HIGH RESOLUTION EMISSION SPECTROSCOPY OF THE VIBRATION-ROTATION BANDS OF HBO AND HBS.

G. LI[a], R.S. RAM, R.J. HARGREAVES, *Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK*; P.F. BERNATH, *Department of Chemistry and Biochemistry, Old Dominion University, Norfolk, VA 23529 USA; Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK*; and H. LI, *State Key Lab of Theoretical and Computational Chemistry, Jilin University, Changchun City, China, 130023*.

The vibration-rotation spectra of HBO and HBS have been investigated at high resolution using a Fourier transform spectrometer. The HBO molecules were produced in a high temperature furnace from the reaction of H_2O vapor with boron by heating a mixture of crystalline boron and boron oxide (B_2O_3) at a temperature $\sim$1350°C. The spectra were recorded in the 1100–2200 cm^{-1} and 1700–4000 cm^{-1} wavenumber regions covering the ν_3 and ν_1 fundamentals, respectively. In total 24 vibrational bands involving 30 vibrational levels of $H^{11}BO$ and 12 bands involving 18 levels of $H^{10}BO$ have been rotationally analyzed. After combining the existing microwave and infrared measurements, the absolute term values have been determined for a number of vibrationally-excited states of $H^{11}BO$ and $H^{10}BO$.

The HBS molecules were formed by the reaction of CS_2 and water vapor with crystalline boron at a temperature $\sim$1300°C. The spectra were recorded in the 850–1500 cm^{-1} and 1750–4000 cm^{-1} wavenumber regions covering the ν_3 and ν_1 frequency regions. In total 29 vibrational bands involving 33 vibrationally-excited levels of $H^{11}BS$ and 9 bands involving 12 vibrational levels of $H^{10}BS$ have been analyzed. The fitted spectroscopic parameters agree very well with the results of our *ab initio* calculations. *L*-resonance interactions observed between the 02^00 (Σ) and 02^20 (Δ) levels of HBO and HBS were analyzed using a 2×2 matrix to yield deperturbed constants.

[a]Current address: Harvard-Smithsonian Center for Astrophysics, Atomic and Molecular Physics Division, MS#50, 60 Garden St., Cambridge, MA, 02138, USA.