The C_2N_2 C^1B_u - $X^1\Sigma_g^+$ Transition: Assignment of the Excited Electronic State, Its Origin and Vibrational Frequencies

Joshua B. Halpern and Yuhui Huang
Department of Chemistry, Howard University, Washington, DC 20059

C_2N_2 has been detected in Titan's atmosphere and may also be present in comets. A new analysis is presented for the VUV C_2N_2 C^1B_u - $X^1\Sigma_g^+$ transition. Contrary to previous studies this is shown to be a linear to bent transition with a trans-bent C^1B_u excited electronic state. The electronic origin is at 59,848 cm^1, about 550 cm^1 lower than previously thought [1]. Vibrational bands between 170 and 145 nm are assigned. The C^1B_u symmetric CN stretching frequency, ν_1, is as previously noted 2050 $\pm$ 20 cm^1 [1]. It has been possible to assign four of the five other vibrational frequencies. The symmetric CC stretching frequency, ν_2, is 926 $\pm$ 20 cm^1. The trans-bending vibrational frequency, ν_3, is 532 $\pm$ 10 cm^1, the torsional bending frequency, ν_4, is 110 $\pm$ 10 cm-1^1 and the cis bending frequency, ν_6, is 140 $\pm$ 10 cm^1. Anharmonicities have also been determined for the various vibrational modes.

References:

. S. Bell, G. J. Cartwright, G. Fish, D. O. O'Hare, R. K. Ritchie, A. D. Walsh and P. A. Warsop, J. Mol. Spectrosc., 30 (1969) 162.

Acknowledgments:

This work was supported by a grant from the National Aeronautics and Space Administration