Supporting Information for publication

Separation of benzene and cyclohexane using deep eutectic solvents with aromatic structure

Mohamed K. Hadj-Kali[1,*], M. Zulhaziman M. Salleh[2,*], Irfan Wazeer[1], Ahmad Alhadid[3], Sarwono Mulyono[1]

[1] Chemical Engineering Department, King Saud University, P.O. Box 800, Riyadh 11421, Saudi Arabia
[2] Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, 43600 Bangi, Selangor, Malaysia
[3] Biothermodynamics, TUM School of Life Sciences, Technical University of Munich, Maximus-von-Imhof-Forum 2, D-85354 Freising, Germany

*Corresponding Authors: mhadjkali@ksu.edu.sa; zulhaziman@ukm.edu.my

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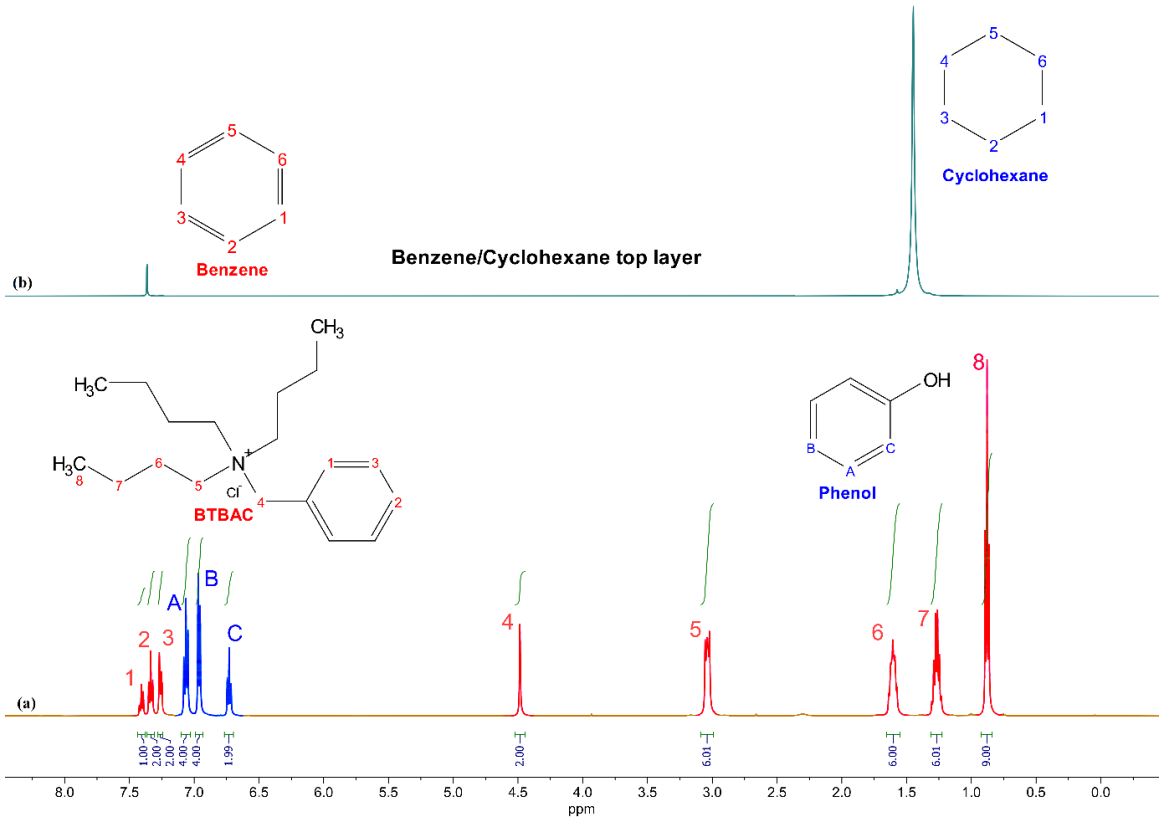

Figure S1. ^{1}H NMR spectra in $CDCl_3$: (a) pure BTBACl:Ph (1:2) DES; (b) top layer.

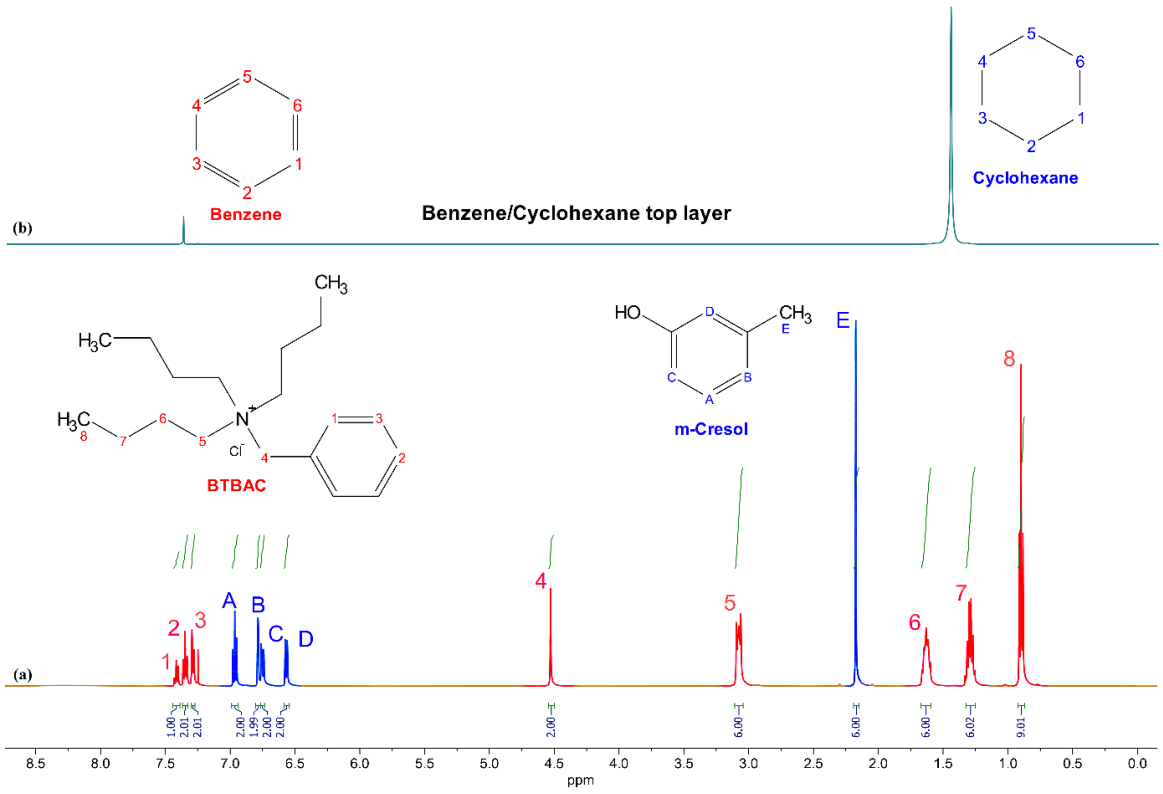

Figure S2. ^{1}H NMR spectra in $CDCl_3$: (a) pure BTBACl:Cre (1:2) DES; (b) top layer.

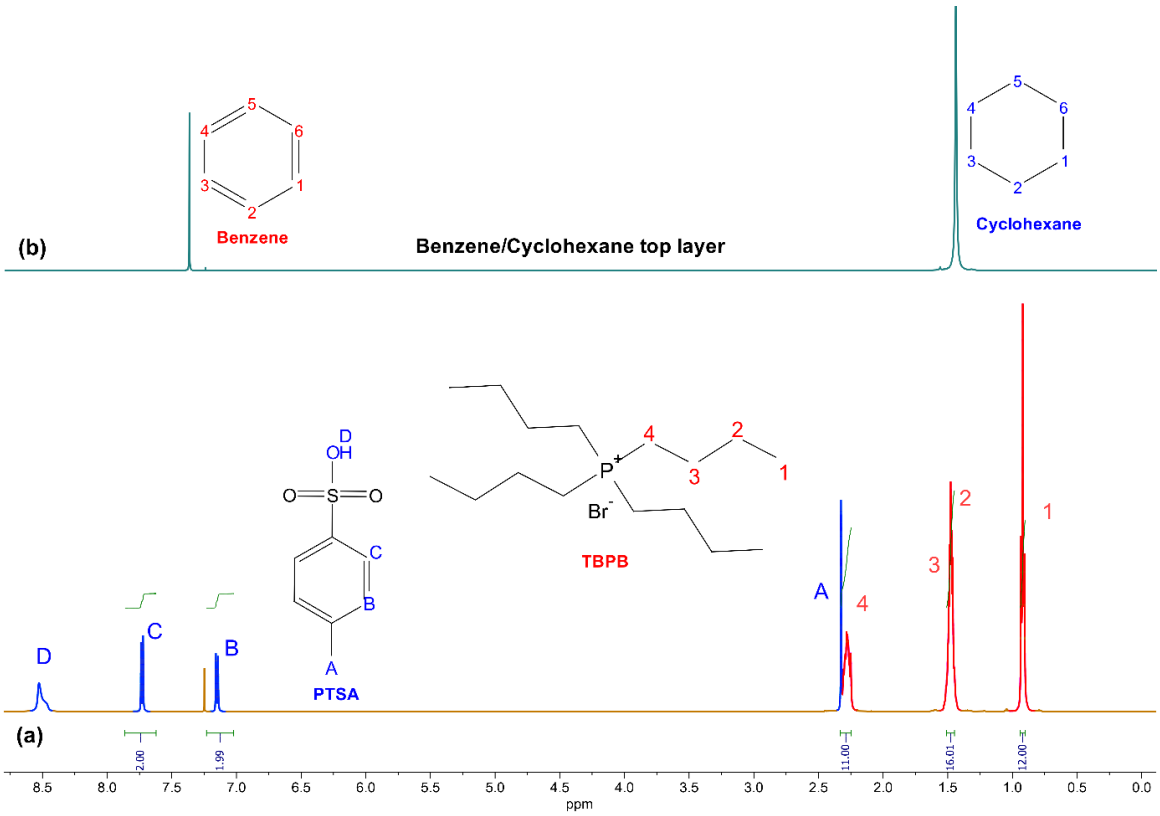

Figure S3. ^{1}H NMR spectra in $CDCl_3$: (a) pure TBPB:PTSA (1:1) DES; (b) top layer.

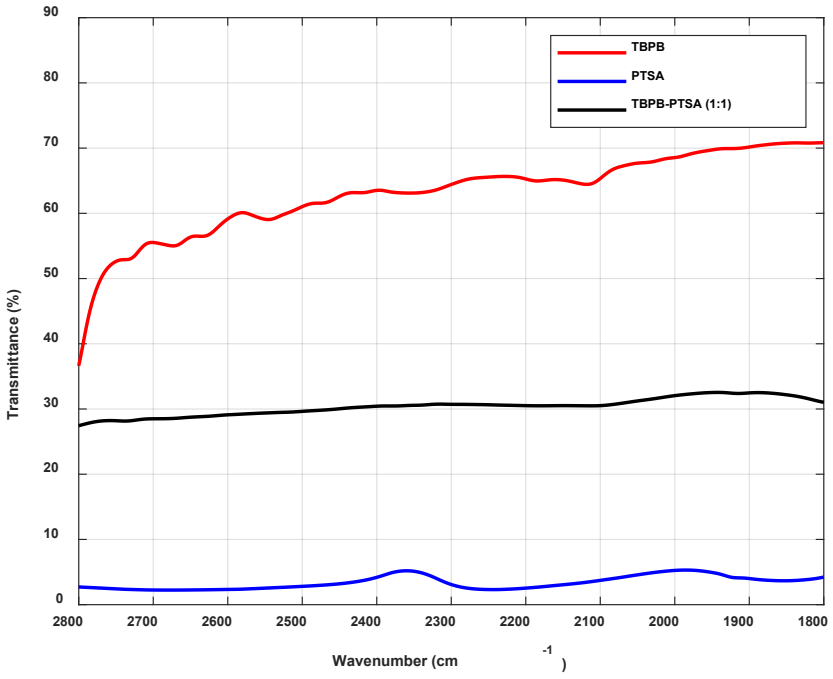

Figure S4: FTIR analysis for DES TBPB:PTSA (1:1). Red line indicates the tetrabutylphosphonium salt, blue indicates p-toluenesulfonic acid and black indicates the DES.

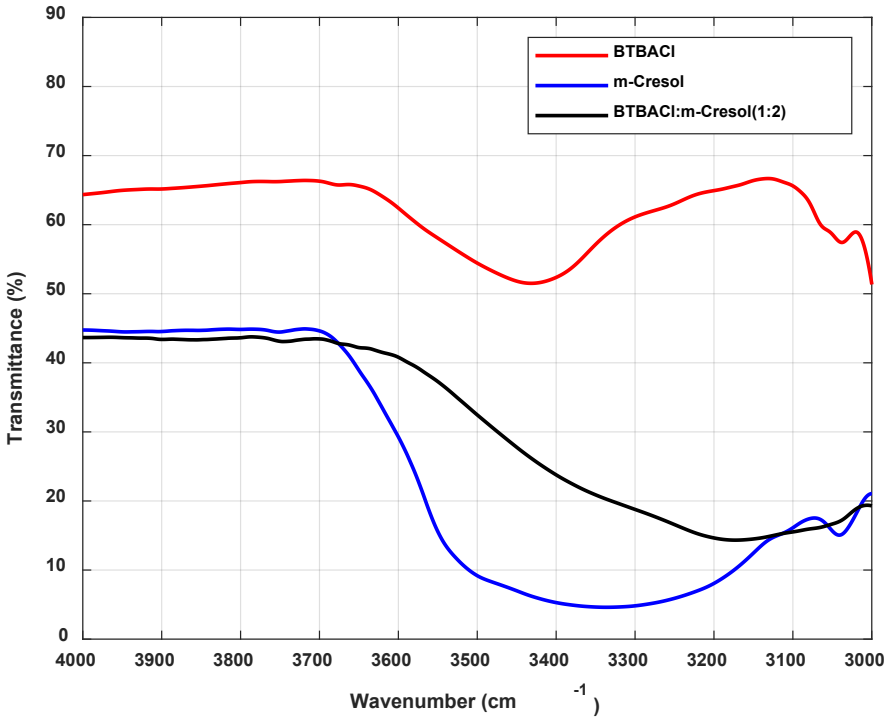

Figure S5: FTIR analysis for DES BTBACl:m-cresol (1:2). Red line indicates benzyltributylammonium chloride, blue indicates m-cresol and black indicates the DES.

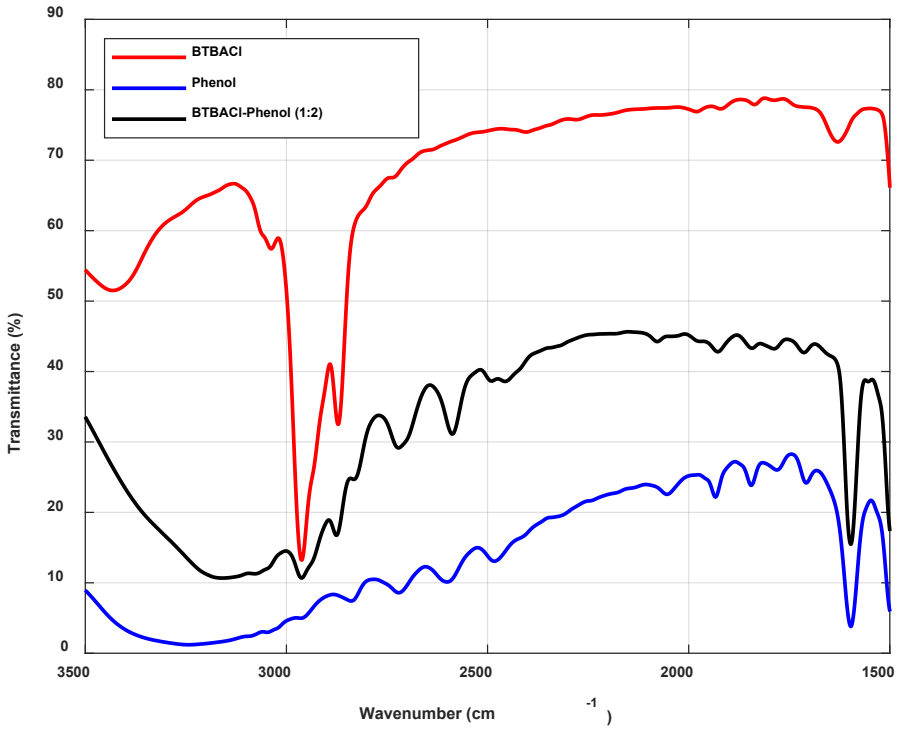

Figure S6: FTIR analysis for DES BTBACl:phenol (1:2). Red line indicates benzyltributylammonium chloride, blue indicates phenol and black indicates the DES.

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Table S1. Some examples of DESs applications in various fields.

Application	Analyte/system	DESs	Refs.
Separation and CO_2 capture			
Liquid-liquid extraction	Heptane/ethaline mixture, removal of volatile fatty acids from aqueous solutions, removal of pertechnate in aqueous media	ChCl[1]:glycerol (1:2), ChCl: levulinic acid (1:2), ChCl:EG[2] (1:2), MTOAC[3]:DA[4] (1:2), MTOB[5]: DA (1:2)	[1-3]
Metal extraction	Removal of various metals including indium, boron, copper, cobalt, manganese, cobalt, nickel and lithium	DA:lidocaine (2:1), thymol: 1-decanol (2:1), thymol:MPD[6] (2:1), menthol: 1-decanol (2:1), menthol:MPD (2:1)	[4-7]
CO_2 capture	solubilization of CO_2	Betaine:lactic acid (1:1), ChCl:guaiacol (1:1), MTPPB[7]/glycerol (1:3), ChCl:urea (1:2), ChCl:EG (1:2)	[8-12]
Electrodeposition			
ionometallurgy	Recovery of gold, tellurium, sulphides and tellurides	ChCl:EG (1:2)	[13]
electrodeposition	electrodeposition of zinc, tin, indium, cobalt, nickel and Samarium	ChCl:EG (1:2), ChCl:urea (1:2)	[14-19]
metal oxides solubility	Various metal oxides	ChCl:EG (1:2), ChCl:urea (1:2), ChCl:malonic acid (1:1)	[20]
Nanotechnology			
Synthesis of nanoparticles	Gold nanoparticles	ChCl:urea (1:2)	[21]
Synthesis of nanoparticles	CuCl nanoparticles	ChCl:urea (1:2)	[22]
Synthesis of nanocrystals	Silver nanocrystals	silver triflate:acetamide (1:4)	[23]
Organic chemistry			
Biochemistry	Glycerol extraction from biodiesel	ChCl:glycerol (1:2), MTPPB:EG (1:3)	[24, 25]
Enzymatic biodiesel production	Triglyceride conversion of miglyol oil	ChCl:urea (1:2), ChCl:glycerol (1:2)	[26, 27]
Solar energy and battery technology			
Vanadium−iron redox flow battery testing	Solubility of vanadium and iron	ChCl:urea (1:2), ChCl:EG (1:2)	[28]
Solar energy	Solar cell	ChCl:glycerol (1:2)	[29, 30]
Electrochemical sensor platform			
Electrochemical sensor	Synthesis of nanoporous gold	ChCl:urea (1:2)	[31]

Electrochemical sensor	Determination of nitrofurazone	ChCl:urea:glycerol (1:1:1)	[32]
Photosynthesis			
Photosynthesis	Photosynthetic reaction centers of rhodobacter sphaeroides	ChCl:EG (1:3), ChCl:malonic acid (1:1)	[33]

[1]Choline chloride,[2]ethylene glycol, [3]methyltrioctylammonium chloride, [4]decanoic acid, [5]methyltrioctylammonium bromide, [6]2-methyl 2,4-pentanediol, [7]methyltriphenylphosphonium bromide

Table S2. Structures of the studied chemicals.

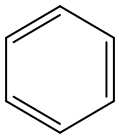
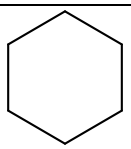
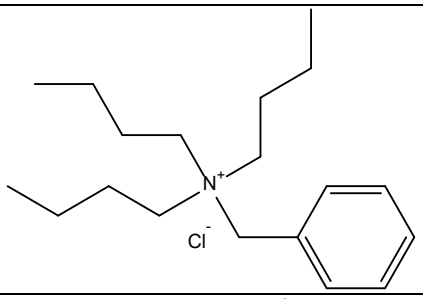
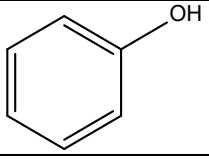
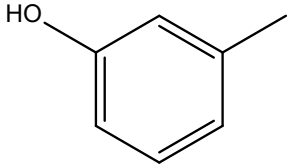
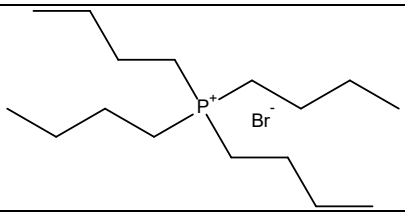
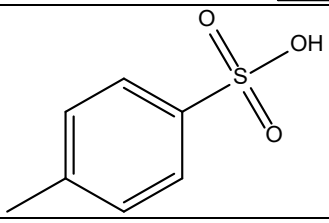
Benzene	
Cyclohexane	
BTBACl	
Phenol	
m-Cresol	
TBPB	
PTSA	

Table S3: Standard deviation (STDEV) on measured solubilities of Benzene (1) / Cyclohexane (2) mixture with BTBACl:Ph (1:2) (3) for mole fractions x: Top layer

Mole fraction			**Average mole fraction**			**STDEV mole fraction**		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0.0784	0.9216	0	0.0789	0.9211	0	0.0005	0.0005	0
0.0793	0.9207	0						
0.0791	0.9209	0						
0.1665	0.8335	0	0.1631	0.8369	0	0.0048	0.0048	0
0.1598	0.8402	0						
0.2450	0.7550	0	0.2429	0.7571	0	0.0018	0.0018	0
0.2422	0.7578	0						
0.2416	0.7584	0						
0.3230	0.6770	0	0.3225	0.6775	0	0.0005	0.0005	0
0.3220	0.6780	0						
0.3224	0.6776	0						
0.4181	0.5819	0	0.4134	0.5866	0	0.0041	0.0041	0
0.4114	0.5886	0						
0.4107	0.5893	0						

Table S4: STDEV on measured solubilities of Benzene (1) / Cyclohexane (2) mixture with BTBACl:Ph (1:2) (3) for mole fractions x: Bottom layer

Mole fraction			**Average mole fraction**			**STDEV mole fraction**		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0.1265	0.3524	0.5211	0.1254	0.3505	0.5241	0.0012	0.0046	0.0045
0.1242	0.3538	0.5220						
0.1254	0.3452	0.5294						
0.2159	0.3417	0.4424	0.2235	0.3317	0.4448	0.0107	0.0142	0.0035
0.2311	0.3217	0.4473						
0.3130	0.3215	0.3655	0.3160	0.3199	0.3641	0.0029	0.0056	0.0043
0.3162	0.3246	0.3592						
0.3188	0.3137	0.3675						
0.4005	0.3004	0.2991	0.4013	0.2989	0.2998	0.0007	0.0016	0.0011
0.4017	0.2989	0.2994						
0.4018	0.2972	0.3010						
0.4716	0.2645	0.2639	0.4729	0.2746	0.2525	0.0011	0.0088	0.0099
0.4734	0.2791	0.2475						
0.4736	0.2803	0.2461						

Table S5: STDEV on measured solubilities of Benzene (1) / Cyclohexane (2) mixture with BTBACl:Cre (1:2) (3) for mole fractions x: Top layer

Mole fraction			**Average mole fraction**			**STDEV mole fraction**		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0.0791	0.9209	0	0.0789	0.9211	0	0.0004	0.0004	0
0.0792	0.9208	0						
0.0785	0.9215	0						
0.1529	0.8471	0	0.1527	0.8473	0	0.0004	0.0004	0
0.1524	0.8476	0						
0.2312	0.7688	0	0.2304	0.7696	0	0.0007	0.0007	0
0.2299	0.7701	0						
0.2301	0.7699	0						
0.3240	0.6760	0	0.3229	0.6771	0	0.0011	0.0011	0
0.3219	0.6781	0						
0.3227	0.6773	0						

Table S6: STDEV on measured solubilities of Benzene (1) / Cyclohexane (2) mixture with BTBACl:Cre (1:2) (3) for mole fractions x: Bottom layer

Mole fraction			**Average mole fraction**			**STDEV mole fraction**		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0.1217	0.4815	0.3968	0.1220	0.4803	0.3977	0.0008	0.0016	0.0009
0.1215	0.4809	0.3976						
0.1230	0.4784	0.3986						
0.2336	0.4605	0.3059	0.2354	0.4531	0.3115	0.0026	0.0105	0.0079
0.2372	0.4457	0.3171						
0.3043	0.4641	0.2316	0.3125	0.4324	0.2551	0.0071	0.0275	0.0204
0.3166	0.4167	0.2667						
0.3166	0.4163	0.2671						
0.3832	0.4081	0.2086	0.3831	0.4111	0.2059	0.0012	0.0050	0.0040
0.3841	0.4082	0.2076						
0.3819	0.4168	0.2013						

Table S7: STDEV on measured solubilities of Benzene (1) / Cyclohexane (2) mixture with TBPB:PTSA (1:1) (3) for mole fractions x: Top layer

Mole fraction			**Average mole fraction**			**STDEV mole fraction**		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0.0900	0.9100	0	0.0893	0.9107	0	0.0011	0.0011	0
0.0900	0.9100	0						
0.0881	0.9119	0						
0.1786	0.8214	0	0.1785	0.8215	0	0.0019	0.0019	0
0.1804	0.8196	0						
0.1766	0.8234	0						
0.2645	0.7355	0	0.2672	0.7328	0	0.0042	0.0042	0
0.2649	0.7351	0						
0.2721	0.7279	0						
0.3557	0.6443	0	0.3593	0.6407	0	0.0038	0.0038	0
0.3590	0.6410	0						
0.3632	0.6368	0						
0.4548	0.5452	0	0.4607	0.5393	0	0.0092	0.0092	0
0.4559	0.5441	0						
0.4713	0.5287	0						
0.5505	0.4495	0	0.5526	0.4474	0	0.0026	0.0026	0
0.5517	0.4483	0						
0.5555	0.4445	0						

Table S8: STDEV on measured solubilities of Benzene (1) / Cyclohexane (2) mixture with TBPB:PTSA (1:1) (3) for mole fractions x: Bottom layer

Mole fraction			**Average mole fraction**			**STDEV mole fraction**		
x_1	x_2	x_3	x_1	x_2	x_3	x_1	x_2	x_3
0.1038	0.2134	0.6827	0.1064	0.2041	0.6895	0.0040	0.0123	0.0139
0.1043	0.1901	0.7056						
0.1111	0.2086	0.6803						
0.2016	0.1921	0.6063	0.2018	0.1899	0.6083	0.0064	0.0048	0.0109
0.1955	0.1845	0.6201						
0.2082	0.1933	0.5986						
0.2989	0.2113	0.4898	0.2925	0.1955	0.5120	0.0111	0.0164	0.0267
0.2989	0.1965	0.5046						
0.2797	0.1786	0.5417						
0.3760	0.1817	0.4423	0.3677	0.1752	0.4571	0.0089	0.0063	0.0152
0.3687	0.1748	0.4565						
0.3583	0.1691	0.4726						
0.4263	0.1641	0.4096	0.4093	0.1565	0.4342	0.0271	0.0103	0.0373
0.4235	0.1607	0.4158						
0.3781	0.1448	0.4771						
0.5158	0.1639	0.3202	0.5116	0.1589	0.3295	0.0050	0.0044	0.0089
0.5129	0.1570	0.3301						
0.5062	0.1558	0.3380						

Table S9: Molar ternary compositions, benzene distribution ratio (D_{Bz}) and solvent selectivity (S) from previous works involving organic solvents, ILs and DESs. x_1, x_2 and x_3 represents the molar composition of benzene, cyclohexane and solvents, respectively.

Top layer			**Bottom layer**			**D_{Bz}**	**S**
x_1	**x_2**	**x_3**	**x_1**	**x_2**	**x_3**		
Benzene (1) + cyclohexane + sulfolane (3)							
0.036	0.963	$1x10^{-3}$	0.015	0.027	0.958	0.417	14.86
0.133	0.856	0.011	0.069	0.037	0.894	0.519	12.00
0.158	0.829	0.013	0.086	0.038	0.876	0.544	11.87
0.217	0.764	0.019	0.118	0.039	0.843	0.544	10.65
0.268	0.701	0.031	0.156	0.05	0.794	0.582	8.16
0.31	0.649	0.041	0.186	0.055	0.759	0.6	7.08
0.356	0.586	0.058	0.225	0.065	0.71	0.632	5.698
0.394	0.53	0.076	0.263	0.078	0.659	0.667	4.54
0.433	0.458	0.109	0.314	0.099	0.587	0.725	3.35
0.457	0.387	0.156	0.361	0.13	0.509	0.79	2.35
Benzene (1) + cyclohexane + ethylene glycol (3)							
0.258	0.74	0.002	0.0348	0.0021	0.965	0.13	47.53
0.464	0.53	0.004	0.086	0.0021	0.912	0.19	46.78
0.66	0.33	0.005	0.172	0.0045	0.823	0.26	19.11
0.831	0.161	0.008	0.221	0.0045	0.774	0.26	9.51
Benzene (1) + cyclohexane + dimethylformamide (3)							
0.0243	0.8907	0.085	0.0219	0.2677	0.7105	0.90123	2.99862
0.0758	0.8112	0.113	0.0652	0.3321	0.6027	0.86016	2.10106
0.1106	0.6542	0.2352	0.1018	0.3752	0.523	0.92043	1.60487
Benzene (1) + cyclohexane (2) + TBABr:Sulf (1:7) (3)							
0.101	0.899	0.000	0.020	0.013	0.967	0.196	13.354
0.194	0.806	0.000	0.041	0.014	0.944	0.212	11.966
0.284	0.716	0.000	0.059	0.015	0.926	0.209	9.859
0.366	0.634	0.000	0.081	0.017	0.902	0.222	8.164
0.471	0.529	0.000	0.104	0.018	0.878	0.222	6.500
0.562	0.438	0.000	0.134	0.021	0.845	0.238	4.902
Benzene (1) + cyclohexane (2) + TBABr:TEG (1:4) (3)							
0.099	0.901	0.000	0.017	0.018	0.965	0.171	8.322
0.203	0.797	0.000	0.028	0.016	0.956	0.136	6.582
0.279	0.721	0.000	0.036	0.019	0.944	0.130	4.831
0.367	0.633	0.000	0.055	0.013	0.931	0.150	7.039
0.478	0.522	0.000	0.070	0.016	0.914	0.145	4.702
0.576	0.424	0.000	0.086	0.015	0.899	0.149	4.257
0.678	0.322	0.000	0.104	0.016	0.880	0.153	3.073
0.774	0.226	0.000	0.128	0.016	0.856	0.166	2.301
Benzene (1) + cyclohexane (2) + MTPPBr:TEG (1:4) (3)							
0.106	0.894	0.000	0.011	0.010	0.979	0.105	12.882
0.197	0.803	0.000	0.023	0.007	0.971	0.115	14.102
0.294	0.706	0.000	0.033	0.009	0.958	0.113	9.220
0.387	0.613	0.000	0.041	0.005	0.954	0.106	12.846
0.492	0.508	0.000	0.054	0.007	0.939	0.109	7.868
0.590	0.410	0.000	0.066	0.006	0.928	0.112	7.630

0.692	0.308	0.000	0.081	0.006	0.914	0.117	6.190
0.828	0.172	0.000	0.103	0.005	0.893	0.124	4.493
Benzene (1) + cyclohexane (2) + MTPPBr:PD (1:4) (3)							
0.110	0.890	0.000	0.010	0.010	0.980	0.093	8.024
0.214	0.786	0.000	0.018	0.010	0.972	0.083	6.578
0.298	0.702	0.000	0.023	0.010	0.967	0.077	5.526
0.403	0.597	0.000	0.033	0.009	0.958	0.081	5.217
0.502	0.498	0.000	0.044	0.009	0.947	0.087	4.630
0.602	0.398	0.000	0.055	0.008	0.938	0.091	4.741
0.703	0.297	0.000	0.061	0.008	0.931	0.087	3.208
0.792	0.208	0.000	0.077	0.009	0.914	0.097	2.186
Benzene (1) + cyclohexane (2) + ChCl:TEG (1:4) (3)							
0.094	0.906	0.000	0.007	0.007	0.986	0.074	9.130
0.197	0.803	0.000	0.014	0.006	0.980	0.070	9.613
0.292	0.708	0.000	0.020	0.004	0.976	0.069	12.091
0.399	0.601	0.000	0.027	0.004	0.969	0.067	9.032
0.502	0.498	0.000	0.032	0.004	0.964	0.064	8.228
0.607	0.393	0.000	0.040	0.004	0.955	0.067	6.100
0.704	0.296	0.000	0.048	0.004	0.948	0.068	4.896
0.809	0.191	0.000	0.057	0.003	0.940	0.071	4.749
Benzene (1) + cyclohexane (2) + [C2mim][Ac] (3)							
0.085	0.915	0.000	0.036	0.021	0.943	0.42	18.34
0.175	0.825	0.000	0.085	0.069	0.847	0.48	10.33
0.264	0.736	0.000	0.140	0.040	0.820	0.53	10.15
0.360	0.640	0.000	0.180	0.034	0.776	0.50	9.56
0.462	0.538	0.000	0.212	0.033	0.755	0.46	7.44
0.561	0.439	0.000	0.218	0.040	0.742	0.39	4.26
Benzene (1) + cyclohexane (2) + [C2mim][SCN] (3)							
0.082	0.918	0.000	0.038	0.010	0.953	0.46	44.71
0.168	0.832	0.000	0.077	0.012	0.910	0.46	31.18
0.259	0.741	0.000	0.114	0.010	0.876	0.44	32.73
0.351	0.649	0.000	0.149	0.009	0.842	0.42	30.94
0.450	0.550	0.000	0.184	0.008	0.808	0.41	26.53
0.553	0.447	0.000	0.222	0.007	0.771	0.40	25.22
Benzene (1) + cyclohexane (2) + [C2mim][N(CN)2] (3)							
0.073	0.927	0.000	0.049	0.020	0.932	0.67	31.85
0.158	0.842	0.000	0.095	0.018	0.886	0.61	27.94
0.247	0.753	0.000	0.141	0.016	0.844	0.57	27.48
0.339	0.661	0.000	0.184	0.015	0.801	0.54	23.51
0.426	0.574	0.000	0.232	0.016	0.752	0.54	19.23
0.522	0.478	0.000	0.275	0.015	0.710	0.53	16.84
Benzene (1) + cyclohexane (2) + [C2mim][Tf2N] (3)							
0.078	0.922	0.000	0.095	0.059	0.846	1.22	19.09
0.157	0.843	0.000	0.185	0.058	0.757	1.18	17.14
0.243	0.757	0.000	0.259	0.057	0.685	1.07	14.28
0.332	0.668	0.000	0.331	0.054	0.615	1.00	12.36
0.417	0.583	0.000	0.396	0.054	0.549	0.95	10.24
0.518	0.482	0.000	0.459	0.054	0.487	0.89	7.91

Benzene (1) + cyclohexane (2) + [C4mim][Tf2N] (3)							
0.04	0.96	0.000	0.066	0.162	0.772	0.168	9.78
0.124	0.876	0.000	0.186	0.156	0.658	0.178	8.42
0.177	0.823	0.000	0.258	0.153	0.589	0.18	7.84
0.23	0.77	0.000	0.301	0.146	0.553	0.19	6.90
0.277	0.723	0.000	0.355	0.139	0.506	0.19	6.67
0.352	0.648	0.000	0.413	0.13	0.457	0.20	5.85
0.439	0.561	0.000	0.478	0.117	0.405	0.21	5.22
0.524	0.476	0.000	0.537	0.104	0.359	0.22	4.69
0.62	0.38	0.000	0.595	0.09	0.315	0.24	4.05
0.784	0.216	0.000	0.705	0.051	0.244	0.24	3.81
Benzene (1) + cyclohexane (2) + [C4mim][PF6] (3)							
0.0392	0.9608	0.000	0.0542	0.0269	0.9189	1.384	49.4
0.0795	0.9205	0.000	0.1098	0.0319	0.8583	1.382	39.9
0.1628	0.8372	0.000	0.1647	0.0368	0.7985	1.012	23
0.2481	0.7519	0.000	0.2375	0.0327	0.7298	0.957	22
0.3507	0.6493	0.000	0.2723	0.0395	0.6882	0.776	12.8
0.449	0.551	0.000	0.324	0.0311	0.6449	0.721	12.8
0.6462	0.3538	0.000	0.4321	0.0245	0.5434	0.669	9.7
0.8724	0.1276	0.000	0.54	0.012	0.448	0.619	6.6
Benzene (1) + cyclohexane (2) + [C4mim][BF4] (3)							
0.046	0.954	0.000	0.031	0.008	0.961	0.67	80.36
0.092	0.908	0.000	0.066	0.012	0.922	0.71	54.28
0.165	0.835	0.000	0.102	0.019	0.879	0.62	27.17
0.245	0.755	0.000	0.153	0.026	0.821	0.62	18.13
0.399	0.601	0.000	0.245	0.034	0.721	0.61	10.85
0.523	0.477	0.000	0.326	0.042	0.632	0.62	7.08
0.682	0.318	0.000	0.465	0.057	0.478	0.68	3.80
0.837	0.163	0.000	0.646	0.039	0.315	0.77	3.22
Benzene (1) + cyclohexane (2) + [C2mim][EtSO4] (3)							
0.054	0.946	0.000	0.034	0.03	0.936	0.63	19.85
0.11	0.89	0.000	0.061	0.031	0.908	0.55	15.92
0.166	0.834	0.000	0.084	0.031	0.885	0.51	13.61
0.223	0.777	0.000	0.112	0.03	0.858	0.50	13.00
0.349	0.651	0.000	0.171	0.026	0.803	0.49	12.27
0.47	0.53	0.000	0.222	0.021	0.757	0.47	11.92
0.591	0.409	0.000	0.273	0.017	0.71	0.46	11.11
0.726	0.274	0.000	0.33	0.011	0.659	0.45	11.32
0.862	0.138	0.000	0.389	0.006	0.605	0.45	10.38
Benzene (1) + cyclohexane (2) + [C4mim][AlCl4] (3)							
0.0438	0.9079	0.0483	0.055	0.0524	0.8926	1.26	21.76
0.0887	0.8616	0.0497	0.1099	0.0498	0.8403	1.24	21.44
0.1444	0.807	0.0486	0.1536	0.0419	0.8045	1.06	20.45
0.1948	0.7533	0.0519	0.2033	0.0457	0.751	1.04	17.20
0.2525	0.6857	0.0618	0.2471	0.0415	0.7114	0.97	16.17
0.3035	0.6214	0.0751	0.2972	0.0366	0.6662	0.98	16.63
0.4122	0.5008	0.087	0.3759	0.0335	0.5906	0.91	13.63

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