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Superposition model analysis of the zero-field splitting parameters of Fe^{3+}: $TLBX_2$ crystals – insight into local distortions and low symmetry aspects

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In this paper we report on our recent studies of the Fe^{3+} centers in single crystals of wide-band gap semiconductors $TlInS_2$, $TlGaS_2$, and $TlGaSe_2$. Superposition model (SPM) calculations were carried out to investigate the local environment around the Fe^{3+} centers. A novel approach based on the ascent in symmetry method is applied to the crystallographic data to quantify the structural approximation from triclinic to orthorhombic and to tetragonal site symmetry. Electron magnetic resonance (EMR) data are reconsidered to provide more meaningful interpretation of the zero-field splitting (ZFS) parameters obtained by fitting EMR spectra. The values of the experimental ZFS parameters are matched with the SPM obtained values to obtain better insight into the local distortions and low symmetry aspects. The SPM results indicate that Fe^{3+} ions substitute for the B^{3+} ions in $TlBX_2$ (B = In, Ga, X = S, Se) crystal here.