INFRARED SPECTROSCOPY OF JET COOLED $ND_2H_2^+$ MOLECULAR IONS: THE SYMMETRIC AND ANTISYMMETRIC NH STRETCH MODES

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Rovibrational progressions in the symmetric (v_6) and antisymmetric (v_1) NH stretching modes of the $ND_2H_2^+$ molecular ion are observed for the first time, exploiting the i) high ion density and ii) high resolution capabilities of our slit jet discharge infrared spectrometer. These isotopomeric ions are generated by striking a modulated (50 KHz) electrical discharge in a mixture of $ND_3/H_2O/H_2$ gases, achieving a modulated ion density suitable for time-gated, lock-in detection in the throat of a long path slit-jet expansion. Assignment of both b-type and c-type bands enables high accuracy determination of the rotational constants (A''=4.85598(19), B''=3.96811(11), and C''=3.44661(40) cm^{-1}), with band origins for v_1 and v_6 modes determined to be 3297.54367(34) and 3337.90456(33) cm^{-1}, respectively. The results prove to be in good agreement with anharmonically corrected predictions from ab initio quartic force fields of Martin and Lee[a].

[a] Jan. M. L. Martin and Timothy J. Lee, Chem. Phys. Lett. 258, 129 (1996)