TIME RESOLVED INFRARED DIODE LASER SPECTROSCOPY OF THE ν_1 BAND OF CONO PRODUCED BY THE ULTRAVIOLET PHOTOLYSIS OF Co(CO)₃NO

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Rovibrational transitions of the ν_1 band (N-O stretch) of CoNO produced by the ultraviolet photolysis of Co(CO)₃NO were observed in the 1775-1800 cm⁻¹ region by time resolved infrared diode laser spectroscopy. In total, 35 absorption lines were assigned to the ν_1 fundamental band, and their J quantum numbers were determined by a simultaneous analysis with millimeter-wave spectroscopy^a. Hotband lines originated from the ν_2 (bending), $2\nu_2$, and ν_3 (Co-N stretch) vibrationally excited states were also observed. Molecular constants, including the band origin ν_0 1796.22371(49) cm⁻¹, the rotational constant B_0 4669.7578(29) MHz, and the vibration rotation constant α_1 31.325(28) MHz, were derived from the observed spectrum. The equilibrium rotational constant B_e (4676.949(51) MHz) was determined with the α_1 value derived in the present study and the α_2 and α_3 values reported by the millimeter-wave spectroscopy^a. The equilibrium bond-length $r_{\text{Co-N}}$ was calculated to be 1.583 Å assuming $r_{\text{NO}} = 1.182$ Å by *ab initio* calculation^b. The absorption lines for the $\nu_1 + \nu_2 \leftarrow \nu_2$ and $\nu_1 + 2\nu_2 \leftarrow 2\nu_2$ bands were split into two components due to the $\Delta l=2$ interaction. The electronic ground state of CoNO was confirmed to be ¹ \Sigma⁺ by this infrared study as reported by our previous millimeter-wave spectroscopy^a.

^aTanaka et al, the 59th OSU International Symposium on Molecular Spectroscopy (2004).

^bM. Zhou and L. Andrews, J. Phys. Chem. A 104, 3915 (2000).