FOURIER TRANSFORM INFRARED EMISSION SPECTROSCOPY AND AB INITIO STUDY OF HBO AND BO

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The Fourier-transform infrared emission spectra of HBO and BO were recorded using a Bruker IFS-125HR Fourier transform spectrometer. HBO molecules were synthesized using a high temperature tube furnace at 1450°C. Our spectra of the HBO molecule in the $1200 - 4000$ cm^{-1} region contain the v_1 and v_3 fundamental vibrational modes plus numerous hot bands. An accurate potential energy surface using the MRCI method with correlation consistent core-valence basis sets aug-cc-PCVnZ (n=3, 4, 5) is being calculated and a vibrational configuration interaction (VCI) calculation based on this surface will be performed to assist in the assignment of the HBO hot bands. BO molecules were produced by applying a DC discharge to the furnace containing HBO. Our spectrum of BO in the $1200 - 2100$ cm^{-1} region contains the fundamental bands of both isotopic species, ^{11}BO, ^{10}BO, and one hot band of the main isotopologue ^{11}BO. The fundamental band of ^{11}BO contains 95 lines roughly equally distributed between the P and R branches. A combined least-squares fit with ground state microwave data was performed to determine the spectroscopic constants. Further results on this ongoing project will be presented.