

PROBING QUANTUM SOLVATION WITH INFRARED SPECTROSCOPY: DOPANT-INDUCED INFRARED ACTIVITY IN SOLID PARAHYDROGEN

ROBERT J. HINDE, *Department of Chemistry, University of Tennessee, Knoxville, TN 37996.*

The infrared absorption spectrum of atom- and molecule-doped solid parahydrogen (pH₂) exhibits weak features near 4160 cm⁻¹ that are absent from the spectrum of pure solid pH₂. These features are associated with the pure vibrational Q₁(0) transitions of pH₂ molecules located near impurities, and represent a rich source of information about the rovibrational dynamics of both molecular impurities and H₂ molecules in doped solid pH₂. Extracting this information could therefore provide insight into the physics of solvation in highly quantum systems. We present the results of diffusion quantum Monte Carlo studies aimed at performing this extraction, and relate the lineshapes of dopant-induced spectral features to the perturbation exerted by the dopant on the vibron bands of the pH₂ crystal.