

The EPR Zero-Field Splitting D and its Pressure and Temperature Dependence for Trigonal Mn^{2+} Centers in $[\text{Zn}(\text{H}_2\text{O})_6](\text{BF}_4)_2:\text{Mn}^{2+}$ Crystal

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The EPR zero-field splitting D ($= b_2^0$) and its pressure and temperature dependence for trigonal Mn^{2+} centers in low and room temperature phases in $[\text{Zn}(\text{H}_2\text{O})_6](\text{BF}_4)_2 : \text{Mn}^{2+}$ crystal are studied by a high-order perturbation formula based on the dominant spin-orbit coupling mechanism. From the studies, the local trigonal distortion angles, the local angular compressibilities and the local angular thermal expansion coefficients for Mn^{2+} centers in both phases of the $[\text{Zn}(\text{H}_2\text{O})_6](\text{BF}_4)_2$ crystal are estimated. The results are discussed.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-Field Theory; Defect Structure and Properties; Mn^{2+} ; $[\text{Zn}(\text{H}_2\text{O})_6](\text{BF}_4)_2$.