Detection of interstellar oxidaniumyl: Abundant H$_2$O$^+$ towards the star-forming regions DR21, Sgr B2, and NGC6334*

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ABSTRACT

Aims. We identify a prominent absorption feature at 1115 GHz, detected in first HIFI spectra towards high-mass star-forming regions, and interpret its astrophysical origin.

Methods. The characteristic hyperfine pattern of the H$_2$O$^+$ ground-state rotational transition, and the lack of other known low-energy transitions in this frequency range, identifies the feature as H$_2$O$^+$ absorption against the dust continuum background and allows us to derive the velocity profile of the absorbing gas. By comparing this velocity profile with velocity profiles of other tracers in the DR21 star-forming region, we constrain the frequency of the transition and the conditions for its formation.

Results. In DR21, the velocity distribution of H$_2$O$^+$ matches that of the [C II] line at 158 μm and of OH cm-wave absorption, both stemming from the hot and dense clump surfaces facing the H$^\text{II}$ region and dynamically affected by the blister outflow. Diffuse foreground gas dominates the absorption towards Sgr B2. The integrated intensity of the absorption line allows us to derive lower limits to the H$_2$O$^+$ column density of 7.2 × 10$^{-14}$ cm$^{-2}$ in NGC 6334, 2.5 × 10$^{-14}$ cm$^{-2}$ in DR21, and 1.1 × 10$^{15}$ cm$^{-2}$ in Sgr B2.


1. Introduction

Oxidaniumyl or oxoniumyl (Connelly et al. 2005), the reactive water cation, H$_2$O$^+$, plays a crucial role in the chemical network describing the formation of oxygen-bearing molecules in UV irradiated parts of molecular clouds (van Dishoeck & Black 1986; Gerin et al. 2010). It was identified at optical wavelengths (Lane et al. 1990; Jakob et al. 2007). The eastern, blue-shifted outflow creates bright photon-dominated (or photo-dissociation) regions (PDRs), visible as clumps of 8 μm emission in Spitzer IRAC maps (Marston et al. 2004) and showing up in emission lines from tracers of irradiated hot gas, such as HCO$^+$, high-J CO, atomic and ionised carbon, and atomic oxygen (Lane et al. 1990; Jakob et al. 2007). The eastern, blue-shifted outflow expands in a blister-like fountain, while the western, red-shifted outflow is confined to a small cone.

2. The sources

We observed three massive Galactic star-forming/HII regions with very different properties. The DR21 star-forming region is embedded in a ridge of dense molecular material that obscures it at optical wavelengths. The embedded cluster drives a violent bipolar outflow and creates bright photon-dominated (or photo-dissociation) regions (PDRs), visible as clumps of 8 μm PAH emission in Spitzer IRAC maps (Marston et al. 2004) and showing up in emission lines from tracers of irradiated hot gas, such as HCO$^+$, high-J CO, atomic and ionised carbon, and atomic oxygen (Lane et al. 1990; Jakob et al. 2007). The eastern, blue-shifted outflow expands in a blister-like fountain, while the western, red-shifted outflow is confined to a small cone.

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The identification with H$_2$O$^+$ because of the simple source velocity structure that cannot be achieved. However, the large centrifugal distortion in H$_2$O$^+$ requires a large set of spectroscopic parameters to reproduce a comparatively small set of data: this may cause problems in the zero-field extrapolation. Moreover, the frequencies of the two fine structure levels of the 1$_{11}$ rotational state in Table V of Mürtz et al. (1998) agree precisely with those of the F$^\prime = J^\prime$, F$'' = J''$ hyperfine transitions. This can only be achieved when the calculated frequencies are lower by 51.56 and 88.05 MHz, respectively, since the respective hyperfine component is the lowest in each case. Correcting the published frequencies of the J = 3/2−1/2 fine structure component by 51.56 MHz improves the agreement with Strahan et al. (1986). The results are summarized in Table 1. Alternatively, we could use the corrected frequencies of Mürtz et al. (1998) and arrive at values that are lower by about 23 MHz. This provides a rough estimate of the uncertainty in the predictions. An H$_2$O$^+$ catalogue entry will be prepared for the CDMS (Müller et al. 2005) by carefully scrutinizing the available IR data summarised in Zheng et al. (2008), and references therein) with ±150 MHz uncertainties.

4. Observations of the 1115 GHz ground-state transition

The H$_2$O$^+$ line was detected in DR21 during performance verification observations of the HIFI instrument, testing spectral scans in the HIFI band 4b. Later science observations of Sgr B2 and NGC 6334 also confirmed the detection in these sources using the identification and frequency assignment from DR21. The main parameters of the observations are summarised in Table 2. At 1115 GHz, the Herschel beam has 21$''$ HPBW.

The identification with H$_2$O$^+$ was straightforward in DR21 because of the simple source velocity structure that cannot be confused with the well resolved, characteristic hyperfine structure of the line. When fitting the line, one has to take into account that the line extinction begins to saturate, with a maximum optical depth of 0.59 for DR21 and 1.55 for Sgr B2 (see below). For
DR21, we fitted the observed profile using an adjusted velocity profile with asymmetric wings. Because of the limited signal-to-noise ratio, the fit was performed manually by adding three Gaussian components of increasing width (see Fig. 2).

The resulting velocity distribution allows us to interpret the origin of the absorbing material by comparing with the velocity distribution of other species observed towards the same position with comparable beam size (see Ossenkopf et al. 2010; Falgarone et al. 2010; van der Tak et al. 2010). Figure 3 shows that the peak H$_2$O$^+$ velocity of $-1.7$ km s$^{-1}$ is not seen in any other tracer. The intrinsic velocity of the DR21 molecular ridge is $-3.0$ km s$^{-1}$, which is matched by the line centres of the H$^{13}$CO$^+$ 1–0, the CO 6–5, and the $^{13}$CO 6–5 transitions. The higher excitation lines of $^{13}$CO, C$^{18}$O, H$_2$O, and the [C II] line exhibit a slightly blue-shifted peak velocity of about $-5.0$ km s$^{-1}$. The H$_2$O$^+$ profile exhibits a prominent, very broad blue wing, but is not present in any of the molecular emission lines, but is found in the [C II] profile and the OH absorption spectrum measured by Guilloteau et al. (1984) towards the same position.

To underline this good match, we have superimposed in Fig. 2 the absorption profile that would be obtained by simply performing the hyperfine superposition of the $6.030$ GHz OH line instead, would provide a larger uncertainty of the order of $6$ MHz.

The identification and the corrected frequencies are then used to analyse the line structures in Sgr B2 and NGC 6334 (Figs. 4 and 5). In Sgr B2, we see absorption at both the velocity of its envelope and the velocities of many foreground clouds, almost saturating the line. NGC 6334 exhibits weak H$_2$O$^+$ absorption at $-13$ km s$^{-1}$. This deviates from the OH absorption profile towards the source measured by Brooks & Whiteoak (2001). At velocities below $-10$ km s$^{-1}$, only some OH maser emission was found. This might indicate that the observed H$_2$O$^+$ is not related to the foreground material, but to hot gas in the direct vicinity of the continuum sources. Alternatively, if we use the predicted frequencies from Strahan et al. (1986) in Table 1, the H$_2$O$^+$ absorption in NGC 6334 is centred on $-9$ km s$^{-1}$, in reasonable agreement with the OH absorption at $-8.2$ km s$^{-1}$ measured toward component F$^1$. At about $-9$ km s$^{-1}$, Beuther et al. (2005) also observed CH$_3$OH and NH$_3$ absorption towards the H II region.

5. Discussion and outlook

That H$_2$O$^+$ shows up in absorption against the dust continuum implies that the excitation of the molecule must be colder than the dust. As a reactive ion (see the discussion by Black 2007; Stäuber & Bruderer 2009), for CO$^+$, H$_2$O$^+$ is not expected to be in thermal equilibrium at the kinetic temperature of the gas. Its excitation reflects either the chemical formation process or the
temperatures well below the upper level energy of 53 K. For Sgr B2, we can clearly identify absorption in multiple transients from foreground clouds. Their densities must be high enough to produce some molecular hydrogen, but low enough not to quickly destroy the H$_2$O$^+$. For NGC 6334, the gas component producing the H$_2$O$^+$ absorption remains unidentified.

With the identification of H$_2$O$^+$ in the interstellar medium, we provide a first step to quantifying an important intermediate node in the oxygen chemical network, connecting OH$^{-}$ in diffuse clouds and at cloud boundaries, through H$_2$O, with water in denser and colder cloud parts. To obtain an estimate for the total H$_2$O$^+$ abundance, we need to measure the excitation temperature of H$_2$O$^+$. Observations of additional transitions of H$_2$O$^+$, such as those at 742 GHz, are therefore essential.

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Fig. 4. Fit of the observed H$_2$O$^+$ line in Sgr B2. The dashed line visualises the velocity structure of the absorbers by plotting the strongest hyperfine component on a linear column density scale, i.e., without optical depth correction.

Fig. 5. Same as Fig. 4, but for NGC 6334.