Theoretical Study of the Spin Hamiltonian Parameters of Vanadium Ions V^{2+} in $CsMgX_3$ (X = Cl, Br, I)

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The spin Hamiltonian *g* factors and the hyperfine structure constants for V^{2+} in $CsMgX_3$ (X = Cl, Br, I) are theoretically studied by using the perturbation formulas of these parameters for a $3d^3$ ion in octahedral symmetry, based on the cluster approach. In such formulas, the contributions from the s-orbitals of the ligands were usually neglected. Here they are taken into account. The theoretical results (particularly the *g* factor for $CsMgI_3$) show a significant improvement compared with those in absence of the ligand s-orbital contributions in the previous studies.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-field Theory; V^{2+}; $CsMgX_3$ (X = Cl, Br, I).