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Theoretical Calculations of g Factors and Hyperfine Structure Constants for Co^{2+} in Cd^{2+}(I) and Cd^{2+}(II) Sites of $CsCdCl_3$ Crystal

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Abstract: The g factors $g_{||}$, $g_{\perp}$ and hyperfine structure constants $A_{||}$, $A_{\perp}$ for two trigonal Co^{2+} centers (i.e., Co^{2+} in Cd^{2+}(I) and Cd^{2+}(II) sites) in $CsCdCl_3$:Co^{2+} crystals are calculated from the high-order perturbation formulas based on the cluster approach. In the calculation, the contributions from covalency effect and configuration interaction effect are considered and the parameters related to both effects are obtained from the optical spectrum and the structure data of the studied system. The results are in good agreement with the observed values.

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