Investigations of the EPR *g* Factors of $NaCrS_2$ and $NaCrSe_2$

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The EPR *g* factors of Cr^{3+} in $NaCrS_2$ and $NaCrSe_2$ crystals are calculated from the high-order perturbation formulas based on the one-spin-orbit (SO)-coupling-parameter (i. e., the SO-coupling-parameter of the central $3d^n$ ion) as well as the two-SO-coupling-parameter (i. e., the SO-coupling-parameter of the $3d^n$ ion and that of ligands) models for $3d^n$ ions in cubic octahedral sites. The calculated results (in particular for $NaCrSe_2$) based on the two-SO-coupling-parameter model are closer to the observed values than those based on the one-SO-coupling-parameter model, suggesting that for calculations of the *g* factor of $3d^n$ ions in covalent crystals the two-SO-coupling-parameter model is preferable to the one-SO-coupling-parameter model. The reasonableness of the calculated results from the two-SO-coupling-parameter model is discussed.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-field Theory; Spin-orbit Coupling; Cr^{3+}; $NaCrS_2$; $NaCrSe_2$.