DISPERSED FLUORESCENCE SPECTRUM OF MATRIX ISOLATED FeCN

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A fluorescence spectrum attributed to FeCN or FeNC was observed from matrices prepared by two different techniques. In the first series of experiments a mixture of $Fe(CO)_5$ diluted in Ar was passed through a microwave discharge, and the products were deposited onto a cold mirror held at 10 K. Trace quantities of nitrogen-containing impurities were present in the mixture. Laser excitation of the matrix at 355 nm yielded the CN B-X and A-X emission systems, along with a new progression of bands that spanned the range from 464 nm to 723 nm. The new bands were assigned to FeCN or FeNC on the basis that they were also observed in the matrices prepared by laser vaporizing an iron target in a flowing BrCN/Ar mixture. Assuming that 355 nm light excites the origin band of the new transition, the dispersed fluorescence spectrum yields lower state vibrational constants of ω_e=2019.9 cm^{-1} and $\omega_e x_e$=11.2 cm^{-1}. These values are consistent with a progression of the CN stretch mode. The upper state emitted with a lifetime of 550 ± 50 ns.

Preliminary electronic structure calcualtions (DFT) yield ground state vibrational constants for the CN stretch of 2126 and 2018 cm^{-1} for FeCN and FeNC, respectively. Isotopic substitution experiments and further calculations are in progress to determine the isomer and the identity of the electronically excited state.