ANALYSIS OF HIGH-RESOLUTION INFRARED SPECTRA OF $^{11}BF_3$

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We have been engaged in the measurement and analysis of high-resolution infrared spectra of enriched samples of $^{11}BF_3$. The Bruker IFS 120HR Fourier transform spectrometer at the Pacific Northwest National Laboratory (PNNL) facilities has been used to obtain measurements that range in resolution from 0.0015 to 0.0035 cm^{-1} with pathlengths of up to 32 m. The fundamental infrared active transitions and many hot bands, overtones and combination bands have been investigated.

A multiple reflection White cell was used to identify a number of weak states not directly visible from the ground state. One of these states, $3\nu_4$, visible as the hot band $3\nu_4 - 2\nu_4$, is involved in a strong Fermi resonance with the ν_3 fundamental and was directly measured for the first time. A rotational perturbation was found to couple the $2\nu_2$ and $\nu_1 + \nu_4$ vibrations through a $\Delta K = 2$, $\Delta l = -1$ interaction constant. The infrared inactive ν_1 symmetric-stretching mode was characterized by two independent routes, one using the transitions $(110^00^0) - (000^00^0)$, $A_2'' - A_1'$ and $(110^00^0) - (100^00^0)$, $A_2'' - A_1'$, and the other using the transitions $(001^10^0) - (000^00^0)$, $E' - A_1'$ and $(001^10^0) - (100^00^0)$, $E' - A_1'$. Since the rovibrational parameters for the ν_1 state are not equilibrium parameters (not parameters from the bottom of the potential well), they are slightly different for $^{11}BF_3$ and $^{10}BF_3$. Rovibrational constants will be presented for a number of combination/overtone states as well as the Hamiltonian used to derive them.