Calculation of the EPR Parameters and the Local Structure for Fe\(^+\) on the Zn\(^{2+}\) Site of ZnSiP\(_2\)

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The zero-field splitting \(D\), \(g\) factors \(g_\parallel\) and \(g_\perp\) and the local structure near Fe\(^+\) on the Zn\(^{2+}\) site of ZnSiP\(_2\) are calculated from high-order perturbation formulas of the EPR parameters for a 3d\(^7\) ion in tetragonally distorted tetrahedra based on the cluster approach. According to these studies, we find that the impurity-ligand bonding angle \(\alpha\)\(_{\text{loc}}\) related to the fourfold axis is about 58.05° in the studied Fe\(^+\) impurity center, which is larger than the metal-ligand bonding angle \(\alpha\)\(_{\text{h}}\) (≈ 56.65°) in pure ZnSiP\(_2\). The EPR parameters based on the above angle \(\alpha\)\(_{\text{loc}}\) agree well with the observed values. The errors of the results are analyzed.

**Key words:** Electron Paramagnetic Resonance (EPR); Defect Structure; Crystal- and Ligand-field Theory; Fe\(^+\); ZnSiP\(_2\).