

Theoretical Studies of the g Factors for Co^{2+} in MgO and CaO Crystals

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Z. Naturforsch. **56 a**, 249–252 (2001); received October 13, 2000

This paper presents a cluster approach to the calculation of the g factors for $3d^7$ ions in cubic octahedral crystals, in which the parameters related to the configuration interaction and the covalency reduction effects are obtained from optical spectra of the studied crystals, and so no adjustable parameters are applied. From the approach, the g factors for $\text{MgO}:\text{Co}^{2+}$ and $\text{CaO}:\text{Co}^{2+}$ are calculated. The calculated results show good agreement with the observed values. The experimental values of $g < 4.333$ (the first order value in absence of configuration and covalency interactions) for $\text{MgO}:\text{Co}^{2+}$ and $g > 4.333$ for $\text{CaO}:\text{Co}^{2+}$ are also explained.

Key words: Electron Paramagnetic Resonance (EPR); Crystal-field Theory; Co^{2+} Ion; MgO; CaO.