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1. Observations and data reduction

The observations of (1) Ceres were carried out using the HIFI[16] instrument aboard the *Herschel Space Observatory*[17]. The ortho 1_{10}-1_{01} H_2O line at 557 GHz ($\lambda = 0.54$ mm) was observed in dual-beam switch (DBS) mode in *HIFI mixers band 1a* (November 2011 and October 2012) or band 1b (March 2013). In the former case, the water line was in the lower side band (LSB) of the Double band receiver, whereas it was in the upper side band (USB) in the latter case. Spectra were acquired with both the Wideband Spectrometer (WBS) and High Resolution Spectrometer (HRS), in the two orthogonal H and V polarizations. Only WBS spectra which have higher signal-to-noise, at the expense of lower spectral resolution (1.1 MHz) are presented. The spectra and maps were processed using the Herschel Interactive Processing Environment (HIPE) with pipeline version 9.0. The resulting Level 2 spectra were exported in the FITS format for subsequent data reduction and analysis using the IRAM GILDAS software package (http://www.iram.fr/IRAMFR/GILDAS).

Because the HIFI receivers are Double band receivers (central frequencies of USB and LSB bands are separated by 11-15 GHz), the continuum measured in the Ceres spectra is equal to twice the thermal radiation from the body at 0.54 mm wavelength. Spectra presented in Fig. 1 and intensities presented in the Extended Data Table 3 refer to recorded H_2O spectra divided by the Ceres thermal radiation.

2. DSMC calculations and radiative transfer

For the simulation of the Ceres' exosphere, we use the Direct Simulation Monte Carlo (DSMC) method[31], where under the effect of mutual collisions and gravity, the evolution of the individual velocity components, the internal energy, and the position coordinates of a large number of "weighted" molecules are monitored. Intermolecular collisions are computed according to the so-called "variable hard sphere" model[31] with internal energy redistribution according to the Larsen–Borgnakke model. A detailed description of these models and parameters is available in Ref. 21.

On the nucleus surface, the flux of emitted particles *F* is given by the analytical expression:

$$F = G exp\left(-\frac{\theta^2}{\theta_0^2}\right)\frac{Q_{H2O}}{\pi R^2}\cos\theta$$

where θ is the solar zenith angle, Q_{H_2O} is the total gas production rate, R is the radius of Ceres, and G is a normalization factor. The active spot is assumed to be at the subsolar point, and its size is specified by θ_0. Calculations show that the depth of the H_2O absorption does not depend strongly on the longitude of the spot with respect to the subsolar point. The surface releases molecules with a half-Maxwellian distribution function at a temperature equal to the nucleus surface temperature T_n. We assume that the surface temperature varies with θ as:

$$T_n = MAX(T_{max}\cos^{0.25}\theta, T_{min})$$

where T_{max}=235 K and T_{min} =168 K.

The molecules striking the surface of Ceres are assumed to be diffusely reflected with complete momentum and energy accommodation. The gravity field is assumed to be spherical with the Ceres gravitational mass M_n= 9.324×10^{20} kg.

To compute the rotational level populations of water molecules we extend our 1D Monte Carlo code[22] to axisymmetric flows. The code that we have elaborated uses the accelerated Monte Carlo algorithm[32]. In the present study we consider the seven lowest rotational levels (which gives nine rotational transitions) of ortho-water and take into account collisions between water molecules, infrared pumping of the vibrational bands by solar radiation, and pumping of the rotational levels by Ceres thermal radiation and 3 K cosmic background. Infrared pumping of the ν_2 vibrational band by Ceres infrared radiation is not significant. The spatial distribution of gas density, velocity and temperature are taken from the gas simulation.

Synthetic spectra were computed with a radiative transfer model which takes into account the Gaussian beam shape (half power beam width of 38.1"). The sub-observer longitude with respect to the longitude of the active spot is a free parameter. To estimate spectra for two active spots (Fig. 2), spectra obtained for the individual spots were added linearly. Indeed, the longitudes of the two active spots considered for the calculations shown in Fig. 2 differ by 100°. Hence, we expect that regions with interaction of flows should not contribute significantly to the spectra.

Synthetic line profiles present both an absorption (negative) component peaking at a negative velocity, and a weaker emission (positive) component, peaking at positive velocity (Fig. 1). The strength of the emission component increases, and that of the absorption component decreases, when the active spot moves towards the limb. Indeed, when the active spot is near the limb, only the rarefied part of the water exosphere is absorbing the Ceres thermal radiation, whereas the densest regions produce increased emission. Water molecules contributing mostly to the absorption of the Ceres thermal radiation are at a few hundred kilometers above the Ceres surface. Their excitation state is intermediate between thermal equilibrium (which becomes less efficient for the 1_{10} and 1_{01} H_2O rotational levels above a few tens of kilometers) and fluorescence equilibrium[22], where essentially the 1_{01} level is populated, hence producing strong absorption.

Due to the contribution of both absorbing and emitting water molecules, the velocity of the center of the absorption feature Δv depends on the position of the active spot with respect to the sub-observer longitude, and is less blue-shifted when the active spot moves towards the limb. For the model parameters of Extended Data Figure 2 ($Q_{H2O} = 10^{26}$ molecules s^{-1}, $\theta_0 = 5°$ corresponding to a 60 km-diameter spot), Δv ranges from -0.65 to -0.45 km s^{-1}, the former value corresponding to the terminal velocity of H_2O molecules along the spot axis (Extended Data Figure 2). These velocities are in good agreement with the measured velocity offsets (Extended Data Table 3).

The width of the observed absorption feature (0.73 ± 0.16 km s^{-1} and 0.68 ± 0.05 km s^{-1} for the 24 October and 6 March spectra, respectively, Extended Data Table 3) is consistent with the width of synthetic line profiles obtained when the sources are near the sub-observer point, 0.76 km s^{-1}, when smoothing to the spectral resolution of the WBS. However, the large line width observed on 11 October (Extended Data Table 3) is unexplained. Detailed data reduction shows that the line width (and velocity offset) changed over the course of the 2 h-long observations. During part of the observations, both the line width and velocity offset were similar to those of the other dates and consistent with computed synthetic line profiles.

Calculations were made with various model input parameters. The strength of the absorption feature does not strongly depend on the size of the spot (for $\theta_0 = 5 - 15$ °) , whereas the strength of the emission feature increases significantly with increasing θ_0. Regarding the dependence with the total water production rate, the strength of the absorption feature is similar for $Q_{H2O} = 10^{26}$ and $Q_{H2O} = 2 \times 10^{26}$ molecules s^{-1}, whereas two times smaller for $Q_{H2O} = 0.3 \times 10^{26}$ molecules s^{-1}. On the other hand, the strength of the emission feature increases with increasing Q_{H2O} in proportion. We also found that the line contrast does not depend much on the assumed surface temperature (in the range 168 − 235 K). The nominal model parameters ($Q_{H2O} = 10^{26}$ molecules s^{-1}, $\theta_0 = 5°$ for each spot) reproduce the spectrum observed on 6 March 2013. The available data set does not allow us better to characterize the active spots.

3. Line polarization

An unexpected aspect of the Ceres data is that the H_2O absorption line appears to be strongly polarized in October 2012 (V/H = 0.40 ± 0.12, 0.38 ± 0.13 for 11 and 24 October, respectively, see Extended Data Table 3, whereas no significant polarization was seen in March 2013 (V/H = 0.74 ± 0.20).

To investigate the possibility of an instrumental artefact, calibration observations of the compact line source AFGL5379 and of the Galactic Centre were obtained with the same instrument settings as the Ceres observations in October 2012, and no polarization is seen for the astronomical sources. Another possibility we investigated is local polarization of the continuum. For a surface that is flat at the size scale of the emission wavelength (0.538 mm for the water ground state line), the continuum emission would be polarized at the limb, with different polarization orientations at the polar and equatorial limb (Fresnel emission)[33]. Indeed, by coincidence the horizontal polarization direction of HIFI was aligned with Ceres' spin axis in both the October 2012 and the March 2013 observations. However, the intensity of the flux decreases towards the limbs when the polarization increases, and it is difficult to obtain a large polarization effect on a strong absorption line in this way. In addition, it would not explain that there is no significant polarization seen in the later observations.

Finally, excitation by anisotropic radiation can yield polarization, as is indeed observed for the fluorescence emission of electronic bands of cometary molecules[34]. This could also be possible for rotational emission (or absorption) of dipolar molecules pumped by infrared radiation in circumstellar envelopes[35]. Generally the polarization from this process is less than seen on Ceres. However, the microwave radiation field acting on the water molecules around Ceres is 2-3 orders of magnitude stronger than the solar radiation that is the usual radiation source acting on water molecules in the solar system. Therefore a stronger polarization in the Ceres case may be plausible. However, since excitation of the water rotational levels from Ceres microwave radiation exceeds other sources of excitation (collisions) and spontaneous decay only in a small region of the inner exosphere, we expect this process to produce little polarization.

Although a more quantitative treatment is beyond the scope of the present paper, the results we have obtained point to this being the first detection of polarization of a water line in observations of a solar system object in the microwave region.

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