( \text{D}_2 \text{H}^+ \)/ortho–\( \text{D}_2 \text{H}^+ \), as well as the upper limit on the ortho-to-para \( \text{D}_2 \text{H}^+ \) ratio. The kinetic temperature is deduced from the line width of both detected ions to be about 10 K, and we varied the molecular hydrogen density between \( 10^5 \) and \( 10^6 \) cm\(^{-3} \). The upper limit on the observed ortho-to-para \( \text{D}_2 \text{H}^+ \) ratio is consistent with the modeling and points to a low (\( \sim 11 \) K) gas kinetic temperature. The detection of the ortho–\( \text{D}_2 \text{H}^+ \) transition in the cold regime is a challenge as an rms of about 9 mK is needed.

3 http://www.ccatobservatory.org/
compared to the 21 mK rms reached by the HIFI instrument in about 5 hours.

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Table 2. Non-LTE computations for the ortho–H$_2$D$^+$, para– and ortho–D$_2$H$^+$ column densities for densities of $10^5$, $5 \times 10^5$ and $10^6$ cm$^{-3}$. The temperature range results from the intersection of the modeling (thin lines in Figure 4) and the non-LTE computation (thick lines in Figure 4).

| $n_{H_2}$ (cm$^{-3}$) | $T_{\text{gas}}$ (K) | $10^7$ | $5 \times 10^7$ | $1 \times 10^8$ |
|------------------------|----------------------|-------|----------------|---------------|
|                        | [12.7 – 15.6]        | [9.9 – 12.2] | [9.4 – 11.2] |
| N(ortho–H$_2$D$^+$)    | [1.4 – 1.9] $\times 10^{13}$ | [1.2 – 1.8] $\times 10^{13}$ | [1.2 – 1.9] $\times 10^{13}$ |
| N(para–D$_2$H$^+$)     | [1.7 – 2.9] $\times 10^{13}$ | [1.1 – 2.4] $\times 10^{13}$ | [1.1 – 2.3] $\times 10^{13}$ |
| N(ortho–D$_2$H$^+$)    | $\leq 1.6 \times 10^{14}$ | $\leq 9.2 \times 10^{14}$ | $\leq 5.1 \times 10^{14}$ |
| [ortho–D$_2$H$^+$]/[para–D$_2$H$^+$] | $\leq 6$ | $\leq 44$ | $\leq 32$ |