Investigation of the Local Lattice Structure and the Effects of the Orbital Reduction Factor on the g Factors of a Trigonal $[Ni(H_2O)_6]^{2+}$ Cluster in $NiTiF_6 \cdot 6H_2O$ and $ZnSiF_6 \cdot 6H_2O$ Crystals at Different Temperatures

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The local octahedral environment of Ni^{2+} in $NiTiF_6 \cdot 6H_2O$ and $ZnSiF_6 \cdot 6H_2O$ crystals with a trigonal distortion has been studied at different temperatures, based on the complete energy matrices. The calculated results showed that the local lattice structure around an octahedral Ni^{2+} centre in $NiTiF_6 \cdot 6H_2O$ and $ZnSiF_6 \cdot 6H_2O$ exhibits a compression distortion. Simultaneously, the orbital reduction effect on the g factors has been studied. The relationship between $\Delta g = g_{\parallel} - g_{\perp}$ and orbital reduction factor k at 4.2, 77 and 298 (302) K has been discussed, suggesting that there is an almost linear relation between k and Δg for the Ni^{2+} ion in $NiTiF_6 \cdot 6H_2O$ and $ZnSiF_6 \cdot 6H_2O$ at each temperature.

Key words: Local Structure; Orbital Reduction Effect; EPR Spectrum; Complete Energy Matrices.