

Investigations of the g Factors of Fe^+ in MgO and CaO

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The g factors of Fe^+ in MgO and CaO are theoretically investigated by the perturbation formula of the g factor of a $3d^7$ ion in cubic octahedral symmetry based on the cluster approach. By considering the partial quenching of the spin-orbit coupling interaction and the effective Landé factor due to the dynamic Jahn-Teller effect (DJTE), the experimental g factors of the studied systems are reasonably interpreted. It can be suggested that the small g factors of the Fe^+ centers in MgO and CaO can be likely attributed to the DJTE, rather than the covalency effect within the scheme of the static crystal-field model.

Key words: Electron Paramagnetic Resonance; Crystal- and Ligand-field Theory; Fe^+ ; MgO ; CaO .