Molecular Interactions in Cumene + Alkan-1-ol Binary Mixtures: Viscometric, Spectroscopic, and DFT Analysis

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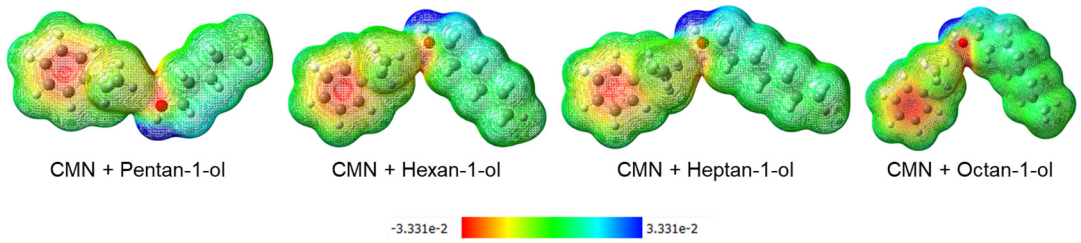
The dynamic viscosity (η) of binary mixtures comprising cumene (CMN) and four alkan-1-ols (pentan-1-ol, hexan-1-ol, heptan-1-ol, and octan-1-ol) have been investigated. Measurements were conducted across a temperature range of 298.15 K to 323.15 K, at 5 K intervals, under atmospheric pressure. From the measured data, deviation in viscosities ($\Delta\eta$), free energies for the activation of viscous flow ($\Delta G^{\neq}$), and their excess ($\Delta G^{\neq E}$) were assessed. Analysis of these properties revealed the influence of several intermolecular forces, including hydrogen bonding, alkyl chain length effects, π-π interactions, dipole-dipole interactions, and geometric fitting, on the behavior of these mixtures. Fourier transform infrared (FT-IR) spectroscopy provided further insights into the specific intermolecular interactions. The measured η and $\Delta G^{\neq}$data were fitted to concentration-dependent polynomial equations, while excess properties ($\Delta\eta$ and $\Delta G^{\neq E}$) were fitted to Redlich-Kister equation. Moreover, the measured viscosity data were fitted with the temperature-dependent Jouyban-Acree model. The correlative abilities of several other viscosity models, including the McAllister three-body, McAllister four-body, and Ausländer models, were also evaluated. Density functional theory calculations were employed to gain a molecular-level understanding of the interactions within the mixtures. The study's findings highlight the complex and composition-dependent nature of molecular interactions in these binary systems.



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