Investigations on the Hyperfine and Superhyperfine Interaction Parameters for $Cs_2GeF_6:Mn^{4+}$

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The hyperfine structure constant A and the superhyperfine interaction parameters A' and B' of $Cs_2GeF_6:Mn^{4+}$ are theoretically studied by the cluster approach. The orbital mixing coefficients and the unpaired spin densities in 2s, $2p_\sigma$ and $2p_\pi$ fluorine orbitals are obtained from the optical spectra and the impurity-ligand distance of the studied system. Based on a uniform scheme, the parameters A, A' and B' (as well as the g factor) are reasonably explained. The results are discussed, and the unpaired spin densities of the 2s, $2p_\sigma$ and $2p_\pi$ orbitals of the ligand F^- are compared with those in previous works.

Key words: Electron Paramagnetic Resonance (EPR); Crystal- and Ligand-field Theory; Hyperfine Interactions; Mn^{4+}; Cs_2GeF_6.