THE C_2N_2 C^1B_u - $X^1\Sigma_g^+$ TRANSITION: ASSIGNMENT OF THE EXCITED ELECTRONIC STATE, ITS ORIGIN AND VIBRATIONAL FREQUENCIES

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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 [a]. 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}. 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 $cm^{-1}$and the cis bending frequency, ν_6, is 140 $\pm$ 10 cm^{-1}. Anharmonicities have also been determined for the various vibrational modes.

[a] S. Bell, et al., Mol. Spectrosc. 30 (1969) 162