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Ortho-To-Para Ratio of Cometary Water and Ammonia

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Abstract. Since the time that the ortho-to-para ratio (OPR) of cometary water was first Determined from observations of Comet Halley, the real meaning of OPR has not been discussed in detail. Here we review the OPRs of water and ammonia and discuss the possibilities that the OPRs were modified in the coma or the nucleus. Our conclusion indicates that the OPRs were not altered after comet nucleus formation, i.e., the OPRs reflect the temperatures in the solar nebula or the pre-solar molecular cloud.

Molecule that have protons at symmetric positions like H_2O, NH_3, and CH_4, can be distinguished into different nuclear spin species ("ortho" and "para", or E, A, and F species) according to the relative orientations of molecular proton spins. The radiative or collisional transitions between ortho and para species are forbidden in the gas phase and the conversion speed between them is probably very slow even in the solid (Mumma et al. 1993; Crovisier 2000). Therefore, even though the rotational distribution of a molecule in the gas phase can be easily changed according to the surrounding environment, the ortho-to-para abundance ratio (OPR) retains the old value. If the OPR was determined in thermal equilibrium, the nuclear spin temperature (Mumma et al. 1987) which is the rotational excitation temperature to reproduce the observed OPR value, is used to infer the temperature condition when the nuclear spins were last equilibrated.

The first determination of the nuclear spin temperature of water in Comet Halley showed about 29 K which was derived from the near infrared observation of the 2.7 μm vibrational bands by the Kuiper Airborne Observatory (Mumma et al. 1987). Three comets were observed in the same vibrational bands after Comet Halley: Comet Wilson with the KAO (Mumma et al. 1993) and Comets Hale-Bopp and Hartley 2 with ISO (Crovisier 2000). Because these water emission bands were hampered by the telluric water vapor, it is difficult to increase the number of samples. The obtained nuclear spin temperature is about 28 — 35 K except for Comet Wilson, which showed > 50 K (this value is considered as the result of cosmic ray damage in the Oort cloud).

Recently, a new technique to derive the OPR of water from ground-based observations has been developed by Dello Russo et al. (2002). They use the vibrational hot band of water. Since the water molecule in the telluric atmosphere is not pumped as much to the vibrational excited levels, the water hot band emissions are not absorbed significantly by the telluric atmosphere. They demonstrated the technique for water OPRs derived from the high-dispersion near infrared spectra of comets (Dello Russo et al. 2002). Their OPR values correspond to spin temperatures of 23 – 26 K.

For another molecule, Kawakita et al. (2001) demonstrated that the OPR of ammonia can be derived from the high-dispersion spectrum of NH_2, which is a photo-dissociation product of ammonia in a comet coma. Based on the same technique, the OPRs of ammonia in four comets have been derived so far (Kawakita et al. 2004). The nuclear spin temperatures of ammonia range from 26 to 32 K in four comets. The nuclear spin temperatures of ammonia are similar to the water values. There are some comets for which the nuclear spin temperature of both ammonia and water were obtained, and the ammonia value is consistent with the water value in each comet. This fact is considered as evidence that the OPRs of water and ammonia were determined in thermal equilibrium (Kawakita et al. 2004). Otherwise, the OPRs of water and ammonia are generally different according to the structures of molecules.

On the other hand, in the case of methane, Gibb et al. (2003) and Weaver et al. (1997) reported the lower limit of the nuclear spin temperature of CH_4 in several comets (25 — 50 K). The nuclear conversion speed of CH_4 may be faster than for water or ammonia and the methane values obtained in the comets were probably affected by the temperature of the nucleus surface (Weaver et al. 1997).

The OPRs of cometary molecules might evolve with time after comet nuclei formed. First, the OPRs might re-equilibrate to the interior temperatures of comet nuclei during their long stay in the Oort cloud or the Kuiper belt. Secondly, the OPRs might re-equilibrated to the surface temperatures of nuclei during sublimation of molecules. Finally, the OPRs might be changed by proton transfer chemical reactions in the inner coma (the nuclear spin temperature reflects the kinetic temperature of the inner coma gas in this case). Here, we check the possibility of these processes based on the present data for water and ammonia molecules (we do not consider methane here).

The nuclear spin temperatures of water and ammonia are about 30 K (except for Comet Wilson as described above) although the orbital periods of the comets vary from only 6 years to several tens of thousands years. Because it is unlikely that the interior temperatures of comet nuclei are the same for all comets, the OPRs didn't equilibrate to their interior temperatures (as pointed out earlier with respect to the OPRs of water by Irvine et al. 2000).

Regarding the second scenario, the observed nuclear spin temperatures of comets are nearly the same and not correlated to the heliocentric distances during their observation. This means that the OPRs did not re-equilibrate to the surface temperatures of the nuclei (the surface temperature depends strongly on the heliocentric distance).

Finally, the possibility of changing the OPR values by the proton transfer reactions in the inner coma is considered. Although the reaction rates of such proton transfer reactions are proportional to the gas density in the inner coma (namely, proportional to gas production rates), there is no correlation between the nuclear spin temperatures and the water production rates during the observations of OPRs. Moreover, the OPRs of ammonia in the inner coma are nearly constant with respect to the nucleocentric distances based on the NH_2 observations. These facts indicate that the OPRs were not altered by chemical reactions. The calculation of inner coma chemistry by Rodgers & Charnley (2002) also supports this conclusion.

Thus, the OPRs of cometary water and ammonia are considered to be fixed in thermal equilibrium, and to be unaltered after the cometary nuclei formed in the solar nebula. Since the nuclear spin temperature must be considered as the physical temperature where the molecules formed or condensed on the cold grain, the OPRs of water and ammonia show that the cometary materials formed or condensed at the temperature of 25 — 35 K in the solar nebula or in the pre-solar molecular cloud. Correlation between the nuclear spin temperature and the molecular abundances should be discussed in future work.

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