

## THE HIGH RESOLUTION RAMAN SPECTRA OF THE $\nu_4$ BAND OF DIBORANE

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Diborane is the simplest of the boro-hydride compounds containing a bridge-hydrogen structure. We report here a study of the high resolution gas phase Raman spectrum of the B··B stretching band,  $\nu_4$  ( $A_g$ ), of this interesting near-prolate asymmetric rotor molecule. The sample contained boron in natural abundance, and therefore, the following isotopomers were present:  $^{11}\text{B}_2\text{H}_6$  (64%),  $^{10}\text{B}^{11}\text{BH}_6$  (32%), and  $^{10}\text{B}_2\text{H}_6$  (4%). The symmetry of the two symmetric isotopomers is  $D_{2h}$  while the other species has  $C_{2v}$  symmetry. The isotopic shift for this vibration is large, however, and the spectra of the two most abundant isotopic species were isolated and recorded. Spectra were recorded with the high resolution inverse Raman spectrometer at Madrid, with an instrumental resolution of  $\sim 0.003\text{ cm}^{-1}$  and accuracy of  $\sim 0.001\text{ cm}^{-1}$ . The cell was filled with 10 mbar of diborane and packed in dry ice, and a triple pass configuration was used to enhance the rather weak signal.

The analysis of the spectrum was not straightforward. For this totally isotropic vibration almost all the band intensity is found in the  $^aQ$ -branch since the  $P$ - and  $R$ -branch transitions are 1 to 2 orders of magnitude weaker in intensity and were not observed in this study. As a result, it was not possible to use combination differences to verify the line assignments. Moreover, the vibrational change in the value of the  $A$  rotational constant is small ( $\sim -0.0022\text{ cm}^{-1}$ ); accordingly, the  $^aQ_K$  sub-branches are completely overlapped, and very few isolated lines are found in the spectrum. However, by fitting higher  $J-K_a$  transitions, an estimate of the upper state rotational constants was obtained, which was refined in an iterative process by comparing simulated and observed spectra. For the spectrum of the  $^{11}\text{B}_2\text{H}_6$  species, a slightly improved fit was obtained by invoking a weak resonance with the  $2\nu_{10}$  state. The band centers obtained were  $790.9829(12)\text{ cm}^{-1}$  and  $804.76985(27)\text{ cm}^{-1}$  for  $^{11}\text{B}_2\text{H}_6$  and  $^{10}\text{B}^{11}\text{BH}_6$ , respectively.

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