I&EC research
Industrial & Engineering Chemistry Research

Article

Cite This: *Ind. Eng. Chem. Res.* 2018, 57, 14242−14253

pubs.acs.org/IECR

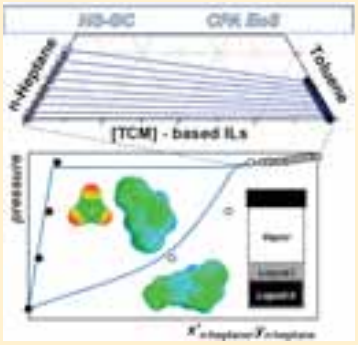
Toluene/*n*-Heptane Separation by Extractive Distillation with Tricyanomethanide-Based Ionic Liquids: Experimental and CPA EoS Modeling

Pablo Navarro,*[,†] Miguel Ayuso,[‡] André M. Palma,[†] Marcos Larriba,[†,‡] Noemí Delgado-Mellado,[‡] Julián García,[‡] Francisco Rodríguez,[‡] João A. P. Coutinho,[†] and Pedro J. Carvalho[†]

[†]CICECO − Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Aveiro 3810-193, Portugal
[‡]Department of Chemical Engineering, Complutense University of Madrid, Madrid E−28040, Spain

Supporting Information

ABSTRACT: This work covers the phase equilibrium characterization of systems containing *n*-heptane, toluene, and two tricyanomethanide-based ionic liquids (ILs), 1-ethyl-3-methylimidazolium tricyanomethanide ([C_2C_1im][TCM]) and 1-butyl-4-methylpyridinium tricyanomethanide ([4-C_4C_1py][TCM]). Aiming at evaluating these ILs for the *n*-heptane/toluene extractive distillation, the vapor−liquid−liquid equilibria (VLLE) and vapor−liquid equilibria (VLE) were determined by headspace-gas chromatography (HS-GC) in the whole composition range at temperatures from 323.2 to 423.2 K and solvent to feed (S/F) ratios of 1, 5, and 10. Experimental results were modeled with the Cubic Plus Association (CPA) Equation of State (EoS). ILs' molecular parameters were regressed through density and heat capacity data and further used to describe the binary and ternary mixtures phase equilibria. Extractive distillation with ILs stands as a powerful approach for the dearomatization of liquid fuels, whereas the combination of HS-GC methodology and CPA EoS has been revealed as an ideal strategy to further exploring this new technology.



Received: August 10, 2018
Revised: September 24, 2018
Accepted: September 28, 2018
Published: September 28, 2018

DOI: 10.1021/acs.iecr.8b03804
Ind. Eng. Chem. Res. 2018, 57, 14242−14253