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.