

## Novel Process to Reduce Benzene, Thiophene, and Pyrrole in Gasoline Based on [4bmpy][TCM] Ionic Liquid

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### Supporting Information

**ABSTRACT:** Regulations on benzene-, nitro-, and sulfur-containing aromatic hydrocarbon content in commercial gasolines are becoming more restrictive due to environmental and health issues. The benzene content in reformulated commercial gasoline is currently around 1%. The reduction of benzene levels to comply with future regulations will imply significant changes in refinery configurations. This paper reports a novel extraction process to simultaneously separate benzene, thiophene, and pyrrole from a gasoline using the 1-butyl-4-methylpyridinium tricyanomethanide ([4bmpy][TCM]) ionic liquid (IL). A distillation sequence is also proposed for the isolation of the three aromatic hydrocarbons. The conceptual design of the whole process has been based on experimental data from the liquid–liquid extraction and vapor–liquid separation of benzene, thiophene, and pyrrole from isooctane using the IL [4bmpy][TCM]. A COSMO-based/Aspen Plus methodology has been used to simulate the conceptual design. The a priori COSMO-based/Aspen Plus approach was validated by comparison with the experimental liquid–liquid extraction results and conventional simulations based on experimental distribution ratios and *K* values. Benzene, thiophene, and pyrrole contents in the gasoline would be reduced from 5.0% to 0.1% using the proposed process with a solvent-to-feed mass ratio of 5.0, and also three streams with high content in each aromatic would be obtained. Increasing the solvent-to-feed mass ratio above 5.0, benzene content in the treated gasoline could be reduced up to 200 ppm.

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