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

V. Ossenkopf$^{1,2}$, H.S.P. Müller$^1$, D.C. Lis$^3$, P. Schilke$^{1,4}$, T.A. Bell$^3$, S. Bruderer$^8$, E. Bergin$^2$, C. Ceccarelli$^6$, C. Comito$^4$, J. Stutzki$^1$, A. Bacmann$^6,7$, A. Baudry$^7$, A.O. Benz$^9$, M. Benedettini$^9$, O. Berne$^{37}$, G. Blake$^1$, A. Boogert$^3$, S. Bottinelli$^{13}$, F. Boulanger$^{10}$, S. Cabrit$^{11}$, E. Caselli$^{12}$, E. Caux$^{13,14}$, J. Cernicharo$^{15}$, C. Codella$^{16}$, A. Coutens$^{13}$, N. Crimier$^{6,15}$, N.R. Crockett$^5$, F. Daniel$^{11,15}$, K. Demyk$^{13}$, P. Dicke$^2$, C. Dominik$^{18,19}$, M.L. Dubernet$^{20}$, M. Emprechtinger$^1$, P. Encinias$^{11}$, E. Falgarone$^{17}$, K. France$^{28}$, A. Fuente$^{21}$, M. Gerin$^{17}$, T.F. Giesen$^1$, A.M. di Giorgio$^9$, J.R. Goicoechea$^{15}$, P.F. Goldsmith$^{22}$, R. Güsten$^1$, A. Harris$^{23}$, F. Helmich$^2$, E. Herbst$^{25}$, P. Hily-Blant$^6$, K. Jacobs$^1$, T. Jacq$^7$, Ch. Joblin$^{13,14}$, D. Johnstone$^{26}$, C. Kahane$^6$, M. Kama$^{18}$, T. Klein$^4$, A. Klotz$^{13}$, C. Kramer$^{27}$, W. Langer$^{22}$, B. Lefloch$^6$, C. Leinz$^4$, A. Lorenzani$^{16}$, S.D. Lord$^3$, S. Marec$^6$, P.G. Martin$^{28}$, J. Martin-Pintado$^{15}$, C. Mccoy$^{29,42}$, M. Melchior$^{30}$, G.J. Melnick$^{31}$, K.M. Menten$^1$, B. Mookerjee$^4$, P. Morris$^3$, J.A. Murphy$^{32}$, D.A. Neufeld$^{53}$, B. Nisini$^{34}$, S. Pacheco$^6$, L. Pagani$^{10}$, B. Parise$^4$, J.C. Pearson$^{22}$, M. Pérault$^{11}$, T.G. Phillips$^3$, R. Plume$^{35}$, S.-L. Quin$^1$, R. Rizzo$^2$, M. Röllig$^1$, M. Salez$^{11}$, P. Saraceno$^9$, S. Schlemmer$^1$, R. Simon$^1$, K. Schuster$^{27}$, F.F.S. van der Tak$^{2,36}$, A.G.G.M. Tielens$^{37}$, D. Teyssier$^{38}$, N. Trappe$^{32}$, C. Vastel$^{13,14}$, S. Viti$^{39}$, V. Wakelam$^7$, A. Walters$^{13}$, S. Wang$^5$, N. Whyborn$^{40}$, M. van der Wiel$^{2,36}$, H.W. Yorke$^{22}$, S. Yu$^{22}$, and J. Zmuidzinas$^3$

*(Affiliations can be found after the references)

Preprint online version: May 17, 2010

ABSTRACT

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.

**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 [CII] line at 158 μm and of OH cm-wave absorption, both stemming from the hot and dense clumps of gas and dust in the HD-The 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 $10^{12}$ cm$^{-2}$ in NGC 6334, $10^{13}$ cm$^{-2}$ in DR21, and $10^{14}$ cm$^{-2}$ in Sgr B2.

**Key words.** Astrochemistry - Line: identification - Molecular data - ISM: abundances - ISM: molecules - ISM: clouds

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 in the tails of comets in the 1970's (Fehrenbach & Arpigny, 1973; Herzberg & Lew, 1974; Wehinger et al., 1974), but its detection in the general interstellar medium has proven elusive.

We report a detection of the ground-state rotational transition of H$_2$O$^+$ in some of the first spectra taken with the HIFI instrument during the ALMA performance verification campaign and early science observations. Section 2 briefly introduces the properties of the sources where H$_2$O$^+$ was detected. Section 3 summarises the spectroscopic data of the molecule. The observations and the line identification are described in Sect. 4 and in Sect. 5 we discuss the physical properties of the H$_2$O$^+$ absorption layer.

2. The sources

We observed three massive Galactic star-forming/Her 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.
Fig. 1. Energy level diagram of the lowest rotational levels of ortho-H$_2$O$^+$ and its radiative transitions. The fine structure transition frequencies are given in GHz.

The Sgr B2(M) and (N) cores are the most massive star-formation sites in our Galaxy. The line of sight, located in the plane of the Galaxy, passes through many spiral arm clouds and the extended envelope of Sgr B2 itself. The foreground clouds display a very rich molecular and atomic spectrum (Polehampton et al., 2007), although they often have very low densities and column densities, characteristic of diffuse or translucent clouds. The envelope of Sgr B2 itself includes hot, low density layers at both the ambient cloud velocity of 64 km s$^{-1}$, and at 0 km s$^{-1}$ (Ceccarelli et al., 2002). Many species detected along this line of sight have not been found elsewhere and the exact origin of the molecular features is often ambiguous because of the overlapping radial velocities (e.g., Comito et al., 2003).

NGC6334 is a nearby molecular cloud complex containing several concentrations of massive stars at various stages of evolution. The far-infrared source “I” contains an embedded cluster of NIR sources (Tapia et al., 1996). Four compact mm continuum sources are located near the geometric centre of the cluster (Hunter et al., 2007). Although NGC6334I is not known to exhibit strong absorption lines, its OH absorption profiles (Brooks & Whiteoak, 2001) reveal two molecular clouds along this line of sight, one with velocities between $-15$ and 2 km s$^{-1}$, and the other near 6 km s$^{-1}$.

### Table 1. Parameters of the hyperfine lines $F' - F''$ in the observed $1_{11} - 0_{00}$, $J = 3/2 - 1/2$ ortho H$_2$O$^+$ transition, including predicted frequencies, Einstein-A and optical depth at low temperatures

<table>
<thead>
<tr>
<th>$F' - F''$</th>
<th>$v_{\text{trans}}^i$ [MHz]</th>
<th>$v_{\text{trans}}^p$ [MHz]</th>
<th>$A_J^i$</th>
<th>$A_J^p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5/2$-$3/2</td>
<td>1115204.1</td>
<td>1115175.8</td>
<td>0.031</td>
<td>23.51</td>
</tr>
<tr>
<td>3/2$-$1/2</td>
<td>1115150.5</td>
<td>1115122.0</td>
<td>0.017</td>
<td>8.67</td>
</tr>
<tr>
<td>3/2$-$3/2</td>
<td>1115263.2</td>
<td>1115235.6</td>
<td>0.014</td>
<td>7.00</td>
</tr>
<tr>
<td>1/2$-$1/2</td>
<td>1115186.2</td>
<td>1115158.0</td>
<td>0.027</td>
<td>6.96</td>
</tr>
<tr>
<td>1/2$-$3/2</td>
<td>1115298.9</td>
<td>1115271.6</td>
<td>0.0035</td>
<td>0.88</td>
</tr>
</tbody>
</table>

- Predictions based on Strahan et al. (1986) and Mürtz et al. (1998).
- Nominal uncertainties are $\pm 2$ MHz but this is inconsistent with the discrepancy between the two predictions so that the actual uncertainty is unknown.
- $\check{c}$ from the matching DR21 OH pattern by Guilleutau et al. (1984) $\check{c}$
- $\int \tau_{\text{HIFI}} / N_{\text{H}2O^+} \, \text{d}v$ in $10^{-14}$ km s$^{-1}$ cm$^{-2}$

### Table 2. Summary of the observational parameters

<table>
<thead>
<tr>
<th>DR21(C)</th>
<th>Sgr B2(M)</th>
<th>NGC 6334</th>
</tr>
</thead>
<tbody>
<tr>
<td>RA (J2000)</td>
<td>20h39m01.1s</td>
<td>17h47m20.3s</td>
</tr>
<tr>
<td>DEC</td>
<td>$-29^\circ37'30''$</td>
<td>$-28^\circ23'03''$</td>
</tr>
<tr>
<td>Mode</td>
<td>Load-chop$^2$</td>
<td>DBS</td>
</tr>
<tr>
<td>$f_{\text{rt}}$</td>
<td>64 s</td>
<td>48 s</td>
</tr>
<tr>
<td>Int. source</td>
<td>0.07 K</td>
<td>0.08 K</td>
</tr>
<tr>
<td>$f_{\text{source}}$</td>
<td>0.08 K</td>
<td></td>
</tr>
</tbody>
</table>

$^1$ at native WBS resolution (1.1 MHz = 0.30 km s$^{-1}$)
$^2$ OFF position=20h37m10s, 42°37'00''

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 $F = J$, $F' = J'$ by fine 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) with $\approx 150$ MHz uncertainties.

### 3. The H$_2$O$^+$ spectroscopy

H$_2$O$^+$ is a radical with a $^2B_1$ electronic ground state and bond lengths and angle slightly larger than H$_2$O. Quantum-chemical calculations (Weis et al., 1989) yield a ground-state dipole moment of 2.4 D. The $B_1$ symmetry of the ground electronic state leads to a reversal of the ortho and para levels relative to water.

The rotational spectrum was measured by laser magnetic resonance (Strahan et al., 1986; Mürtz et al., 1998). Predictions of the $N_{3K} = 1_{11} - 0_{00}$, $J = 3/2 - 1/2$ fine structure component near 1115 GHz using the new parameters by Mürtz et al. (1998) are between 27.3 and 28.5 MHz higher than those calculated from Strahan et al. (1986), even though both articles claim to have reproduced the experimental data to $\approx 2$ MHz. The reanalysis of equivalent measurements of SH$^+$, by Brown & Müller (2009), shows that this accuracy is in principle achievable.

### 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 $^{13}$CO$^+$ 1-0, the CO 6-5, and the $^{12}$CO 6-5 transitions. The higher excitation lines of $^{13}$CO, C$^{18}$O, H$_2$O, and the [C n] 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. This is not present in any of the molecular emission lines, but is found in the [C n] 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 absorption profile. The match is as good as that achieved with the analytic profile and even reproduces the small excursions at 1115.22 and 1115.27 GHz. This indicates that OH and H$_2$O$^+$ occur in the same region and under the same physical conditions. The displacement of the fitted profile relative to the [C n] and OH profiles of about 4.0 km s$^{-1}$ is within the discrepancies between the different predictions of the line frequency. The astronomically determined line rest frequencies from comparison with the OH line fall 15 MHz below the predicted frequencies. As the line peak is very sharp, the accuracy of the frequency is
V. Ossenkopf, H.S.P. Müller, D. Lis, P. Schilke et al.: Detection of interstellar oxidaniumyl

W3 IRS5 and AFGL2591 by Benz et al. (in prep.) seems to favor the predicted frequencies from Strahan et al. (1986) in Table 1, the was found. This might indicate that the observed H$_2$O$^+$ is not file 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 NGC6334 is centred on -9 km s$^{-1}$, in reasonable agreement with the OH absorption at -8.2 km/s measured toward component F1. 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 radiative coupling with the environment. From a single absorption line, one can only provide a lower limit to the H$_2$O$^+$ column density, assuming a low excitation temperature where basically all H$_2$O$^+$ resides in the ground state, which is applicable to temperatures well below the upper level energy of 53 K.

Table 1 provides the integral over the optical depth of the hyperfine components in the low temperature limit. For the overall $J = 3/2-1/2$ line structure transition, we obtain an integrated optical depth of $\int \tau dv/N_{H_2O^+} = 4.70 \times 10^{-13}$ km s$^{-1}$ cm$^2$ per molecule, resulting in a lower limit to the H$_2$O$^+$ ground-state column densities of $7.2 \times 10^{12}$ cm$^{-2}$ for NGC 6334, 2.3 $\times 10^{13}$ cm$^{-2}$ for DR21, and 1.1 $\times 10^{15}$ cm$^{-2}$ for Sgr B2.

These values are lower limits not only because of the low-temperature approximation, but also because they assume that the absorption occurs in front of the continuum source and not within the dusty cloud, where the line absorption is partially compensated by dust emission. There may also be additional amounts of H$_2$O$^+$ in the para species that would not contribute to the 1115 GHz line. Altogether, the total H$_2$O$^+$ column density could be much higher than the lower limits given here.

The excellent correlation between the H$_2$O$^+$ profile and the OH absorption profile in DR21 indicates that both species occur in the same thin layer of hot gas (Jones et al., 1994) that directly faces the H II region at the blue-shifted blister outflow. There is no obvious correlation with the distributions of CO, H$_2$O, or HCO$^+$. For Sgr B2, we can clearly identify absorption in multiple translucent 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 NGC6334, 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 cooler 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.

References

Black 2007, in Molecules in Space and Laboratory, by J.L. Lemaire & F. Combes (eds.), S. Diana publ, p.90
de Graauw, Th., et al. 2010, A&A this volume
Ossenkopf, V.; Röllig, M.; Simon, R. et al. 2010, A&A this volume
Pilbratt, G.; et al. 2010, A&A this volume
van der Tak, F. F. S.; Marselle, M. G.; Herpin, F. 2010, A&A this volume
Acknowledgements. HIFI has been designed and built by a consortium of institutes and university departments from across Europe, Canada and the United States under the leadership of SRON Netherlands Institute for Space Research, Groningen, The Netherlands and with major contributions from Germany, France and the U.S. Consortium members are: Canada: CSA, U.Waterloo; France: CESR, LAB, LERMA, IRAM; Germany: KOSMA, MPIfR, MPS; Ireland, NUI Maynooth; Italy: ASI, IFSI-INAF, Osservatorio Astrofisico di Arcetri- INAF; Netherlands: SRON, TUD; Poland: CAMK, CBK; Spain: Observatorio Astronómico Nacional (IGN), Centro de Astrobiología (CSIC-INTA); Sweden: Chalmers University of Technology - MC2, RSS & GARD; Umeå University - Onsala Space Observatory; Swedish National Space Board, Stockholm University - Stockholm Observatory; Switzerland: ETH Zurich, FHNW; USA: Caltech, JPL, NHSC.

This work was supported by the German Deutsche Forschungsgemeinschaft, DFG project number Os 177/1-1. HSPM is grateful to the Bundesministerium für Bildung und Forschung (BMBF) for financial support aimed at maintaining the Cologne Database for Molecular Spectroscopy, CDMS. This support has been administered by the Deutsches Zentrum für Luft- und Raumfahrt (DLR). D.C.L. is supported by the NSF, award AST-0540882 to the Caltech Submillimeter Observatory. A portion of this research was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space administration.