

Accurate Vibrational–Rotational Parameters and Infrared Intensities of 1-Bromo-1-fluoroethene: A Joint Experimental Analysis and Ab Initio Study

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The medium-resolution gas-phase infrared (IR) spectra of 1-bromo-1-fluoroethene ($\text{BrFC}=\text{CH}_2$, 1,1- $\text{C}_2\text{H}_2\text{BrF}$) were investigated in the range 300–6500 cm^{-1} , and the vibrational analysis led to the assignment of all fundamentals as well as many overtone and combination bands up to three quanta, thus giving an accurate description of its vibrational structure. Integrated band intensity data were determined with high precision from the measurements of their corresponding absorption cross sections. The vibrational analysis was supported by high-level ab initio investigations. CCSD(T) computations accounting for extrapolation to the complete basis set and core correlation effects were employed to accurately determine the molecular structure and harmonic force field. The latter was then coupled to B2PLYP and MP2 computations in order to account for mechanical and electrical anharmonicities. Second-order perturbative vibrational theory was then applied to the thus obtained hybrid force fields to support the experimental assignment of the IR spectra.

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