Theoretical Study of the Local Lattice Structure and the Site Symmetry of Fe^{3+} in $ZnGa_2O_4$:Fe^{3+}

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The site symmetry of Fe^{3+} in $ZnGa_2O_4$:Fe^{3+} and the local lattice structure around the impurity ion have been studied by diagonalizing the complete energy matrices for a d^5 configuration ion in a trigonal ligand-field, and calculating the EPR parameters D and $(a - F)$. The calculation indicates that when the local lattice structure of Fe^{3+} located at an octahedral site is distorted slightly, the site symmetry for Fe^{3+} is still D_{3d}, but not C_{3v}. – PACS numbers: 71.70.Gm Exchange interactions; 71.70.Ch Crystal and ligand-fields.

Key words: Space Group; EPR; Local Lattice Structure; Site Symmetry.