Defect Structure of Co^{2+} Center in α-$LiIO_3$ Crystal

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In this paper we establish the formulas of EPR g factors $g_{||}$, $g_{\perp}$ for $3d^7$ ions in trigonal octahedral crystals from a cluster approach. In these formulas, the contributions from configuration interaction- and covalency-effects are considered. The parameters related to both effects can be determined from the optical spectra and the structural parameters of the studied crystal. With these formulas, the defect structure of a Co^{2+} center in α-$LiIO_3$ crystal is studied. It is found that, to reach good fits between the calculated and observed $g_{||}$, $g_{\perp}$, the O^{2-} ions between Co^{2+} and Li^+ vacancy (V_{Li}) should shift away from the V_{Li} by about 0.49 Å. The displacement direction is consistent with those obtained for Cr^{3+}, Fe^{3+}, and Mn^{2+} centers in α-$LiIO_3$ crystals as well as with the expectation based on the electrostatic interaction model.

Key words: Electron Paramagnetic Resonance (EPR); Crystal-field Theory; Defect Structure; Co^{2+}; α-$LiIO_3$ Crystal.