Studies of the Zero-field Splitting for Mn$^{2+}$ in 6H-RbMgF$_3$ Crystal

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By using the spin-orbit coupling mechanism and the empirical superposition model, the zero-field splittings $D$ of Mn$^{2+}$ ions on both Mg$^{2+}$ sites in hexagonal 6H-RbMgF$_3$ crystal are calculated from the structural data of both Mg$^{2+}$ sites. The calculated results of both methods confirm the suggestion that Mn$^{2+}$ in 6H-RbMgF$_3$ occupies the Mg$^{2+}$ (I) site (which has D$_{3d}$ site symmetry) and the zero-field splitting $D$ of 6H-RbMgF$_3$: Mn$^{2+}$ is explained reasonably.

Key words: Electron Paramagnetic Resonance; Crystal-Field Theory; Superposition Model; Mn$^{2+}$; 6H-RbMgF$_3$. 