NUCLEAR SPIN CONVERSION OF CH₃D IN SOLID PARAHYDROGEN

ANH H. M. NGUYEN, IBRAHIM MUDDASSER, DAVID T. ANDERSON, Department of Chemistry, University of Wyoming, Laramie, WY, USA.

Nuclear spin symmetry conservation provides strong selection rules in radiative transitions, inelastic collisions, and chemical reactions 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 (CH₃D) trapped in solid parahydrogen (pH₂) samples at approximately 1.7 K via high-resolution Fourier transform infrared spectroscopy. CH₃D doped pH₂ crystals are prepared using a rapid vapor deposition technique to co-deposit room temperature CH₃D and precooled pH₂ gases onto a cold substrate. This project focuses on the ν₂ (CD stretch) and ν₀ (CH₃ 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, CH₃F, CH₃OH, and CH₃CCH isolated in pH₂ display a range of time constants. By systematically studying the NSC of methyl containing molecules trapped in solid pH₂ 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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