Theoretical Investigations of the Local Structure and the EPR Parameters of Mn^{4+} in LiF:U:Mn Crystal

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The local structure and the EPR parameters (zero-field splitting D, g factors $g_{\parallel}$ and $g_{\perp}$ and hyperfine structure constants $A_{\parallel}$ and $A_{\perp}$) of Mn^{4+} in LiF:U:Mn crystal have theoretically been investigated by using the perturbation formulas of the EPR parameters for a $3d^3$ ion in trigonally distorted octahedra. In this trigonal Mn^{4+} center, three U^{6+} ions locate on (1,1,0), (1,0,1) and (0,1,1) sites, each surrounded by six O^{2-} ions. Thus, the studied system is characterized as the Mn^{4+} associated with one host F^- triangle, one O^{2-} triangle and an additional equivalent F'^- triangle containing the three U^{6+} ions, i.e. an $[MnF_3O_3F'_3]^{8-}$ cluster. The central Mn^{4+} impurity is found to shift towards the oxygen triangle along the C_3 (or [111]) axis by an amount ΔZ (≈ 0.29 Å) due to the strong electrostatic attraction between the Mn^{4+} and the oxygen triangle (and also the additional equivalent F'^- triangle), which increases the trigonal distortion of the Mn^{4+} center considerably. The calculated EPR parameters based on the above displacement ΔZ agree reasonably with the observed values.

Key words: Defect Structure; Electron Paramagnetic Resonance (EPR); Crystal-field Theory; Mn^{4+}; LiF.