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 $Fe(CO)_5$ and $(CN)_2$ in an AC discharge and could also be produced using metal vapor and $(CN)_2$ 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 v_2 bending mode. The Ω = 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.