Investigation of the Spin-Hamiltonian Parameters and the Local Structure of Ni^{2+} Ions in $CsMgX_3$ (X = Cl, Br, I) Crystals

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Z. Naturforsch. **63a,** 188 – 192 (2008); received September 17, 2007

Taking into account spin-spin (SS), spin-other-orbit (SOO), and orbit-orbit (OO) interactions in addition to general spin-orbit (SO) interactions, the local structures of Ni^{2+} in $CsMgX_3$ (X = Cl, Br, I) are theoretically investigated by using the complete diagonalization method (CDM). On this basis, it is found that the local angles, at the Ni^{2+} centres are larger than those, at the hosts. The contributions to the spin-Hamiltonian parameters from spin triplets and slight magnetic interactions are discussed.

Key words: Spin-Hamiltonian Parameters; Local Structure; Ni^{2+}; $CsMgX_3$ (X = Cl, Br, I).