

ANALYSIS OF HIGH-RESOLUTION INFRARED SPECTRA OF $^{11}\text{BF}_3$ FOR VIBRATIONAL STATES BETWEEN 1600 AND 4300 cm^{-1}

ARTHUR MAKI, 15012 24th Ave. S.E., Mill Creek WA, 98012; TONY MASIELLO, THOMAS A. BLAKE, Pacific Northwest National Laboratory, P.O. Box 999, Mail Stop K8-88, Richland, WA 99352 (PNNL is operated for the US Department of Energy by the Battelle Memorial Institute under contract DE-AC05-76RL01830).

Last year at this Symposium (RX02) we presented spectroscopic measurements and ro-vibrational analysis for vibrational states of $^{11}\text{BF}_3$ below 1600 cm^{-1} . This year we present measurements and analysis for vibrational states of $^{11}\text{BF}_3$ up to 4300 cm^{-1} . Measurements were made of an isotopically enriched sample using a Bruker IFS 120HR Fourier transform spectrometer located at the Pacific Northwest National Laboratory. Spectra were recorded with resolutions ranging from 0.0015 to 0.0035 cm^{-1} and pathlengths up to 32 m. The combination states in the following sets of interacting states have been either observed directly from a transition or determined indirectly by its perturbative effects on observed states: $102^2 0^0$ (3783.85162(8) cm^{-1}), $102^0 0^0$ (3756.085 cm^{-1}), $101^{-1} 3^3$ (3763.14(16) cm^{-1}), $002^0 2^2$ (3830.233(50) cm^{-1}); $200^0 1^1$ (2240.94976(3) cm^{-1}), $120^0 0^0$ (2264.327(10) cm^{-1}); $300^0 1^1$ (3118.20602(6) cm^{-1}), $220^0 0^0$ (3141.688(13) cm^{-1}); $110^0 1^1$ (2050.11053(7) cm^{-1}), $030^0 0^0$ (2081.12683(6) cm^{-1}); $010^0 2^0$ (1652.35840(7) cm^{-1}), $010^0 1^2$ (1652.73764(5) cm^{-1}); $101^1 0^0$ (2336.2009(29) cm^{-1}), $100^0 3^{1,3}$ (2311.519(15) cm^{-1}); $201^1 0^0$ (3216.2986(13) cm^{-1}), $200^0 3^{1,3}$ (3188.650(76) cm^{-1}); $(001^1 1^1)^{0,2}$ (1931.87377(14) cm^{-1}), $(000^0 4^{0,2,4})$ (1921.996(11) cm^{-1}); $(101^1 1^1)^{0,2}$ (2810.69018(8) cm^{-1}), $(100^0 4^{0,2,4})$ (2787.31 cm^{-1}); $(201^1 1^1)^{0,2}$ (3687.1503(10) cm^{-1}). The $003^1 0^0 - 000^0 0^0$ transition was observed near 4310 cm^{-1} and was treated as an unperturbed perpendicular band except for the l -type resonance between the $k = 1, l = 1$ and $k = -1, l = -1$ levels. Effects from other perturbations are thought to be too small to be observed. An infrared forbidden transition $011^1 0^0 - 000^0 0^0, E'' - A'_1$, was also observed near 2140 cm^{-1} . The transitions obey electric dipole allowed selection rules $\Delta k = \pm 2, \Delta l = \mp 1$. Intensity comes from a term in the dipole moment operator that governs the intensity of the $002^2 0^0 - 000^0 0^0$ transition and to a lesser extent from terms that govern the intensity of the $001^1 1^1 - 000^0 0^0$ transition and the fundamentals. A detailed discussion of the interactions and the fit spectroscopic constants will be presented for the vibrational states as well as the Hamiltonian used to derive them.