# Effects of Concentration, Temperature and Hydrostatic Pressure on the Local Lattice Structure of $Ni^{2+}$ Doped $Zn(BF_4)_2 \cdot 6H_2O$ Crystal

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Z. Naturforsch. **64a,** 511 – 517 (2009); received October 9, 2008 / revised December 29, 2008

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 $Zn(BF_4)_2 \cdot 6H_2O$ crystal have been studied. Our results show that the local lattice structures of $[Ni(H_2O)_6]^{2+}$ 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 $Zn(BF_4)_2 \cdot 6H_2O$ 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; $Zn(BF_4)_2 \cdot 6H_2O$:$Ni^{2+}$ System; Complete Energy Matrices.