

EPR and optical study of Mn²⁺ doped lithium hydrogen oxalate monohydrate single crystals

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EPR study of Mn²⁺ doped lithium hydrogen oxalate monohydrate single crystals are done at room temperature. The Mn²⁺ spin Hamiltonian parameters are evaluated employing a large number of resonant line positions observed for different orientations of the external magnetic field. The values of g , A , B , D , E and a are 1.9942 ± 0.0002 , $114 \pm 2 \times 10^{-4} \text{ cm}^{-1}$, $103 \pm 2 \times 10^{-4} \text{ cm}^{-1}$, $180 \pm 2 \times 10^{-4} \text{ cm}^{-1}$, $57 \pm 2 \times 10^{-4} \text{ cm}^{-1}$ and $7 \pm 1 \times 10^{-4} \text{ cm}^{-1}$, respectively. The optical absorption study of the crystal is also done. The observed bands are assigned as transitions from the ${}^6A_{1g}(S)$ ground state to various excited quartet levels of Mn²⁺ ion in a cubic crystalline field. These bands are fitted with four parameters, inter-electronic repulsion parameters (B and C), crystal field parameter (Dq) and Tree's correction (α). The values found for the parameters are $B=814 \text{ cm}^{-1}$, $C=2255 \text{ cm}^{-1}$, $Dq=780 \text{ cm}^{-1}$, and $\alpha=76 \text{ cm}^{-1}$. On the basis of the data obtained the surrounding crystalline field and the nature of metal-ligand bonding are discussed.

Keywords: *spin Hamiltonian, crystal field, fine structure, percentage covalency, hyperfine coupling.*

PACS No. : 76.30

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