Electronic Supplementary Material

Extractive desulfurization of model fuels with a nitrogen-containing heterocyclic ionic liquid

Guojia Yu, Dongyu Jin, Xinyu Li, Fan Zhang, Shichao Tian, Yixin Qu, Zhiyong Zhou (✉), Zhongqi Ren (✉)

College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 100029, China

E-mails: renzq@mail.buct.edu.cn (Ren Z); zhouzy@mail.buct.edu.cn (Zhou Z)

FT-IR spectrum

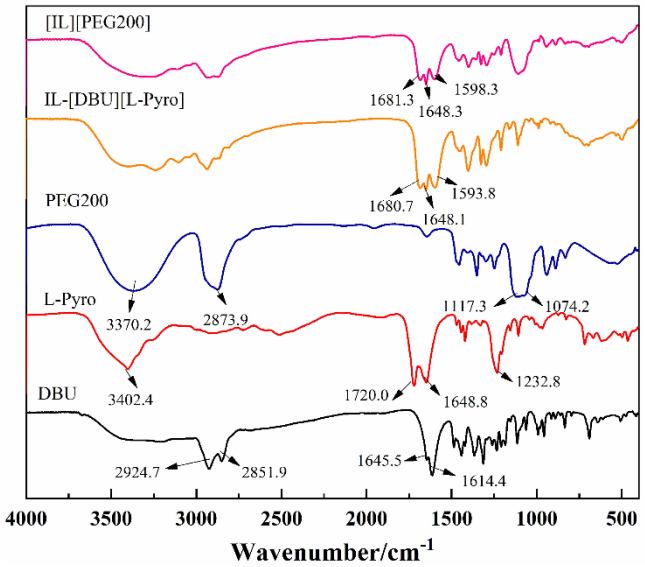


Fig. S1 FI-IR spectra of ILs and corresponding reactants.

In Figure S1, the absorption peaks of DBU molecule at 1614.4 cm^{-1}, 2851.9 cm^{-1} and 2924.7 cm^{-1} correspond to -C=N, and -CH_2-cycloalkane stretching vibrations. The absorption peaks of L-Pyro at 3402.4 cm^{-1}, 1720.0 cm^{-1}, 1684.8 cm^{-1}, 1232.8 cm^{-1} correspond to -OH, -C=O stretching vibrations in -COOH, ketone group of -C=O on the ring and -CN stretching peak, respectively. Comparing the peaks of DBU and L-Pyro molecule, IL-[DBU][L-Pyro] had peak shift change, where -C=O stretching vibration in -COOH shifted from 1720 to 1680.7 cm^{-1}, -C=N shifted from 1614.4 to 1593.8 cm^{-1}. The absorption peaks of PEG200 were at 3370.2 cm^{-1} (-OH characteristic absorption peak), 2873.9 cm^{-1} (-CH_2-symmetric stretching vibration), 1117.3 cm^{-1} and 1074.2 cm^{-1} (-C-O-C stretching vibration). The characteristic peak of PEG200 appeared in [IL][PEG200].

^{1}H NMR spectrum

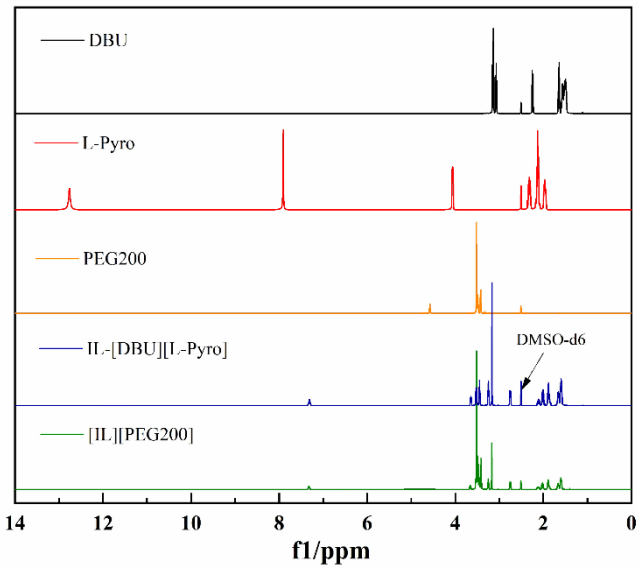


Fig. S2 ^{1}H NMR spectra (DMSO-d6, 500 MHz) of ILs and corresponding reactants.

The H signal at 12.76 ppm represents the -COOH active hydrogen of the hydroxyl group contributed by L-Pyro in Figure S2. After protonation, the -COOH

active hydrogen in [DBU][L-Pyro] disappeared. And the shift peaks of PEG200 existed in the spectrum of [IL][PEG200].

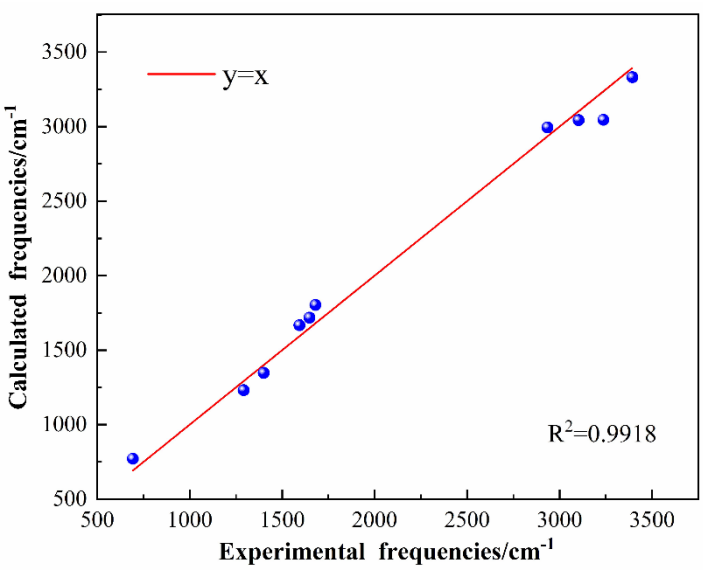


Fig. S3 High linear correlations between calculated and experimental infrared vibrational frequencies.

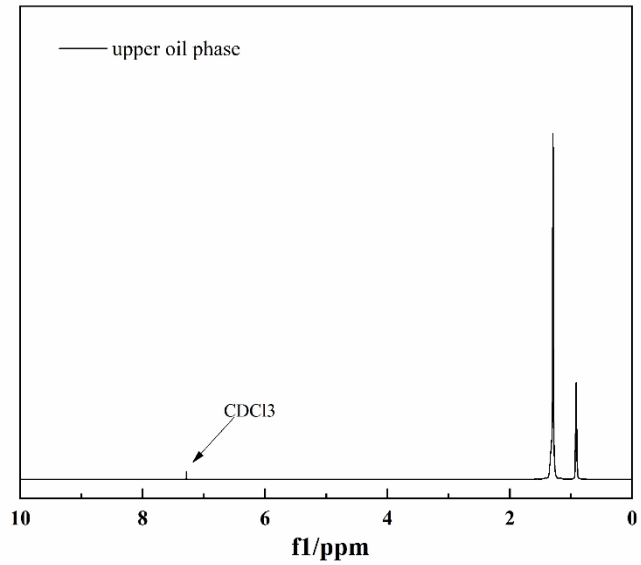
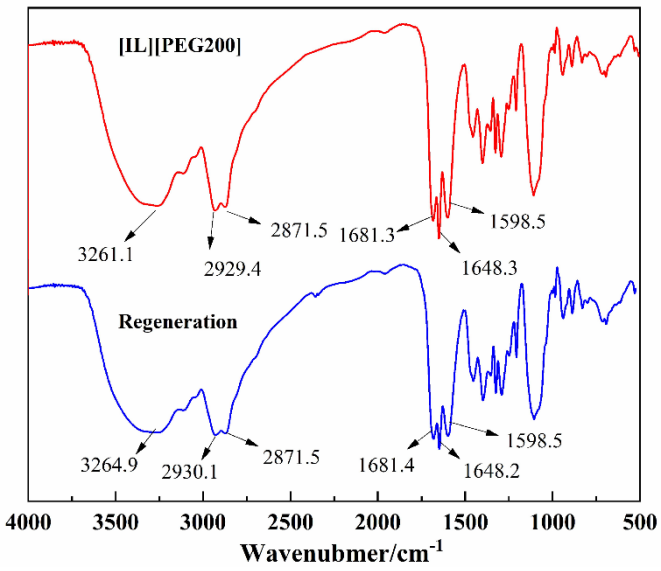
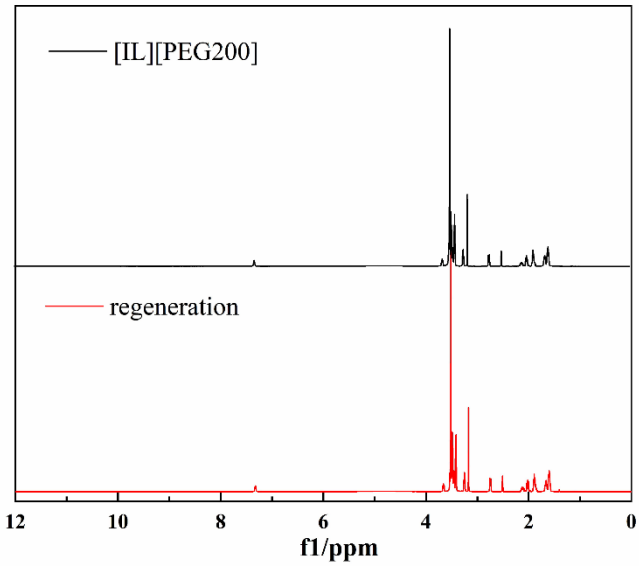


Fig. S4 ^{1}H NMR spectrums ($CDCl_3$, 500 MHz) of upper liquid after the EDS process.

Figure S4 showed that there were no impurities in the supernatant, indicating that [IL][PEG200] would not contaminate the simulated oil.



(a)



(b)

Fig. S5 (a) Infrared and (b) ^{1}H NMR ($CDCl_3$, 500 MHz) characterization before and after the extractive desulfurization process.