EXPERIMENTAL AND THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE AND BONDING OF THE BeAl MOLECULE

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The electronic structure of the BeAl molecule formed by laser ablation of a beryllium-aluminum alloy and cooled by free jet expansion was investigated by laser induced fluorescence (LIF) and resonance enhanced multiphoton ionization (REMPI) spectroscopy. In agreement with recent ab initio studies the molecule has a $^2\Pi_{1/2}$ ground state, and transitions to two low lying electronic states $(2)^2\Pi_{1/2}(v) \leftarrow X^2\Pi_{1/2}(v=0)$ and $(1)^2\Delta(v) \leftarrow X^2\Pi_{1/2}(v=0)$ are observed and rotationally analyzed. [Ribas et al. Chem. Phys. **330** (2006) 295]. Additional band systems are observed in the near ultraviolet, 28000-32000 cm^{-1} region, one of them exhibiting an unusual pattern of vibrational levels resulting from an avoided crossing of the $(4)^2\Sigma_{1/2}$ and $(5)^2\Sigma_{1/2}$ electronic states. The ionization energy of 48124(80) cm^{-1} is determined for BeAl from photoionization efficiency (PIE) curves. Fine structure in the PIE curve is attributed to resonances with Rydberg series correlating with vibrational states of the $BeAl^+$ ion, and in good agreement with theory a vibrational frequency of 240(20) cm^{-1} is determined for $BeAl^+$. To interpret the UV spectra, new multi-reference configuration interaction (MRCI) calculations are carried out, and also the influence of spin-orbit coupling is investigated.