THE PURE ROTATIONAL SPECTRUM OF THE MOLECULAR ION FeO^+ ($X^6\Sigma^+$)

D. T. HALFEN and L. M. ZIURYS, *Department of Chemistry, Department of Astronomy, and Steward Observatory, University of Arizona, Tucson, AZ, 85721.*

The pure rotational spectrum of the FeO^+ ($X^6\Sigma^+$) molecular ion has been measured using millimeter-wave direct absorption techniques incorporating velocity modulation methods. This work is the first measurement of high-resolution spectra for this ion. This species was created by the reaction of gas-phase $Fe(CO)_5$ and N_2O in the presence of argon carrier gas and an AC glow discharge. The strengths of the signals due to FeO^+ were over 50 times less intense than those of FeO. Nine rotational transitions were measured in the frequency range of 300 to 544 GHz. Each transition was found to be split into six fine-structure components, a result of spin-rotation and spin-spin interactions, over a range of 4 GHz. The data have been fit with a case (b) Hamiltonian, and rotational and fine-structure constants were determined. The bond length in FeO^+ appears to be similar to its neutral counterpart (1.641 Å vs. 1.619 Å), not unexpected given that the two electron configurations differ by a single δ electron. FeO^+ is a powerful catalytic oxidant in the gas phase, and has been shown to convert methane into methanol.