

# Experimental and CPA EoS Description of the Key Components in the BTX Separation from Gasolines by Extractive Distillation with Tricyanomethanide-Based Ionic Liquids

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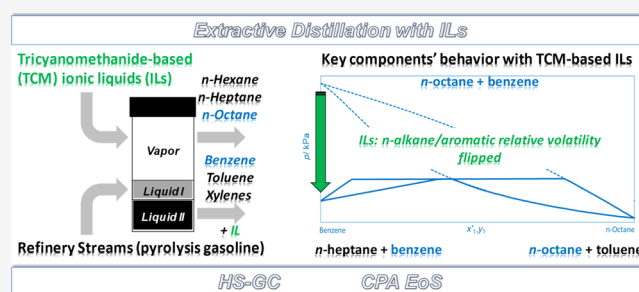
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**ABSTRACT:** Two tricyanomethanide-based ionic liquids (ILs), namely, 1-ethyl-3-methylimidazolium tricyanomethanide ( $[\text{C}_2\text{C}_1\text{im}][\text{TCM}]$ ) and 1-butyl-4-methylpyridinium tricyanomethanide ( $[\text{4-C}_4\text{C}_1\text{py}][\text{TCM}]$ ), have been recently reported as effective solvents for the benzene, toluene, and xylene (BTX) extractive distillation from pyrolysis gasoline. The vapor–liquid or vapor–liquid–liquid equilibria (VLE/VLLE) of several {aliphatic + aromatic + [TCM]-based ILs} ternary systems related to pyrolysis gasoline were extensively determined by headspace gas chromatography on a wide range of temperatures and solvent-to-feed ratios. The cubic plus association equation of state (CPA EoS) was used to predictively describe the experimental VLE/VLLE from binary interaction parameters regressed from {hydrocarbon + IL} binary systems. Here, the VLE/VLLE related to the separation of the pyrolysis gasoline key components (*n*-octane and benzene) and other aliphatic/aromatic challenging mixtures in terms of aliphatic/aromatic relative volatility are reported. Specifically, the VLE/VLLE data for {*n*-octane + benzene + IL}, {*n*-heptane + benzene + IL}, and {*n*-octane + toluene + IL} ternary systems were determined. The CPA EoS accuracy, robustness, and transferability between different systems are verified, with the advantages and limitations shown in previous works. Overall, the results obtained in this work lay the foundation for the implementation of the CPA EoS parameterization in a commercial simulator to rigorously simulate the multicomponent BTX extractive distillation from pyrolysis gasoline with ILs.



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