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Effect of rare gas matrix confinement on water nuclear spin conversion

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The properties of the nuclear spin isomers of the water molecule are of great interest in astrophysics since the ortho:para ratio (OPR) is assumed to provide insight into the formation mechanism and history of comets as well as other celestial bodies [1,2]. Technological advances are also foreseen for ortho-water enriched samples in magnetic resonance applications, in analogy with hyperpolarisation experiments relying on para-hydrogen. Motivated by these perspectives, technological bottlenecks need to be overcome: the development of an efficient separation methodology and the improvement in storage strategies through a better understanding of their inter-conversion mechanism [3-5]. Recent investigations of the inter-conversion kinetics in isolated water molecules, trapped in rare gas matrices at cryogenic temperatures, may provide important clues of the underlying mechanism [6]. In particular, the inter-conversion rates accelerate dramatically in the heavier water isotopologues H217O and H218O compared the normal water. This may provide insight into the role played by intramolecular (i.e., spin-rotation and spin-spin) as well as intermolecular (i.e., rotation-translation, inter-molecular spin-spin) couplings in the inter-conversion between the ortho and para-water nuclear spin isomers which are at play in the evolution of H2O nuclear spin states in all phases of water including ice.

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Significance statement

First study of water isotopomers nuclear spin conversion confined in rare gas matrix.

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