

Investigation of the Spin Hamiltonian Parameters of a Tetragonal VO^{2+} Center in $(\text{NH}_4)_2\text{SbCl}_5$

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The spin Hamiltonian parameters g_{\parallel} and g_{\perp} and the hyperfine structure constants A_{\parallel} and A_{\perp} of a tetragonal VO^{2+} center in $(\text{NH}_4)_2\text{SbCl}_5$ are investigated, using the perturbation formulas for a $3d^1$ ion in tetragonally compressed octahedra. In these formulas, the contributions to the spin Hamiltonian parameters from the s- and p-orbitals as well as the spin-orbit coupling coefficient of the Cl^- ligand are taken into account, based on the cluster approach. According to these studies, compression of the ligand octahedra results from the strong axial crystal-fields due to the short $\text{V}^{4+}\text{-O}^{2-}$ bond in the $[\text{VOCl}_4]^{2-}$ cluster. The obtained spin Hamiltonian parameters agree well with the experimental data and need fewer adjustable parameters than the previous studies. The covalency of the studied system is also discussed.

Key words: Electron Paramagnetic Resonance; Crystal-Fields and Spin Hamiltonians; VO^{2+} ; $(\text{NH}_4)_2\text{SbCl}_5$.