MILLIMETER-WAVE SPECTROSCOPY OF CoNO IN THE GROUND ($X^1\Sigma$) STATE

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Infrared spectrum of CoNO has been measured in low temperature Ar matrix and the ν_1 and ν_3 band origins were reported to be 1761.0 and 620.1 cm^{-1} respectively. [a] Recent DFT calculations suggested that the linear form ($X^1\Sigma$) and bent form (X^3A') of CoNO have almost the same energies.[a] In the present study, the pure rotational spectrum of CoNO generated in a supersonic jet expansion by ultraviolet photolysis of $Co(CO)_3NO$ was observed in the millimeter-wave region. This is the first observation of the rotationally resolved spectrum of the transition metal nitrosyl in the gas phase. Seven rotational transitions (from $J = 6 - 5$ to $12 - 11$) were measured in the frequency region of $56 - 112$ GHz. Each rotational transition was split into $8-11$ components due to hyperfine interaction of the Co ($I = 7/2$) nucleus. The spectrum was analyzed to determine molecular constants, including the rotational constant *B*, centrifugal distortion constant *D*, nuclear quadrupole interaction constant *eQq*, and nuclear spin-rotation interaction constant C_I. From the observed spectral pattern, it is confirmed that CoNO has a linear structure and the electronic ground state is $^1\Sigma$. The Co−N bond length was calculated to be 1.588 Å from the rotational constant, which is by 0.1 Å shorter than the Co−C bond length of CoCO. Measurement of rotational transitions in the ν_2 vibrationally excited state is in progress.

[a] Mingfei Zhou and Lester Andrews, *J. Phys. Chem.*, **A104,** 3915 (2000)