

THE PURE ROTATIONAL SPECTRUM OF FeNC ($X^6\Delta_i$): IT HAD TO BE THERE!

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The pure rotational spectrum of FeNC has been measured in its ground electronic and vibrational state using direct absorption methods. The radical was synthesized from gas-phase $\text{Fe}(\text{CO})_5$ and $(\text{CN})_2$ in an AC discharge and could also be produced using metal vapor and $(\text{CN})_2$ in a Broida oven. Eighteen rotational transitions have been recorded in the frequency range 150-505 GHz, many containing all six spin components. In addition, Renner-Teller effects have been observed for the excited vibrational ν_2 bending mode. The $\Omega = 3/2, 1/2,$ and $-1/2$ spin states appear to exhibit significant Λ -doubling. Preliminary results from isotopic substitution of ^{54}Fe , observed in natural abundance, indicate that the ground state structure is likely the linear isocyanide with a rotational constant near 4.1 GHz. Substitution of ^{13}C is underway and will yield a definitive structure. The data are currently being analyzed with a case (a) Hamiltonian, and spectroscopic constants for rotation, fine structure, and Λ -doubling are being established.