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Multifaceted analysis of intermolecular interactions in α-terpineol-halobenzenes binary mixtures: Insights from thermophysical, acoustical, and spectral techniques, supported by quantum computational approaches

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This study examines the thermophysical, acoustical, and spectral properties of binary mixtures of α-terpineol with fluorobenzene, chlorobenzene, and bromobenzene under standard atmospheric pressure at 303.15 K, 308.15 K and 313.15 K. Molar volume (V_m), excess molar volume (V_m^E), partial molar volume ($\bar{V}_{m,i}^o$), excess partial molar volume ($\bar{V}_{m,i}^{o,E}$), apparent molar volume ($V_{m,\Phi,i}$), deviation in speed of sound (Δu), isentropic compressibility (κ_s), deviation in isentropic compressibility ($\Delta\kappa_s$), acoustical impedance (z), deviation in acoustical impedances (Δz), intermolecular free length (L_f), partial molar isentropic compression ($\bar{K}_{s,m,i}^o$), excess partial molar isentropic compression ($\bar{K}_{s,m,i}^{o,E}$), and apparent molar isentropic compression ($K_{s,m,\Phi,i}$) have been measured. Parameters such as infinite dilution apparent molar volume ($V_{m,\Phi,1}^o$), infinite dilution apparent molar isentropic compression ($K_{s,m,\Phi,1}^o$) have also been determined. The Redlich-Rosenberg-Mayer equation for empirical coefficients and applied theoretical models to analyze speed of sound and deviation properties have been used. FT-IR spectral analysis has been performed on binary mixtures at 298.15 K, while computational investigations include gas phase optimization, Mulliken charges, vibrational frequencies, NCI, ELF, LOL, and NBO analyses using DFT. These studies elucidate intermolecular interactions, their strengths, and variations with temperature and halobenzene concentration.

Keywords: Binary mixtures, Density, Speed of sound, FT-IR, DFT