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

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The infrared absorption spectrum of atom- and molecule-doped solid parahydrogen (pH_2) exhibits weak features near 4160 cm^{-1} that are absent from the spectrum of pure solid pH_2. These features are associated with the pure vibrational $Q_1(0)$ transitions of pH_2 molecules located near impurities, and represent a rich source of information about the rovibrational dynamics of both molecular impurities and H_2 molecules in doped solid pH_2. 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 pH_2 crystal.