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-$RbMgF_3$.