Theoretical Study of the Spin Hamiltonian Parameters of Vanadium Ions 
\( V^{2+} \) in \( \text{CsMgX}_3 \) (X = Cl, Br, I) 

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Z. Naturforsch. 60a, 145 – 148 (2005); received January 10, 2005  

The spin Hamiltonian \( g \) factors and the hyperfine structure constants for \( V^{2+} \) in \( \text{CsMgX}_3 \) (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 \( \text{CsMgI}_3 \)) 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; \( V^{2+} \); \( \text{CsMgX}_3 \) (X = Cl, Br, I).