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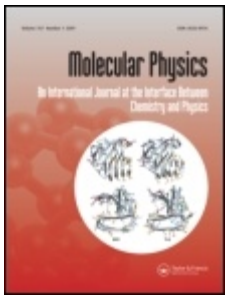

ESR and optical study of Cu^{2+}-doped bis-(5,5′-diethylbarbiturato)bis picoline Zn(II)

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Abstract

ESR studies were conducted on Cu^{2+}-doped bis-(5,5′-diethylbarbiturato)bis picoline Zn(II). Two Cu^{2+} lattice sites, Cu^{2+}(I) and Cu^{2+}(II), were identified. These sites exhibit two sets of four hyperfine lines in all directions. The g factor and hyperfine splitting were calculated from ESR absorption spectra: $g_x = 2.0201 \pm 0.002$, $g_y = 2.0900 \pm 0.002$, $g_z = 2.1634 \pm 0.002$, $A_x = (30 \pm 2) \times 10^{-4}\ \mathrm{cm}^{-1}$, $A_y = (40 \pm 2) \times 10^{-4}\ \mathrm{cm}^{-1}$ and $A_z = (154 \pm 2) \times 10^{-4}\ \mathrm{cm}^{-1}$. It was found that Cu^{2+} enters the lattice substitutionally. The ground-state wavefunction of the Cu^{2+} ion in this lattice was determined from the spin

Hamiltonian constants obtained from the ESR studies. With the help of an optical absorption study, the nature of the bonding in the complex is also discussed.

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Keywords

- ESR,
- spin Hamiltonian,
- absorption,
- angular variation,
- rhombic symmetry

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