

Electronic Supplementary Information (ESI)

**Concentration-dependent Apparent Partition Coefficients of Ionic
Liquids Possessing Ethyl- and Bi-sulphate Anions**

Preeti Jain, Anil Kumar*

Physical and Materials Chemistry Division

CSIR-National Chemical Laboratory

Pune-411 008, India

a.kumar@ncl.res.in

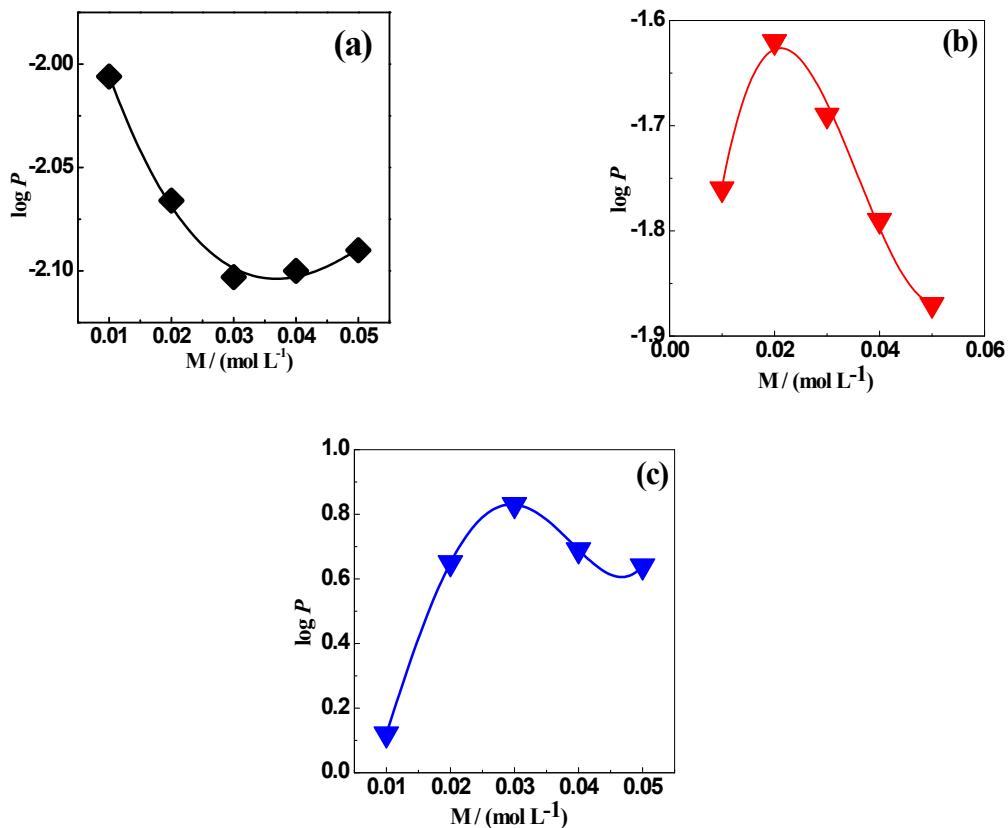


Fig. S1 Variation of $\log P$ with concentration (a) for [BMIM][HSO₄], (b) for [HMIM][EtSO₄], and (c) for [OMIM][EtSO₄].

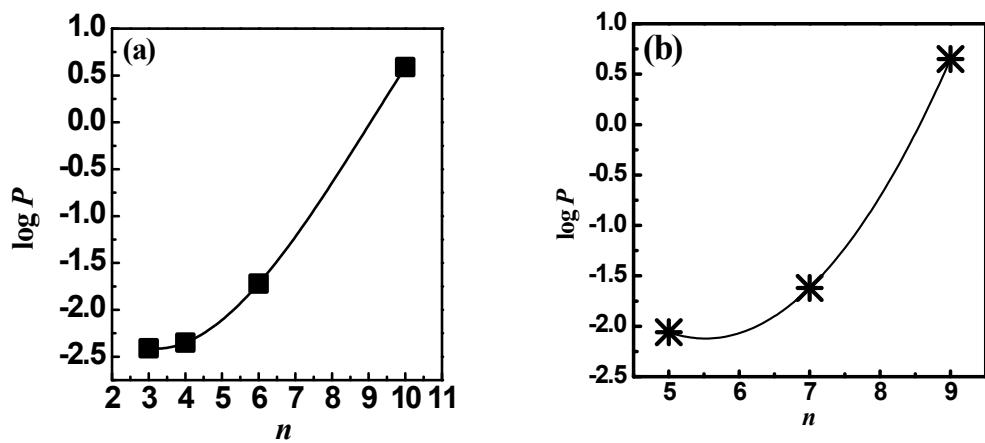


Fig. S2 Variation of $\log P$ with the number of carbon atoms in alkyl groups attached to the cationic ring of ionic liquids (a) [EtSO₄]⁻-based ionic liquids, and (b) [HSO₄]⁻-based ionic liquids.

Table S1. Apparent Partition Coefficient ($\log P$) Values of $[\text{EtSO}_4]^-$ -based Ionic Liquids as a Function of Concentration at 298 K.

Conc (M)/ (mol L ⁻¹)	Log P			
	[EMIM] [EtSO ₄]	[dEIM] [EtSO ₄]	[EBIM] [EtSO ₄]	[EOIM] [EtSO ₄]
0.01	-2.04 ± 0.13	-2.12 ± 0.08	-1.64 ± 0.02	0.19 ± 0.02
0.02	-2.41 ± 0.02	-2.35 ± 0.05	-1.72 ± 0.02	0.59 ± 0.05
0.03	-2.55 ± 0.05	-2.45 ± 0.03	-1.76 ± 0.00	0.95 ± 0.07
0.04	-2.62 ± 0.06	-2.51 ± 0.02	-1.84 ± 0.00	1.32 ± 0.03
0.05	-2.82 ± 0.03	-2.63 ± 0.03	-1.92 ± 0.00	1.65 ± 0.01

Table S2. Apparent Partition Coefficient ($\log P$) Values of $[\text{HSO}_4]^-$ -based Ionic Liquids as a Function of Concentration at 298 K.

Conc (M) / (mol L ⁻¹)	Log P		
	[Bmim][HSO ₄]	[HMIM][HSO ₄]	[OMIM][HSO ₄]
0.01	-2.01 ± 0.02	-1.76 ± 0.02	0.12 ± 0.02
0.02	-2.07 ± 0.03	-1.62 ± 0.02	0.66 ± 0.02
0.03	-2.11 ± 0.02	-1.69 ± 0.02	0.83 ± 0.04
0.04	-2.10 ± 0.00	-1.79 ± 0.01	0.69 ± 0.01
0.05	-2.09 ± 0.00	-1.87 ± 0.02	0.64 ± 0.02

Table S3. Apparent Partition Coefficient ($\log P$) Values of Pyridinium-based Ionic Liquids as a Function of Concentration at 298 K.

Conc (M) / (mol L ⁻¹)	Log P	
	[BPy][HSO ₄]	[OPy][HSO ₄]
0.01	-2.45 ± 0.02	-0.39 ± 0.02
0.02	-2.63 ± 0.01	0.20 ± 0.01
0.03	-2.51 ± 0.01	0.40 ± 0.07
0.04	-2.44 ± 0.00	0.86 ± 0.03
0.05	-2.42 ± 0.00	1.22 ± 0.09

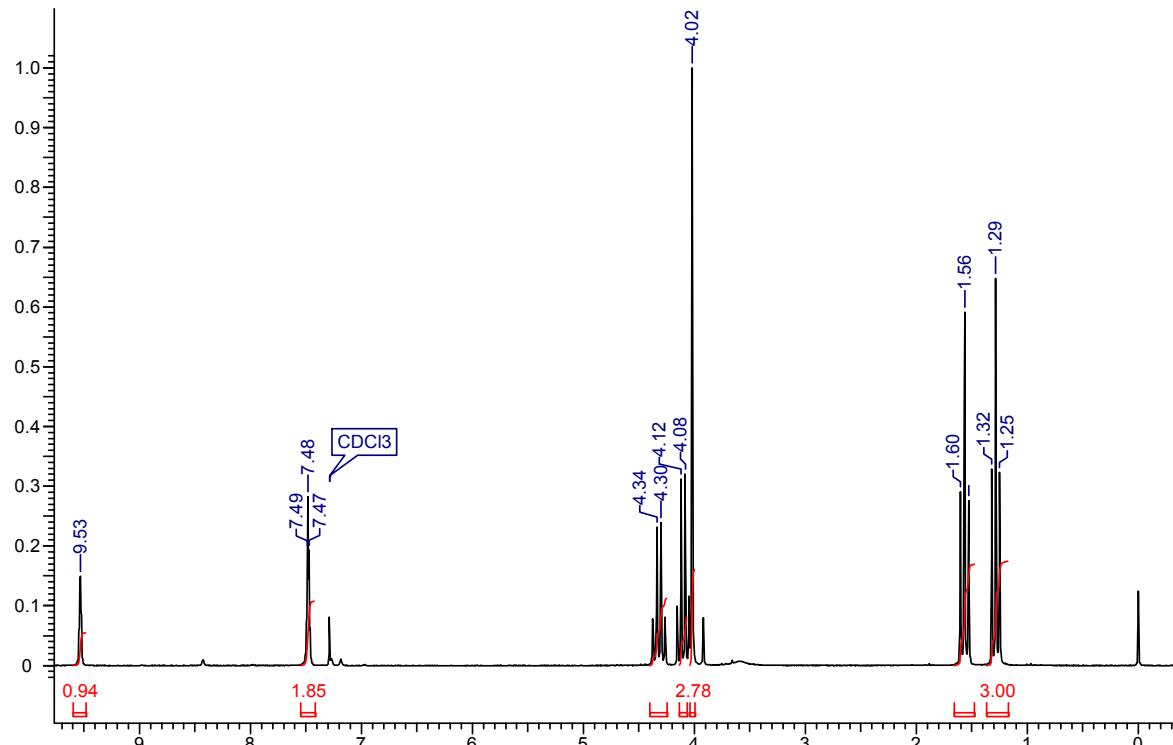
Table S4. Log P of Ionic Liquids having different Anion and Cationic Ring as a Function of Concentration at 298 K.

Conc (M)/ (mol L ⁻¹)	Log P			
	[Bmim] [HSO ₄]	[BMIM] [BuSO ₄]	[OMIM] [HSO ₄]	[OPy] [HSO ₄]
0.01	-2.01 ± 0.02	-0.59 ± 0.04	0.12 ± 0.02	-0.39 ± 0.02
0.02	-2.07 ± 0.03	-0.69 ± 0.05	0.66 ± 0.02	0.20 ± 0.01
0.03	-2.11 ± 0.02	-0.76 ± 0.03	0.83 ± 0.04	0.40 ± 0.07
0.04	-2.10 ± 0.00	-0.70 ± 0.03	0.69 ± 0.01	0.86 ± 0.03
0.05	-2.09 ± 0.00	-0.67 ± 0.02	0.64 ± 0.02	1.22 ± 0.09

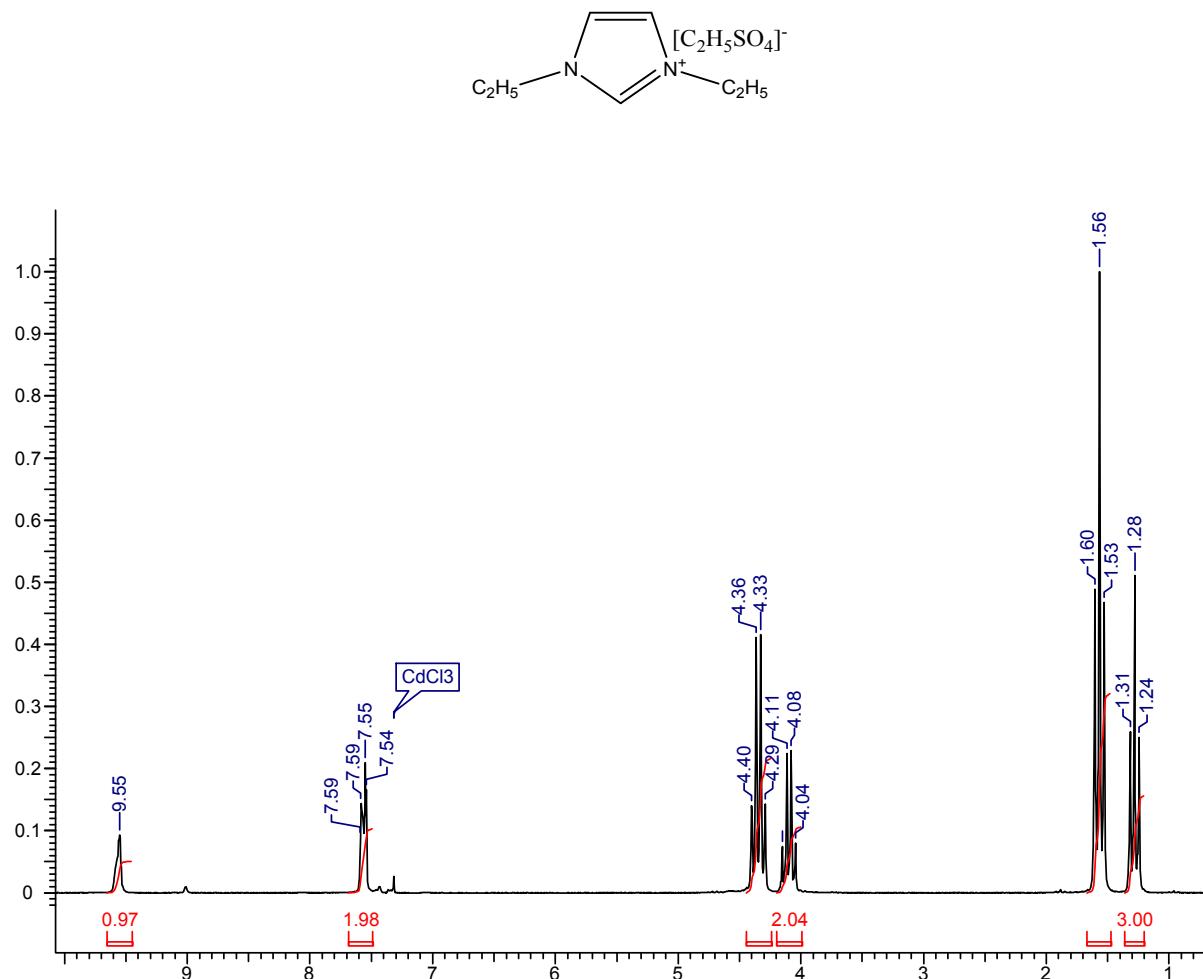
Table S5. Molar Absorption Coefficient Values of Ionic Liquids in Saturated *n*-Octanol and Saturated Water.

Name of ILs	ε in saturated <i>n</i> -octanol (mol ⁻¹ L cm ⁻¹)	ε in saturated water (mol ⁻¹ L cm ⁻¹)
[EMIM][EtSO ₄]	1570.00 ± 27.84	4115.4 ± 72.119
[dEIM][EtSO ₄]	2767.08 ± 139.46	4132.90 ± 113.92
[EBIM][EtSO ₄]	3955.08 ± 78.01	4227.08 ± 156.87
[EOIM][EtSO ₄]	3801.25 ± 74.19	3973.34 ± 91.18
[BMIM][HSO ₄]	3096.67 ± 124.98	-
[HMIM][HSO ₄]	4074.15 ± 212.87	-
[OMIM][HSO ₄]	4704.15 ± 299.31	-
[BMIM][BuSO ₄]	4280.42 ± 100.65	4151.25 ± 52.82
[BPy][HSO ₄]	4995.00 ± 155.38	4934.16 ± 225.02
[OPy][HSO ₄]	3455.00 ± 196.50	3287.08 ± 99.45

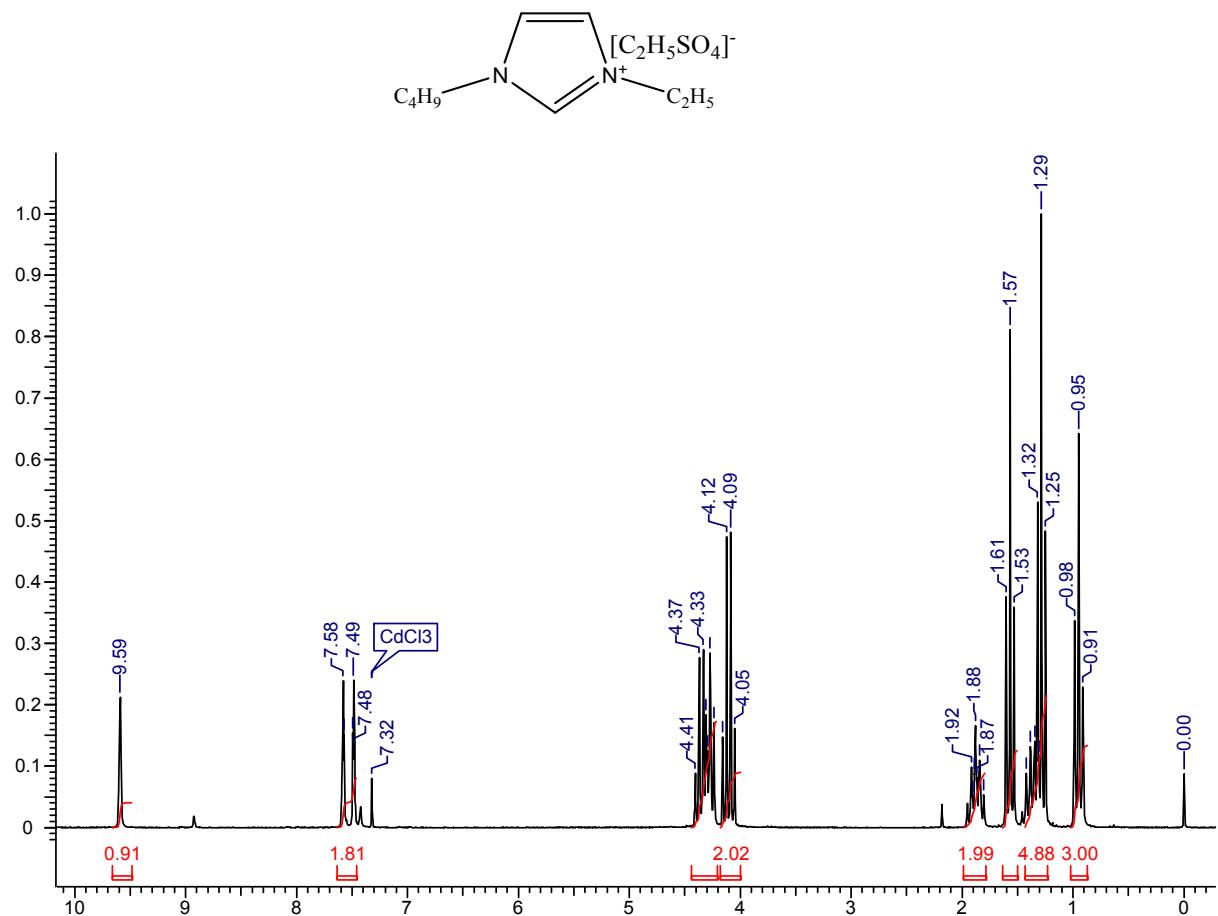
1. [EMIM][EtSO₄] - ¹H NMR, 200 MHz, CDCl₃



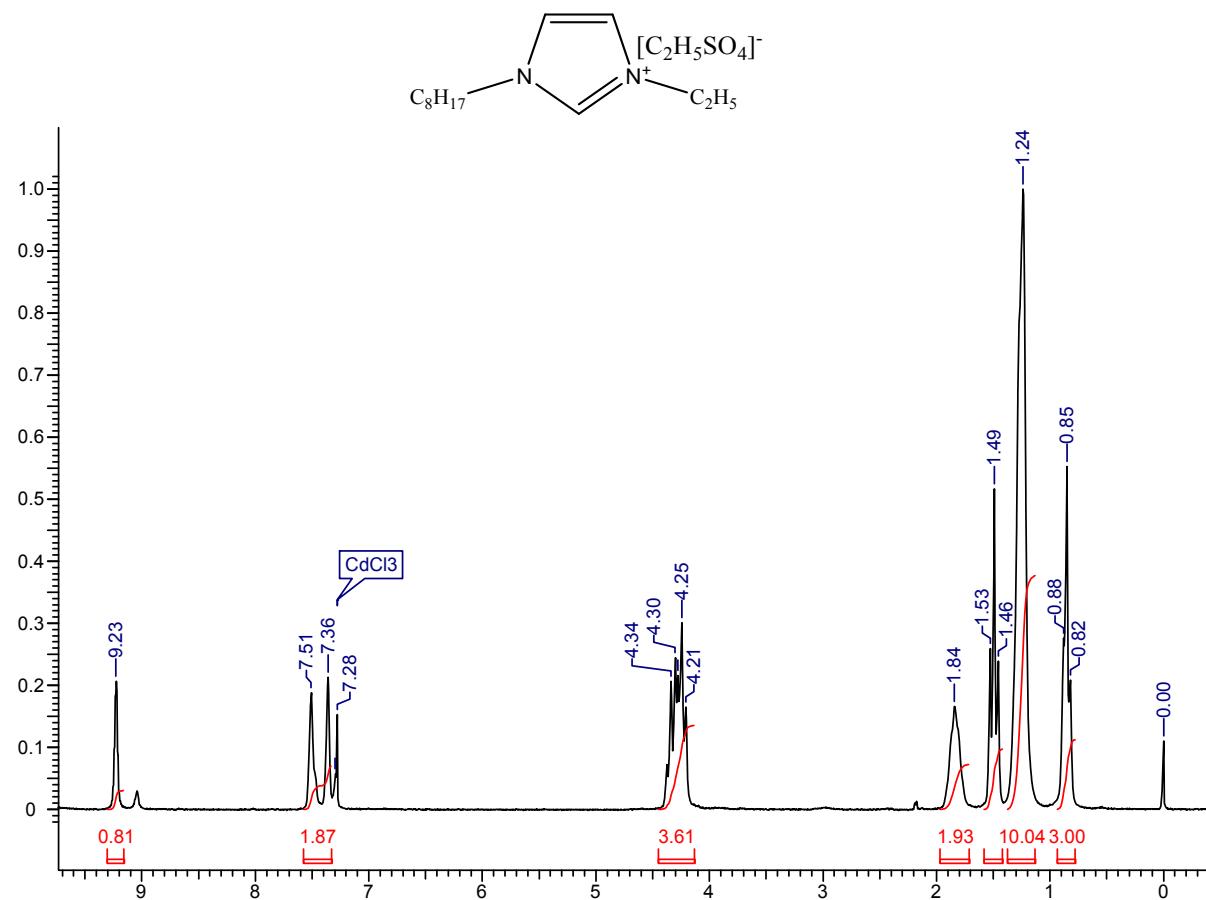
2. [dEIM][EtSO₄] - ¹H NMR, 200 MHz, CDCl₃



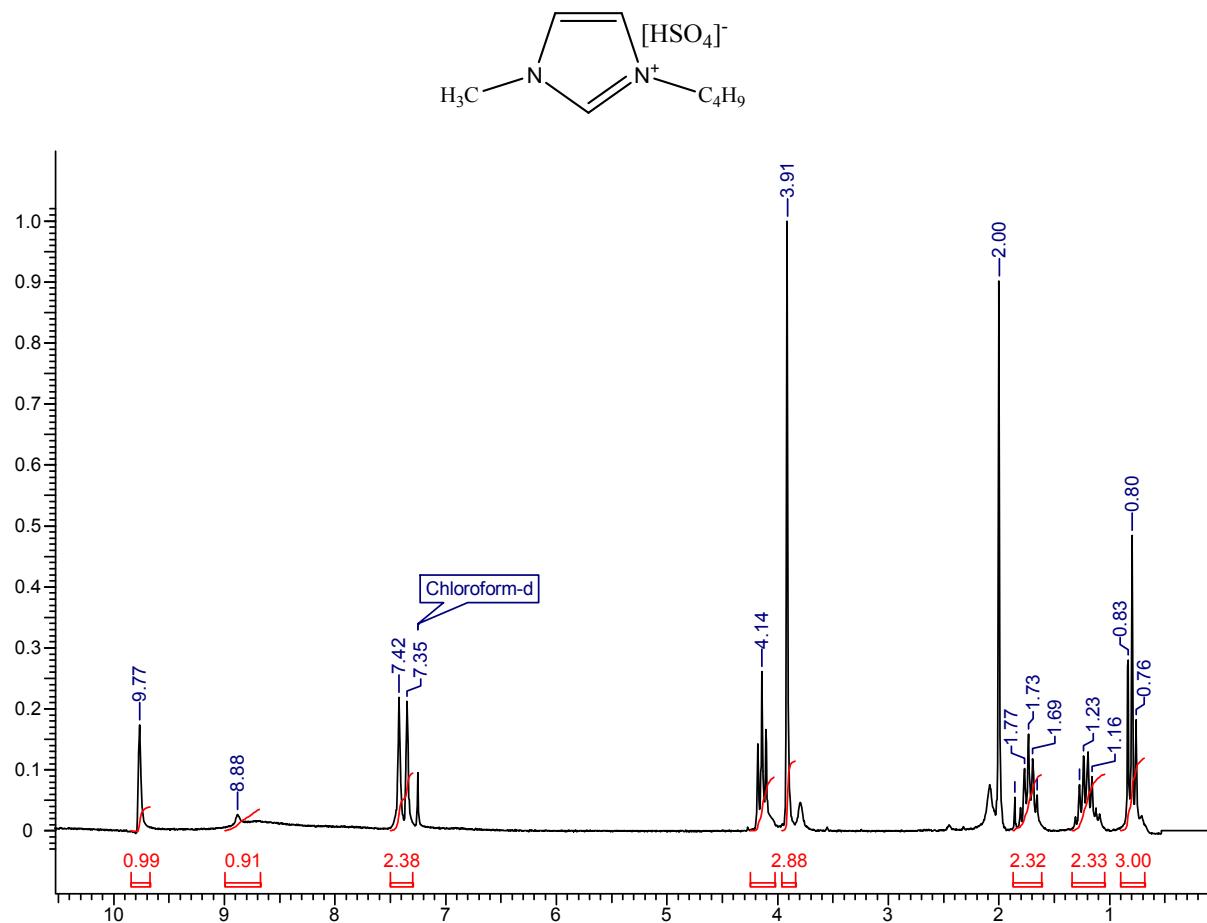
3. [EBIM][EtSO₄] - ¹H NMR, 200 MHz, CDCl₃



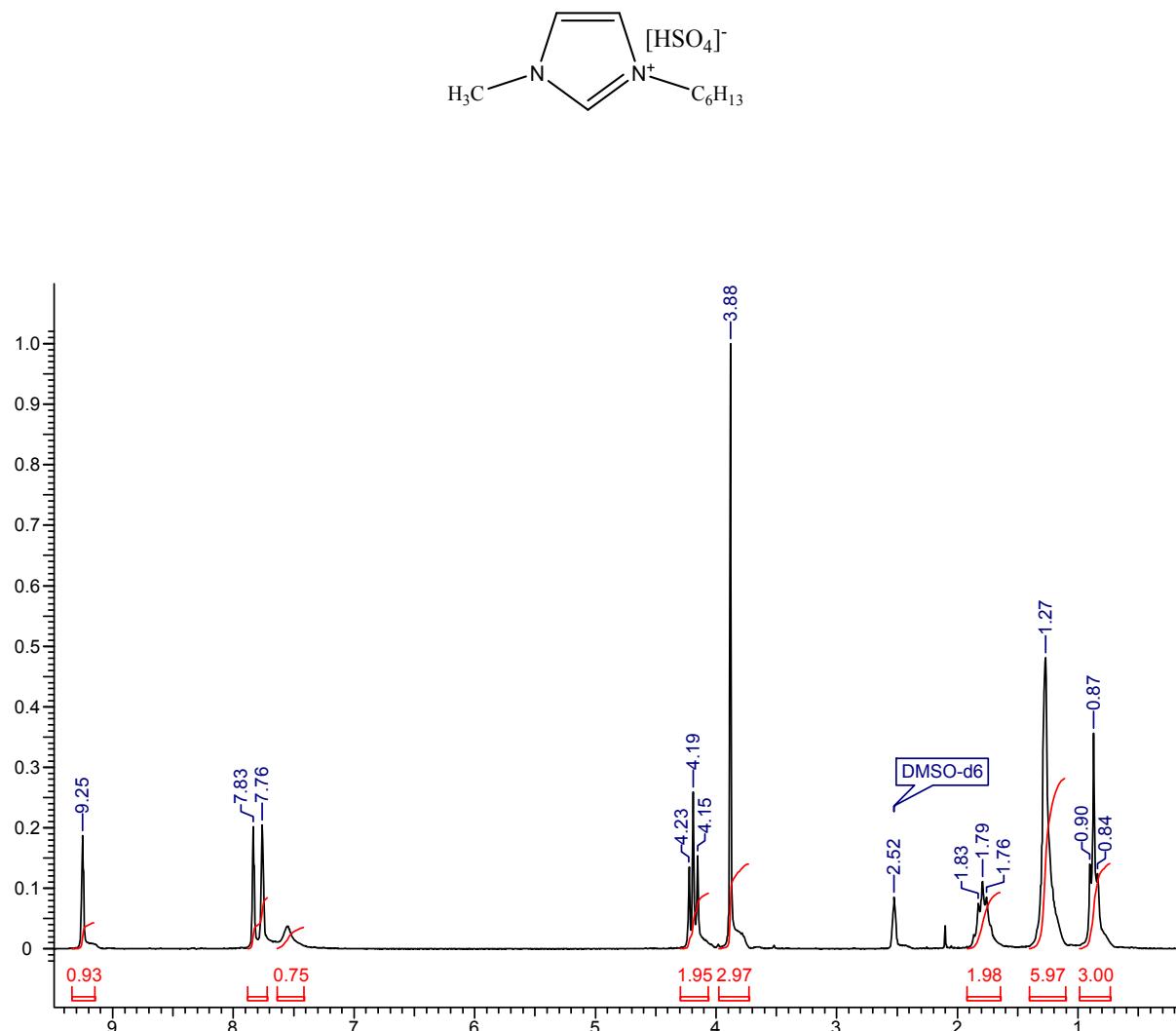
4. [EOIM][EtSO₄] - ¹H NMR, 200 MHz, CDCl₃



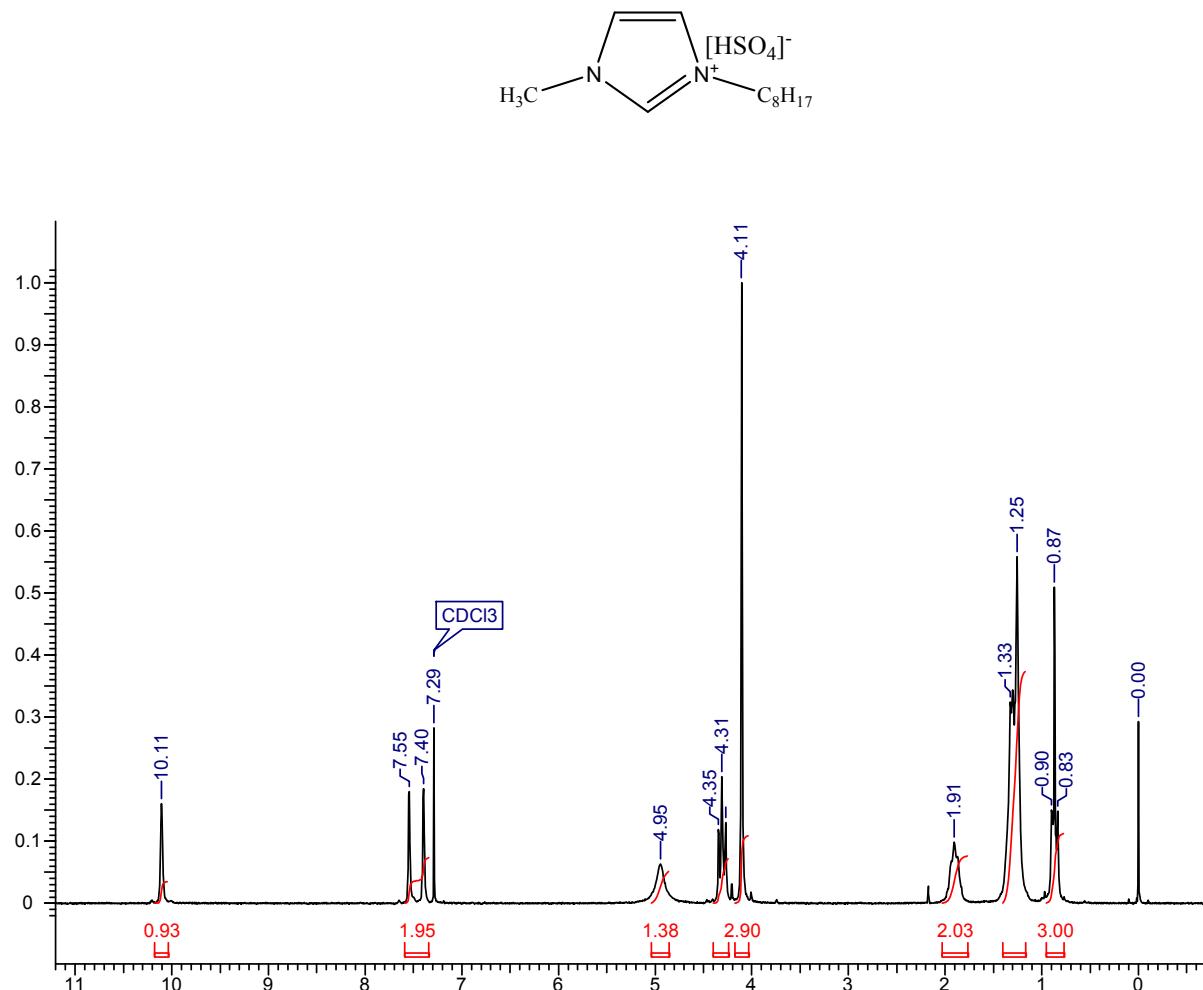
5. [BMIM][HSO₄] - ¹H NMR, 200 MHz, CDCl₃ +DMSO-d6



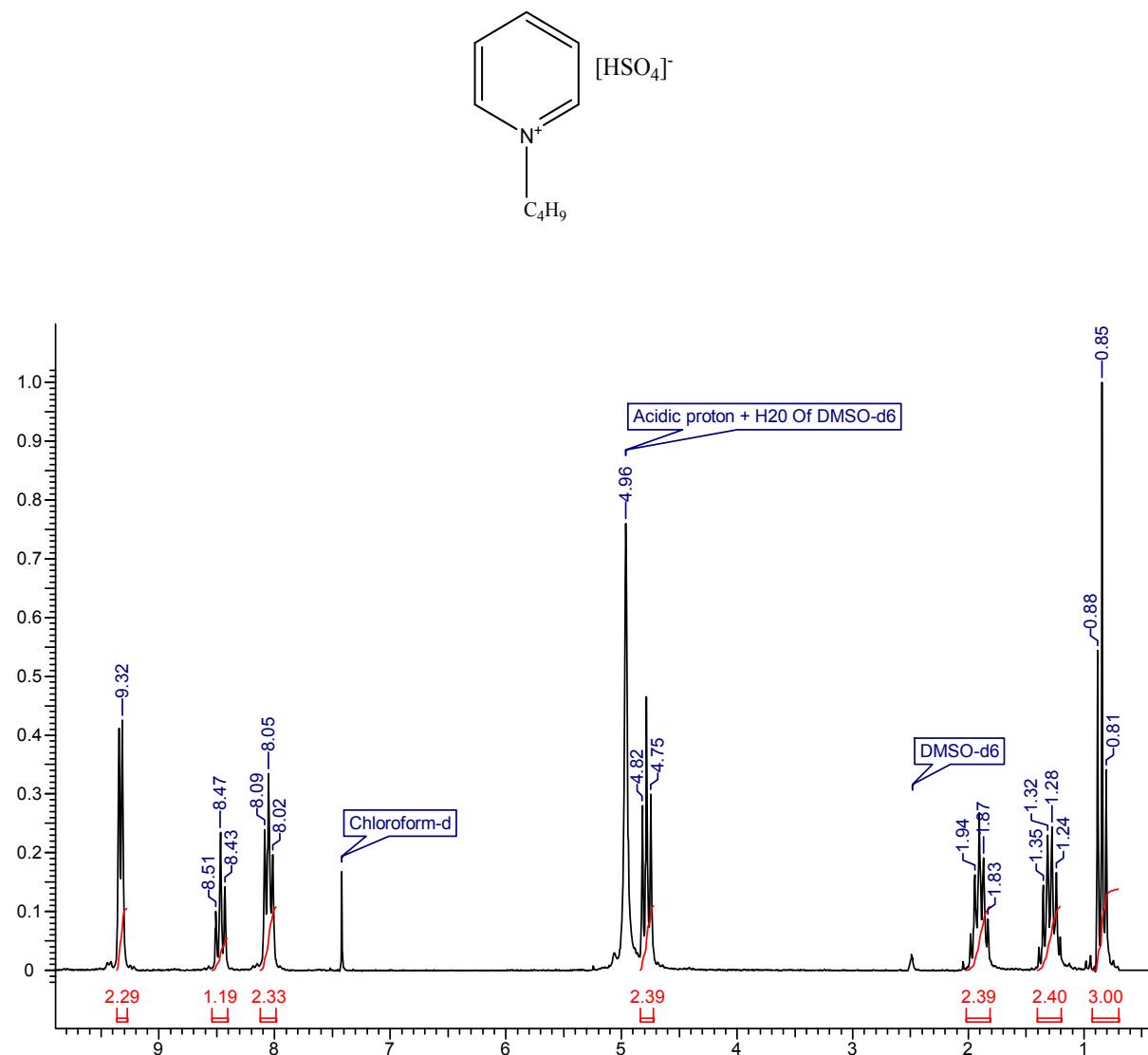
6. [HMIM][HSO₄] - ¹H NMR, 200 MHz, CDCl₃ +DMSO-d6



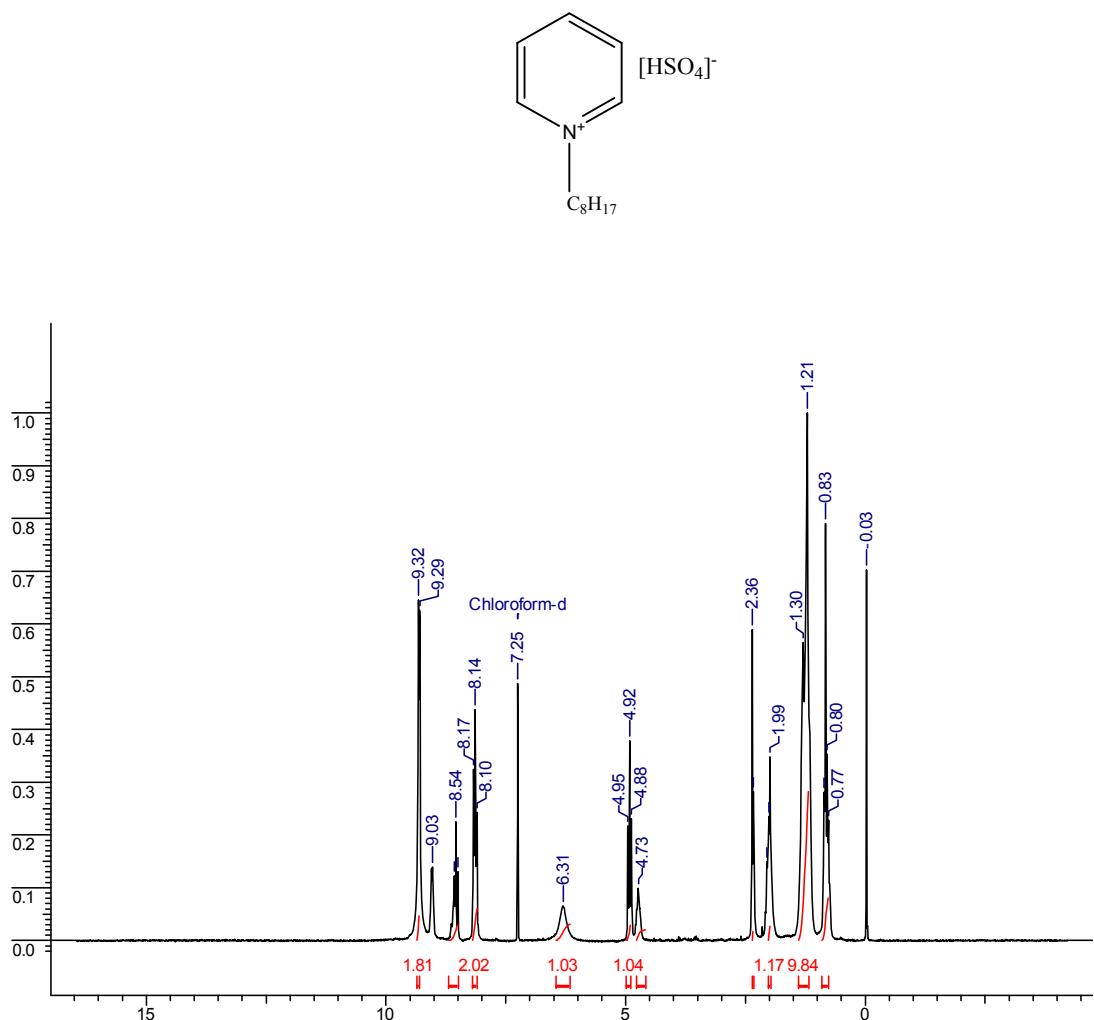
7. [OMIM][HSO₄] - ¹H NMR, 200 MHz, CDCl₃



8. [BPy][HSO₄] - ¹H NMR, 200 MHz, CDCl₃ +DMSO-d6



9. [OPy][HSO₄] - ¹H NMR, 200 MHz, CDCl₃



10. [BMIM][BuSO₄] - ¹H NMR, 200 MHz, CDCl₃ +DMSO-d6

