

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

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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 $\text{Fe}(\text{CO})_5$ 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.