

Theoretical Studies of the EPR g Factors and the Hyperfine Structure Constants of Cr^{3+} in MgS and SrS

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The EPR g factors and the hyperfine structure constant A factors for Cr^{3+} in MgS and SrS are theoretically studied by using the two-spin-orbit (S.O.)-coupling-coefficient formulas for a $3d^3$ ion in octahedra based on the cluster approach. In these formulas, both the contributions due to the S.O. coupling coefficient of the central $3d^3$ ion and that of ligands are taken into account. Based on these studies, the g and A factors of Cr^{3+} in both MgS and SrS are satisfactorily explained. The results are discussed.

Key words: EPR; Crystal- and Ligand-fields; Cr^{3+} ; MgS; SrS.