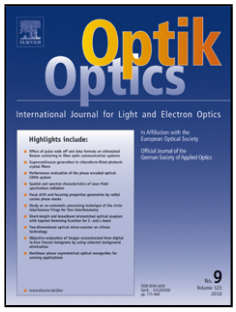

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Authors: B. Srinivasa, R.Vijaya kumar, Abdul Hameed, G. Ramadevudu, M. Narasimha Chary, Md. Shareefuddin

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Experimental and Theoretical Electron Paramagnetic Resonance and Optical studies of Cu^{2+} spin probe in BaO-TeO_2-Bi_2O_3-B_2O_3 glass system

B.Srinivas [a], R.Vijaya kumar [b], Abdul Hameed [a], G.Ramadevudu [c], M.Narasimha Chary [a] and Md.Shareefuddin [a]

[a] *Department of Physics, Osmania University, Hyderbad-500007, Telangana state, India.*
[b] *School of Physics, University of Hyderabad, Hyderbad-500046, Telangana state, India.*
[c] *Vasavi College of Engineering(A), Ibrahimbagh, Hyderbad-500031, Telangana state, India.*

Corresponding author email: srinivas.physicsscholar@gmail.com, mobile no: +919948303303

Abstract:

Boro-bismuth glasses containing BaO-TeO_2 in varying proportions were prepared by the conventional melt quenching method. One mol% of CuO was integrated as the spin probe to the glass systems. The prepared glasses were transparent, bubble-free and light blue in color. The optical absorption spectra revealed two absorption bands corresponding to the transitions $^2B_{1g} \rightarrow {}^2B_{2g}$ and $^2B_{1g} \rightarrow {}^2E_{2g}$ respectively. A large anisotropy ($\Delta g = g_{\parallel} - g_{\perp}$) due to the distortion around the Cu^{2+} site by the ligands was observed. Experimental and theoretical EPR results have shown that $g_{\parallel} > g_{\perp} > g_e$ (=2.0023) and $A_{\parallel} > A_{\perp}$. The ligand field around Cu^{2+} ions is tetragonally elongated octahedral with $d_{x^2-y^2}$ ($^2B_{1g}$) ground state. The decreased peak-to-peak linewidth (ΔB) with increasing BaO content is attributed to decrease in dipolar interaction between the copper ions. The number of EPR active copper ions (N) and the paramagnetic susceptibility (χ) were computed. EPR and optical data were used to determine the bonding parameters α^2, β^2, β_1^2, τ_π and τ_σ. Theoretical investigations were performed using the high order perturbation formulae for $3d^9$ ions in tetragonally elongated octahedra to determine the spin-Hamiltonian parameters (SHP) and d-d transition bands. The variation of BaO content in the glass matrix had affected the orbital reduction factor, spin-orbit coupling coefficient, cubic and tetragonal field parameters. The Cu^{2+}-O^{2-} octahedron experiences 0.50% elongation along C_4 axis. The theoretical and experimental results are well in coincidence within the error limits.

Keywords: EPR, spin-Hamiltonian parameters, Optical absorption, Molecular Orbital (MO) coefficients.