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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 $\text{Cu}^{2+}$ spin probe in $\text{BaO-TeO}_2\text{-Bi}_2\text{O}_3\text{-B}_2\text{O}_3$ glass system

B.Srinivas <sup>a</sup>, R.Vijaya kumar <sup>b</sup>, Abdul Hameed <sup>a</sup>, G.Ramadevudu <sup>c</sup>, M.Narasimha Chary <sup>a</sup> and Md.Shareefuddin <sup>a</sup>

<sup>a</sup> Department of Physics, Osmania University, Hyderabad-500007, Telangana state, India.

<sup>b</sup> School of Physics, University of Hyderabad, Hyderabad-500046, Telangana state, India.

<sup>c</sup> Vasavi College of Engineering(A), Ibrahimbagh, Hyderabad-500031, Telangana state, India.

Corresponding author email: [srinivas.physicsscholar@gmail.com](mailto:srinivas.physicsscholar@gmail.com), mobile no: +919948303303

## Abstract:

Boro-bismuth glasses containing  $\text{BaO-TeO}_2$  in varying proportions were prepared by the conventional melt quenching method. One mol% of  $\text{CuO}$  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  $^2\text{B}_{1g} \rightarrow ^2\text{B}_{2g}$  and  $^2\text{B}_{1g} \rightarrow ^2\text{E}_{2g}$  respectively. A large anisotropy ( $\Delta g = g_{\parallel} - g_{\perp}$ ) due to the distortion around the  $\text{Cu}^{2+}$  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  $\text{Cu}^{2+}$  ions is tetragonally elongated octahedral with  $d_{x^2-y^2}$  ( $^2\text{B}_{1g}$ ) ground state. The decreased peak-to-peak linewidth ( $\Delta B$ ) with increasing  $\text{BaO}$  content is attributed to decrease in dipolar interaction between the copper ions. The number of EPR active copper ions ( $N$ ) and the paramagnetic susceptibility ( $\chi$ ) were computed. EPR and optical data were used to determine the bonding parameters  $\alpha^2$ ,  $\beta^2$ ,  $\beta_1^2$ ,  $\tau_{\pi}$  and  $\tau_{\sigma}$ . 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  $\text{BaO}$  content in the glass matrix had affected the orbital reduction factor, spin-orbit coupling coefficient, cubic and tetragonal field parameters. The  $\text{Cu}^{2+}\text{-O}^{2-}$  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.

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