

Abstract Submitted
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Phase behavior and mixing-demixing transitions in binary liquid mixtures with spherical and non-spherical interactions¹ ENRIQUE DIAZ-HERRERA, Depto. de Fisica, UAM-I (MEXICO), GUILLERMO RAMIREZ-SANTIAGO, Instituto de Fisica, UNAM (MEXICO), J. ANTONIO MORENO-RAZO, Depto. de Fisica, UAM-I (MEXICO) — We have carried out extensive equilibrium molecular dynamics simulations to study the temperature versus density phase diagrams and the mixing-demixing transition line in fluid equimolar binary mixtures modeled by: (i) Lennard-Jones, (ii) Stock-Mayer, and (iii) Gay-Berne molecular interactions. These studies are performed as function of miscibility parameter, $\alpha = \epsilon_{AB}/\epsilon_{AA}$, where $\epsilon_{AA} = \epsilon_{BB}$ and ϵ_{AB} stand for the parameters related to the attractive part of the intermolecular interactions for similar and dissimilar particles, respectively. When the miscibility of the Lennard-Jones mixture varies in the range $0 < \alpha < 1$, a continuous critical line of consolute points $T_{\text{cons}}(\rho)$, appears. This line intersects the liquid-vapor coexistence curve at different positions depending on the values of α , yielding mainly three different topologies for the phase diagrams. These results are in qualitative agreement to those found previously for square well and hard-core Yukawa binary mixtures. We also carry out a detailed study of the liquid-liquid interfacial and liquid-vapor surface tensions, as function of temperature and miscibility as well as its relationship to the topologies of the phase diagrams. Similar studies and analysis are also performed for Stock-Mayer and Gay-Berne binary mixtures.

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