THE HIGH-RESOLUTION INFRARED SPECTRUM OF DIBORANE

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We are in the process of recording and analyzing all of the infrared active bands of B_2H_6, the simplest of the hydrogen-bridged borane compounds, with the goal of determining the frequencies of the IR forbidden modes in this very symmetric (D_{2h}) molecule by means of anharmonic interactions. The spectra were obtained on a Bruker 120HR FT spectrometer with a spectral resolution of 0.002 cm^{-1}. The sample contained boron in natural abundance (~80% ^{11}B; 20% ^{10}B) and, therefore, the abundance of $^{11}B_2H_6$, $^{10}B^{11}BH_6$ and $^{11}B_2H_6$ was 64%, 32% and 4% respectively. With the resolution available, the spectra of the two most abundant isotopomers were readily assignable. At this point, the ν_{14} (c-type) and ν_{17} (a-type) bands have been assigned for both the $^{11}B_2H_6$ and $^{11}B^{10}BH_6$ isotopic species and ground state and upper state constants obtained. Both bands exhibit small perturbations. A mixed r_s-r_0 structure for diborane has been obtained.