

## NUCLEAR SPIN CONVERSION OF CH<sub>3</sub>D IN SOLID PARAHYDROGEN

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Nuclear spin symmetry conservation provides strong selection rules in radiative transitions, inelastic collisions, and chemical reactions<sup>a</sup> and yet when a molecule is trapped in a cryocrystal at low temperatures, nuclear spin symmetry conversion is observed. In this study we report observations of the nuclear spin conversion (NSC) of monodeuterated methane (CH<sub>3</sub>D) trapped in solid parahydrogen (pH<sub>2</sub>) samples at approximately 1.7 K via high-resolution Fourier transform infrared spectroscopy. CH<sub>3</sub>D doped pH<sub>2</sub> crystals are prepared using a rapid vapor deposition technique to co-deposit room temperature CH<sub>3</sub>D and precooled pH<sub>2</sub> gases onto a cold substrate. This project focuses on the  $\nu_2$  (CD stretch) and  $\nu_6$  (CH<sub>3</sub> rock) modes corresponding to parallel and perpendicular rovibrational bands, respectively. The temporal changes in peak intensities extracted from the IR spectra are characteristic of NSC and can be used to assign peaks originating from the ortho ( $J, K = 0, 0, I = 3/2$ ) and para ( $J, K = 1, 1, I = 1/2$ ) nuclear spin states. Measurements performed on as-deposited and annealed samples show comparable first-order NSC dynamics with an average time constant  $\tau = 311(33)$  min. The measured NSC time constants for a variety of methyl containing molecules, CH<sub>3</sub>F, CH<sub>3</sub>OH, and CH<sub>3</sub>CCH isolated in pH<sub>2</sub> display a range of time constants.<sup>bcd</sup> By systematically studying the NSC of methyl containing molecules trapped in solid pH<sub>2</sub> we hope to better understand how solvation/confinement of the molecule results in a breakdown of the nuclear spin symmetry conservation rules.

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<sup>a</sup>V. Horka-Zelenkova, G. Seyfang, P. Dietiker and M. Quack, *J. Phys. Chem. A*, 2019, 123, 6160-6174.

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<sup>c</sup>Y.-P. Lee, Y.-J. Wu, R. M. Lees, L.-H. Xu and J. T. Hougen, *Science*, 2006, 311, 365-368.

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