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FAR-INFRARED DETECTION OF H_2D^+ TOWARD SGR B2[1]

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Abstract

We report on the first far–IR detection of H_2D^+, using the *Infrared Space Observatory*, in the line of sight toward Sgr B2 in the galactic center. The transition at λ=126.853 μm connecting the ground level of o-H_2D^+, $1_{1,1}$, with the the $2_{1,2}$ level at 113 K, is observed in absorption against the continuum emission of the cold dust of the source. The line is broad, with a total absorption covering 350 km s^{-1}, i.e., similar to that observed in the fundamental transitions of H_2O, OH and CH at ∼179, 119 and 149 μm respectively. For the physical conditions of the different absorbing clouds the H_2D^+ column density ranges from 2 to 5×10^{13} cm^{-2}, i.e., near an order of magnitude below the upper limits obtained from ground based submillimeter telescopes. The derived H_2D^+ abundance is of a few 10^{-10}, which agrees with chemical models predictions for a gas at a kinetic temperature of $\simeq$20 K.

Subject headings: Astrochemistry — molecular processes — line : identification — ISM : molecules — ISM : individual (Sgr B2) — infrared : ISM

1. INTRODUCTION

The H_3^+ molecular ion is a key molecule for the gas phase chemistry in interstellar clouds (Herbst & Klemperer 1973; Watson 1973). Produced by the fast reaction of H_2 with H_2^+, it reacts with almost all neutral atoms and molecules, and thus it is the precursor of a large number of complex neutral and ionic molecular species. Initially suggested to be present in molecular clouds by Martin et al. (1961), there is a long history behind the search for this crucial molecule. Due to its lack of permanent dipole moment, H_3^+ must be observed in the near–IR through its ro-vibrational transitions (Oka 1980). The first searches only provided upper limits to the H_3^+ column density (Geballe & Oka 1989; Black et al., 1990). However, H_3^+ has been finally detected toward GL2136 and the W33A clouds (Geballe & Oka 1996). In addition, H_3^+ has also been detected toward the diffuse interstellar medium (ISM) by McCall et al. (1998), and more recently in the line of sight toward several galactic center clouds (Oka et al. 2005). Unfortunately, these observations only provide information on the H_3^+ abundance in the most diffuse and warm external layers of molecular clouds, and are limited to lines of sight with bright near-IR background sources.

A different approach to study H_3^+ in denser regions obscured by dust extinction is to observe the asymmetrical species H_2D^+ and HD_2^+, which do have a rotational spectrum. These species play a crucial role in the deuteration enhancement of many molecular species in clouds with kinetic temperatures below $\simeq$30 K (see, e.g., Gerlich et al., 2002 and references therein). In particular, the H_2D^+/H_3^+ abundance ratio is expected to dramatically increase above the elemental D/H ratio as the gas cools down. The first calculation of the H_2D^+ rotational spectrum was reported by Dalgarno et al. (1973), who suggested that it could be detectable in dense and cold clouds. The H_2D^+ $1_{1,0}$-$1_{1,1}$ transition has been observed in the laboratory at 372.42134 GHz (Bogey et al. 1984; Warner et al. 1984). This precise measurement opened the quest for the detection of H_2D^+ in dense molecular clouds. Initial searches for the o-H_2D^+ $1_{1,0}$-$1_{1,1}$ line, and also the p-H_2D^+ $1_{0,1}$-$0_{0,0}$ (at 1370 GHz), performed with the *Kuiper Airborne Observatory* (Phillips et al., 1985; Pagani et al., 1992a; Boreiko & Betz, 1993), and with the *Caltech Submillimeter Observatory* (van Dishoeck et al., 1992) were, however, unsuccessful. Fortunately, H_2D^+ has finally been detected toward the young low-mass protostar NGC1333-IRAS4A (Stark et al. 1999), and in several dark clouds (Caselli et al. 2003; Vastel et al., 2004, 2006a,b; Hogerheijde et al., 2006; Harju et al., 2006), and tentatively in protoplanetary disks (Ceccarelli et al., 2004; see also Guilloteau et al., 2006).

Observational evidence for the crucial role of H_2D^+, HD_2^+ (Vastel et al., 2004), and even of D_3^+, in the deuteration processes of the ISM have been widely probed by the detection of double and triple deuterated species such as D_2CO (Turner, 1990; Ceccarelli et al., 1998), NHD_2 (Roueff et al., 2000; Loinard et al., 2001; Gerin et al. 2006), ND_3 (van der Tak et al., 2002; Lis et al., 2002), CHD_2OH (Parise et al., 2002), CD_3OH (Parise et al., 2004), D_2CS (Marcelino et al., 2005).

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Ground-based observations of H_2D^+ and HD_2^+ have always been performed toward very dense and cold cores as the high Einstein coefficients of the involved transitions require high volume densities to produce significant emission. Therefore, it is difficult to estimate the H_2D^+ abundance in lower density regions through submillimeter observations. In this Letter, we report on the first detection of H_2D^+ in the far-IR spectrum of Sgr B2 observed with the *Infrared Space Observatory* (ISO). The observed transition connects the ground state, $1_{1,1}$, with the $2_{1,2}$ level at 113.4 K, and has a wavelength of 126.853 μm. This detection opens the possibility to detect H_2D^+ in clouds with moderate volume density in which the $1_{0,1}$-$1_{1,1}$ transition at 372 GHz will be subthermally excited and its intensity too weak to be detected with currently available radio telescopes. It also opens the quest to detect H_2D^+ toward far-IR luminous galaxies and high redshift objects.

2. OBSERVATIONS

The data presented in this paper are based on the final calibration analysis of the high spectral resolution line survey of Sgr B2 obtained with the Long Wavelength Fabry-Pérot Spectrometer (LWS/FP) on board ISO in its L03 mode (Polehampton 2002; Polehampton et al., 2007). The data for NH_2, which are necessary to interpret the H_2D^+ absorption reported in this paper, were previously presented by Goicoechea et al. (2004). The spectral resolution of the LWS/FP spectrometer is $\simeq$ 35 km s^{-1}. The telescope was pointed toward α(2000)=17^h 47^m 21.75^s; δ(2000)=-28^o 23' 14.1". The H_2D^+ and NH_2 data are presented in Figs. 1 and 2.

The procedure to reduce the LWS/FP data have been described in detail by Polehampton et al. (2007). This provides a significant improvement over the previous reduction of Goicoechea et al. (2004), who did not apply any interactive processing to the standard pipeline data products except for the removal of glitches, averaging of individual scans and removal of baseline polynomials. The improvements applied in the full spectral survey reduction include determination of accurate detector dark currents (including stray light), improved instrumental response calibration (including a correction to account for adjacent FP orders) and interactive shifting of individual miniscans (to correct for uncertainty in the angle of the LWS grating). The signal-to-noise ratio was also enhanced by including every available observation in the survey (in this case 2 independent observations). The broad absorption feature shown in Figure 1 was previously assigned only to p-NH2 (Goicoechea et al., 2004; transition $2_{2,1}$-$1_{1,0}$ J=5/2-3/2). However, the final reduction of the LWS/FP survey toward Sgr B2 shows that the broadening is real. The feature appears in 2 independent observations : ISO TDT number 50601112, observed on 1997 April 5 with LWS detector LW2; and ISO TDT number 50800515, observed on 1997 April 7 with LWS detector LW3. The fact that the feature appears on 2 separate detectors rules out any spurious instrumental broadening of the p-NH2 line.

Taking into account the latest data reduction, the broad feature detected at $\sim$126 μm cannot be due to p-NH_2 alone. In fact, NH_2 far-IR lines are narrow and appear only at the velocity of Sgr B2 (see, van Dishoeck et al., 1993, for the detection of NH_2 in the submm).

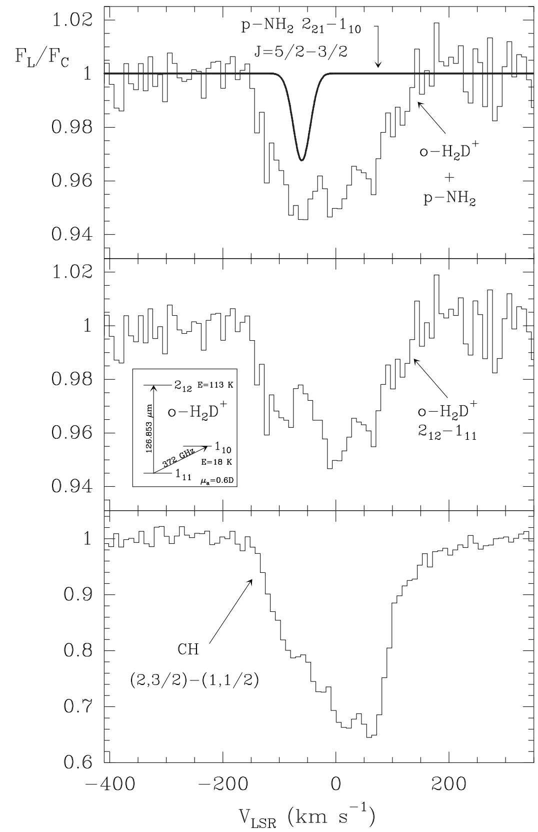

FIG. 1.— Observed ISO spectrum at 126.853 μm toward Sgr B2. The upper panel shows the data and the expected contribution of p-NH_2 (see Figure 2). The middle panel shows the o-H_2D^+ line profile after subtracting the contribution from p-NH_2. Finally, the lower panel shows the absorption of CH for comparison purposes.

Only a few lines remain unidentified in the ISO far-IR line survey of SgrB2. The feature discussed in this paper must correspond to a line arising from a low energy level or to a blend of lines. However, molecules heavier than H_2D^+ could have other lines in the far-IR domain. We have considered the possibility of b-type transitions from slightly asymmetric rotors like HNCO and $HOCO^+$. Both have one transition at similar wavelengths. However, the line of HNCO involves two high energy levels and can be easily ruled out. $HOCO^+$ has several other lines in the 120-127 μm range involving low energy levels. None of which are detected in the far-IR line survey of Sgr B2 (Polehampton et al., 2007). Hence, we are confident that the broad feature detected at 126.853 μm corresponds to H_2D^+.

The intensity scale in figures 1 and 2 was obtained by dividing the observed flux by a fitted continuum as described by Polehampton et al. (2007). Hence, it is directly related with the line opacity convolved with the instrumental spectral profile of the LWS/FP spectrometer. The velocity scale in Figure 1 has been obtained assuming λ_{rest}=126.853 μm (2363.325 GHz), i.e., the wavelength of the o-H_2D^+ 2_{12}-1_{11} transition (Amano & Hirao, 2005). The expected error on the frequency of this transition is $\simeq$ 5 MHz, i.e., a velocity uncertainty $<$ 2 km s^{-1} (3σ), which is much lower than the spectral resolution of the LWS/FP spectrometer. The p-NH_2 $2_{2,1}$-$1_{1,0}$ J=5/2-3/2 line is separated by $\simeq$-123 km s^{-1} with respect to the 2_{12}-1_{11} line of o-H_2D^+.

3. RESULTS AND DISCUSSION

The upper panel of Figure 2 shows the three spin–rotational components of the o-NH_2 $2_{2,0}$-$1_{1,1}$ transition at $\sim$117 μm (Goicoechea et al. 2004). In order to compute the expected contribution of the p-NH_2 $2_{2,1}$-$1_{1,0}$ triplet at $\simeq$126 μm we have modeled the NH_2 absorption assuming a rotational temperature of 20 K, an intrinsic linewidth of 10 km s^{-1}, a total NH_2 column density of 1.2×10^{15} cm^{-2} (Goicoechea et al. 2004), and an ortho/para ratio of 3. NH_2 wavelengths and line strengths are from the Cologne Database for Molecular Spectroscopy (Müller et al. 2001). The NH_2 hyperfine structure is unresolved by the LWS/FP. The synthetic spectrum, convolved with the LWS/FP spectral resolution, is shown in Figure 2. The expected contribution from p-NH_2 to the absorption feature is shown as a continuous line in the upper panel of Figure 1. The middle panel of this Figure shows the same data with the expected contribution from p-NH_2 removed. The remaining absorption feature is broad and has several absorption velocity peaks, which are similar to those found in unsaturated ground–state transitions of light species such as the (2,3/2)-(1,1/2) line of CH (see bottom panel of Figure 1). Therefore, in the following, we assign this unidentified broad feature to the o-H_2D^+ $2_{1,2}$-$1_{1,1}$ line.

H_2D^+ is an asymmetric molecule with $\mu_a \simeq$0.6 D (Dalgarno et al., 1973). It has two different species, ortho (Ka=odd), and para (Ka=even), with a spin weight ratio of 3:1. The three lowest energy levels, $1_{1,1}$, $1_{1,0}$ and $2_{1,2}$, which are at 0, 17.9 and 113.4 K (see insert in the middle panel of Figure 1), are enough to compute the partition function (F_{par}) at low temperatures. Hence, $F_{par}(T_r) \simeq 3(1+e^{-17.8/T_r})$ is a good approximation for $T_r < 30$ K, where T_r is the rotational temperature. For example, F_{par}(3 K)= 3.004 (all molecules in the ground state), while F_{par}(30 K)=4.8. Although the $1_{1,0}$ level starts to be populated in this case, the $2_{1,2}$ one is still unpopulated. Consequently, if there is a strong continuum source behind or inside the source, we could expect to see the $2_{1,2}$-$1_{1,1}$ transition of o-H_2D^+ in absorption. The same behavior is observed in CH toward Sgr B2, where only the ground-state line is observed with the line profile shown in the bottom panel of Figure 1 (Goicoechea et al. 2004; Polehampton et al. 2007).

The Einstein coefficient of the o-H_2D^+ $2_{1,2}$-$1_{1,1}$ transition is large, 1.7×10^{-2} s^{-1}, which implies that the rotational temperature of the line will be extremely low in most relevant cases (or close to the dust temperature if continuum emission is optically thick), even when the $1_{1,0}$-$1_{1,1}$ transition is already collisionally excited (its Einstein coefficient is two orders of magnitude lower). Therefore, in order to derive a column density from absorption measurements of the $2_{1,2}$-$1_{1,1}$ line, we can assume that all molecules are in the $1_{1,1}$ ground level, and that the transition has a low rotational temperature in absence of infrared pumping. The opacity of the $2_{1,2}$-$1_{1,1}$ line can be written as $\tau(T_r) \simeq 0.067(N/10^{13})(10/\Delta v)/F_{par}(T_r)$, where Δv is the linewidth at half intensity in km s^{-1}, and N is the column density of o-H_2D^+ in cm^{-2}. If N(o-H_2D^+)=10^{13} cm^{-2} and Δv=10 km s^{-1}, $\tau(2_{1,2}$-$1_{1,1})$ would be 0.024 for T_r=3 K and 0.014 for T_r=30 K respectively. For comparison purposes, the opacity of the $1_{1,0}$-$1_{1,1}$ transition at 372 GHz would be 0.024 and 0.006 for T_r=3 and 30 K respectively.

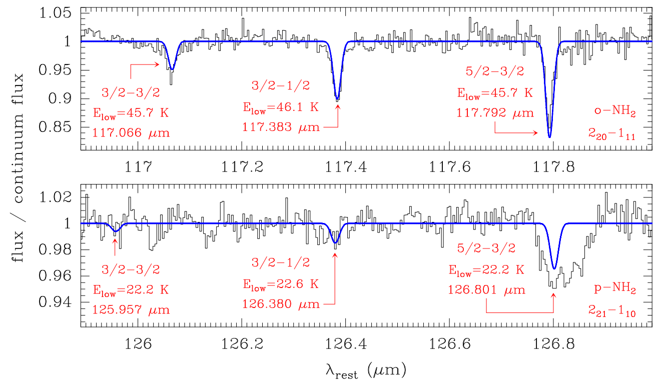

FIG. 2.— Rest ISO/LWS/FP spectrum of Sgr B2 around 117 and 126 μm, corrected by the averaged velocity of far–IR lines toward the source (62.7 km s^{-1}). Lines due to o-NH_2 (upper panel) and p-NH_2 plus o-H_2D^+ (lower panel) are shown. The expected NH_2 absorption is shown by continuous lines in both panels (see text). An NH_2 ortho/para ratio of 3 has been assumed. Note that the NH_2 lines show absorption only at the velocity of Sgr B2.

The interpretation of the absorption produced by o-H_2D^+ in Sgr B2 requires knowledge of the rotational temperature of the transition. The cloud has a large dust opacity in the far-IR, $\tau_d(100\mu m)$=3.5 (Cernicharo et al. 1997, 2006; Goicoechea et al. 2004). Hence, infrared photons cloud play an important role in the pumping of the molecular levels of o-H_2D^+. In addition, the fraction of the cloud depth that is "seen" at this wavelength corresponds only to its external layers, where $\tau_d(127\ \mu m)\simeq$1, i.e., N(H_2)$\simeq3\times10^{23}$ cm^{-2}, rather than the $\geq10^{24}$ cm^{-2} corresponding to the total column density along the line of sight ($\tau_d(127\ \mu m)\simeq$3). In order to estimate the radiative and collisional effects on the excitation of the $2_{1,2}$-$1_{1,1}$ transition, we have assumed de-excitation collisional rates $\sigma(1_{1,0}$-$1_{1,1})$=$\sigma(2_{1,2}$-$1_{1,0})$= 10^{-10} cm^3 s^{-1}, and $\sigma(2_{1,2}$-$1_{1,1})$=5×10^{-11} cm^3 s^{-1}. For a gas at 30 K purely excited by collisions with N(o-H_2D^+)= 10^{13} cm^{-2}, and Δv=10 km s^{-1}, the rotational temperature varies from 9 to 12 K for H_2 densities of 10^5 and 10^6 cm^{-3} respectively. Reducing the collisional rates by a factor 10 produces rotational temperatures of 6 and 8 K for the same volume densities.

The role of radiative pumping by far–IR dust photons can be estimated assuming that the gas we observe in absorption, $\tau_d(127\mu m)$=1, surrounds a region with $\tau_d(127\mu m)$=2.0 and T_d=30 K. If the radius of the absorbing shell is twice that of the region emitting the bulk of the infrared emission, R_{abs}/R_{cont}=2, we obtain an excitation temperature of 17 K, with a little dependency on the assumed collisional rates. For R_{abs}/R_{cont}=3 and 1.5, the rotational temperature is 15 and 20 K respectively. In the following we assume T_r=10-20 K, and we use these values to derive upper and lower limits to the opacity of the H_2D^+ $2_{1,2}$-$1_{1,1}$ line. Assuming a linewidth of 10 km s^{-1} we obtain $\tau(2_{1,2}$-$1_{1,1})$=0.18 and 0.36 for T_r=10 and 20 K respectively. The corresponding column densities are $\simeq 9\times10^{13}$ and 2.3×10^{14} cm^{-2}, and the abundance of o-H_2D^+, for a total gas column density of 3×10^{23} cm^{-2}, is $\simeq 3\times10^{-10}$ for T_r=10 K and 9×10^{-10} for T_r=20 K. The latter can be ruled out from the upper limit obtained by Pagani et al (1992a) for the emission of the $1_{1,0}$-$1_{1,1}$ line at 372 GHz, N(o-

H_2D^+)<1.1×10^{14} cm^{-2}. Hence, a low rotational temperature, $T_r \simeq 10$ K, and an abundance of 3×10^{-10} are the best fit to the o-H_2D^+ absorption at the velocity of Sgr B2.

For the other absorbing clouds which are not directly associated to Sgr B2, it is reasonable to assume radiative thermalization with the cosmic background, $T_r \simeq 3$ K, i.e., no significant collisional excitation or infrared pumping. Assuming an intrinsic line width of 10 km s^{-1}, the observed absorption features at -100, 10 and 120 km s^{-1} have opacities of of 0.1, 0.15 and 0.06 and column densities of $\simeq$ 4.5, 6.7, and 2.7 10^{13} cm^{-2} respectively. These clouds have low volume densities and total gas column densities of a few 10^{22}-10^{23} cm^{-2}. The associated o-H_2D^+ abundances are of a few 10^{-10}–10^{-9}.

The derived abundance of o-H_2D^+ in Sgr B2 corresponds to the predictions of chemical models for T_K <20 K (see Pagani et al., 1992b; Walmsley et al., 2004; Flower et al., 2006). These models predict that the para species could be more abundant than the ortho one for that temperature and the expected density of the gas (a few 10^4-10^5 cm^{-3}). Hence, the fundamental line of p-H_2D^+ could produce significant absorption at 218.8 μm in the direction of Sgr B2. The abundances observed toward the other clouds in the line of sight of Sgr B2 indicate lower kinetic temperatures, $T_K \simeq 10$ K. In these clouds the predicted ortho/para abundance ratio favors the ortho species. Due the high dependency of the ortho/para ratio with the gas temperature, simultaneous observation of both the 126.853 μm (o-H_2D^+) and the 218.8 μm (p-H_2D^+) lines will provide a direct measurement of the efficiency of the reactions of H_2D^+ with H_2 and of the conversion of ortho–to–para H_2D^+ and viceversa, i.e., to check chemical models.

Due to the poor spectral and angular resolution of ISO, and due to the limited sensitivity of the LWS/FP instrument, the o–H_2D^+ line at 126.853 μm could only be expected in sources with a large column density of cold gas with broad linewidths in the line of sight. As an example, a broad absorption feature has been also reported in the bright IR galaxy Arp220 at 127 μm by González-Alfonso et al. (2004) using the LWS grating spectrometer (spectral resolution more than 20 times lower than the LWS/FP). These authors assigned it to NH_3. While several lines of NH and NH_3 have been observed in this source, no lines have been assigned to NH_2 so far. Hence, the broad absorption feature assigned to NH_3 by González-Alfonso et al., could also contain some contribution from o-H_2D^+. The detection of H_2D^+ presented in this work, shows that far–IR ortho– and para–H_2D^+ lines can be used to trace the deuteration fractionation of H_3^+ in galaxies (see also Ceccarelli and Dominik, 2006). Therefore, far–IR observations with the PACS instrument on board Herschel satellite (or in the future with SOFIA), will be an important tool to understand the cold ISM chemistry in distant galaxies where the D/H ratio will be different and the gas temperature affected by the local cosmic background temperature.

Finally, the opacity of the $2_{1,2}$-$1_{1,1}$ transition for a dark cloud with Δv=0.5 km s^{-1} (see Vastel et al., 2004), N(o-H_2D^+)=10^{12} cm^{-2}, and T_r= 3 K is $\simeq$0.05. While the expected emission in the $1_{1,0}$-$1_{1,1}$ transition at 372 GHz will be negligible, the expected absorption at 126.853 μm will be 5%, i.e., easy to detect with the expected sensitivities of the high spectral resolution instruments planned for SOFIA. Dark clouds (see, e.g., Nisini et al., 1999), prestellar cores, and protoplanetary disks (see Wyatt et al., 2003) have enough continuum emission in the far-IR, hence, the $2_{1,2}$-$1_{1,1}$ transition can be used as a key observing tool to trace column densities of o-H_2D^+ larger than a few 10^{11} cm^{-2}, and to understand the deuterium fractionation at large spatial scales in cold dark clouds. Observations of the fundamental lines of p-HD_2^+ at 691.6605 GHz and o-HD_2^+ 203.03 μm will provide additional constraints on these deuteration processes in molecular clouds and protoplanetary disks.

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