DIRECT SPECTRAL EVIDENCE OF SINGLE-AXIS ROTATION AND ORTHO-HYDROGEN-ASSISTED NUCLEAR SPIN CONVERSION OF CH_3F IN SOLID PARA-HYDROGEN

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Numerous studies have shown that methane and its various deuterated isotopologs $CH_{4-n}D_n$ $(n = 0 - 4)$ can rotate relatively freely in solid parahydrogen. Less is known, however, of whether methyl groups can also carry out rotation (or internal rotation) in *p*-H_2, and even less is known of whether other large-amplitude motions involving hydrogen atoms (e.g., inversion or H transfer) can occur easily. The present talk, which is part of an attempt to systematically investigate these latter questions in National Chiao Tung University, presents infrared spectra for the nondegenerate (ν_1, ν_2, ν_3) and doubly degenerate (ν_4, ν_5, ν_6) vibrational fundamentals of CH_3F, together with a theoretical analysis strongly suggesting that CH_3F does indeed rotate about its symmetry axis (*a* axis) in *p*-H_2, but does not rotate about axes perpendicular to the symmetry axis. The theoretical analysis makes use of the fact that *a*-axis rotation is expected to give rise: (i) to energy levels of the form $E = AK^2$, (ii) to first-order Coriolis interactions in degenerate vibrational states (E states), and (iii) to different nuclear spin functions for rovibrational A $(K = 0)$ and E $(K = 1$ and $2)$ states. Experimental values for the relatively slow E $\rightarrow$ A conversion rate in *p*-H_2 have also been determined. The results for CH_3F will be compared with our earlier results for CH_3OH.