

HIGH RESOLUTION INFRARED SPECTROSCOPY OF DIBORANE DISPERSED IN SOLID PARAHYDROGEN

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Few polyatomic molecules have been the subject of more *ab initio* studies than B₂H₆, diborane. The earliest studies were focused on elucidating the structure of its prototypical three-center, two-electron “banana” bonds. Information about the force field and motion of atoms in B₂H₆ can be most directly derived from its vibrational frequencies. However, with eight atoms, high symmetry, and significant vibrational anharmonicities, an exclusively spectroscopic determination of its anharmonic force field is nearly an intractable problem. However, with advances in *ab initio* methods and the development of methods to treat vibrational frequencies and intensities beyond the harmonic approximation, this challenging system is now amenable to deeper understanding. We decided to use parahydrogen (pH₂) matrix isolation infrared spectroscopy to measure the vibrational wavenumbers and intensities of as many infrared absorptions of B₂H₆ as possible in the 800 to 5000 cm⁻¹ region to compare with more recent *ab initio* studies by Ziegler and Rauhut that go beyond the double harmonic approximation.^a Our studies show nearly quantitative agreement between theory and experiment for the allowed infrared vibrational modes in the surveyed region. We devised a scheme to assign peaks in our spectra that then can be compared directly with computational predictions. Indeed, earlier spectroscopic assignments were hampered by not knowing the anharmonic contributions to the measured vibrational frequencies. We are currently investigating the analogous spectra of the B₂D₆ isotopolog and will present our latest findings and comparisons with available theory at the meeting.

^aB. Ziegler, G. Rauhut, *J. Phys. Chem. A* **123**, 3367 (2019).