Theoretical Studies of the EPR $g$ Factors and Optical Spectra for Tetragonal Ce$^{3+}$ Centers in CaF$_2$ and SrF$_2$ Crystals

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By using the irreducible tensor operator technique, the complete energy matrix including the admixture between $J = 7/2$ and $J = 5/2$ manifolds and the covalency reduction effect for 4f ion in tetragonal symmetry is established. Based on this, the electron paramagnetic resonance (EPR) $g$ factors for the tetragonal Ce$^{3+}$ centers in CaF$_2$ and SrF$_2$ crystals are reasonably explained and some levels of the $J = 5/2$ manifold for these centres are estimated. The results are discussed.

Key words: Crystal- and Ligand-field Theory; Electron Paramagnetic Resonance (EPR); Optical Spectra; Ce$^{3+}$; CaF$_2$; SrF$_2$. 