Effects of Concentration, Temperature and Hydrostatic Pressure on the Local Lattice Structure of Ni$^{2+}$ Doped Zn(BF$_4$)$_2 \cdot 6$H$_2$O Crystal

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A theoretical method for studying the inter-relationship between electronic and molecular structure is presented by means of complete energy matrices. As an application, the effects of temperature, concentration and hydrostatic pressure on the local structures of Ni$^{2+}$ doped Zn(BF$_4$)$_2 \cdot 6$H$_2$O crystal have been studied. Our results show that the local lattice structures of [Ni(H$_2$O)$_6$]$^{2+}$ coordination complex have expansion distortions as the temperature rises. Meanwhile, we find that the local structure parameter $\theta$ becomes smaller with the increasing concentration of Ni$^{2+}$ ions doped in Zn(BF$_4$)$_2 \cdot 6$H$_2$O crystal. Furthermore, the pressure dependence of $\theta$ and anisotropic $g$-factors are discussed and the relationship between zero-field splitting parameter $D$ and $\Delta g$ is determined.

Key words: Local Structure; Zn(BF$_4$)$_2 \cdot 6$H$_2$O:Ni$^{2+}$ System; Complete Energy Matrices.