

Choline Chloride-Based Deep Eutectic Solvents in the Dearomatization of Gasolines

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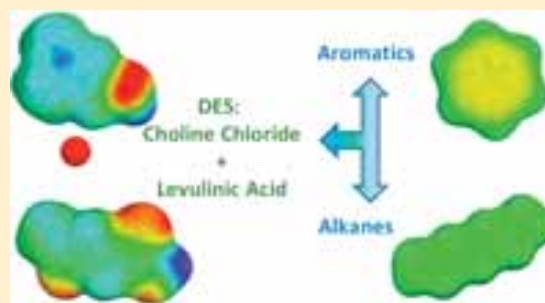
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Supporting Information

ABSTRACT: The extraction of aromatic hydrocarbons from reformer and pyrolysis gasolines is currently performed by liquid–liquid extraction using organic solvents. Deep eutectic solvents (DES) are being widely studied as environmentally benign alternatives to conventional solvents since DES can be prepared using nontoxic and renewable chemicals. In this work, we have studied for the first time the application of DES in the extraction of aromatic hydrocarbons from reformer and pyrolysis gasolines. We have tested six choline chloride-based DES formed by ethylene glycol, glycerol, levulinic acid, phenylacetic acid, malonic acid, and urea as hydrogen bond donors. COSMO-RS method was employed to predict the performance of the DES in the extraction of aromatics, whereas experimental results indicate that DES formed by choline chloride and levulinic acid has exhibited the most adequate extractive and physical properties. Afterward, the simulation and optimization of the whole process for extraction of aromatics, recovery of extracted hydrocarbons, and regeneration of the solvent have been performed. The proposed process of dearomatization could work at moderate temperatures using a cheap, sustainable, and nontoxic solvent.

KEYWORDS: Extraction of aromatic hydrocarbons, Reformer and pyrolysis gasolines, Deep eutectic solvents, COSMO-RS, Process simulation



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