FAR-INFRARED DETECTION OF H_3O^+ IN SAGITTARIUS B2¹

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ABSTRACT

We report the first far-infrared detection of the hydronium ion (H_3O^+) toward the Sagittarius B2 molecular cloud, near the Galactic center. Using the *Infrared Space Observatory* Long-Wavelength Spectrometer, we have detected three lines arising from the ν_2 ground-state inversion mode ($0^+ \rightarrow 0^-$) at 55.3 cm^{-1} . All transitions are observed in absorption against the optically thick infrared continuum emission of the dust. Two different absorption regions can be distinguished, the H_3O^+ associated with the Sgr B2 extended envelope and that of foreground gas along the line of sight. The derived abundances for both components are rather similar, $\lesssim 1 \times 10^{-9}$, and may explain the high water abundance found in the low-density gas toward Sgr B2 as its dissociative recombination leads to the formation of important molecules OH and H_2O . Contribution of the $Q(1, 1)$ line of para- H_3O^+ to the $2_{12}-1_{01}$ line of H_2^{18}O is also analyzed. This allows a better determination of water abundance from far-infrared observations. The corrected H_2O abundances are $\lesssim 10^{-6}$ for the diffuse clouds along the line of sight and a few times 10^{-6} for the gas associated with the Sgr B2 envelope, in good agreement with water vapor observations from the *Submillimeter Wave Astronomy Satellite*.

Subject headings: infrared: ISM: lines and bands — ISM: individual (Sagittarius B2) — ISM: molecules — line: identification — molecular data

1. INTRODUCTION

H_3O^+ is a saturated molecular ion that plays an important role in the oxygen chemistry network (Sternberg & Dalgarno 1995) and is believed to be present in gas-phase reactions occurring in both the diffuse and dense interstellar medium (ISM). Its dissociative recombination (DR) leads to the formation of the abundant species OH and H_2O (Bates 1986; Galloway & Herbst 1991) with an imprecise branching ratio for each channel of the dissociation. However, this ratio is a crucial parameter for the interstellar chemistry (Sternberg, Dalgarno, & Leep 1987) and for the modeling of molecular clouds. In recent years, ab initio molecular calculations of dissociation pathways and potential energy curves of $\text{H}_3\text{O}^+ + e^-$ (Ketvirtis & Simons 1999; Park 1999) have improved our knowledge about reaction mechanisms and electronic states of the neutral products formed. On the other hand, laboratory experiments using different techniques have been carried out in order to determine this branching ratio (Williams et al. 1996; Vejby-Christensen et al. 1997).

Water itself is one of the most important and abundant molecules (after H_2 and CO) in the ISM. It plays a critical role in the radiative cooling of dense molecular gas (Neufeld, Lepp, & Melnick 1995), from star-forming regions to envelopes of evolved stars. Hence, the determination of its abundance, distribution, and formation is decisive for our understanding of chemical and physical processes taking place in a great variety of astronomical environments. Before the launch of the *Infrared Space Observatory* (ISO; Kessler et al. 1996), some ground-based and airborne observations of H_2O maser transitions were performed (Cheung et al. 1969; Cernicharo et al. 1990, 1994; Menten & Melnick 1991; González-Alfonso et al. 1999) but do not provide accurate information about abundances. Infrared

and submillimeter observations of thermal transitions confirm that the presence of water vapor is ubiquitous in the direction of star-forming molecular clouds like Orion (Cernicharo et al. 1994; Wright et al. 2000) or Sagittarius B2 (Cernicharo et al. 1997, hereafter Cer97; Neufeld et al. 2000) with abundances as high as 10^{-4} . Moreover, the emission/absorption appears to be extended. In this way, studying the appearance of its parental molecule, H_3O^+ , we will also be getting insight into the H_2O chemistry.

In this Letter, we report the first far-IR H_3O^+ absorption lines in the ISM. The three detected lines arise from the lowest rotational levels of $K = 0$ (ortho) and 1 (para) ladders of the ν_2 ground-state inversion mode ($0^+ \rightarrow 0^-$) at ≈ 100 and $\approx 181 \text{ } \mu\text{m}$. These transitions can be observed only from airborne or space-based observatories. We have used the ISO Long-Wavelength Fabry-Perot spectrometer (LWS/FP; Clegg et al. 1996) to search for the hydronium ion in the Sgr B2 molecular cloud, where we know water vapor and OH to be very abundant.

2. OBSERVATIONS AND RESULTS

All the results presented here were taken in the direction of Sgr B2 molecular cloud. The complex is an active star-forming region close to the Galactic center (GC). Due to its high column density, $N(\text{H}_2) \approx 10^{23}\text{--}10^{24} \text{ cm}^{-2}$ (Lis & Goldsmith 1991), it is a very opaque source at optical but with high luminosities in far-IR, millimeter, and radio wavelengths. Because of its physical and chemical complexity (clumped structure, extended envelope, hot cores, ultracompact H II regions, etc.), it is a unique object for spectroscopy studies and for the searching of new molecules.

The ISO LWS/FP data of Sgr B2 were obtained during revolutions 462 and 508 in 1997 February and April. The number of scans for each spectrum was 18 and three, with integration times of 3664 and 5040 s, respectively. The spectral resolution was $0.015 \text{ } \mu\text{m}$. The measured FP continuum flux level varied from 10% to 25% over each wavelength range. When compared with the grating observation, the mean FP continuum flux of

¹ Based on observations with ISO, an ESA project with instruments funded by ESA member states (especially the PI countries: France, Germany, the Netherlands, and the UK) and with participation of ISAS and NASA.

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each line deviates by $\lesssim 20\%$, similar to the grating flux calibration errors (Swinyard et al. 1998). The propagation of these systematic uncertainties are always larger than the statistical errors derived from the line signal-to-noise ratios. The continuum level of the FP data was corrected to coincide with the grating data. Then, a polynomial baseline was removed from all FP spectra. The resulting lines are shown in Figure 1.

The LWS grating observations ($43\text{--}196.7\ \mu\text{m}$) of Sgr B2 were obtained during revolution 287 in 1996 August (see Baluteau et al. 1997 and Cer97 for complementary analysis). The spectral resolution is $0.29\ \mu\text{m}$ for the $43\text{--}93\ \mu\text{m}$ range and $0.6\ \mu\text{m}$ for the $80\text{--}196\ \mu\text{m}$ range. The integration time was 2836 s. Up to 16 scans were taken in the direction of the Sgr B2 central position, at $\alpha = 17^{\text{h}}47^{\text{m}}21^{\text{s}}.75$, $\delta = -28^{\circ}23'14''.1$ (J2000). The *ISO* database observation numbers are 46201123 and 50800416 for the FP and 28701401 for the grating. The spectra were analyzed using the *ISO* spectrometer data reduction package ISAP³ to remove glitches and fringes. Small shifting factors have been used for each detector in order to have a smooth grating spectrum. FP and grating data were processed with versions 9.5 and 9 of the pipeline.

H_3O^+ is an oblate symmetric molecule, isoelectronic to NH_3 with the same physical structure, i.e., pyramidal geometry. Like ammonia, it has a double minimum vibrational potential so that the oxygen can tunnel through the plane of the hydrogen atoms. In such a molecule (also AsH_3 and PH_3), this leads to an inversion splitting of the rotational levels that can be observed from radio to infrared wavelengths depending on the potential barrier height (Pitzer 1939). Surprisingly, the inversion splitting of H_3O^+ is very large, $\approx 55\ \text{cm}^{-1}$ (Liu & Oka 1985), and its fundamental transitions of the ν_2 (umbrella) mode lie at much higher frequencies than those of the NH_3 splitting ($\approx 1\ \text{cm}^{-1}$). Due to the small H_3O^+ inversion barrier, rotation inversion (Plummer, Herbst, & De Lucia 1985; Bogey et al. 1985) and pure inversion transitions (Verhoeve et al. 1989) have been observed in the laboratory in the submillimeter and far-IR domains, respectively. Interstellar H_3O^+ was tentatively detected (Wootten et al. 1986; Hollis et al. 1986; Timmermann et al. 1996) and finally confirmed (Wootten et al. 1991; Phillips, van Dishoeck, & Keene 1992, hereafter PhvDK) as an abundant molecular ion.

Figure 1 shows the detected transitions: $2_1^- \leftarrow 1_1^+$ and $2_0^- \leftarrow 1_0^+$ (rotation inversion) and $1_1^- \leftarrow 1_1^+$ (pure inversion). We note that the alternative notation for these transitions is $R(1, 1)$, $R(1, 0)$, and $Q(1, 1)$, respectively. The $Q(1, 1)$ line is blended with the $2_{12}-1_{01}$ transition of isotopical water, H_2^{18}O , at $181.053\ \mu\text{m}$ (see below). Here we will determine the contribution of each molecule to the feature seen in the spectrum. In addition, we present detections of the $2_{20}-1_{11}$ and possibly $5_{14}-4_{23}$ H_2O lines.

All H_3O^+ lines are observed in absorption against the far-IR continuum of the cloud opposite of what is found with submillimeter transitions (PhvDK). Line velocities appear to be $\approx 45 \pm 5\ \text{km s}^{-1}$, in agreement with the velocity of water vapor far-IR transitions detected also with the LWS/FP in Sgr B2 (J. Cernicharo et al. 2001, in preparation). Taking into account the absolute wavelength calibration of the FP instrument ($\pm 15\ \text{km s}^{-1}$), these velocities could correspond to the systemic $\approx 60\ \text{km s}^{-1}$ expected for the Sgr B2 cloud in the spectral resolution limit.

Anyway, radial velocities close to $50\ \text{km s}^{-1}$ are also as-

FIG. 1.—LWS/FP observations of H_3O^+ in Sgr B2 and rest wavelengths. The intensity scale corresponds to the continuum normalized flux. The abscissa corresponds to the LSR velocity. *Top*: Broad $R(1, 1)$ absorption line. *Middle*: $Q(1, 1)$ transition and $2_{12}-1_{01}$ transition of H_2^{18}O . *Bottom*: $R(1, 0)$ and two water vapor features.

sociated with gas surrounding most of the continuum sources. The region of the cloud covered by our observations presents several clumps of absorbing gas at these velocities (Martín-Pintado et al. 1990). H_3O^+ absorption may come mainly from these regions. The three features show absorption at more negative velocities than those of Sgr B2 complex, i.e., H_3O^+ is present in the molecular gas along the line of sight toward Sgr B2. The same behavior is observed in H_2O and OH rotational transitions also coming from the ground state (Storey, Watson, & Townes 1981; Cer97).

2.1. Possible Blending with Other Molecules

We have carried out a detailed study of possible overlapping with other molecular transitions with significant line strength. This is necessary to determine the exact contribution of each line and to be sure about the H_3O^+ assignments. Lines such as *b*-type transitions of slightly asymmetrical molecules are known to be present in the cloud and might contribute to the absorption features.

³ The *ISO* Spectral Analysis Package (ISAP) is a joint development by the LWS and SWS instrument teams and data centers. Contributing institutes are CESR, IAS, IPAC, MPE, RAL, and SRON.

1. For the $\sim 100.5 \mu\text{m}$ feature, the formyl radical, HCO, has a rotational line (10_8-9_{19}) at $100.579 \mu\text{m}$. This transition arises from an energy state of 217 K. According to the HCO column density of $(1.21-1.22) \times 10^{13} \text{ cm}^{-2}$ observed by Hollis & Churchwell (1983) in Sgr B2, we have computed the predicted absorption for this carrier. The expected line opacity is not large enough to produce appreciable absorption in the cloud. Also the $5_{14}-4_{23}$ transition of H^{17}_2O lies at $100.562 \mu\text{m}$. Nevertheless, this line has a lower energy level at 574 K. Only hotter gas would excite this transition, so it is unlikely to have any contribution from isotopical water. Therefore, we attribute this feature to the $R(1, 1)$ transition of para- H_3O^+ at $100.577 \mu\text{m}$.

2. For the $\sim 100.8 \mu\text{m}$ feature, only the protonated form of CO_2 can contribute with a rotational line ($29_{2,27}-28_{1,28}$) at $100.858 \mu\text{m}$. Millimeter observations of HOCO^+ by Minh, Irvine, & Ziurys (1988) in Sgr B2 proved its extended emission with a column density of $\approx 2 \times 10^{14} \text{ cm}^{-2}$. With these parameters and the b -type dipole moment derived by Green et al. (1976) we have calculated the expected absorption for the far-IR line. Again, the resulted small opacity excludes an HOCO^+ contribution for the observed absorption. Hence, we assign this feature to the $R(1, 0)$ line of ortho- H_3O^+ at $100.869 \mu\text{m}$.

3. The $\sim 181.05 \mu\text{m}$ feature has been generally attributed entirely to the $2_{12}-1_{01}$ transition of ortho- H_2^{18}O at $181.053 \mu\text{m}$ from which water abundance can be estimated. However, in regions of high H_2O column density and low excitation temperatures, a significant contribution of H_3O^+ cannot be excluded. The $Q(1, 1)$ transition of para- H_3O^+ at $181.054 \mu\text{m}$ involves the lowest allowed rotational energy level of H_3O^+ and may be excited by a suitable far-IR background source. This is possibly the case of gas toward Sgr B2. In § 3, we analyze this contribution.

3. DISCUSSION

DR of H_3O^+ leads to the formation of water and OH. Last ion-storage experiments for low-energy electron collisions (Vejby-Christensen et al. 1997) determine that water dissociation channel will occur with a branching ratio of 0.33 at those impact energies, in agreement with the usually adopted theoretical value. On the other hand, laboratory experiments are not sensitive to the electronic states in which final products are formed. Thus, is impossible to explain why most exothermic ground-state product channel, $\text{H}_2\text{O}(X^1A_1) + \text{H}$, is not the dissociation pathway of the largest branching ratio. Ab initio calculations studying ground and valence-to-Rydberg excited states of H_3O suggest that an excess of internal energy in the H_2O formed may allow a subsequent decay to produce $\text{OH}(X^2\Pi) + 2\text{H}$ (Ketvirtis & Simons 1999). Moreover, energetically inaccessible states such as $\text{OH}(A^2\Sigma)$ can be produced as the electron energies increase. The most striking result of last year's studies on H_3O^+ DR is that if hydronium is an abundant astronomical ion, H_2O will be a dominant molecule in space.

3.1. Column Densities and H_3O^+ Abundance

The small H_3O^+ inversion potential barrier allows its detection in molecular cloud far-IR spectra. As other new molecules detected by us in this spectral range, C_3 , NH (Cernicharo, Goicoechea, & Caux 2000), and NH_2 (Goicoechea & Cernicharo 2001) lines are seen in absorption against the continuum emission of dust. This means that detected lines come from regions where excitation temperatures are lower than the dust temperature ($T_{\text{exc}} \leq T_d$). In the case of Sgr B2 (see Fig. 2), the max-

FIG. 2.—ISO/LWS spectrum of the Sgr B2 central position between 43 and $196 \mu\text{m}$, with main detected features labeled. Inset: Graybody fit to the continuum dust emission.

imum dust thermal emission peaks at $\sim 80 \mu\text{m}$, and the shape resembles a Planck distribution. A graybody fitting to the grating observations (inset) suggests that dust is relatively cold ($T_d \sim 30 \text{ K}$) and that far-IR continuum is optically thick even at $180 \mu\text{m}$ (see also Cer97). Such high dust opacities are equivalent to a visual extinction of $A_V \sim 200-1000 \text{ mag}$ or $N_T(\text{H}_2) \approx 2 \times 10^{23}-10^{24} \text{ cm}^{-2}$. Thus, the far-IR continuum emission is coming mostly from dust located in the outer regions of the cloud and not in the hot dense cores where extinction is much larger. Our ISO/LWS observations of H_3O^+ are sensitive only to those regions in front of the infrared continuum sources. Hence, the H_3O^+ absorption lines originating in the ground state must come from the moderate density and extended envelope so that collisions are less important and can be neglected as a first approximation. Due to the strong dust emission and high continuum opacity at the inversion wavelengths, the excitation of the molecule is dominated by far-IR photons. Here we consider radiative pumping by the dust and thus excitation temperatures slightly lower than the dust temperature ($T_{\text{exc}} = 20-27 \text{ K}$). Ortho and para ladders are considered separately. To compute the Einstein coefficients, we have used the theoretical dipole moment of 1.44 D derived by Botschwina, Rosmus, & Reinsch (1983). Considering that lines are optically thin, the $R(1, 1)$ absorption leads to a column density of $N(\text{para-}\text{H}_3\text{O}^+) \approx (9 \pm 2) \times 10^{13} \text{ cm}^{-2}$, which is a factor $\approx (1.25 \pm 0.5)$ larger than the ortho- H_3O^+ column density obtained from the $R(1, 0)$ line. This suggests that the ortho-to-para (OTP) ratio differs from its equilibrium value. It seems that at the low gas temperatures and densities of the envelope, para- H_3O^+ is more abundant than the ortho species. The OTP ratio is a critical parameter in the treatment of interstellar H_3O^+ . For the same cloud, Wootten et al. (1991) assumed a value of 3 while PhvDK used a ratio of unity, which holds for temperatures $T \geq 50 \text{ K}$ if H nuclei exchange reactions are fast enough. Assuming that the OTP ratio is just $R(1, 0)/R(1, 1)$, we derive a fractional H_3O^+ abundance of $\sim 1 \times 10^{-9}$ within a factor of 2 error due to the T_{exc} -range considered and the calibration error propagation. Detailed chemical models predict a fractional H_3O^+ abundance of $(1-4) \times 10^{-9}$ (see, e.g., Millar et al. 1991).

Of course, the ground-state lines we detect should influence the population of the levels observed in the submillimeter. PhvDK suggested that IR pumping could play a role in the intensity of the para- $\text{H}_3\text{O}^+ 3_2^+ \rightarrow 2_2^-$ line at 364 GHz. Our ob-

servations indicate that the IR pumping will also affect the intensities of all submillimeter lines. In particular, the 307 GHz line arises from the 1_1^- level, which is, from our data, essentially populated by the absorption of IR photons from the 1_1^+ ground level. In addition, the submillimeter lines could be tracing a different gas than the IR lines. The advantage of far-IR observations is that we can trace more extended and lower density gas. In this context, a preliminary analysis of the grating raster maps around Sgr B2 indicate the presence of several H_3O^+ lines arising from the ground inversion rotation ortho and para states over large spatial scales around that source (J. R. Goicoechea et al. 2001, in preparation).

The $R(1, 1)$ and $R(1, 0)$ line profiles in Figure 1 also show an absorption of $\sim 5\%$ for gas at more negative velocities than those related to Sgr B2. The derived abundance for the foreground gas between -50 and 20 km s^{-1} remains similar to that in the Sgr B2 envelope if the diffuse clouds along the line of sight have $N_T(\text{H}_2) \leq 3 \times 10^{22} \text{ cm}^{-2}$.

With these values, we now determine the contribution of the $Q(1, 1)$ line of H_3O^+ to the observed feature blended with the $2_{12}-1_{01}$ transition of H_2^{18}O . Assuming also the same excitation temperatures and fixating the para- H_3O^+ column density, we conclude that $\leq 40\%$ of the absorption associated with Sgr B2 at $181.05 \mu\text{m}$ corresponds to hydronium ion. For the foreground gas, the contribution is $\geq 40\%$. This difference is due to an enhanced H_2^{18}O abundance toward the GC and to radiative excitation differences between both components. For a given column density, the H_3O^+ contribution to the $181.05 \mu\text{m}$ ab-

sorption decreases with increasing line T_{exc} . In the Sgr B2 envelope, T_{exc} is higher than in the foreground gas because dust emission increases the T_{exc} to values close to T_d . Using the same model for water absorption as Cer97 and assuming the H_3O^+ contamination in the H_2^{18}O feature, we derive an H_2O abundance of $\leq 10^{-6}$ for the diffuse clouds along the line of sight and a few times 10^{-6} for the gas associated with the Sgr B2 envelope. Hence, far-IR observations are in good agreement with the last results from the *Submillimeter Wave Astronomy Satellite* (Melnick et al. 2000; Neufeld et al. 2000). Besides, the similar H_3O^+ abundance both in the foreground gas and in the Sgr B2 envelope could explain the enhanced water abundances found in this line of sight.

Ground-state lines of other important light molecules (H_2O , OH, CH ...) can also be observed through absorption in the far-IR. A detailed analysis of the *ISO* database is under study in order to characterize the cold gas toward the GC. The high-frequency resolution of future heterodyne instruments, such as HIFI on board the *Herschel Space Observatory*, will allow a separated detection of H_3O^+ and H_2^{18}O lines at $\approx 181 \mu\text{m}$. This will provide a definitive determination of both molecule abundances along the line of sight of Sgr B2 and other molecular clouds.

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