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Influence of nuclear spin conversion of H2 molecules on the chemistry of the interstellar medium - Experiment and modelling

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Hydrogenated molecules like H2 and H2O exist in several nuclear spin configurations due to the Pauli exclusion principle. These configurations are called ortho (parallel proton spins) and para (antiparallel proton spins). The ortho and para populations have been regularly determined by observations in different regions of space in far UV absorption (Copernicus, FUSE) and in IR and sub-mm emission (ISO, Spitzer, Herschel). The ortho/para ratio (OPR) depends on physico-chemical processes in these environments such as chemical formation, reactive collisions, adsorption and desorption effects of molecules on ice grains and could be a tracer of the history of molecules. In order to interpret the astronomical observations, it is important to confront the observations with the outputs of the more complete astrochemical model. H2 is the most abundant molecule in the interstellar medium and is known to be the main reactant involved in the reaction chain to form hydrogenated molecules (Van Dishoeck et al. 2013), the ortho/para ratio of H2 then plays a role in the chemical evolution of molecules like water (Bron et al. 2016, Dislaire et al. 2012).
For this purpose, we update the Meudon PDR code to take into account selective ortho/para chemistry in the gas and on grains. A gas-phase chemical network which takes into account the ortho/para aspect of the species (like the UGAN network developed by IPAG- Grenoble) is implemented to compare the models in PDRs with and without ortho/para
species. Moreover, the ortho/para ratio of H2 in gas phase could be affected by desorption processes on interstellar grains in cold regions and has to be implemented in the PDR Code. It is then necessary to know the characteristic time for the equilibration of the nuclear spin states of H2 on solid water at low temperature and the relative abundances of the nuclear spin states during desorption. To address these questions, we are currently developing a new laboratory experiment (COSPINU 2) in an ultra-high vacuum chamber to perform in situ measurements of the nuclear spin conversion of H2 deposited on H2O ices using Fourier transform infrared spectroscopy.
First results obtained with the new version of the Meudon PDR code using a chemical network restricted to a few ortho/para species will be presented for the water chemistry.
Measurements reported in the literature on the characteristic time of the nuclear spin conversion of H2 on solid water have shown large discrepancies - ranging from minutes to hours - (Ueta et al. 2016, Chehrouri et al. 2011, Sugimoto and Fukutani. 2011). We will present how the recent results obtained with COSPINU 2 fit into this context.

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