



## Synthesis and Structural Characterization of Bimetallic malonatoZinc(II) and its Copper(II) doped Complex

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Received on 19<sup>th</sup> March and finalized on 15<sup>th</sup> May 2013.

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### ABSTRACT

The crystal structure of Zinc(II) malonato $[Zn(H_2O)_2(Zn(mal)_2(H_2O)_2)]_n$  complex has been investigated by X-ray diffraction technique. Electron paramagnetic resonance, optical, FTIR and powder XRD studies have been carried out on Cu(II) doped Zinc(II) malonato complex to get information about the effect of dopant. Angular variation of copper hyperfine lines in EPR study shows the presence of a single site with  $g$  and  $A$  values as:  $g_{xx} = 2.101$ ,  $g_{yy} = 2.068$ ,  $g_{zz} = 2.365$  and  $A_{xx} = 4.32$  mT,  $A_{yy} = 3.55$  mT,  $A_{zz} = 12.60$  mT. The direction cosines of principle  $g$  and  $A$  values suggest that electric field around the impurity is rhombic and it is present substitutionally through metal carboxylate oxygen bond of the host lattice. The low value of  $A_{||}$  has been explained by taking account of considerable admixture between the ground and excited states of copper (II) such as  $d_{x^2-y^2}$  and  $d_z^2$ , with admixture coefficients of  $a = 0.144$ ,  $b = 0.988$ ,  $c = 0.052$ ,

$d = 0.019$  and  $e = -0.019$ , where coefficients  $a$  and  $b$  correspond to coefficients for  $d_z^2$  and  $d_{x^2-y^2}$  orbitals respectively. Few other calculated parameters such as  $\kappa = 0.37$ ,  $P = 290 \times 10^{-4} \text{ cm}^{-1}$ ;  $\alpha = 0.88$  and  $\alpha' = 0.53$  indicate considerable covalence.

**Keywords:** Bimetallic zinc, malonato, copper, admixture coefficient, EPR, optical.

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