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Does nuclear-spin temperature of water molecules in comet coma reflect the formation temperature of the cometary ice?

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The nuclear-spin temperature (T_{spin}) is derived from the ortho-to-para ratio (OPR) of molecules such as H_2 or H_2O, which contains two protons with spin of 1/2; thus, its total spin state can be either 0 (singlet, para) or 1 (triplet, ortho). In the case of H_2O, the OPR is equal to 3 in statistical equilibrium, which is achieved at temperatures above ˜50 K.

T_{spin} of interstellar H_2O molecules has been observed, because they are suggested to be indicators of these molecules' physical and chemical histories. In cometary coma, T_{spin} of H_2O has been derived to be typically ˜30 K. Recently, it was found that there has been a wide range of the observed values of T_{spin} of H_2O from 13.5 K to ˜50 K in interstellar space.

Since nuclear-spin conversion is unlikely to occur for isolated molecules in the gas phase. These values have been implicated as the temperature of cold grains at molecular condensation or formation in a molecular cloud, or in the solar nebula, for example. However, the real meaning of the observed T_{spin} remains a topic of continuing debate. For a proper interpretation of T_{spin} of molecules observed in interstellar space or cometary coma, the correlation between T_{spin} and temperatures of ice at condensation, formation, and desorption needs to be investigated. Even T_{spin} of thermally desorbed H_2O from water ice condensed or formed at low temperature is yet to be experimentally measured.

The present study measured the T_{spin} of H_2O thermally desorbed from pure amorphous solid water (ASW) deposited at 8 K by employing a combination of temperature programmed desorption and resonance-enhanced multiphoton ionization (REMPI) methods. We also produced ASW at 8 K by photolysis of a CH_4/O_2 mixture (photoproduced ASW) for the idea that T_{spin} of H_2O molecules formed at a low temperature relates to the formation environment.

As a result, thermally desorbed H_2O molecules at 150 K from all ice samples prepared at 8 K showed T_{spin} almost at the statistical high-temperature limit (>˜30 K). T_{spin} of desorbed H_2O from vapor-deposited pure ASW is almost at the statistical high-temperature limit (>˜30 K), while its value was almost the same after leaving it for 9 days at 8 K. These results suggest that the T_{spin} of gaseous H_2O molecules thermally desorbed from ice does not necessarily reflect the surface temperature at which H_2O molecules condensed or formed. We discuss the possibility of nuclear-spin conversion of H_2O in water ice.

Keywords: comet, nuclear-spin temperature, ortho-to-para ratio, interstellar molecules, laboratory experiment