MOLECULAR BEAM STUDY of $AlND_3$ COMPLEX: STRUCTURE, VIBRATIONAL FREQUENCIES, and IONIZATION POTENTIAL.

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$AlND_3$ 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, $Al^{14}NH_3$, $Al^{15}NH_3$, $Al^{14}ND_3$, $Al^{14}NHD_2$, and $Al^{14}NH_2D$, are observed. Only the $AlND_3$ 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(4*s*)+$ND_3(^1A_1')$ and Al(3*p*)+$ND_3(^1A_1')$ asymptotes, respectively. The $AlND_3$ 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-ND_3 stretch), ν_4 (AlN-D_3 symmetric stretch), and ν_6 (Al-ND_3 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 $AlND_3$ complex is measured by photoionization efficiency technique as equal 39710±10 cm^{-1}. Rydberg series converging to various levels of the Al^+-ND_3 stretching mode of the $AlND_3^+$ cation are observed. The ν_3^+ frequency is determined to be 322 cm^{-1}. The structure determination of the neutral and monopositive complex and assignment of vibrational modes are aided by $ab\,initio$ calculation.