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Spectroscopic characterization of the ionization energy, $^3\Sigma_u^+$, $(2)^3\Pi_g$, and $(3)^3\Pi_g$ states of Be_2 JEREMY MERRITT, Department of Chemistry, Emory University, Atlanta GA 30322, VLADIMIR BONDYBEY, Institut fur Physikalische and Theoretische Chemie der TU Munchen, Garching, Germany, MICHAEL HEAVEN, Department of Chemistry, Emory University, Atlanta GA 30322 — Low-lying electronic states of beryllium dimer are investigated by laser induced fluorescence (LIF) and resonance enhanced multiphoton ionization (REMPI) spectroscopies. Be_2 is formed by pulsed laser ablation and free jet expansion into vacuum. Comparing 1+1 REMPI and LIF spectra for the $X^1\Sigma_g^+$ (v=0) -> $B^1\Sigma_u^+$(v) bands we find significant perturbations in the REMPI spectra, which are interpreted as autoionizing resonances in the ionization continuum. Photoionization efficiency (PIE) measurements yield an accurate value for the ionization energy, namely 7.40 eV, which is considerably larger than previous theoretical predictions. New CASSCF/MRCI calculations are presented which accurately reproduce the experimental IP. Rotationally resolved spectra for the $(1)^3\Sigma_u^+ -> (2)^3\Pi_g$ and $(1)^3\Sigma_u^+ -> (3)^3\Pi_g$ band systems of Be_2 have also been measured for the first time providing further experimental benchmarks for recent ab initio calculations. PIE measurements are also used to accurately determine the $X^1\Sigma_g^+ <-> (1)^3\Sigma_u^+$ interval.

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