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Electron Paramagnetic Resonance of Mn²⁺-Doped Cadmium Formate Dihydrate Single Crystals

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Abstract

An electron paramagnetic resonance (EPR) study on Mn²⁺ doped Cadmium formate dihydrate single crystals is carried out. The EPR spectrum at room temperature exhibits only one out of five fine structural transitions which split into six hyperfine lines in all directions. The spectrum is simulated using the EasySpin program and evaluated spin Hamiltonian parameters. The simulated EPR spectrum is in good agreement with the experiment. By comparing direction cosines of spectroscopic splitting factor g and the direction cosines of different bonds determined by the crystal structure data it is found that Mn²⁺ enters the lattice substitutionally and only one Mn²⁺ site is identified. The obtained g and the

hyperfine interaction constant A achieved are $g = 2.006 \pm 0.002$, $A = (98 \pm 2) \times 10^{-4} \text{ cm}^{-1}$ and the second-order axial zero-field splitting parameter $D = (60 \pm 2) \times 10^{-4} \text{ cm}^{-1}$.

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