Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2023

# **Supplementary Information**

## Deep extractive and catalytic oxidative desulfurization of liquid fuels by using iron(III)

## based dication ionic liquids

Anham Zafar<sup>ab</sup>, Imtiaz-ud-Din<sup>a</sup>, Saadia Batool<sup>a</sup>, Robert G. Palgrave<sup>b</sup>, Sammer Yousuf<sup>c</sup>,

- a. Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan
- b. Chemistry Department, University College London, 20 Gordon Street, London, WC1E 0AJ, UK
- c. H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan

#### **Table of Contents**

NMR Spectrometry(I <sub>1</sub> -I <sub>5</sub> )	2
Mass Spectrometry (1-5)	7
Raman spectroscopy (1-5)	9
X-ray photoelectron spectroscopy (1-5)	10







**Fig.S2.** <sup>13</sup>C NMR spectrum for  $I_1$ 



Fig.S4. <sup>13</sup>C NMR spectrum for I<sub>2</sub>



Fig.S5. <sup>1</sup>H NMR spectrum for I<sub>3</sub>



Fig.S6. <sup>13</sup>C NMR spectrum for  $I_3$ 











Fig. S9. <sup>1</sup>H NMR spectrum for I<sub>5</sub>



Fig.S10. <sup>13</sup>C NMR spectrum for  $I_5$ 

#### Mass Spectrometry (1-5)



Fig.S11. ESI<sup>+</sup> mass spectrum for (1)











Fig.S14. ESI<sup>+</sup> mass spectrum for (4)



Fig.S15. ESI<sup>+</sup> mass spectrum for (5)

Raman spectroscopy (1-5)



Fig.S16. Raman Spectra of DcILs (1-5)





Fig.S17. High resolution XP spectra of 1 showing (a) full survey spectra, (b) peak fitted C 1s with structural assignment, (c) Br 3d, (d) Cl 2p, (e) N 1s and (f) Fe 2p



Fig.S18. High resolution XP spectra of (2) showing (a) full survey spectra, (b) peak fitted C 1s with structural assignment, (c) Br 3d, (d) Cl 2p, (e) N 1s and (f) Fe 2p



Fig.S19. High resolution XP spectra of (3) showing (a) full survey spectra, (b) peak fitted C 1s with structural assignment, (c) Br 3d, (d) Cl 2p, (e) N 1s and (f) Fe 2p



Fig.S20. High resolution XP spectra of (4) showing (a) full survey spectra, (b) peak fitted C 1s with structural assignment, (c) Br 3d, (d) Cl 2p, (e) N 1s and (f) Fe 2p



Fig.S21. High resolution XP spectra of (5) showing (a) full survey spectra, (b) peak fitted C 1s with structural assignment, (c) Br 3d, (d) Cl 2p, (e) N 1s and (f) Fe 2p