

MOLECULAR BEAM STUDY of AlND₃ COMPLEX: STRUCTURE, VIBRATIONAL FREQUENCIES, and IONIZATION POTENTIAL.

ZYGMUNT J. JAKUBEK and BENOIT SIMARD, *Stacie Institute for Molecular Sciences, National Research Council of Canada, Ottawa, ON, Canada K1A 0R6.*

AlND₃ complexes are produced in a Smalley-type laser ablation source and probed by resonance 2-photon ionization technique. In the range 18500-23500 cm⁻¹, several vibronic bands for five isotopomers, Al¹⁴NH₃, Al¹⁵NH₃, Al¹⁴ND₃, Al¹⁴NHD₂, and Al¹⁴NH₂D, are observed. Only the AlND₃ complex is studied in detail. The spectrum is assigned to the $\tilde{B}^2A_1-\tilde{X}^2E$ electronic transition, with the \tilde{B}^2A_1 and \tilde{X}^2E states correlating to the Al(4s)+ND₃(¹A₁') and Al(3p)+ND₃(¹A₁') asymptotes, respectively. The AlND₃ complex has approximate C_{3v} symmetry in both states. The origin band of the $\tilde{B}^2A_1-\tilde{X}^2E$ transition is located at 18532.5±1.0 cm⁻¹. The spin-orbit splitting of the ground state is determined to be 55.7 ± 0.4 cm⁻¹. Frequencies of the ν_3 (Al-ND₃ stretch), ν_4 (AlN-D₃ symmetric stretch), and ν_6 (Al-ND₃ bend) vibrations in the \tilde{B}^2A_1 state are measured to be 315.7 ± 0.6 cm⁻¹, 2657±1 cm⁻¹, and 411±1 cm⁻¹, respectively. Partially resolved rotational structure of some of the bands is observed and analyzed. The adiabatic ionization potential of the AlND₃ complex is measured by photoionization efficiency technique as equal 39710±10 cm⁻¹. Rydberg series converging to various levels of the Al⁺-ND₃ stretching mode of the AlND₃⁺ cation are observed. The ν_3^+ frequency is determined to be 322 cm⁻¹. The structure determination of the neutral and monpositive complex and assignment of vibrational modes are aided by *ab initio* calculation.