

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

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Rovibrational transitions of the ν_1 band (C-O stretch) of the CoCO radical produced by the ultraviolet photolysis of Co(CO)₃NO were observed in 1949-1991 cm⁻¹ region by the time resolved infrared diode laser spectroscopy. The electronic ground state was confirmed to be $X^2\Delta_i$ by the analysis as predicted by the density functional theory calculation.^a More than 140 absorption lines were assigned to the $\Omega = 5/2$ spin component of the ν_1 fundamental band in the $X^2\Delta_i$ state. No lines of the $\Omega = 3/2$ component were observed due to the large spin-orbit interaction constant A (-500 cm⁻¹). Effective molecular constants for the $\Omega = 5/2$ spin component, including the band origin ν_0 and the rotational constant B , were derived from observed transitions. Hot band lines originated from the ν_2 (Co-C-O bending) and ν_3 (Co-C stretch) vibrational excited states were observed. Absorption lines for the ν_2 hot band were split into two components because of the vibronic interaction between the ν_2 state and other nearby electronic excited states. The effective equilibrium rotational constant B_e and the vibration rotation constants, α_1 , α_2 and α_3 were determined from the analysis of the fundamental band and hot bands.

^aM. Zhou, L. Andrews, *J. Phys. Chem. A* **102**, 10250 (1998)