

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

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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.