Supporting Information

Tuning Task-Specific Ionic Liquids for the Extractive Desulfurization of Liquid Fuel

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Table S1 Names, abbreviations, sources, and densities of ionic liquids

#	Name	Abbreviation	Source	Density, g/mL (1 atm, 25 ºC)
Imidazolium-based ILs				
1	1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[BMIM][Tf_2N]	Prepared by precipitation reaction[1] (see ESI[2])	1.44[3]
2	1-butyl-3-methylimidazolium bis(pentafluoroethylsulfonyl)imide	[BMIM][beti]	Prepared following ref. [4]	1.51[5]
3	1-butyl-3-methylimidazolium tetrafluoroborate	[BMIM][BF_4]	Alfa Aesar (L19087), 98+%	1.20[6]
4	1-butyl-3-methylimidazolium dicyanamide	[BMIM][dca]	Alfa Aesar (H59175), 97%	1.06[3]
5	1-butyl-3-methylimidazolium trifluoromethanesulfonate	[BMIM][OTf]	Alfa Aesar (L19765), 99%	1.30[7]
6	1-butyl-3-methylimidazolium thiocyanate	[BMIM][SCN]	Aldrich (724408), ≥95%	1.07[8]
7	1-butyl-3-methylimidazolium nitrate	[BMIM][NO_3]	Prepared by anion-exchange (see ESI[2])	1.16[9]
8	1-butyl-3-methylimidazolium methylsulfate	[BMIM][$MeSO_4$]	Alfa Aesar (H27754), 99%	1.21[10]
9	1-butyl-3-methylimidazolium dimethylphosphate	[BMIM][Me_2PO_4]	Prepared following Refs.[11, 12]	1.16[13]
10	1-butyl-3-methylimidazolium trifluoroacetate	[BMIM][CF_3COO]	Prepared by anion-exchange (see ESI[2])	1.21[14]
11	1-butyl-3-methylimidazolium acetate	[BMIM][OAc]	Prepared by anion-exchange[15] (see ESI[12])	1.05[16]
12	1-butyl-3-methylimidazolium formate	[BMIM][HCOO]	Prepared by anion-exchange[15] (see ESI[12])	0.94 [a]
13	1-butyl-3-methylimidazolium 1-butanesulfonate	[BMIM][$BuSO_3$]	Prepared following	1.26 [a]

			ref.[4]	
14	1-butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	[BMIM][$Me(OCH_2CH_2)_2SO_4$]	Sigma-Aldrich (67421), ≥95.0%	1.18[17]
15	1-ethyl-3-methylimidazolium hydrogensulfate	[EMIM][HSO_4]	Fluka (56486), ≥95%	–[b]
16	1-ethyl-3-methylimidazolium acetate	[EMIM][OAc]	Prepared by anion-exchange[15] (see ESI[12])	1.11[18]
17	1-hexyl-3-methylimidazolium acetate	[HMIM][OAc]	Prepared by anion-exchange[15] (see ESI[12])	1.05[a]
18	1-hexyl-3-methylimidazolium hexafluorophosphate	[HMIM][PF_6]	Prepared following ref.[4]	1.29[19]
19	1-methyl-3-octylimidazolium tetrafluoroborate	[OMIM][BF_4]	Prepared by anion-exchange (see ESI[2])	1.11[20]
20	1-benzyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[BzMIM][Tf_2N]	Prepared by following ref.[21]	1.49[22]
21	1-(cyclohexylmethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[ChxmMIm][Tf_2N]	Prepared by following ref.[21]	1.42[22]
Pyridinium-based ILs				
22	1-hexylpyridinium bis(triflurommethylsulfonyl)imide	[C_6Py][Tf_2N]	Prepared following ref.[23]	1.39[24]
23	1-hexylpyridinium thiocyanate	[C_6Py][SCN]	Additional details provided below	1.07[a]
24	1-hexylpyridinium dicyanamide	[C_6Py][dca]	Prepared following ref.[25]	1.11[a]
25	1-octylpyridinium bis(trifluoromethylsulfonyl)amide	[C_8Py][Tf_2N]	Prepared following ref.[26]	1.33[27]
26	1-dodecylpyridinium bis(trifluoromethylsulfonyl)imide	[C_{12}Py][Tf_2N]	Prepared following ref.[28]	1.25[27]
27	1-benzylpyridinium bis(trifluoromethylsulfonyl)imide	[BzPy][Tf_2N]	Prepared by following ref.[21]	1.44[a]
28	1-(cyclohexylmethyl)pyridinium bis(trifluoromethylsulfonyl)imide	[ChxmPy][Tf_2N]	Prepared by following ref.[21]	1.26[a]

Ammonium-based ILs				
29	cholinium bis(trifluoromethylsulfonyl)imide	[Choline][Tf_2N]	Prepared by precipitation reaction[1] (see ESI[2])	1.53 [a]
30	tributylmethylammonium bis(trifluoromethylsulfonyl)imide	[N4441][Tf_2N]	Prepared following ref.[29]	1.26[30]
31	hexyltrimethylammonium bis(trifluoromethylsulfonyl)imide	[N6111][Tf_2N]	Prepared following ref.[29]	1.31[29]
32	methyltrioctylammonium bis(trifluoromethylsulfonyl)imide	[N8881][Tf_2N]	Prepared following ref.[29]	1.08[29]
33	decyltrimethylammonium bis(trifluoromethylsulfonyl)imide	[N10,111][Tf_2N]	Prepared following ref.[29]	1.23[29]
34	isopropyldimethylpropylammonium bis(trifluoromethylsulfonyl)imide	[C_3Me_2iPrN][Tf_2N]	Prepared following ref.[31]	1.38 [a]
35	isopropyldimethyl(3-bromopropyl)ammonium bis(trifluoromethylsulfonyl)imide	[N11iPrC_3Br][Tf_2N]	Prepared following ref.[31]	1.47 [a]
36	(*n*-hexyl)isopropyldimethylammonium bis(trifluoromethylsulfonyl)imide	[C_6Me_2iPrN][Tf_2N]	Prepared following ref.[31]	1.16 [a]
37	(3-chloro-2-hydroxypropyl)trimethylammonium bis(trifluoromethylsulfonyl)imide	[3Cl_2OHPropN111][Tf_2N]	Metathesis of commercial chloride salt (Sigma-Aldrich, 348287) using reported methods[4]	1.21 [a]
38	silver(I)/*n*-propylamine bis(trifluoromethylsulfonyl)imide	[Ag(*n*-$PrNH_2)_2$][Tf_2N]	Prepared following ref.[32]	1.46 [a]
39	silver(I)/isopropylamine bis(trifluoromethylsulfonyl)imide	[Ag(*i*-$PrNH_2)_2$][Tf_2N]	Prepared following ref.[32]	1.61 [a]
Pyrrolidinium-based ILs				
40	1-methyl-1-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_3MPyrr][Tf_2N]	Prepared following ref.[31]	1.41 [a]
41	1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_4MPyrr][Tf_2N]	Prepared following ref.[31]	1.39[33]
42	1-methyl-1-pentylpyrrolidinium	[C_5MPyrr][Tf_2N]	Prepared following	1.36[34]

	bis(trifluoromethylsulfonyl)imide		ref.[31]	
43	1-hexyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_6MPyrr][Tf_2N]	Prepared following ref.[31]	1.34[35]
44	1-methyl-1-octylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_8MPyrr][Tf_2N]	Prepared following ref.[31]	1.21 [a]
45	1-decyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_{10}MPyrr][Tf_2N]	Prepared following ref.[31]	1.27 [a]
46	1-dodecyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_{12}MPyrr][beti]	Prepared following ref.[31]	– [b]
47	1-butyl-1-methylpyrrolidinium tetracyanoborate	[C_4MPyrr][$B(CN)_4$] [c]	EMD Chemicals Inc., 99%	0.98 (20 ºC),[36] 1.01 [a]
48	1-(cyclohexylmethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[ChxmMPyrr][Tf_2N]	Prepared by following ref.[21]	1.42 [a]
Phosphonium-based ILs				
49	trihexyltetradecylphosphonium bis(pentafluoroethylsulfonyl)imide	[P14,666][beti]	Prepared by ion exchange[37]	1.07 [a]
50	trihexyltetradecylphosphonium L-lactate	[P14,666][L-Lact]	Prepared by ion exchange[37]	– [b]
51	trihexyltetradecylphosphonium perfluoropentanoate	[P14,666][$C_4F_9CO_2$]	Prepared by ion exchange[37]	1.09 [a]
Other types of ILs				
52	1-butyl-1-methylpiperidinium bis(trifluoromethanesulfonyl)imide	[C_4MPip][Tf_2N]	Prepared following an earlier study[4]	1.38[38]
53	Lithium(triglyme) bis(trifluoromethanesulfonyl)imide	[Li(G3)][Tf_2N]	Prepared as reported previously[39]	1.51 [a]
54	1-octyl-1,4-diazabicyclo[2.2.2]octan-1-ium bis(trifluoromethylsulfonyl)imide	[DAB8][Tf_2N]	Additional details provided below	– [b]
55	2,3,4,6,7,8-hexahydropyrrolo[1,2-*a*]pyrimidinium acetate	[DBNH][OAc]	Prepared following an earlier study[40]	1.23 [a]
56	2,3,4,6,7,8-hexahydropyrrolo[1,2-*a*]pyrimidinium trifluoroacetate	[DBNH][CF_3COO]	Prepared following an earlier study[40]	1.30 [a]
57	*N*,*N*,*N*',*N*'-tetramethyl-*N*''-ethylguanidinium	[Me_4Etguan][FAP]	EMD Chemicals	1.66 [a]

	tris(perfluoroethyl)trifluorophosphate		Inc., 98%	
Deep eutectic solvents (DES)				
58	Choline chloride/glycerol (1:2)	Choline chloride/glycerol (1:2)	Prepared following our earlier study[41]	1.18 (20 ºC)[42]
59	Choline acetate/glycerol (1:1.5)	Choline acetate/glycerol (1:1.5)	Prepared following our earlier study[41]	– [b]
Alkoxy- or hydroxy-functionalized ILs				
60	1-(2-hydoxyethyl)-3-methylimidazolium bis(trifluoromethanesulfonyl)imide	[HO-EMIM][Tf_2N]	Prepared following ref.[31]	1.63 [a]
61	1-(2-methoxyethyl)-3-methylimidazolium bis(trifluoromethanesulfonyl)imide	[$MeOCH_2CH_2$-MIM][Tf_2N]	Prepared following ref.[31]	1.59 [a]
62	1-ethyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)imidazolium bis(trifluoromethanesulfonyl)imide	[$Me(OCH_2CH_2)_3$-Et-Im][Tf_2N]	Prepared in our earlier studies[2, 12]	1.20 [a]
63	1-butyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)imidazolium acetate	[$Me(OCH_2CH_2)_3$-Bu-Im][OAc]	Prepared in our earlier studies[2, 12]	1.15 [a]
64	1-ethyl-3-(2-(2-methoxypropyloxy)propyloxy)propyl)imidazolium acetate	[$Me(OPr)_3$-Et-Im][OAc]	Prepared in our earlier studies[2, 12]	1.07 [a]
65	triethyl (2-(2-methoxyethoxy)ethoxy)ethylammonium acetate	[$Me(OCH_2CH_2)_3$-Et_3N][OAc]	Prepared in our earlier studies[2, 12]	1.10 [a]
66	triethyl (2-(2-methoxyethoxy)ethoxy)ethylammonium bis(trifluoromethanesulfonyl)imide	[$Me(OCH_2CH_2)_3$-Et_3N][Tf_2N]	Prepared in our earlier studies[2, 12]	1.36 [a]
67	triethyl (2-(2-methoxyethoxy)ethoxy)ethylammonium formate	[$Me(OCH_2CH_2)_3$-Et_3N][HCOO]	Prepared in our earlier studies[2, 12]	1.08 [a]
68	triethyl (2-(2-methoxyethoxy)ethoxy)ethylammonium bromide	[$Me(OCH_2CH_2)_3$-Et_3N]Br	Prepared in our earlier studies[2, 12]	1.29 [a]
69	1-ethyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)piperidinium acetate	[$Me(OCH_2CH_2)_3$-Et-Pip][OAc]	Prepared in our earlier studies[2, 12]	1.08 [a]
70	1-ethyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)piperidinium bis(trifluoromethanesulfonyl)imide	[$Me(OCH_2CH_2)_3$-Et-Pip][Tf_2N]	Prepared in our earlier studies[2, 12]	1.40 [a]

71	1-ethyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)piperidinium bromide	$[Me(OCH_2CH_2)_3\text{-Et-Pip}]Br$	Prepared in our earlier studies[2, 12]	1.23 [a]
72	(2-hydroxyethyl)dimethylammonium acetate	$[Me_2NH(CH_2CH_2OH)][OAc]$	Bioniqs (York, UK), batch #07/10232	1.23 [a]
73	bis(2-methoxyethyl)ammonium acetate	$[(CH_3OCH_2CH_2)_2NH_2][OAc]$	Bioniqs (York, UK), batch #07/10233	1.10 [a]

Note: [a] The density at 20 °C was estimated in this study following these procedures: a small vial containing IL was placed on a balance which was then zeroed; the vial was removed from the balance, and 50 μL of IL was withdrawn using a pipette; the vial was placed back to the balance to determine the mass loss due to IL removal; the density was calculated using the mass loss and the volume (50 μL). [b] The density cannot be determined by the method described above; in this case, the IL is too viscous and volumetric withdrawal using a micropipette is not reproducible. Therefore, the density was assumed to be 1.2 g mL^{-1} for the purposes of calculating the Nernst sulfur partition coefficient. [c] This IL (**47**) tends to crystallize at room temperature over time; suggesting that its fluid state is a supercooled liquid.

Additional Synthetic Details:

1-hexylpyridinium thiocyanate, $[C_6Py][SCN]$: In a 100 mL round bottom flask, 5 g (20.5 mmol) of $[C_6Py][Br]$ was dissolved in 25 mL of dry acetone, followed by addition of 2.42 g (1.0 eq) of potassium thiocyanate (KSCN) which resulted in a white, milky suspension. After stirring the reaction for 2 days, the white suspension was allowed to settle overnight and then stored in a freezer for 24 h. The reaction was filtered via gravity filtration to remove NaBr. The filtrate was collected and the solvent removed by rotary evaporation to give a slightly yellow liquid. ^1H NMR (500 MHz, $CDCl_3$): δ 9.57 (d, 2H), 8.52 (t, 1H), 8.14 (t, 2H), 4.99 (t, 2H), 2.03 (m, 2H), 1.33 (m, 2H), 1.27 (m, 4H), 0.82 (t, 3H).

1-octyl-1,4-diazabicyclo[2.2.2]octan-1-ium bis(trifluoromethylsulfonyl)imide, $[DAB8][Tf_2N]$: In a 100 mL round bottom flask, 5 g (16.3 mmol) of [DAB8][Br] was dissolved in 25 mL of deionized water, followed by addition of 4.70 g (1.0 eq) of lithium bis(trifluoromethylsulfonyl)imide ($LiTf_2N$) which resulted in the formation of a dense colorless bottom liquid phase. The reaction was washed with water five times and dried under vacuum for 2 days. ^1H NMR (500 MHz, D_2O): δ 3.21 (m, 14 H), 1.70 (m, 2H), 1.30 (m, 10 H), 0.87 (t, 3H).

Table S2 Miscibility between selected ILs and *n*-octane or *n*-dodecane

#	IL	***n*-octane**	***n*-dodecane**
4	[BMIM][dca]	Im	Im
6	[BMIM][SCN]	Im	Im
22	[C_6Py][Tf_2N]	Im	Im
23	[C_6Py][SCN]	Im	Im
25	[C_8Py][Tf_2N]	Im	Im
26	[C_{12}Py][Tf_2N]	Im	Im
29	[Choline][Tf_2N]	Im	M
30	[N4441][Tf_2N]	Im	M
31	[N6111][Tf_2N]	Im	M
32	[N8881][Tf_2N]	Im	M
33	[N10,111][Tf_2N]	Im	M
38	[Ag(*n*-PrNH_2)$_2$][Tf_2N]	Im	M
39	[Ag(*i*-PrNH_2)$_2$][Tf_2N]	Im	M
40	[C_3MPyrr][Tf_2N]	Im	M
41	[C_4MPyrr][Tf_2N]	Im	M
42	[C_5MPyrr][Tf_2N]	Im	M
43	[C_6MPyrr][Tf_2N]	Im	M
44	[C_8MPyrr][Tf_2N]	Im	M
45	[C_{10}MPyrr][Tf_2N]	Im	M
46	[C_{12}MPyrr][beti]	Im	M
47	[C_4MPyrr][B(CN)$_4$]	Im	Im
48	[ChxmMPyrr][Tf_2N]	Im	Im
49	[P14,666][beti]	M	M
50	[P14,666][L-Lact]	M	M
51	[P14,666][$C_4F_9CO_2$]	M	M
64	[Me(OPr)$_3$-Et-Im][OAc]	Im	Im
67	[Me(OCH_2CH_2)$_3$-Et$_3$N][HCOO]	Im	Im
68	[Me(OCH_2CH_2)$_3$-Et$_3$N]Br	Im	Im
73	[(CH_3OCH_2CH_2)$_2$NH_2][OAc]	Im	Im

Note: Im = immiscible, M = miscible.

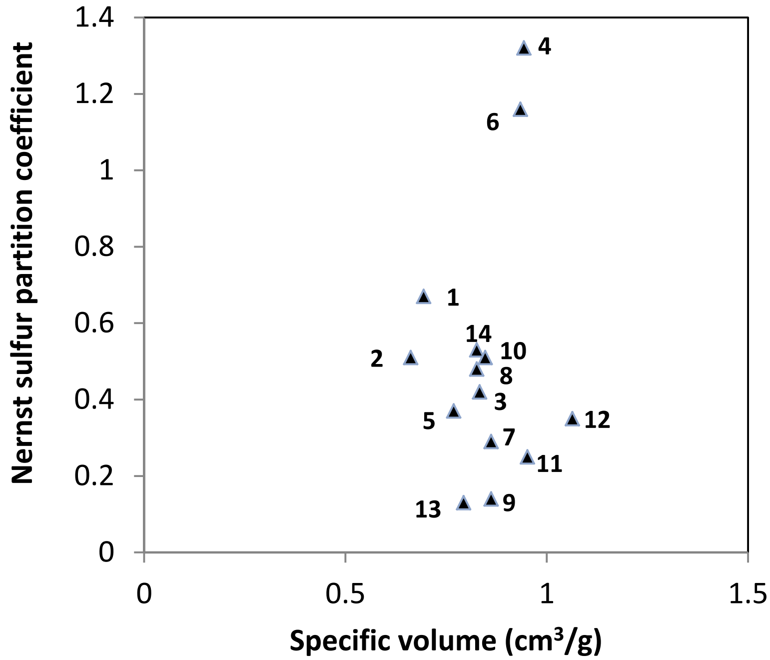

Figure S1. Correlation between the DBT partition coefficient and the specific volume of the ILs (specific volume = 1/density).

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