Hot, metastable hydronium ion in the Galactic centre: formation pumping in X-ray-irradiated gas?

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With a 3.5 m diameter telescope passively cooled to approximately 80 K, and a science payload comprising two direct detection cameras/medium resolution imaging spectrometers (PACS and SPIRE) and a very high spectral resolution heterodyne spectrometer (HIFI), the Herschel Space Observatory is providing extraordinary observational opportunities in the 55–670 μm spectral range. HIFI has opened for the first time to high-resolution spectroscopy the submillimetre band that includes the fundamental rotational transitions of interstellar hydrides, the basic building blocks of astrochemistry. We discuss a recent HIFI discovery of metastable rotational transitions of the hydronium ion (protonated water, H₃O⁺), with rotational level energies up to 1200 K above the ground state, in absorption towards Sagittarius B2(N) in the Galactic centre. Hydronium is an important molecular ion in the oxygen chemical network. Earlier HIFI observations have indicated a general deficiency of H₃O⁺ in the diffuse gas in the Galactic disc. The presence of hot H₃O⁺ towards Sagittarius B2(N) thus appears to be related to the unique physical conditions in the central molecular zone, manifested, for example, by the widespread presence of abundant H₂⁺. One intriguing theory for the high rotational temperature characterizing the population of the H₃O⁺ metastable levels may be formation pumping in molecular gas irradiated by X-rays emitted by the Galactic centre black hole. Alternatively, the pervasive presence of enhanced turbulence in the central molecular zone may give rise to shocks in the lower-density medium that is exposed to energetic radiation.

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1. Introduction

The submillimetre band, broadly defined as a decade of wavelengths between 1 mm and 100 μm, gives access to cold, dust-enshrouded objects that are often hidden from view at shorter wavelengths. Dust continuum sources with temperatures of order 30 K peak near 100 μm. In colder sources, such as prestellar cores before the onset of star formation, the emission is shifted to even longer wavelengths. A complex network of chemical reactions takes place in these cold environments, including both gas-phase and grain-surface processes. High-resolution heterodyne techniques provide velocity-resolved ($R \gtrsim 10^6$) spectra of the rotational lines of abundant gas-phase molecules. Such observations give invaluable information about the chemical composition, kinematics (infall, outflow, rotation) and the physical conditions (temperature, density, UV field intensity, ionization fraction) at the onset of star formation. The line forest of heavy organic species that dominates the line spectrum at longer millimetre wavelengths gradually gives way to fundamental rotational transitions of light hydrides and deuterides in the submillimetre. Atomic fine structure lines of abundant elements (C, O and N), neutral or ionized, are also present and are important coolants of the gas.

The Herschel Space Observatory [1] is the fourth ESA cornerstone mission, the first space facility to completely cover the 60–670 μm spectral range. It consists of a 3.5 m diameter telescope, passively cooled to approximately 80 K, in a Lissajous orbit around the Lagrangian point L2, behind the Moon—a very stable and low-background orbit. The satellite was launched by Ariane 5 on 14 May 2009 from the Centre Spatial Guyanais in Kourou, French Guiana. It carries three cryogenically cooled instruments: two imaging cameras, PACS and SPIRE, both using bolometer detectors, and the heterodyne instrument, HIFI [2]. HIFI covers the 625–240 μm wavelength range using state-of-the-art SIS mixers, as well as the 212–157 μm wavelength range using HEB mixers. The instrument has a wide instantaneous IF bandwidth (4 GHz in two polarizations for SIS mixers and 2.4 GHz in two polarizations for HEB mixers), a high-frequency resolution (1 MHz over the full IF band and up to 140 kHz over a portion of the band) and a near-quantum-limit sensitivity.

The HIFI science can be broadly described as the ‘life cycle of gas and dust’. One of the main science themes is ‘unbiased spectral line surveys’, which provide a complete census of molecules in star-forming regions. The fundamental rotational transitions of light hydrides and deuterides that dominate the submillimetre spectrum often have very high critical densities and the excited energy levels are difficult to populate by collisions at the typical conditions characteristic of the interstellar medium. However, the dust continuum flux steeply increases at short submillimetre wavelengths (figure 1). This offers an opportunity to probe even relatively diffuse regions, characterized by several magnitudes of visual extinction, by means of absorption spectroscopy. Lines of sight towards distant dust continuum sources, such as Sagittarius B2 in the Galactic centre, often intersect several Galactic spiral arms, thus allowing detailed investigations of the physics and chemistry of the foreground gas in clouds with a wide range of physical conditions. The Herschel guaranteed time key programme HEXOS (Herschel/HIFI observations of EXtra-Ordinary Sources: the Orion and Sagittarius B2 star-forming regions; [3]) is devoted primarily to

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spectral line surveys. One of the sources studied is Sagittarius B2(N)—a line of sight that shows a rich, complex molecular emission and absorption spectrum (figure 1).

Hydronium is an important molecular ion in the oxygen molecular network (e.g. [4] and references therein). It is isoelectronic with ammonia, like ammonia it is a symmetric rotor, and it also has the characteristic inversion splitting of its rotational levels. However, in the case of H$_3$O$^+$, the inversion splitting is very large, comparable to the rotational-level spacing, and lines occur in the THz frequency range [5] (see the energy-level diagram in figure 2). Just like in the case of ammonia, H$_3$O$^+$ has ortho and para spin variants. Levels with $K = 0$ and $3n$ are ortho and those with $K = 3n + 1$ and $3n + 2$ para. Because there are no allowed radiative transitions between different $K$ ladders, the lowest energy levels in each ladder are metastable, connected only by collisions, and their relative populations can be used to derive an estimate of the gas kinetic temperature (e.g. [6,7] for NH$_3$). Transitions connecting to these metastable levels are referred to here as ‘metastable transitions’.

2. Observations

Herschel/HIFI observations presented here were carried out between September 2010 and April 2011, using the HIFI single point dual beam switch (DBS) observing mode. The source coordinates are: $\alpha_{J2000} = 17^h47^m19.88^s$, $\delta_{J2000} = -28^\circ22'18''.4$. The DBS reference beams lie approximately 3’ east and west (i.e. perpendicular to the roughly north–south elongation of the source). We used the HIFI wide-band spectrometer providing a spectral resolution of 1.1 MHz over a 2.5 GHz IF bandwidth of the high-frequency HEB receivers. The spectra

Figure 1. Herschel/HIFI spectral scan of Sagittarius B2(N). A complex spectrum of emission and absorption features is seen, with absorption dominating the spectrum above about 1THz. The HIFI point source sensitivity is 464–506 Jy K$^{-1}$ at frequencies 480–1910 GHz and the full width at half maximum beam size varies between 44” and 11”, respectively. (Online version in colour.)
Figure 2. The $\text{H}_3\text{O}^+$ energy-level diagram. Transitions connecting to the ground-state level in each $K$ ladder, which are discussed in this study, are marked in red. Other millimetre-wave transitions previously studied from the ground are marked in black (these are typically seen in emission). Transitions are labelled with the corresponding line frequency in GHz. The ‘plus’ and ‘minus’ signs denote parity of the levels. All levels for which collisional rates are available in the LAMDA database (www.strw.leidenuniv.nl/~moldata/) are included in the figure, but the $\text{H}_3\text{O}^+$ transitions detected with HIFI extend well beyond what is shown, up to approximately 1200 K in energy. (Online version in colour.)

Presented here are averages of the H and V polarizations, with equal weighting, reduced using HIPE [8] with pipeline version 5.1. The double sideband spectra were subsequently deconvolved into single sideband spectra, using the technique described in Comito & Schilke [9].

3. Discussion

The $\text{H}_3\text{O}^+$ absorption spectra towards Sagittarius B2(N) are shown in figure 3. Metastable transitions up to (11,11), with a lower level energy of 1219 K, are covered in the HIFI spectra, and clear signatures of $\text{H}_3\text{O}^+$ absorption are detected. The (1,1) ground state para transition at 1655.831 GHz is blended with the $2_{1,2}^{-1}_{0,1}$ transition of $\text{H}_2^{18}\text{O}$ at 1655.868 GHz and cannot be used in the excitation analysis. However, all the remaining metastable transitions, as well as the ground state $0^-1^+$ ortho line at 984.709 GHz, are clean from line contamination.
Figure 3. Spectra of H$_3$O$^+$ absorption towards Sgr B2(N), normalized to the continuum. The 0$^+$−1$^+$, (3,3), (6,6) and (9,9) lines are ortho and the remaining lines are para. The (1,1) line is blended with the 2$_{1,2}$−1$_{0,1}$ transition of H$_2^{18}$O and cannot be used in the analysis. Lower right: the H$_3$O$^+$ population diagram for the sum of the 65 and 80 km s$^{-1}$ components. A local thermodynamic equilibrium ortho/para ratio of 2 : 1 is assumed. (Online version in colour.)

Figure 4 shows a uniformly weighted average of the H$_3$O$^+$ (2,2) to (11,11) metastable transitions, with lower level energies greater than 43 K (figure 4a) and the H$_3$O$^+$ 0$^+$−1$^+$ transition (figure 4b; shifted down by 0.4 to avoid overlap). At least four H$_3$O$^+$ absorption components can be identified in the averaged spectrum of the metastable transitions, with central local standard of rest velocities of −75, 6, 65 and 80 km s$^{-1}$. The first two velocity components correspond to foreground gas on the line of sight, but still in the Galactic centre region, while the latter two are associated with the Sagittarius B2 cloud itself. The 65 km s$^{-1}$ component is also seen towards the nearby source Sagittarius B2(M), whereas the 80 km s$^{-1}$ component is local to Sagittarius B2(N). Although the signal-to-noise ratio of the top spectrum is limited, it appears that −104 and −40 km s$^{-1}$ components, which are quite prominent in other molecular tracers, such as ammonia (figure 4c, shifted down by 0.8), are weak or absent in the metastable H$_3$O$^+$ transitions. However, weak absorption at these velocities can be seen in H$_3$O$^+$ 0$^+$−1$^+$ spectrum (figure 4b)—in this case, the absorption originates from the ground state ortho-H$_3$O$^+$ level. Figure 4d shows a spectrum of H$_3^+$ R(1,1)$^l$ absorption at 3.715 μm on a nearby line of sight, 2M17470898-2829561, between Sagittarius B2 and Sagittarius B1 [10]. All the velocity components seen in the metastable H$_3$O$^+$ transitions can also be identified in the H$_3^+$
Figure 4. (a) A uniformly weighted average of the H$_3$O$^+$ (2,2) to (11,11) spectra; (b) the H$_3$O$^+$ 0$^+$–1$^+$ spectrum; (c) the 2$_1$–1$_1$ spectrum of para-NH$_3$ towards Sagittarius B2(N); and (d) the R(1,1)$^l$ spectrum of H$_3^+$ (multiplied by 5) [10] for a nearby line of sight, 2M1747, between Sagittarius B2 and Sagittarius B1. The four spectra have been shifted vertically to avoid overlap. Green lines show multi-component Gaussian fits to the H$_3$O$^+$ spectra. The strong 3$_{11}$–2$_{10}$ line of NH$_3$, present in the (9,9) spectrum at about $-110$ km s$^{-1}$, has been removed before averaging the spectra of the metastable transitions. Spectra of OH$^+$ and H$_2$O$^+$ on the same line of sight are also available, but not shown here, because complex hyperfine patterns do not allow one to easily isolate individual velocity components. (Online version in colour.)

spectrum, which shows, however, many additional velocity components—notably, the strongest H$_3^+$ absorption is seen at $-40$ km s$^{-1}$, which comes from the 3 kpc arm [11], outside the Galactic centre. The differences between the H$_3^+$ and H$_3$O$^+$ absorption patterns may be partly due to the limited signal-to-noise ratio of the high-frequency HIFI spectra. However, it appears that H$_3$O$^+$ is strongly enhanced only in some of the H$_3^+$ velocity components—H$_3$O$^+$ probes denser clouds, which are localized, whereas H$_3^+$ probes mostly diffuse clouds, which are ubiquitous.

The H$_3$O$^+$ population diagram for the sum of the 65 and 80 km s$^{-1}$ components is shown in figure 3, lower-right panel. It can be described by a two-component excitation model, with rotational temperatures of 162 and 519 K. For a 30 per
cent calibration uncertainty, the uncertainty in the rotational temperature of the hot component is about 100 K. The H$_3$O$^+$ column densities associated with the two temperature components are estimated to be $5 \times 10^{14}$ and $4 \times 10^{14}$ cm$^{-2}$, respectively. The two-component fit presented here provides only an approximate description of the H$_3$O$^+$ population distribution. In particular, in the case of formation pumping (see below), temperatures derived from the rotation diagram may not correspond to the kinetic temperature of the gas, as the rotational levels are likely not thermalized.

The detection of H$_3$O$^+$ absorption in multiple metastable transitions, with lower level energies up to approximately 1200 K, is surprising. Earlier Herschel/HIFI observations towards W31C and W49N, outside of the Galactic centre [12,13] (see also [14]) have shown strong OH$^+$ and H$_2$O$^+$ absorption, but only weak H$_3$O$^+$. These observations probe primarily diffuse gas, with low molecular fractions. Neufeld et al. [13] argue that if the ratio of electron density to H$_2$ is sufficiently large, the pipeline leading from O$^+$ to OH$^+$, to H$_2$O$^+$, to H$_3$O$^+$ can be leaky, with the flow of ionization reduced at each step by the dissociative recombination of OH$^+$ and H$_2$O$^+$. In dense molecular clouds, by contrast, the ionized hydrogen abundance and temperature are both too low for O$^+$ production by charge transfer to be efficient, and the dominant source of OH$^+$ is the reaction of H$_3^+$ with O. Once again, the chemistry is driven by cosmic ray ionization—the original source of H$_3^+$—but now the conversion of OH$^+$ to H$_2$O$^+$, and to H$_3$O$^+$ via reactions with H$_2$ proceeds with almost 100 per cent efficiency, because of the low density of electrons. In this context, the non-detection of H$_3$O$^+$ towards Orion KL by Gupta et al. [15] is interesting. On this line of sight, the column densities of the three oxygen-bearing ions are up to an order of magnitude lower than those towards W31C and W49N. These comparatively low column densities may be explained by a higher gas density, despite the assumption of a very high ionization rate.

The sightline towards Sagittarius B2 is different from the sightlines previously studied by HIFI in that it probes the molecular gas in the central molecular zone, characterized by higher density, degree of turbulence, as well as increased rates of cosmic ray and X-ray fluxes [16]—the environment typically found in active galactic nuclei. In the following we discuss how these factors may affect H$_3$O$^+$ abundance and excitation.

(a) Shocks

Ceccarelli et al. [17] carried out an unbiased spectral scan towards Sagittarius B2, using the ISO long wavelength spectrometer (LWS) and detected absorption signatures of 21 ammonia transitions covering a wide range of energy levels between 65 and 720 K, including metastable and non-metastable levels of both ortho and para species. They concluded that the absorption occurs in a thin, hot foreground layer, with a kinetic temperature of $700 \pm 100$ K and a density lower than $10^4$ cm$^{-3}$. Earlier ground-based observations of the ammonia inversion lines at radio wavelengths [18,19] have been explained by the presence of shocked gas on the line of sight towards Sagittarius B2, and the ISO LWS observations

$^1$A large-scale shock in Sagittarius B2, caused by a cloud–cloud collision, has also been postulated by Hasegawa et al. [20], on the basis of the observed morphology and kinematics of $^{13}$CO emission.
of Ceccarelli et al. [17] are consistent with this explanation. The angular extent of the absorbing layer is estimated to be approximately 30″ (although the 60 km s\(^{-1}\) component is seen towards both N and M sources, which are separated by 45″). Assuming an ammonia abundance of 10\(^{-6}\) (appropriate for shocked gas, but highly uncertain), the corresponding H\(_2\) column density in the hot layer is approximately 3 \times 10^{22} \text{ cm}^{-2}.

The rotational temperature of hot H\(_3\)O\(^+\) towards Sagittarius B2 is consistent with the earlier ammonia estimates, given the uncertainties of the two measurements. A natural explanation would thus be that H\(_3\)O\(^+\) comes from the same shocked layer as ammonia. In this case, the H\(_3\)O\(^+\) abundance would be 1.3 \times 10^{-8}. However, the main source of ionization in J-shocks are UV photons, and models have shown that the H\(_3\)O\(^+\) abundance in UV-irradiated regions does not exceed 3 \times 10^{-9}, even for extreme cosmic ray ionization rates (5 \times 10^{-15} \text{ s}^{-1}) [21]. C-shocks do not produce their own ionizing radiation, but preliminary models we made in an environment where additional ionization is provided by cosmic rays or X-rays indicate that the observed abundances and column densities of ammonia, water and H\(_3\)O\(^+\) could be explained by such a scenario. This needs to be investigated further, however. A detailed analysis of the H\(_3\)O\(^+\) excitation under the conditions characteristic of the shocked layer is hampered by the lack of collisional cross sections, which are available only for the low-energy H\(_3\)O\(^+\) rotational levels shown in figure 2.

The kinematics of the hot layer poses another intriguing question, as the velocities of the absorbing components are the same as those of the dense cores in Sagittarius B2, while low-density gas is present throughout the cloud envelope over a wide range of velocities, between 0 and 100 km s\(^{-1}\). This and the small angular extent derived from ISO observations indicate that the absorbing gas may be associated with the region in the immediate vicinity of the dense cores. Rolffs et al. [22] have detected signatures of the reversal of infall in Sagittarius B2(M) in ground-based and HIFI spectra of HCN transitions, with infall dominating in the colder, outer regions and expansion dominating in the warmer, inner regions. It is possible that a shock may be present at the interface between these two regimes. However, one would then expect a much higher density in the shocked gas than that derived from the ammonia observations.

Wilson et al. [23] detected the (18,18) inversion line of ammonia, with a lower level energy of 3130 K above the ground state, in absorption towards Sagittarius B2(M) and (N). The rotation temperature between the (18,18) and (12,12) levels, more than 1300 K, is significantly higher than the approximately 700 K value derived by Hüttemeister et al. [19] and Ceccarelli et al. [17], on the basis of observations of lower-energy transitions. This indicates that a range of excitation temperatures is present, which may not be representative of the kinetic temperature of the gas. Wilson et al. [23] consider two equally plausible scenarios explaining the (18,18) ammonia absorption towards Sagittarius B2: (i) an extended low-density envelope surrounding Sagittarius B2(M) and (N) or (ii) much more compact, dense clouds associated with the hot cores of this star-forming region. They also consider heating by shocks, X-rays, UV, cosmic rays and the dissipation of supersonic cloud motions, and exclude the latter three mechanisms. In the absence of detailed models of X-ray heating, they favour the shock explanation.
As an alternative, Wirström et al. [24] modelled Odin observations of water and ammonia absorption lines towards Sagittarius B2 and concluded that the non-local thermodynamic equilibrium excitation of ammonia in the environment of Sagittarius B2 could be explained without invoking a hot molecular layer in addition to the warm envelope gas. In this scenario, ammonia is formed by exothermic gas-phase reactions with a formation temperature in excess of 1000 K. In addition, Wirström et al. [24] conclude that a hot layer is not required to explain the line profiles of water isotopologues observed by Odin.

(b) Cosmic rays

In a recent study, Meijerink et al. [25] modelled the effect of cosmic rays and mechanical heating on molecular abundances in environments characteristic of active galactic nuclei. In the Meijerink et al. [25] models, the H$_3$O$^+$ abundance can reach values as high as $1 \times 10^{-8}$ at hydrogen column densities in excess of $1 \times 10^{22}$ cm$^{-2}$ in a relatively high-density gas (a few $\times 10^5$ cm$^{-3}$), exposed to strong UV field ($G_0$ approx. $10^5$). The H$_3$O$^+$/H$_2$O ratio predicted by these models is typically approximately $10^{-2}$. The H$_2$O column density towards Sagittarius B2 in the relatively large SWAS beam is approximately $2.4 \times 10^{16}$ cm$^{-2}$ [26]. The observed H$_3$O$^+$/H$_2$O ratio is thus in the correct range. The high gas density required to produce the enhanced H$_3$O$^+$ abundances is consistent with that present in the central $5 \times 10^{pc}$ core of Sagittarius B2 [27], but again appears inconsistent with the value derived for the hot ammonia layer.

(c) X-rays

X-rays can be an important source of ionization and energy input, leading to the formation of H$_3$O$^+$ via reaction of H$_3^+$+O, followed by H$_2$O$^+$+H$_2$, or by H$_3^+$+H$_2$O, and models suggest that H$_3$O$^+$ abundances of $10^{-8}$ and beyond are likely to occur in X-ray-dominated regions (XDRs) [21]. It is also straightforward to obtain H$_3$O$^+$/H$_2$O ratios as high as $10^{-2}$ in XDRs, whereas photon-dominated region (PDR) model ratios are generally $10^{-3}$ or less. The H$_3$O$^+$ abundance and the H$_3$O$^+$/H$_2$O ratio towards Sagittarius B2 are thus in the range predicted by XDR models.

The presence of strong 6.4 keV iron fluorescence and hard X-ray emission has led to the suggestion that giant molecular clouds in the Galactic centre, in particular Sagittarius B2, have been recently illuminated by an X-ray flash [28,29]. Terrier et al. [30] have shown clear observational evidence that the X-ray emission of Sagittarius B2 is now fading. The characteristic time scale for the decay is approximately 8 years, compatible with the light crossing time of the molecular cloud core. On the basis of this fast variability, Terrier et al. [30] rule out alternative explanations of the origin of the iron line and continuum emission, such as inverse bremsstrahlung from sub-relativistic ions and low-energy cosmic ray electrons, and conclude that Sagittarius B2 is likely to be an X-ray reflection nebula. The location of the illuminating source is yet to be determined, but the most likely explanation is a period of high activity of the massive black hole at the centre of the Galaxy, associated with the radio continuum source Sagittarius A*, which ended about 100 years ago.

X-ray-driven chemistry thus offers an intriguing explanation for the observed hot, metastable H$_3$O$^+$ towards Sagittarius B2. In the context of X-ray models, the high rotational temperature observed may be naturally explained by the
H$_3$O$^+$ formation pumping—H$_3$O$^+$ molecules are formed in highly excited states, and quickly decay radiatively to populate the metastable levels probed by our HIFI observations. The reaction H$_2$O$^+$ + H$_2$ → H$_3$O$^+$ + H has an exothermicity of 1.694 eV and H$_3^+$ + H$_2$O → H$_3$O$^+$ + H$_2$ of 2.814 eV. It is not known how this excess energy is distributed between the reaction products and one may expect that the light H and H$_2$ carry most of the excess energy. However, in principle, a lot of excess energy is available to populate excited H$_3$O$^+$ levels. The population would then get trapped in the metastable levels that are probed by our HIFI observations.

While this explanation is appealing, given our understanding of the physical conditions in the Sagittarius B2 environment, detailed model calculations are required, as formation pumping is relatively inefficient. While XDR models may be able to easily reproduce the required column density of H$_3$O$^+$, explaining the observed excitation requires that the collisional relaxation time is long relative to that required for recombination/reformation of H$_3$O$^+$ molecules (molecules have to be produced efficiently in highly excited states before they have time to relax through collisions and typical reaction rates are of order $10^{-9}$ s$^{-1}$, only a factor of a few larger than typical collisional de-excitation rates). Ammonia observations would also have to be explained by the same model, and one may expect that ammonia, being chemically more stable than H$_3$O$^+$, would have more time to relax through collisions, and should thus display a lower rotation temperature. Observations do not indicate higher rotational temperatures of H$_3$O$^+$, when compared with ammonia, but the uncertainties of the two measurements are relatively large.

(d) Extragalactic H$_3$O$^+$

The Galactic centre can be viewed as the closest active galactic nucleus. In this context, our observations are relevant for extragalactic applications. Aalto et al. [31] have observed H$_3$O$^+$ towards the centres of seven active galaxies to investigate the impact of starburst and active galactic nucleus activity on the chemistry of the interstellar medium. They find high H$_3$O$^+$ abundances, in excess of $10^{-8}$, in four galaxies: NGC 253, NGC 1068, NGC 4418 and NGC 6240. Only in IC 342 is the H$_3$O$^+$ abundance an order of magnitude lower, and here a standard PDR chemistry can explain the observed H$_3$O$^+$ abundance. The temperature of the H$_3$O$^+$-emitting gas is not constrained by the present observations. While the large H$_3$O$^+$ columns derived towards the four galaxies are generally consistent with predictions of XDR models, Aalto et al. [31] also consider an alternative scenario, in which H$_3$O$^+$ can be formed from H$_2$O evaporating from dust grains and reacting with HCO$^+$ in a warm, dense gas. Shocks would help remove water molecules from grain mantles, resulting in an enhanced gas-phase water abundance. Detailed modelling of the H$_3$O$^+$ excitation towards Sagittarius B2, in conjunction with HIFI observations of water isotopologues on the same line of sight, may help distinguish between these scenarios. We note, however, that earlier SWAS and HIFI observations [26,32,33] indicate enhanced water abundance on the line of sight towards Sagittarius B2, as predicted by the shock evaporation models. As water, unlike hydronium, has no metastable levels, it is challenging to observationally distinguish between water in the warm envelope and water in the hot layer.
4. Concluding remarks

The H$_3$O$^+$ results presented here should be considered preliminary, as significant improvements are expected for the pipeline processing of the HIFI HEB bands in the recently released version 8 of the HIPE software. The resulting improvement in the signal-to-noise ratio in the spectra should increase the accuracy of the population diagrams, and possibly allow the determination of the rotation temperature for the individual velocity components in the H$_3$O$^+$ absorption spectra (figure 4).

H$_3$O$^+$ formation pumping in X-ray irradiated gas seems to naturally explain our observations, but detailed models are needed to support this hypothesis and exclude equally plausible alternative explanations, such as shocks or cosmic rays. Given the observed decrease in the X-ray flux, these models should be time-dependent and should explain simultaneously both the hydronium ion and ammonia observations.

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