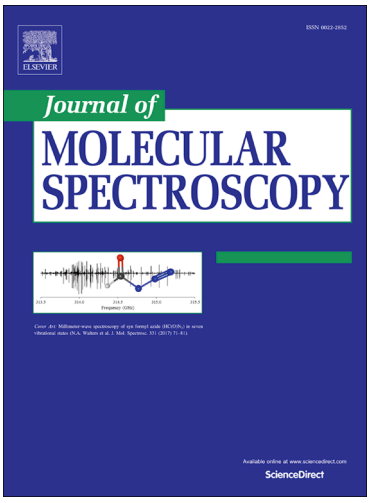

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Infrared Spectroscopy of Propene in Solid para-Hydrogen and Helium Droplets: the Role of Matrix Shifts in the Analysis of Anharmonic Resonances

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Abstract

The infrared spectrum of propene in the CH stretching region is complicated by anharmonic resonance polyads associated with the coupling of CH stretch fundamentals to overtones and combinations of CH_n bends and CC stretches. We report the spectra of propene isolated in both helium nanodroplets (HENDI) and solid *para*-hydrogen (*p*-H_2). Spectral assignments and anharmonic polyad memberships are obtained with a VPT2+K effective Hamiltonian. In the 2800 to 3120 cm^{-1} region, the average differential matrix shift in going from HENDI to *p*-H_2 is ~4.4 cm^{-1} to the red, with a standard deviation of 1.9 cm^{-1}. Moreover, the choice of matrix environment influences the positions and intensity ratios of transitions within the resonance polyads. Two-state interaction models are used to confirm that differential matrix shifts less than 10 cm^{-1} are sufficient to account for the observed differences.

Keywords

para-Hydrogen matrix isolation, Helium nanodroplet isolation, Propene infrared spectroscopy, Anharmonic resonance polyads, Effective Hamiltonian calculations