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Three-body interactions in liquid and solid hydrogen: Evidence from vibrational spectroscopy ROBERT HINDE, Univ. of Tennessee — In the cryogenic low-density liquid and solid phases of H_2 and D_2 , the H_2 and D_2 molecules retain good rotational and vibrational quantum numbers that characterize their internal degrees of freedom. High-resolution infrared and Raman spectroscopic experiments provide extremely sensitive probes of these degrees of freedom. We present here fully-first-principles calculations of the infrared and Raman spectra of liquid and solid H_2 and D_2 , calculations that employ a high-quality six-dimensional coupled-cluster H_2 - H_2 potential energy surface and quantum Monte Carlo treatments of the single-molecule translational degrees of freedom. The computed spectra agree very well with experimental results once we include three-body interactions among the molecules, interactions which we also compute using coupled-cluster quantum chemical methods. We predict the vibrational spectra of liquid and solid H_2 at several temperatures and densities to provide a framework for interpreting recent experiments designed to search for superfluid behavior in small H_2 droplets. We also present preliminary calculations of the spectra of mixed H_2/D_2 solids that show how positional disorder affects the spectral line shapes in these systems.

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