THE IONIZATION ENERGY OF Be_2, AND SPECTROSCOPIC CHARACTERIZATION OF THE $(1)^3\Sigma_u^+$, $(2)^3\Pi_g$, and $(3)^3\Pi_g$ STATES

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Beryllium dimer is formed by pulsed laser ablation of Be metal in the presence of helium carrier gas, followed by free jet expansion into vacuum. Its low-lying electronic states are investigated by laser induced fluorescence (LIF) and resonance enhanced multiphoton ionization (REMPI) techniques. Differences between the 1+1 REMPI and LIF spectra of the $B^1\Sigma_u^+(v) \leftarrow X^1\Sigma_g^+(v = 0)$ bands observed in the ionization continuum are due to resonances with Rydberg series correlating with vibrations of the ion. Photoionization efficiency (PIE) measurements yield an accurate value of 7.418(5) eV for the ionization energy (IE), in good agreement with the results from multi-reference configuration interaction (MRCI) theory. By fitting the Rydberg progressions and making use of this IE, the Be_2^+ vibrational frequency and binding energy of 498(20) and 16076(40) cm^{-1}, respectively, are determined, again in agreement with MRCI calculations. Rotationally resolved spectra of the $(2)^3\Pi_g \leftarrow (1)^3\Sigma_u^+$ and $(3)^3\Pi_g \leftarrow (1)^3\Sigma_u^+$ Be_2 transitions provide further experimental benchmarks for ab initio calculations. PIE measurements also yield an accurate value for the $(1)^3\Sigma_u^+ \leftrightarrow X^1\Sigma_g^+$ interval. Rotationally resolved spectra for the $A^1\Pi_u(v = 15 - 18) \leftarrow X^1\Sigma_g^+(v = 0)$ transitions in Be_2 have also been observed allowing for a more precise determination of the $A^1\Pi_u$ potential energy surface. New MRCI calculations are described in order to refine the theoretical IE as well as to quantify the role of spin-orbit coupling in the $(2)^3\Pi_g$ and $(3)^3\Pi_g$ states.