Onsala Proposal

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Distribution of molecular ions in cometary comae

Semester: feb2025   **Science Cat.: Solar system**

Abstract

Comets are remnant bodies from a time when the solar system was formed. Hence, the cometary chemical composition reflects the conditions prevailing in the early solar nebula. While there has been many studies regarding the neutral molecular gas ejected from the comet, essentially nothing is known of the molecular ion structure in the inner coma except what is known from space probe fly-bys (eg. Giotto). We here propose to resolve the line profiles of the two most abundant molecular ions, H2O+ and H3O+. Our modelling work shows that lines (at 307 GHz and in the 600 GHz band) from these two molecular ions are readily detectable with APEX for a comet (at 1 AU distance from us and 1 AU from the Sun) with a water production rate of Q(H2O) = 10^(29) molecules/s.

Applicants

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Is this a long term proposal: No

Overall scheduling requirements

This is a ToO proposal

Observing runs

run	telescope	instrument	time request (minimal)	frequency (GHz)	weather (pwv)	LST range	comments/constraints
A	APEX	SEPIA345 (277-371 GHz)	8h (4h)	307	0.5-1 mm		LSB
B	APEX	SEPIA660 (581-727 GHz)	5h (5h)	606	< 0.5mm		LSB
C	APEX	SEPIA660 (581-727 GHz)	5h (5h)	633	< 0.5mm		USB

Targets

Source	RA	Dec	Epoch	Vlsr (km/s)	Duration (min)	Runs	Comments
ToO	00:00:00.00	+00:00:00.0	J2000	0.0	1080	A B C	

This proposal is a **resubmission** of several previous ToO proposals (`O-0102.F-9309`, `O-0103.F-9306`, `O-0104.F-9300`, `O-0105.F-9307`, and `O-0113.F-9306`) that have not been observed in depth since no suitable comet, with $Q(\mathrm{H_2O}) \geq 10^{29}$ molecules/s, appeared during Swedish observing time.

Scientific Rationale

Comets were formed in the young solar nebula and can be considered as left-overs from a time when our planetary system was formed. Their chemical composition reflect conditions that prevailed then. Water ice is believed to be the major constituent of the volatile material in comet nuclei, accounting for some 80%-90% of the ejected material. Hence, the most abundant molecule in (the inner) cometary coma is $\mathrm{H_2O}$, and thus the outgassing activity of a comet is expressed using the water production rate, $Q(\mathrm{H_2O})$. The production rate is typically, for long-periodic comets, of the order of 10^{29} water molecules per sec. Other molecules, such as CO, HCN and $\mathrm{CH_3OH}$, have substantially lower production rates.

Although comet tails and their solar-wind interactions have long been studied through low-resolution UV/visible spectroscopy of molecular ions, much less is known about the ionization in cometary comae. This is where APEX can make an important contribution. Observation of the dominant ions $\mathrm{H_2O^+}$ and $\mathrm{H_3O^+}$ will test the existing ionization models. Comparison of their line profiles with that of a common neutral ($\mathrm{CH_3OH}$) will probe whether the kinematics of ions and neutrals begin to differ already in the coma, before the ions reach the tail where they interact with the solar wind.

The neutral part of the coma extends to a radius where the photoionization, caused by the solar radiation field, starts to convert the neutral gas (mainly water) into $\mathrm{H_2O^+}$ and $\mathrm{H_3O^+}$ by the routes

$$\mathrm{H_2O} + h\nu \rightarrow \mathrm{H_2O^+} + e$$

$$\mathrm{H_2O^+} + \mathrm{H_2O} \rightarrow \mathrm{H_3O^+} + \mathrm{OH}$$

At this radius, the so called contact radius (located at a few 100 km to a few 1000 km depending on the activity), the ions formed start to decouple from the radial outflow of the neutrals and instead they get deflected toward the tail. This was indeed demonstrated in quite some detail, using the Giotto fly-by data of comet 1P/Halley, see Ip & Axford (1990) and Rubin et al. (2009). The latter study also performed detailed chemical modelling from which it is evident that the electron density, $n(e)$, is essentially given by

$$n(e) \approx n(\mathrm{H_2O^+}) + n(\mathrm{H_3O^+})$$

The radial electron density distribution is an important aspect for the excitation of the remaining neutrals through collisions (Xie & Mumma 1992, Bergman et al. 2022). In the innermost part of the coma, collisions with water molecules is the dominating excitation mechanism for all neutrals (including water itself, eg. Bensch & Bergin 2004, Bergman et al. 2022). Further out, collisions with electrons is the dominating excitation mechanism, while in the outer part of the coma (outside the contact surface) radiative excitation (by solar radiation field) is governing the molecular excitation. Since the electron-neutral collisional excitation is important for cometary comae it is crucial to know the electron density distribution throughout the coma cloud. Apart from the in-situ molecular ion measurements[1] by Giotto and Rosetta, one has to rely on estimates from models (see, for example, Bensch & Bergin 2004). Observations of the dominant molecular ions will therefore directly yield the electron density as well as the dynamics of the ion flow (which differ from the neutral ~ 1 km/s flow outside the contact surface, see the Rosetta results

[1]Vibronic bands of $\mathrm{H_2O^+}$ near 5900 Å have been observed in comets from ground but they are affected by line blending and limited velocity resolution, eg. Schmidt (2015)

Table 1: Lines to be observed

Molecule	Frequency GHz	Expected intensity K km/s	Notes
$p\text{−H}_3\text{O}^+$ $1_{1-} - 2_{1+}$	307.2	0.076	75% of $n(e)$ and an o/p of 2
$p\text{−H}_2\text{O}^+$ $1_{10,2} - 1_{01,1}$	604.7	0.165	20% of $n(e)$ and an o/p of 3
$p\text{−H}_2\text{O}^+$ $1_{10,2} - 1_{01,2}$	607.2	0.791	
$p\text{−H}_2\text{O}^+$ $1_{10,1} - 1_{01,1}$	631.7	0.326	
$p\text{−H}_2\text{O}^+$ $1_{10,1} - 1_{01,2}$	634.3	0.167	

of 67P/Churyumov-Gerasimenko by Vigren et al. (2017) where the ion velocity is in the range 2-8 km/s).

We here propose to observe the molecular ions H_2O^+ and H_3O^+ using the APEX telescope for a comet with a water production rate of about 1.0×10^{29} s^{-1} (or higher). There is no candidate comet known now, and thus we only ask for observing time should a suitable comet become available during 2024. To estimate the expected ion line intensities we have run comet radiative transfer models for $Q(H_2O) = 10^{29}$ mol/s and assuming a comet distance to the Sun of 1 AU and a distance between the comet and Earth of 1 AU. Moreover, based on the work by Rubin et al. (2009), we fix the abundances of the ions H_3O^+ and H_2O^+ relative to electrons of 75% and 20%, respectively. The expansion velocity is set to 0.85 km/s and the temperature of the comet nuclei surface is 40 K. For these parameters, the radius of the contact surface becomes about 1000 km. The model results are presented in Table (1) and Fig. 1. Near the $p\text{−H}_3\text{O}^+$ line at 307 GHz there are several CH_3OH lines that can be used to probe the neutral coma.

Observing Requirements

All four H_2O^+ lines can be observed in two frequency settings with SEPIA660. The SEPIA660 observations require a pwv of 0.5 mm (or better). We opt for an RMS of 50 mK and a velocity resolution of 0.2 km/s to resolve the line profiles for the strongest transitions (at 607 and 632 GHz). From the online calculator, we find that for the 632/634 GHz observations we need 1.7 hrs, and for the 605/607 GHz setup we need 7.5 hrs since the atmosphere is more opaque here. For the 307.2 GHz line (see Fig. 1 right), we need 10 mK rms using the velocity resolution of 0.2 km/s to secure a line profile. This requires 5.7 hrs of observing time in pwv 2.0 mm weather. Thus, we ask for 18 hrs in total (10 hrs SEPIA660, 8 hrs SEPIA345) when also accounting for pointing, focussing, tuning, receiver changes.

Observing plan and special requirements

This is a ToO-proposal. Comet observations require special care at APEX. The ephemeris from JPL Horizons will be supplied.

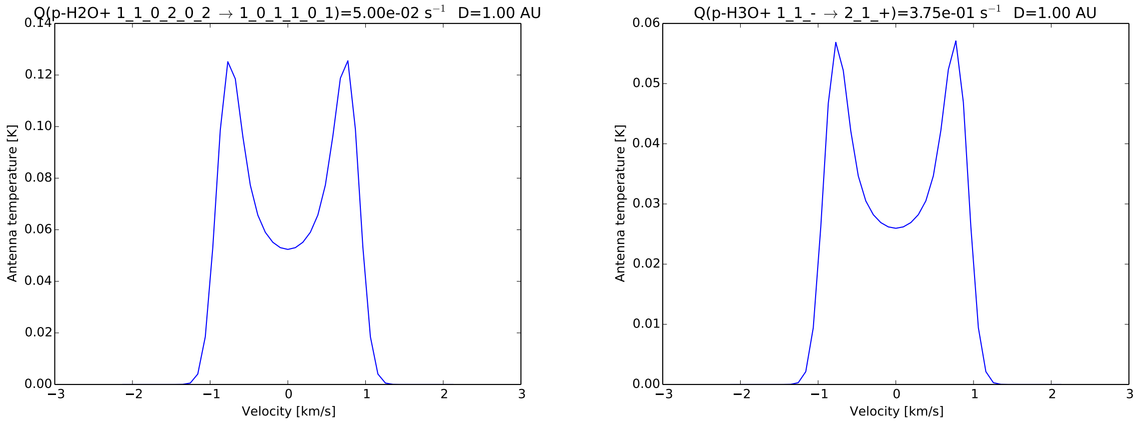

Figure 1: Model comet spectra of $p{-}H_2O^+$ (left, line at 604.7 GHz) and $p{-}H_3O^+$ (right, line at 307.2 GHz). These spectra are calculated assuming the ions expand in the same way as the neutral gas. Outside of the contact surface, the ions will be deviated towards the tail and this will affect the line profiles (the impact on the integrated line intensities is expected to be low because of optically thin emission).

References

[1] Bensch, F. & Bergin, E. A. 2004, ApJ 615, 531

[2] Bergman, P., Lerner, M. S., Olofsson, A. O. H., et al. 2022, A&A 660, 118B

[3] Ip, W.-H., & Axford, W. I. 1992, in *Physics and Chemistry of Comets*, ed F. Huebner, (Berlin: Springer), 177

[4] Rubin, M., Hansen, K. C, Gombosi, T. I., et al. 2009, Icarus 199, 505

[5] Schmidt, C. 2015, Icarus 265, 35

[6] Vigren, E., André, M., Edberg, N. J. T., et al. 2017, MNRAS 469, 142

[7] Wirström, E. S., Lerner, M. S., Källström, P., Levinsson, A., Olivefors, A., Tegehall, E. 2016, A&A 588, A72

[8] Xie, X., & Mumma, M. J. 1992, ApJ 386, 720

Figures

No PhD Students involved

Linked proposal submitted to this TAC: No

Linked proposal submitted to other TACs: No

Relevant previous Allocations: Yes

see science justification

No additional remarks

Observing run info :