FOURIER TRANSFORM INFRARED EMISSION SPECTRA OF BeH/BeD AND BeH_2/BeD_2

A. SHAYESTEH, K. TERESZCHUK, and P. F. BERNATH, *Department of Chemistry, University of Waterloo, Waterloo, ON, N2L 3G1, Canada*; R. COLIN, *Laboratoire de Chimie Physique Moleculaire, Universite Libre de Bruxelles, C.P. 160/09, 50 av. F.D. Roosevelt, 1050 Brussels, Belgium*.

We have recorded the first vibration-rotation spectra of gaseous BeH/BeD and BeH_2/BeD_2 in emission using a furnace-discharge source. The molecules were generated at 1500°C and 333 mA discharge current with beryllium and a mixture of helium and hydrogen or deuterium gases. The recorded spectra contained several emission bands, as well as the absorption of atmospheric H_2O and CO_2. The highest signal-to-noise ratio for BeH lines was about 350. The vibrational bands v=1-0 to v=4-3 of BeH/BeD were observed in the spectra. The bands were rotationally analyzed, and the spectroscopic constants for v=0 to 4 levels of BeH and BeD, as well as the Dunham constants and the Born-Oppenheimer breakdown constants, were obtained. The antisymmetric stretching mode (ν_3) of BeH_2/BeD_2 and several hot bands involving ν_1, ν_2 and ν_3 were found and rotationally analyzed to yield the spectroscopic constants. For BeH and BeD, we determined the equilibrium rotational constants (B_e) to be 10.31959(3) cm^{-1} and 5.68829(2) cm^{-1}, respectively, while the equilibrium vibrational constants (ω_e) are 2061.416(3) cm^{-1} and 1529.956(3) cm^{-1}. We also determined B_e for BeH_2 to be 4.75366(2) cm^{-1}. Using the B_e values of BeH and BeH_2, the equilibrium Be-H bond distances (R_e) were calculated for BeH and BeH_2 to be 1.342436(2) Å and 1.326407(3) Å, respectively.