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Selective Extractive Desulfurization of Simulated Straight-Run Diesel with Imidazole-Based Deep Eutectic Solvents

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INTRODUCTION

Given the current situation of excess diesel production capacity in China and the widespread adoption of renewable energy, selective desulfurization of diesel is a key method for achieving the resource utilization of its components. Based on the principle of polarity similarity and solubility, this study designed and synthesized a series of imidazole-based deep eutectic solvents (DESs) for the selective extractive desulfurization of simulated straight-run diesel. By evaluating the performance parameters of the extractants, it was determined that the deep eutectic solvent composed of 1-ethyl-3-methylimidazole chloride (EmimCl) as the hydrogen bond acceptor (HBA) and 2-imidazolidinone (IMD) as the hydrogen bond donor (HBD) is the optimal extractant.

Under optimized, the removal efficiency of sulfides reached 61.77%, while that of aromatic compounds was significantly lower (6.87%). This high selectivity (sulfide/aromatic = 15.44) was predominantly attributed to the effective extraction of bicyclic aromatics such as 1-methylnaphthalene, in contrast to the minimal removal of monocyclic species (e.g., tetrahydronaphthalene and butylbenzene). Quantum chemical calculations based on an implicit solvent model further revealed that differences in solvation free energy, governed by solvent polarity and van der Waals interactions, strengthen the selectivity between sulfides and aromatic compounds.

DESIGN AND SCREENING OF EXTRACTANTS

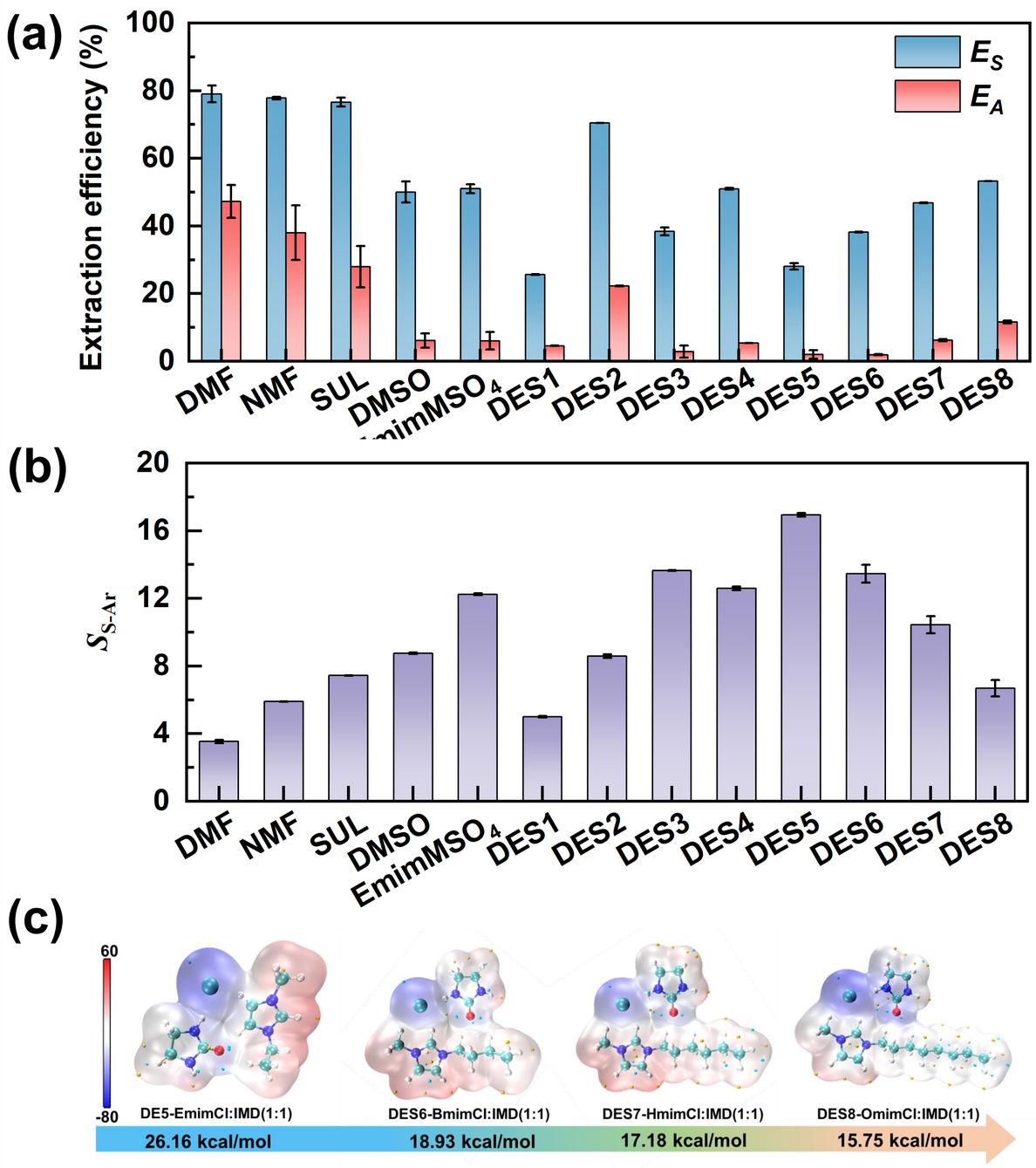

Figure 1 (a) Desulfurization and dearomatization performance of different extractants; (b) Extraction selectivity of different solvents; (c) ESP images and MPI of different extractants.

RESULTS & DISCUSSION

- **Optimization of extraction conditions**

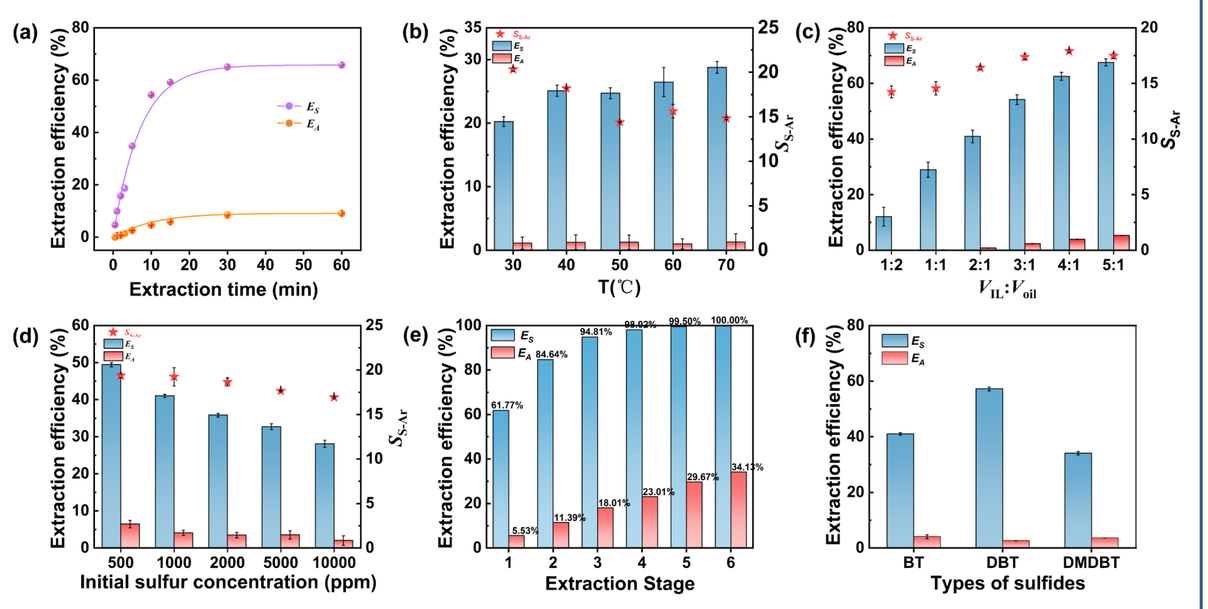

Figure 2. Effect of experimental parameters on the extraction performance. (a) extraction time; (b) extraction temperature; (c) DES/oil ratio; (d) initial aromatic concentration; (e) the number of extraction stages; (f) different sulfides.

- **Recycling of DES**

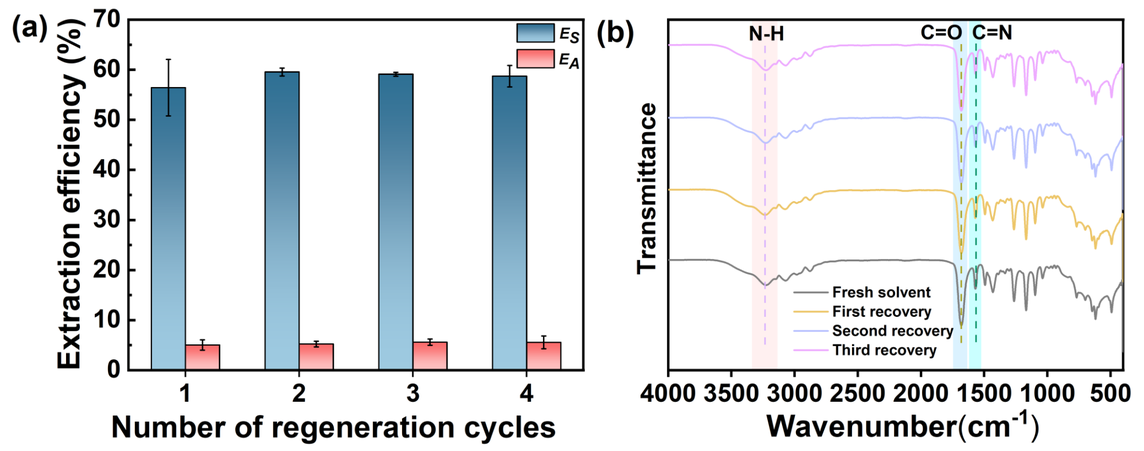

Figure 3. (a) Effect of regeneration cycles on the extraction performance; (b) FTIR spectra of fresh and recycled DES.

- **Extraction mechanism**

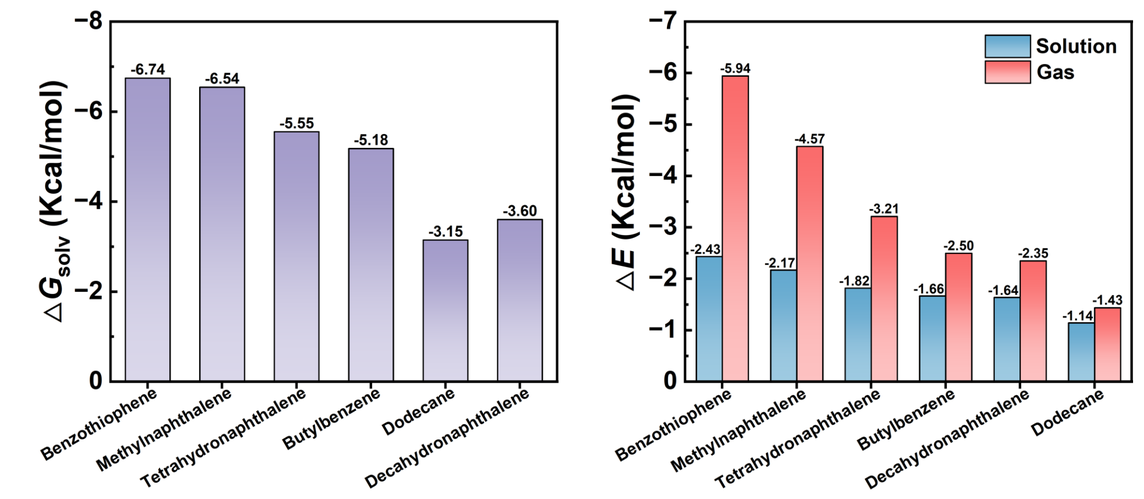

Figure 4. (a) Solvation free energy and (b) interaction energy between DES and different component.

CONCLUSION

- Through systematic screening of extractants, the DES composed of EmimCl as the hydrogen bond acceptor and IMD as the hydrogen bond donor was identified as the optimal extractant.
- Combined computational and experimental analyses reveal that the selectivity originates from differences in molecular polarity and specific noncovalent interactions.