IONIZATION ENERGY MEASUREMENTS AND SPECTROSCOPY OF THE BeOBe MOLECULE

J. M. MERRITT, V. E. BONDYBEY, and M. C. HEAVEN, *Department of Chemistry, Emory University, Atlanta, GA 30322*.

The Be_2O^+ cation was observed some fifty years ago in mass spectroscopic studies of vapors above heated beryllium oxide. From temperature and electron energy dependence of the ion abundance, Theard and Hildebrand (JCP 41, 3416 (1964)) deduced a value of -8±10 kcal/mole for the enthalpy of formation of neutral Be_2O in the gas phase. Such strong bonding of the second Be atom to BeO was, at the time, somewhat surprising given the initial view of a double bond in BeO, such that Be donates two electrons and the O atom would have a filled valence shell. More recent electronic structure calculations have shown that the bonding of BeO is intermediate between a single and double bond and thus can form a strong bond with a second Be atom. Calculations have also predicted that the ground electronic state of BeOBe is multi-reference in nature, thus accurate characterization of this molecule can be used to benchmark high-level multiconfigurational theoretical methods.

The electronic structure of the BeOBe molecule has been investigated using laser induced fluorescence (LIF) and resonance enhanced multiphoton ionization (REMPI) tenchniques in the 27000-33000 cm^{-1} range. The BeOBe molecule has been stabilized in the gas phase using pulsed laser vaporization of Beryllium metal, and subsequent free jet expansion into vacuum. Vibrational progressions assigned to excitations of the symmetric and antisymmetric stretches in the excited state are observed and analyzed. Rotationally resolved spectra are found to exhibit nuclear spin statistics which confirm the ground electronic state of BeOBe has $^1\Sigma_g^+$ symmetry. A BeO bond length of 1.399(3) Angstrom has been determined for the ground state. Photoionization efficiency curves were also recorded to determine an accurate ionization energy for BeOBe of 8.12(1) eV. Comparisons with electronic structure calculations will also be presented.