COMPLETING THE STUDY OF THE 3d FLUORIDES: PURE ROTATIONAL SPECTROSCOPY OF ZnF ($X^2\Sigma^+$)

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Although the 3d transition metal fluorides have been studied by many spectroscopic techniques, ZnF has never been investigated by gas-phase methods. In order to complete the 3d series, the pure rotational spectrum of ZnF has been recorded. This radical was synthesized by the reaction of zinc vapor with a mixture of 10% F_2 in helium. Transitions arising from five isotopomers of ZnF were measured in the frequency range 175 - 530 GHz in the ground (v=0) and excited vibrational (v=1,2,3) states. The spectral pattern clearly indicates that the ground electronic state of ZnF is $^2\Sigma^+$. Fluorine hyperfine interactions were resolved in three isotopomers and hyperfine structure arising from the ^{67}Zn nucleus was present for ^{67}ZnF. The spectra were analyzed with a case (b) Hamiltonian, and rotational, spin, and hyperfine constants were determined. Equilibrium parameters were also established, and the dissociation energy D_E of 3.123 eV for ZnF was found to be in close agreement with that predicted by Harrison, Field, and Jarrold. The bond length of ZnF is calculated to be 1.767657(21) Å. Based on the hyperfine constants, it is estimated that the unpaired electron is in a σ orbital that is approximately 90% Zn^+ and 10% F in nature.