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LETTER TO THE EDITOR

HIFI observations of water in the atmosphere of comet C/2008 Q3 (Garradd)*

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ABSTRACT

High-resolution far-infrared and sub-millimetre spectroscopy of water lines is an important tool to understand the physical and chemical properties of cometary atmospheres. We present observations of several rotational ortho- and para-water transitions in comet C/2008 Q3 (Garradd) performed with HIFI on *Herschel*. These observations have provided the first detection of the 2_{12}–1_{01} (1669 GHz) ortho and 1_{11}–0_{00} (1113 GHz) para transitions of water in a cometary spectrum. In addition, the ground-state transition 1_{10}–1_{01} at 557 GHz is detected and mapped. By detecting several water lines quasi-simultaneously and mapping their emission we can constrain the excitation parameters in the coma. Synthetic line profiles are computed using excitation models which include excitation by collisions, solar infrared radiation, and radiation trapping. We obtain the gas kinetic temperature, constrain the electron density profile, and estimate the coma expansion velocity by analyzing the map and line shapes. We derive water production rates of 1.7–2.8×10^{28} s^{-1} over the range $r_{\rm h}$ = 1.83–1.85 AU.

Key words. Comets: individual: C/2008 Q3 (Garradd) – radiative transfer – radio lines: solar system – submillimetre – techniques: spectroscopic

1. Introduction

Comets spend most of their lifetime in the outer Solar System and therefore have not undergone considerable thermal processing. Line emission is useful to study the physical and chemical conditions of cometary atmospheres, and their relation to other bodies in the Solar System (Biver et al. 2002; Bockelée-Morvan et al. 2004).

Water molecules in cometary atmospheres are excited due to collisions with other molecules and radiative pumping of the fundamental vibrational levels by the solar infrared flux. The 1_{10}–1_{01} ortho-water transition at 557 GHz is one of the strongest lines in cometary comae, but it cannot be detected directly from the ground due to absorption in the Earth's atmosphere (Bockelée-Morvan 1987). Water vapour production has been estimated previously from the ground through measurements of its photodissociation product, the OH radical (see e.g. A'Hearn 1982), and water high vibrational bands (Bockelée-Morvan et al. 2004). The 1_{10}–1_{01} rotational transition of ortho-water at 557 GHz has been observed using heterodyne techniques by the Submillimeter Wave Astronomical Satellite (SWAS) (Neufeld et al. 2000; Chiu et al. 2001), and later with Odin (Lecacheux et al. 2003; Biver et al. 2007, 2009).

ESA's *Herschel* Space Observatory was successfully launched on May 14, 2009 and entered a Lissajous orbit around the L_2 Lagrangian point (Pillbratt et al. 2010). The Heterodyne Instrument for the Far-Infrared (HIFI) onboard *Herschel* has continuous coverage in five frequency bands in the 480–1150 GHz range, and an additional dual frequency band covering the 1410–1910 GHz range that are not observable from the ground (de Graauw et al. 2010). HIFI's submillimetre frequency coverage is of great importance to observe water vapour in Solar System objects such as cometary comae with unique sensitivity and the required high spectral resolution to resolve the emission lines.

Comet C/2008 Q3 (Garradd) is a long-period comet (P = 1.9×10^5) with a highly eccentric orbit (e = 0.99969). It passed perihelion on June 23, 2009 at a distance of 1.7982 AU from the Sun and was observed with HIFI in July 2009 as part of the *Herschel* guaranteed time key project "Water and related chemistry in the Solar System" (Hartogh et al. 2009). In this letter, we describe the observations of water and the analysis of part of the data set. Water production rates derived from our radiative transfer models are presented.

2. *Herschel* HIFI observations

Comet C/2008 Q3 (Garradd) was observed with HIFI about one month post-perihelion in the period July 20–27 2009, when the comet was at $r_{\rm h} \simeq 1.8$ AU from the Sun and $\Delta \simeq 1.9$ AU from *Herschel* (Table 1). HIFI's submillimetre high-resolution heterodyne spectrometer is designed to have noise levels close to the quantum limit (de Graauw et al. 2010). The spectral resolution is

* *Herschel* is an ESA space observatory with science instruments provided by European-led Principal Investigator consortia and with important participation from NASA.

1.1 MHz and 140 KHz provided by the Wideband Spectrometer (WBS) and the High Resolution Spectrometer (HRS), enabling HIFI to resolve spectrally cometary line shapes.

We present a summary of the HIFI observations in Table 1. These HIFI observations constitute the first detection of the 2_{12}–1_{01} transition of ortho-water at 1669.9 GHz, and the 1_{11}–0_{00} transition of para-water at 1113.3 GHz in cometary coma. In addition, the ground-state transition 1_{10}–1_{01} at 557 GHz is detected. Multi-line observations can provide more reliable water production rates using molecular excitation codes.

The data were acquired using the standard frequency switching and position switching observing modes. In the latter mode, a reference cold sky position separated from the comet by 0.5° was observed for the same amount of time and subtracted from the on-source observations. Three additional on-the-fly (OTF) maps were obtained at 557 GHz with the standard observational modes (the OTF mode was not released at that time). The *Herschel* telescope has a diameter of 3.5 m, with a corresponding HIFI Half Power Beam Width (HPBW) of 12.7″, 19.2″, and 38.1″ at 1669, 1113, and 557 GHz, respectively. This represents projected distances of $1.7–5.1 \times 10^4$ km at the comet. The JPL's HORIZONS system[1] is used to calculate the ephemerides and the relative motion of the comet with respect to the satellite.

The data were reduced to a level 2 product using the standard *Herschel* Interactive Processing Environment (HIPE) routines for HIFI (de Graauw et al. 2010). The frequency scale of the observed spectra was corrected for the geocentric velocity of the comet and the spacecraft orbital velocity. We scaled the main beam brightness temperature using the beam efficiency of the *Herschel* telescope, ranging between 0.65–0.75 at different frequencies. Integrated line intensities and velocity offsets in the comet rest frame are given in Table 1.

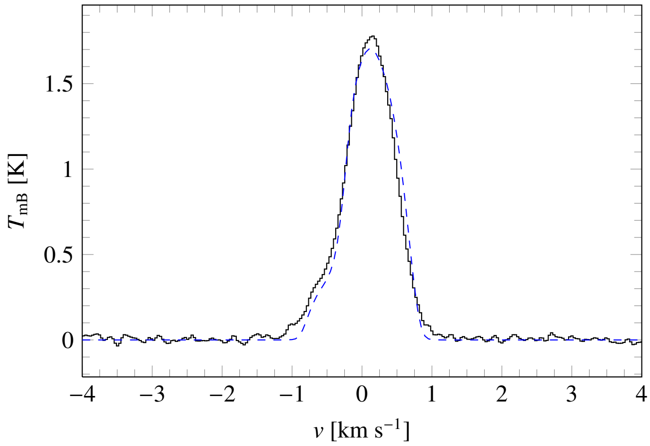

Fig. 1. Spectrum of the 1_{10}–1_{01} ortho-water line at 556.936 GHz in comet C/2008 Q3 (Garradd) obtained by the HRS on July 20.94 UT in FSw mode. The velocity scale is given with respect to the comet rest frame. The dashed line shows a synthetic profile computed with the Monte Carlo model for isotropic outgassing at $v_{\rm exp} = 0.55$ km s^{-1}, $T = 15$ K, and $x_{n_e} = 0.2$.

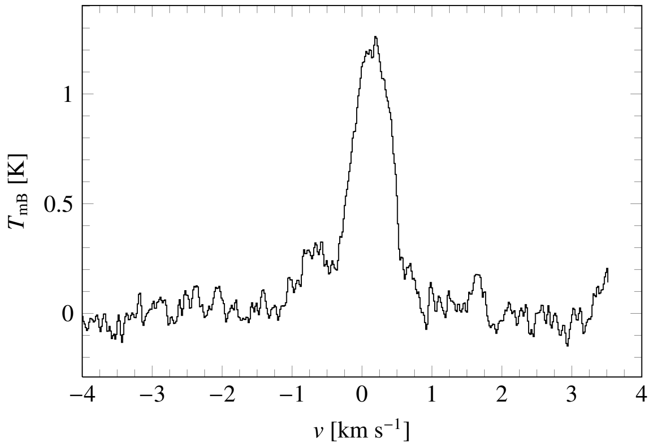

Fig. 2. Average of the HRS frequency-switched observations of the 1_{11}–0_{00} para-water line at 1113.343 GHz in comet C/2008 Q3 (Garradd) obtained on July 22.34 and 27.78 UT.

3. Data analysis

3.1. Water line emission

Figure 1 shows the spectrum of the 1_{10}–1_{01} ortho-water line, corresponding to a long integration in frequency switching mode with a throw of 18 MHz. Here the signal-to-noise ratio is very high. This line is optically thick and slightly asymmetric due to self-absorption effects in the coma. From the width of the non-self-absorbed redshifted side of the line we obtain an estimate of 0.55 km s^{-1} for the coma expansion velocity. Values in the range $v_{\rm exp} = 0.5 - 0.8$ km s^{-1} are typical for relatively weak comets with total water production rate $Q_{\rm H_2O} < 10^{29}$ s^{-1} at $r_{\rm h} > 1.2$ AU.

Figure 2 shows the water spectrum of the 1_{11}–0_{00} para-water line at 1113.3 GHz observed in frequency switching mode. We averaged over two dates to increase the signal-to-noise ratio. The 2_{12}–1_{01} ortho-water line at 1669.9 GHz is detected in the HRS and WBS data (Fig. 3). There are standing waves in the spectrum due to the frequency switching observing mode. The line intensity is strongly baseline-dependent. Figure 4 shows the on-the-fly integrated intensity map of water emission at 557 GHz. The outer regions beyond ∼ 10″ (13 000 km) from the nucleus are dominated by infrared fluorescence.

3.2. Modelling

We adopted the publicly available Accelerated Monte Carlo radiative transfer code *ratran* (Hogerheijde & van der Tak 2000) to calculate water line emission in cometary coma. We used the one-dimensional version of the code following the work of Bensch & Bergin (2004). A water excitation model based on the Sobolev escape probability method was also considered (Bockelée-Morvan 1987; Biver 1997). These two approaches provide very similar results (Zakharov et al. 2007).

The radial gas density profile for water was obtained using the standard spherically symmetric Haser distribution (Haser 1957). The expansion velocity is assumed to be constant in the coma. We use a constant neutral gas kinetic temperature throughout the coma and the electron temperature profile given by Biver (1997) (see also Bensch & Bergin 2004). We assume an ortho-to-para water abundance ratio of 3 (see e.g., Crovisier et al. 1997). The few number of observed water lines, their non-simultaneity, and the different beam sizes for each line prevented us to derive useful constraints on the ortho-to-para ratio. Molecular data for ortho- and para-water have been obtained from the current version of the LAMDA database [2] (Schöier et al. 2005).

[1] `http://ssd.jpl.nasa.gov/?horizons`

[2] `http://www.strw.leidenuniv.nl/~moldata/`

Table 1. Summary of HIFI observations of comet C/2008 Q3 (Garradd) and retrieved water production rates. The observations were conducted using standard frequency switching (FSw), position switching (PSw) and on-the-fly spectral maps (OTF) observing modes. The error bars in line intensity, velocity shift and production rate are the statistical errors.

Obs. ID	UT start date [mm/dd.ddd]	Δ [AU]	r_h [AU]	Band	Obs. mode	ν_{ij} [GHz]	Integration [s]	Intensity [K km s^{-1}]	Velocity shift [m s^{-1}]	Q_{H_2O} [10^{28}s^{-1}]
1342180461	07/20.908	1.865	1.831	1a	FSw	557	2181	1.594 ± 0.009	+56 ± 3	2.73 ± 0.01
1342180462	07/20.933	1.865	1.831	1a	PSw	557	381	1.717 ± 0.023	+55 ± 10	2.81 ± 0.03
1342180463	07/20.936	1.865	1.831	1a	OTF	557	2725			
1342180557	07/22.338	1.901	1.836	4b	FSw	1113	2802	1.206 ± 0.022	+24 ± 13	1.82 ± 0.03
1342180813	07/27.726	2.037	1.850	6b	FSw	1669	3018	1.597 ± 0.104	+283 ± 28	2.12 ± 0.30
1342180815	07/27.782	2.039	1.850	4b	FSw	1113	2802	0.994 ± 0.023	+42 ± 15	1.70 ± 0.03

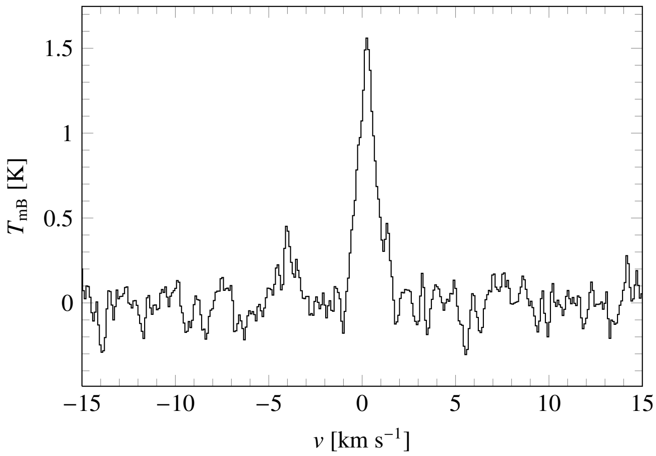

Fig. 3. WBS frequency-switched observation of the 2_{12}–1_{01} ortho-water line at 1669.905 GHz towards comet C/2008 Q3 (Garradd) obtained on July 27.73 UT.

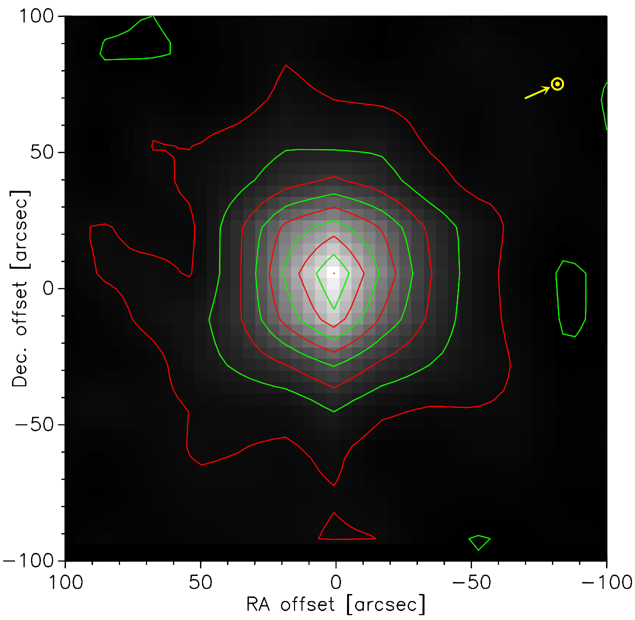

Fig. 4. On-the-fly map of the 557 GHz ortho line obtained by HRS on July 20.95 UT. The contour step is 0.2 K km s^{-1} in brightness temperature, from 0 to 1.8 K km s^{-1}. The map width is 3×10^5 km projected at the comet. The direction towards the Sun is indicated by the arrow in the upper right corner.

The electron density profile is derived from the 1P/Halley in situ measurements scaled to the water production rate and heliocentric distance of comet C/2008 Q3 (Garradd) (Biver 1997; Bensch & Bergin 2004). A scaling factor to this electron density profile, x_{n_e}, is introduced as a free parameter to the model (Biver 1997). Observations of the 557 GHz line in comets with Odin have shown that the radial profiles of the line brightness are best explained with x_{n_e} = 0.2 (Biver et al. 2007). For the Monte Carlo code, the water-electron collision rates from Faure et al. (2004) are used.

Infrared pumping of vibrational bands by solar radiation contributes to the excitation in the outer coma where the gas and electron densities are low (Bockelée-Morvan 1987). We use the effective pumping rates for the lowest rotational levels of the ground vibrational state of ortho-water from Zakharov et al. (2007). Effective pumping rates for para-water were computed as described in Zakharov et al. (2007).

The relative level population of the lowest levels of para-water is shown in *online* Fig. 5. In the inner coma, frequent collisions between water molecules lead to a thermal equilibrium distribution, and electrons are cooled down close to the neutral gas temperature (e.g Bensch & Bergin 2004). Given the beam sizes (between 17 000 and 51 000 km projected on the comet), molecules from the outer coma contribute to the detected emission. The line excitation in this region is dominated by water-electron collisions and infrared fluorescence.

Once the level populations are calculated, we solve the radiative transfer equation along different lines of sight through the comet atmosphere covering 2.5×HPBW, and compute the beam averaged emission at the distance of the comet. By comparing to the observed line emission, we deduce the water production rate.

3.3. Water production rates

Mapping observations shown in Fig. 4 can be used to constrain the neutral gas kinetic temperature and the electron density scaling factor x_{n_e}. We constrained these model parameters by minimizing the radial variation of the water production rate deduced from the intensity at different offset positions. Hence, deviations from the Haser law due, e.g., to sublimating grains or structures induced by the rotation of the nucleus are not considered. We used the HRS data with the two orthogonal polarisations. We averaged radially the line intensity using bins of 10″ to 20″. In Fig. 6, we show the retrieved water production rate as a function of offset for an isotropic model with an expansion velocity v_{exp} = 0.55 km s^{-1}, T = 15 K, and x_{n_e} = 0.2 and 1. We found that a constant production rate is obtained for excitation parameters in the range T = 15–25 K and x_{n_e} = 0.1–0.2. The best-fit synthetic line profile computed using the Monte Carlo code with v_{exp} = 0.55 km s^{-1}, T = 15 K, and x_{n_e} = 0.2 is shown

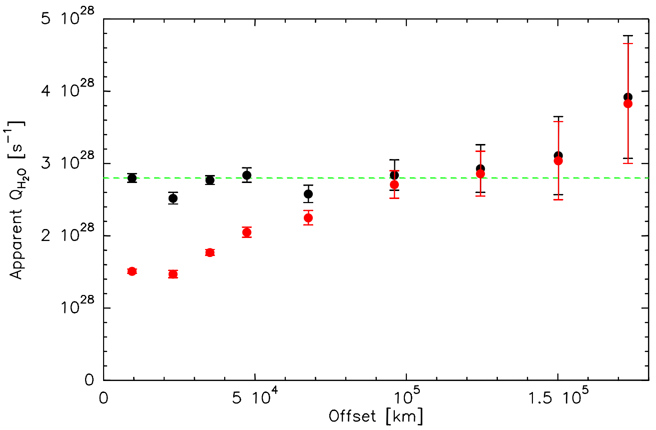

Fig. 6. Apparent water production rates as a function of offset deduced from the 557 GHz map shown in Fig. 4. Isotropic outgassing at $v_{\rm exp}$ = 0.55 km s^{-1}is assumed. Results for x_{n_e} = 0.2 and 1 are shown with black and red symbols, respectively. The dashed horizontal line shows the mean water production rate.

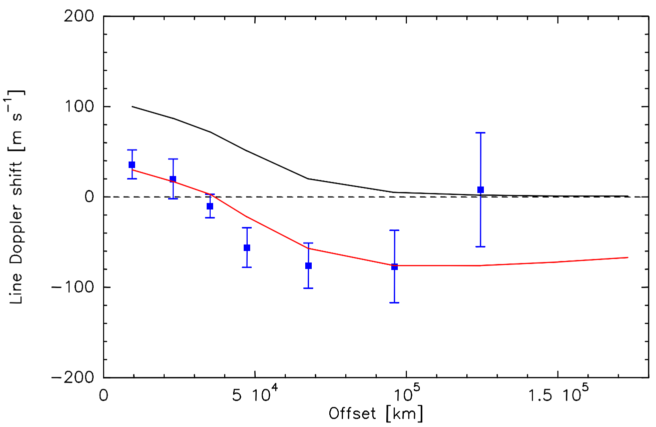

Fig. 7. 557-GHz line Doppler shift as a function of position offset for models considering isotropic outgassing (black line) and anisotropic outgassing concentrated in a ±130° cone (red line). The blue squares indicate the observed line Doppler shift.

in Fig. 1. This model explains satisfactorily the observed line shape. A similar spectrum is obtained with the escape probability method. Both models differ by less than 5% in the calculated line intensities.

We also investigated an anisotropic model with the outgassing restricted to a ±130° cone centered in the direction towards the Sun and expansion velocity of 0.60 km s^{-1}. The anisotropic model provides a better fit to the evolution of the line mean Doppler shift (Fig. 7). This suggests a day/night asymmetry in the comet outgassing which may affect production rate determinations.

The water production rates derived from different lines are in the range 1.7–2.8 × 10^{28} s^{-1}. Those derived from the 1113 and 1669 GHz lines observed on the same day are consistent. A decrease of the comet activity from July 20.9 to 27.8 UT is suggested. However, this needs to be confirmed from a proper consideration of the outgassing asymmetry and possible pointing offsets related to the comet ephemeris.

4. Conclusions

The *Herschel* Space Observatory provides unique new capabilities for the detection of water in the Solar System. HIFI's spectral range and high resolution allowed for the direct detection of several water lines almost simultaneously. High spectral resolution is crucial to resolve the line shape and asymmetries due to self-absorption.

On 20-27 July 2009, comet C/2008 Q3 (Garradd) was observed with HIFI. The high-resolution spectra of HIFI allows us to detect for the first time several rotational water lines in cometary spectra. A water production rate of ∼ 2 × 10^{28} s^{-1} was derived at heliocentric distance of 1.8 AU using radiative transfer numerical codes which include collisional effects and infrared fluorescence by solar radiation.

In future studies, HIFI will be able to detect water isotopes, and determine the D/H ratio in active comets.

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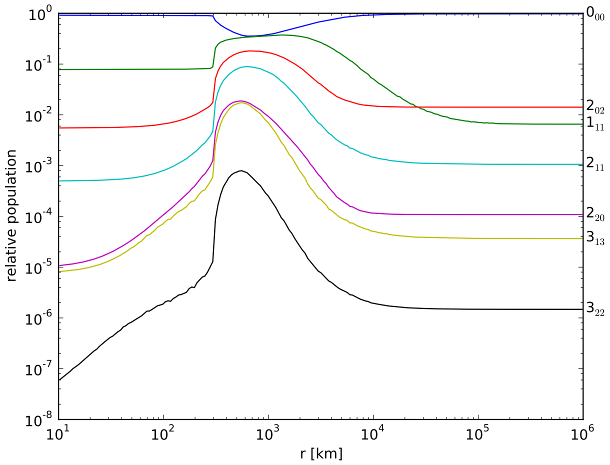

Fig. 5. Level population of para-water as a function of distance to the nucleus for $Q_{H_2O} = 1.7\times10^{28}$ s^{-1}, $r_h = 1.83$ AU, $T = 15$ K, and $x_{n_e} = 0.2$.