



INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: Molecular Modeling and Thermodynamic Studies on the Selective Extraction of Poly Aromatic Hydrocarbons from Fuel oil using Deep Eutectic Solvents

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SHORT ABSTRACT

Poly aromatic hydrocarbon (PAH) along with nitrogen and sulfur heteroatoms are the main impurities in the fuel oil. These PAHs are the primary cause for air pollution due to the release of SO_x and NO_x during combustion of fuel oil. The thesis aims to extract the nitrogen based PAH from fuel oil through Liquid Liquid Extraction (LLE). Green solvents such as Deep Eutectic Solvent (DES) have been used as extractive solvent. The DES here is synthesized by mixing hydrogen bond donor (HBD: ethylene glycol) with hydrogen bond acceptor (HBA: methyltriphenylphosphonium bromide) at an appropriate molar ratio. Fourier transform infrared (FTIR) and thermo gravimetric analysis (TGA) analysis were then carried out to understand the functional groups along with their thermal stability. The LLE experiments were then performed for the extraction of quinoline and indoline as model PAH from fuel oil. Molecular dynamics study were carried out to understand the molecular insights within the extraction phenomena. Further degradation pathways for quinoline using Reactive Force Field (ReaxFF) simulations were also carried out. Overall, DES are environmentally benign and offers several advantages over conventional catalytic extraction process in terms of efficiency and cross-contamination.