VAPOR PHASE INFRARED SPECTROSCOPY AND ANHARMONIC AB INITIO FUNDAMENTAL FREQUENCIES OF AMMONIA BORANE

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Ammonia borane (NH_3BH_3) has garnered considerable interest in recent years as a solid state hydrogen storage material for fuel cells. While many papers have been published on its physical and chemical properties, its vapor phase infrared spectrum has not yet been reported. A 1973 paper by Smith, Seshardi, and White [a] reported the matrix isolation spectrum of ammonia borane and this has been used as the infrared spectrum of the fundamental modes of the isolated molecule since. Using a White cell with an optical path set to 68 meters and a room temperature sample, an adequate pressure-pathlength burden was achieved that allowed the moderate resolution spectrum of ammonia borane to be recorded using a Bruker IFS 120HR Fourier transform spectrometer. Additionally, first principles CCSD(T) and MP2 electronic structure calculations of the fundamental mode frequencies were performed. The harmonic frequencies were computed at the CCSD(T) level whereas anharmonic corrections were estimated at the MP2 levels of theory. The molecule has an ethane-like structure (eclipsed conformation) of C_{3v} symmetry with five A_1 symmetry vibrational modes, an inactive A_2 torsional mode and six degenerate E symmetry modes. Of the five A_1 modes, four were observed: sym. B−H stretch at 2298.6 cm^{-1} (2444 cm^{-1} calculated); sym. NH_3 deformation 1281.8 (1271); sym. BH_3 deformation 1176.5 (1182); B−N stretch 610 (593). The B−N stretch mode is very weak. Of the six E symmetry modes, four were observed: asym. N−H stretch 3419.2 (3376); asym. B−H stretch 2407.9 (2369); asym. NH_3 deformation 1613.8 (1531); and the asym. BH_3 deformation 1042.2 (1127).

[a] J. Smith, K.S. Seshadri and D. White, J. Molec. Spectrosc. 45 327 (1973).