SPECTROSCOPIC CHARACTERIZATION OF Be₂⁺ X²Σₜ⁺ AND THE IONIZATION ENERGY OF Be₂

I. O. ANTONOV, B. J. BARKER, V. E. BONDYBEY, M. C. HEAVEN, Department of Chemistry, Emory University, Atlanta, GA 30322.

Rotationally resolved spectra for Be₂⁺ were recorded with PFI-ZEKE technique. Vibrational levels v⁺=0-6 were observed. The symmetry of the ground state was determined as ²Σₜ⁺. The bond energy was found to be Dₑ⁺ = 16348(5) cm⁻¹ and the equilibrium distance Rₑ⁺ = 2.211(8) Å. The ionization energy for Be₂ was refined at 59824(2) cm⁻¹. Comparisons with high-level theoretical calculations indicate that the bonding in Be₂⁺ is adequately described by MRDCI calculations with moderately large basis sets.