INFRARED PHOTODISSOCIATION SPECTROSCOPY OF HYDROGEN CLUSTERS

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Highly fluxional ${H_5}^+$ and ${D_5}^+$ ions are generated via arc discharge in a pulsed supersonic expansion source and analyzed by infrared photodissociation spectroscopy. A breakdown in the harmonic approximation because of the delocalized and highly anharmonic shared-proton stretch mode has caused uncertainty with previous attempts by Lee and coworkers to assign the peaks. An improvement in quality of the spectra along with good agreement with frequencies from a new fixed-node diffusive Monte Carlo calculation method help assign the peaks to their corresponding vibrational modes.