

Supporting Information for publication

# Deep Eutectic Solvents for the Separation of Toluene/1-hexene via Liquid-liquid Extraction

Mohamed K. Hadj-Kali <sup>1,\*</sup>, Lahssen El Blidi <sup>1</sup>, Sarwono Mulyono <sup>1</sup>, Irfan Wazeer <sup>1</sup>, Emad Ali <sup>1</sup> and Jagan Rallapalli <sup>2</sup>

<sup>1</sup> Chemical Engineering Department, King Saud University, P.O. Box 800, Riyadh 11421, Saudi Arabia

<sup>2</sup> Functional Chemicals, Sabic Technology Centre, Riyadh, Saudi Arabia

\* Correspondence: mhadjkali@ksu.edu.sa

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Table S1. Summary of performance extraction of toluene/heptane using DESs

No.	DESs	T(°C)	Ratio	D <sub>toluene</sub>	Selectivity	Ref
1	ETPI/EG	50	1/10	0.11-0.22	20.6-65.3	[1]
2	ETPI/SUL	30	1/6	0.38-0.57	12.7-44.2	[1]
3	MTPB/EG	35	1/4	0.23-0.29	12.6-47.1	[2]
4	MTPB/GL	35	1/4	0.18-0.22	1.2-21.6	[2]
5	ChCl/LA	25	1/2	0.01-0.13	9.4-23.9	[3]
6	BCC/LA	25	1/2	0.15-0.34	12.3-39.1	[3]
7	TBAC/LA	25	1/2	0.48-0.74	0.6-13.4	[3]
8	ChlCl/LA	25	1/2	0.095-0.127	9.47-23.90	[4]
9	BzChlCl :LA	25	1/2	0.158-0.337	12.31-39.11	[4]
10	N <sub>444</sub> Cl :LA	25	1/2	0.480-0.742	0.60-13.41	[4]

Table S2: COSMO-RS screening results

No.	DES (HBA:HBD)	$C^\infty$	$S^\infty$	$PI^\infty$
1	BzTPPCL:TEG (1:8)	1.975	0.538	1.063
2	TBABr:TEG (1:3)	0.988	0.580	0.573
3	MTPPBr:TEG (1:4)	0.941	0.481	0.453
4	TBABr:LA (1:3)	0.604	0.472	0.285
5	TBABr:LA (1:2)	0.515	0.492	0.254
6	MTPPBr:LA (1:4)	0.439	0.343	0.150
7	TBABr:EG (1:2)	0.418	0.566	0.236
8	TBPBr:EG (1:2)	0.412	0.565	0.233
9	TEABr:LA (1:3)	0.330	0.368	0.121
10	MTPPBr:EG (1:5)	0.323	0.405	0.131
11	ChC:TEG (1:3)	0.320	0.481	0.154
12	ChCl:TA (2:1)	0.274	0.418	0.115
13	ChCl:1,4-BD (1:4)	0.270	0.509	0.138
14	TBACl:MalA (1:3)	0.262	0.436	0.114
15	BzTMACl:LA (1:4)	0.257	0.332	0.085
16	TEACl:Gly (1:2)	0.241	0.498	0.120
17	Capr:Im (1:1)	0.192	0.436	0.084
18	EmimCl:EG (1:2)	0.191	0.421	0.080
19	Capr:Act (1:1)	0.190	0.487	0.092
20	ChCl:Phe (1:4)	0.178	0.315	0.056
21	TMACl:EG (1:3)	0.158	0.423	0.067
22	ChCl:PD2 (1:4)	0.151	0.470	0.071
23	Carn:Phe (1:3)	0.150	0.320	0.048
24	ChCl:LA (1:3)	0.138	0.327	0.045
25	ChCl:DEG (1:2)	0.134	0.414	0.056
26	ChCl:1,4-BD (1:2)	0.133	0.460	0.061
27	ChCl:1,3-BD (1:2)	0.129	0.457	0.059
28	ChCl:1,6-HD (1:2)	0.122	0.508	0.062
29	ChCl:PhPA (1:2)	0.121	0.346	0.042
30	ChCl:EG (1:2)	0.119	0.431	0.051
31	TMACl:Gly (1:2)	0.111	0.413	0.046
32	ChCl:AcA (1:2)	0.110	0.354	0.039
33	ChCl:2,3-BD (1:2)	0.110	0.456	0.050
34	ChCl:LA (1:2)	0.105	0.335	0.035
35	TMACl:Gly (1:5)	0.102	0.394	0.040
36	TMACl:PAA (1:2)	0.101	0.299	0.030
37	ChCl:1,2-BD (1:2)	0.099	0.446	0.044
38	TMACl:Gly (1:4)	0.089	0.391	0.035
39	ChCl:PhAA (1:2)	0.088	0.308	0.027
40	ChCl:BzA (1:2)	0.082	0.296	0.024
41	ChCl:Gly (1:4)	0.075	0.392	0.030
42	ChCl:Ur (1:2)	0.072	0.318	0.023
43	ChCl:Xy (1:1)	0.067	0.410	0.028
44	ChCl:Gly (1:2)	0.066	0.399	0.026
45	ChCl:MalA (1:1)	0.056	0.313	0.018
46	ChCl:Sorb (1:1)	0.049	0.388	0.019
47	ChCl:MA (1:1)	0.044	0.313	0.014
48	ChCl:OA (1:1)	0.039	0.281	0.011
49	ChBr:Ur (1:2)	0.029	0.266	0.008
50	ChCl:CA (1:1)	0.025	0.271	0.007
51	ChCl:GA (1:3)	0.023	0.237	0.005
52	ClChCl:Ur (1:2)	0.021	0.221	0.005
53	ChCl:TUr (1:2)	0.005	0.159	0.001

Table S3: Standard deviation STDEV on measured solubilities of 1-hexene (1) / Toluene (2) mixture with DES #1 (3) for mole fractions x: Top layer

Mole Fraction			Average Mole Fraction			STDEV Mole Fraction		
X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
0.9241	0.0759	0.0000	0.9233	0.0767	0.0000	0.0365	0.0030	0.0000
0.9226	0.0774	0.0000						
0.8373	0.1627	0.0000	0.8381	0.1619	0.0000	0.0323	0.0062	0.0000
0.8385	0.1615	0.0000						
0.8385	0.1615	0.0000						
0.7393	0.2607	0.0000	0.7386	0.2614	0.0000	0.0281	0.0099	0.0000
0.7383	0.2617	0.0000						
0.7383	0.2617	0.0000						
0.6556	0.3444	0.0000	0.6535	0.3465	0.0000	0.0248	0.0131	0.0000
0.6530	0.3470	0.0000						
0.6519	0.3481	0.0000						
0.5684	0.4316	0.0000	0.5684	0.4316	0.0000	0.0215	0.0163	0.0000
0.5653	0.4347	0.0000						
0.5714	0.4286	0.0000						
0.4578	0.5422	0.0000	0.4679	0.5321	0.0000	0.0177	0.0202	0.0000
0.4788	0.5212	0.0000						
0.4670	0.5330	0.0000						
0.3645	0.6355	0.0000	0.3625	0.6375	0.0000	0.0138	0.0243	0.0000
0.3598	0.6402	0.0000						
0.3632	0.6368	0.0000						
0.2413	0.7587	0.0000	0.2440	0.7560	0.0000	0.0094	0.0291	0.0000
0.2418	0.7582	0.0000						
0.2490	0.7510	0.0000						
0.1280	0.8720	0.0000	0.1254	0.8746	0.0000	0.0050	0.0349	0.0000
0.1265	0.8735	0.0000						
0.1216	0.8784	0.0000						

Table S4: Standard deviation STDEV on measured solubilities of 1-hexene (1) / Toluene (2) mixture with DES #1 (3) for mole fractions x: bottom layer

Mole Fraction			Average Mole Fraction			STDEV Mole Fraction		
X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
0.0663	0.0304	0.9033	0.0675	0.0291	0.9034	0.0019	0.0008	0.0260
0.0687	0.0277	0.9036						
0.0594	0.0582	0.8824	0.0578	0.0596	0.8827	0.0016	0.0017	0.0248
0.0585	0.0604	0.8811						
0.0555	0.0601	0.8844						
0.0462	0.0795	0.8743	0.0453	0.0778	0.8769	0.0017	0.0030	0.0334
0.0451	0.0770	0.8779						
0.0445	0.0768	0.8787						
0.0494	0.1249	0.8257	0.0474	0.1198	0.8328	0.0018	0.0045	0.0316
0.0472	0.1186	0.8342						
0.0457	0.1158	0.8386						
0.0543	0.1808	0.7649	0.0519	0.1795	0.7685	0.0020	0.0068	0.0262
0.0508	0.1730	0.7762						
0.0507	0.1848	0.7645						
0.0842	0.2190	0.6968	0.0768	0.2322	0.6910	0.0029	0.0088	0.0262
0.0799	0.2547	0.6655						
0.0663	0.2231	0.7106						
0.0588	0.2629	0.6783	0.0570	0.2560	0.6870	0.0022	0.0098	0.00262
0.0549	0.2469	0.6982						
0.0574	0.2582	0.6844						
0.0483	0.2974	0.6543	0.0482	0.3048	0.6470	0.0019	0.0117	0.0249
0.0438	0.2883	0.6679						
0.0524	0.3288	0.6187						
0.0306	0.4074	0.5620	0.0327	0.4066	0.5607	0.0013	0.0162	0.0244
0.0365	0.4307	0.5328						
0.0309	0.3817	0.5874						

Table S5: Standard deviation STDEV on measured solubilities of 1-hexene (1) / Toluene (2) mixture with DES #2 (3) for mole fractions x: Top layer

Mole Fraction			Average Mole Fraction			STDEV Mole Fraction		
X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
0.9152	0.0848	0.0000	0.9150	0.0850	0.0000	0.0362	0.0034	0.0000
0.9149	0.0851	0.0000						
0.8236	0.1764	0.0000	0.8228	0.1772	0.0000	0.0317	0.0068	0.0000
0.8222	0.1778	0.0000						
0.8228	0.1772	0.0000						
0.7278	0.2722	0.0000	0.7280	0.2720	0.0000	0.0277	0.0104	0.0000
0.7269	0.2731	0.0000						
0.7292	0.2708	0.0000						
0.6345	0.3655	0.0000	0.6344	0.3656	0.0000	0.0240	0.0139	0.0000
0.6326	0.3674	0.0000						
0.6361	0.3639	0.0000						
0.5508	0.4492	0.0000	0.5506	0.4494	0.0000	0.0208	0.0170	0.0000
0.5509	0.4491	0.0000						
0.5500	0.4500	0.0000						
0.4578	0.5422	0.0000	0.4679	0.5321	0.0000	0.0177	0.0202	0.0000
0.4788	0.5212	0.0000						
0.4670	0.5330	0.0000						
0.3685	0.6315	0.0000	0.3652	0.6348	0.0000	0.0139	0.0242	0.0000
0.3643	0.6357	0.0000						
0.3629	0.6371	0.0000						
0.2572	0.7428	0.0000	0.2571	0.7429	0.0000	0.0099	0.0286	0.0000
0.2591	0.7409	0.0000						
0.2551	0.7449	0.0000						
0.1280	0.8720	0.0000	0.1254	0.8746	0.0000	0.0050	0.0349	0.0000
0.1265	0.8735	0.0000						
0.1216	0.8784	0.0000						

Table S6: Standard deviation STDEV on measured solubilities of 1-hexene (1) / Toluene (2) mixture with DES #2 (3) for mole fractions x: bottom layer

Mole Fraction			Average Mole Fraction			STDEV mole Fraction		
X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
0.0239	0.0103	0.9658	0.0228	0.0099	0.9673	0.0007	0.0003	0.0278
0.0217	0.0095	0.9688						
0.0194	0.0245	0.9561	0.0219	0.0234	0.9547	0.0006	0.0007	0.0269
0.0160	0.0202	0.9637						
0.0175	0.0222	0.9603						
0.0305	0.0525	0.9170	0.0309	0.0532	0.9159	0.0012	0.0020	0.0348
0.0292	0.0499	0.9209						
0.0331	0.0571	0.9098						
0.0253	0.0700	0.9046	0.0254	0.0697	0.9049	0.0010	0.0027	0.0343
0.0230	0.0633	0.9137						
0.0278	0.0758	0.8965						
0.0371	0.1417	0.8212	0.0363	0.1408	0.8229	0.0014	0.0054	0.0311
0.0353	0.1411	0.8236						
0.0366	0.1394	0.8240						
0.0382	0.1897	0.7721	0.0430	0.2177	0.7392	0.0016	0.0083	0.0279
0.0490	0.2473	0.7036						
0.0419	0.2161	0.7420						
0.0396	0.2733	0.6870	0.0396	0.2651	0.6953	0.0014	0.0097	0.0270
0.0399	0.2631	0.6970						
0.0393	0.2588	0.7019						
0.0305	0.3216	0.6479	0.0290	0.3186	0.6524	0.0011	0.0124	0.0250
0.0293	0.3248	0.6459						
0.0274	0.3093	0.6634						
0.0321	0.4280	0.5398	0.0343	0.4270	0.5386	0.0014	0.0172	0.0214
0.0383	0.4512	0.5105						
0.0325	0.4019	0.5656						

Table S7: Standard deviation STDEV on measured solubilities of 1-hexene (1) / Toluene (2) mixture with DES #3 (3) for mole fractions x: Top layer

Mole Fraction			Average Mole Fraction			STDEV Mole Fraction		
X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
0.9280	0.0720	0.0000	0.9267	0.0733	0.0000	0.0365	0.0029	0.0000
0.9264	0.0736	0.0000						
0.9258	0.0742	0.0000						
0.8434	0.1566	0.0000	0.8419	0.1581	0.0000	0.0324	0.0061	0.0000
0.8412	0.1588	0.0000						
0.8412	0.1588	0.0000						
0.7401	0.2599	0.0000	0.7417	0.2583	0.0000	0.0282	0.0098	0.0000
0.7424	0.2576	0.0000						
0.7424	0.2576	0.0000						
0.6414	0.3586	0.0000	0.6418	0.3582	0.0000	0.0243	0.0136	0.0000
0.6408	0.3592	0.0000						
0.6432	0.3568	0.0000						
0.5412	0.4588	0.0000	0.5415	0.4585	0.0000	0.0205	0.0173	0.0000
0.5412	0.4588	0.0000						
0.5421	0.4579	0.0000						
0.4504	0.5496	0.0000	0.4537	0.5463	0.0000	0.0172	0.0207	0.0000
0.4522	0.5478	0.0000						
0.4585	0.5415	0.0000						
0.3548	0.6452	0.0000	0.3530	0.6470	0.0000	0.0134	0.0246	0.0000
0.3503	0.6497	0.0000						
0.3539	0.6461	0.0000						
0.2413	0.7587	0.0000	0.2407	0.7593	0.0000	0.0093	0.0293	0.0000
0.2425	0.7575	0.0000						
0.2383	0.7617	0.0000						
0.1248	0.8752	0.0000	0.1260	0.8740	0.0000	0.0050	0.0349	0.0000
0.1254	0.8746	0.0000						
0.1280	0.8720	0.0000						



Table S8: Standard deviation STDEV on measured solubilities of 1-hexene (1) / Toluene (2) mixture with DES #3 (3) for mole fractions x: bottom layer

Mole Fraction			Average Mole Fraction			STDEV mole Fraction		
X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>
0.0783	0.0315	0.8902	0.0736	0.0299	0.8965	0.00755	0.0030	0.0182
0.0740	0.0295	0.8965						
0.0685	0.0286	0.9029						
0.0683	0.0599	0.8718	0.0692	0.0584	0.8724	0.0064	0.0054	0.0162
0.0719	0.0580	0.8701						
0.0674	0.0573	0.8753						
0.0458	0.0590	0.8952	0.0463	0.0611	0.8926	0.0062	0.0081	0.0238
0.0469	0.0623	0.8908						
0.0461	0.0620	0.8918						
0.0388	0.0707	0.8905	0.0365	0.0702	0.8933	0.0048	0.0093	0.0237
0.0363	0.0685	0.8952						
0.0345	0.0714	0.8941						
0.0343	0.0841	0.8816	0.0327	0.0835	0.8838	0.0042	0.0108	0.0228
0.0321	0.0825	0.8854						
0.0318	0.0839	0.8842						
0.0370	0.1198	0.8432	0.0374	0.1260	0.8367	0.0043	0.0144	0.0192
0.0356	0.1217	0.8428						
0.0395	0.1365	0.8240						
0.0373	0.1677	0.7950	0.0358	0.1618	0.8024	0.0038	0.0172	0.0171
0.0341	0.1537	0.8123						
0.0360	0.1641	0.8000						
0.0240	0.1970	0.7790	0.0230	0.1928	0.7842	0.0024	0.0199	0.0162
0.0241	0.2005	0.7754						
0.0210	0.1808	0.7982						
0.0164	0.2508	0.7328	0.0155	0.2508	0.7337	0.0015	0.0243	0.0142
0.0154	0.2475	0.7370						
0.0147	0.2541	0.7312						

Table S9: GC data of top and bottom layers for 1-hexene (1) / Toluene (2) mixture with DES #1 (3)

Wt% toluene in feed	Top layer		Bottom layer	
	1-hexene	Toluene	1-hexene	toluene
10	2346568	309964	83223	61353
	1041680	140527	141374	91712
20	518892	162141	525260	826862
	524752	162490	488334	810974
	545867	168991	468694	816142
30	696467	394760	343462	951168
	674344	384311	341709	938617
	664799	378918	346372	961425
40	681345	575438	266120	1082307
	704553	601944	262361	1060544
	725439	622763	255626	1041870
50	434803	530828	1843486	9859058
	704581	870878	5357930	29363850
	720820	869356	4709757	27575003
60	1240628	2361763	4554387	19036242
	1332569	2332486	3226574	16543014
	1434402	2632137	3384544	18303735
70	1225494	3435163	2743218	19723114
	158503	453490	1883959	13632466
	100056	282083	2062792	14916277
80	305360	1543868	2272189	22469452
	349403	1761013	2358634	24977719
	332659	1613147	2255746	22740627
90	601632	6587985	676229	14474408
	442235	4910885	1248822	23660394
	514839	5980839	1067590	21200917

Table S10: GC data of top and bottom layers for 1-hexene (1) / Toluene (2) mixture with DES #2 (3)

Wt% toluene in feed	Top layer		Bottom layer	
	1-hexene	Toluene	1-hexene	toluene
10	1020478	152101	1741381	1205387
	928250	138797	1732928	1220943
20	528892	182141	615260	1086862
	524752	182490	588334	990974
	545867	188991	568694	956142
30	656467	394760	343462	951168
	636344	384311	341709	938617
	634799	378918	346372	961425
40	621345	575438	266120	1182307
	644553	601944	262361	1160544
	655439	602763	255626	1121870
50	404803	530828	1343486	8259058
	664581	870878	2857930	18363850
	660820	869356	2709757	16575003
60	1240628	2361763	219338	1751341
	1332569	2332486	211129	1712058
	1434402	2632137	205524	1703940
70	446889	1231340	1020034	11314252
	520303	1459892	1202844	12763811
	564997	1594842	1205283	12768610
80	1117424	5187259	1004546	17038912
	909464	4181025	762231	13594066
	1067067	5008836	768292	13955369
90	601632	6587985	676229	14474408
	442235	4910885	1248822	23660394
	514839	5980839	1067590	21200917

Table S11: GC data of top and bottom layers for 1-hexene (1) / Toluene (2) mixture with DES #3 (3)

Wt% toluene in feed	Top layer		Bottom layer	
	1-hexene	Toluene	1-hexene	toluene
10	884383	110275	1284226	831655
	571224	73001	1138825	728883
	778522	100248	1273355	854301
20	739970	220956	1391245	1963106
	748137	227003	1288498	1670836
	775669	235496	1241452	1696565
30	901003	508554	1281354	2651407
	754683	420919	1192861	2547351
	711757	397070	1589852	3436345
40	1080530	971137	1301629	3815013
	84873	76498	1497300	4546840
	614794	548182	1200713	4001474
50	352618	480619	1417466	5592309
	388029	528881	1663025	6874833
	348345	472991	1291480	5480716
60	456092	894693	1368473	7119410
	438049	852972	1303299	7162792
	540682	1026570	1553966	8639721
70	548411	1603591	1441316	10425991
	589507	1757899	1674859	12146097
	555617	1630710	1529954	11222349
80	246983	1248788	1070100	14092322
	19232	96580	1105686	14769126
	185025	950719	958624	13293137
90	212147	2392059	385644	9475734
	159769	1792212	479760	12378643
	114053	1249340	468826	13048903

Table S12: Summary of performance extraction of toluene/heptane using organic solvents and ILs

No.	Solvents	T (°C)	D <sub>toluene</sub>	Selectivity	Ref.
Organic solvents					
1	Ethylene carbonate	30	0.16-0.49	3.6-16.9	[5]
2	Ethylene carbonate	40	0.22-0.61	1.9-13.3	[5]
3	Triethylene glycol	25	0.06-0.17	37.2-85.5	[6]
4	Propylene carbonate	25	0.35-0.44	5.9-14.0	[6]
5	Sulfolane	25	0.30-0.50	1.7-38	[7]
6	Ethylene glycol	30	0.02-0.04	7.1-39.8	[8]
ILs					
7	[BMIM][SCN]	40	0.19-0.20	46.5-101.6	[9]
8	[BMIM][SCN]	40	0.34-0.46	17.8-53.2	[9]
9	[BMIM][HSO <sub>4</sub> ]	30	0.25-0.49	1.4-48.6	[10]
10	[HMIM][HSO <sub>4</sub> ]	30	0.20-0.37	1.2-40.4	[10]
11	[C <sub>3</sub> (MIM) <sub>2</sub> ][(HSO <sub>4</sub> ) <sub>2</sub> ]	30	0.23-0.67	8.9-77.6	[10]
12	[C <sub>6</sub> (MIM) <sub>2</sub> ][(HSO <sub>4</sub> ) <sub>2</sub> ]	30	0.30-0.80	6.4-91.8	[10]
13	[EMim][ESO <sub>4</sub> ]	25	0.21-0.25	8.4-30.7	[11]

Table S13: Composition of the NRTL tie-lines (mole fraction), for the ternary system {1-hexene (1) + Toluene (2) + DES #1 (3)} at 298.15 K and 101.325 kPa.

Top layer			Bottom Layer		
$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
0.909	0.087	0.004	0.085	0.010	0.905
0.820	0.177	0.004	0.075	0.032	0.893
0.728	0.269	0.003	0.066	0.067	0.867
0.645	0.353	0.003	0.059	0.109	0.832
0.558	0.440	0.002	0.052	0.161	0.787
0.471	0.527	0.002	0.044	0.217	0.739
0.382	0.617	0.002	0.035	0.276	0.689
0.276	0.723	0.001	0.025	0.343	0.632
0.151	0.848	0.001	0.012	0.414	0.574

Table S14: Composition of the NRTL tie-lines (mole fraction), for the ternary system {1-hexene (1) + Toluene (2) + DES #2 (3)} at 298.15 K and 101.325 kPa.

Top layer			Bottom Layer		
$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
0.913	0.086	0.001	0.022	0.007	0.971
0.821	0.177	0.002	0.021	0.023	0.957
0.727	0.271	0.002	0.020	0.052	0.928
0.641	0.357	0.002	0.020	0.091	0.889
0.552	0.445	0.003	0.021	0.142	0.837
0.464	0.532	0.003	0.021	0.200	0.779
0.372	0.624	0.004	0.020	0.268	0.713
0.271	0.724	0.005	0.017	0.344	0.640
0.151	0.842	0.008	0.011	0.434	0.555

Table S15: Composition of the NRTL tie-lines (mole fraction), for the ternary system {1-hexene (1) + Toluene (2) + DES #3 (3)} at 298.15 K and 101.325 kPa.

Top layer			Bottom Layer		
$x_1$	$x_2$	$x_3$	$x_1$	$x_2$	$x_3$
0.900	0.096	0.004	0.099	0.005	0.896
0.804	0.193	0.003	0.080	0.017	0.903
0.715	0.282	0.002	0.065	0.034	0.901
0.627	0.371	0.002	0.052	0.057	0.890
0.538	0.460	0.002	0.042	0.088	0.871
0.453	0.546	0.001	0.033	0.122	0.846
0.361	0.639	0.001	0.024	0.162	0.814
0.255	0.745	0.001	0.015	0.211	0.774
0.139	0.861	0.000	0.007	0.262	0.731

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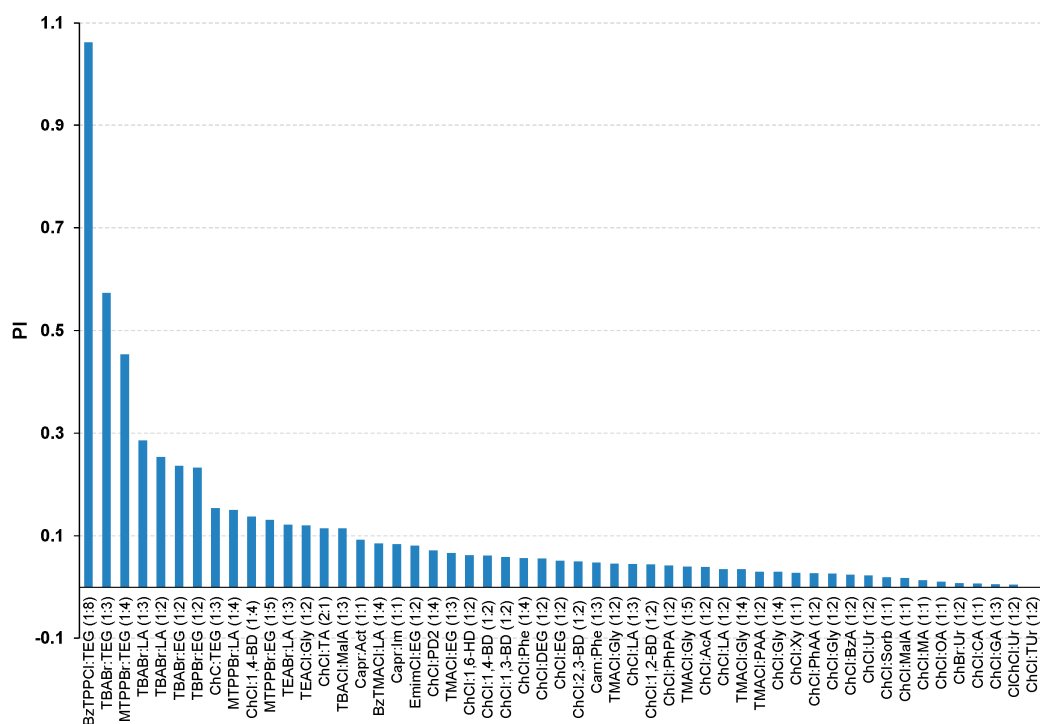


Figure S1: Performance index of the selected DESs at infinite dilution

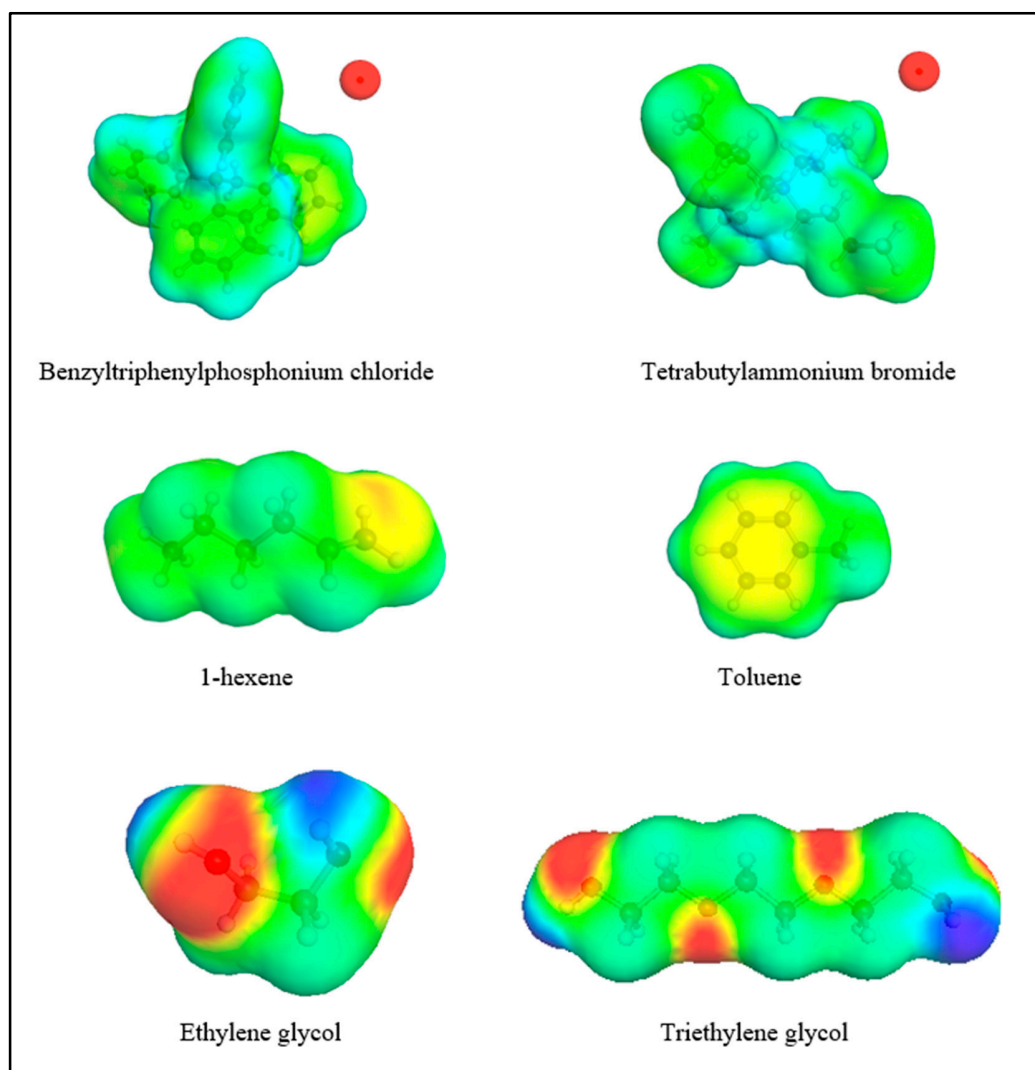


Figure S2: Sigma surfaces of different HBA, HBD investigated in this work both with those of toluene and 1-hexene



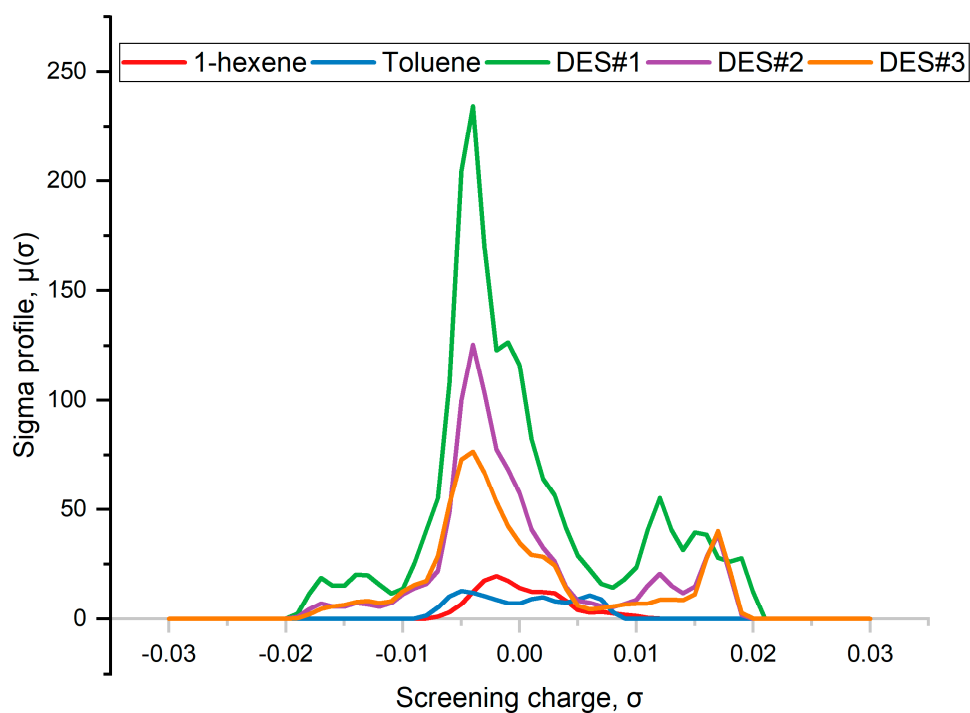


Figure S3: Sigma ( $\sigma$ ) profiles of species in the toluene-hexene systems using three DESs.

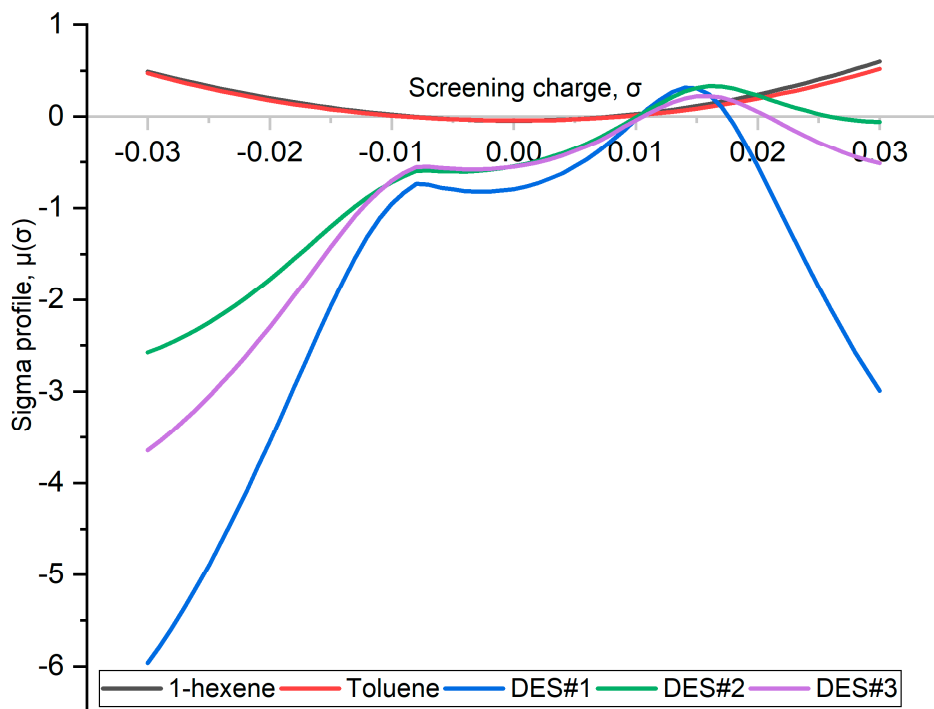


Figure S4: Sigma ( $\sigma$ ) potential of species in the toluene-hexene systems using three DESs.

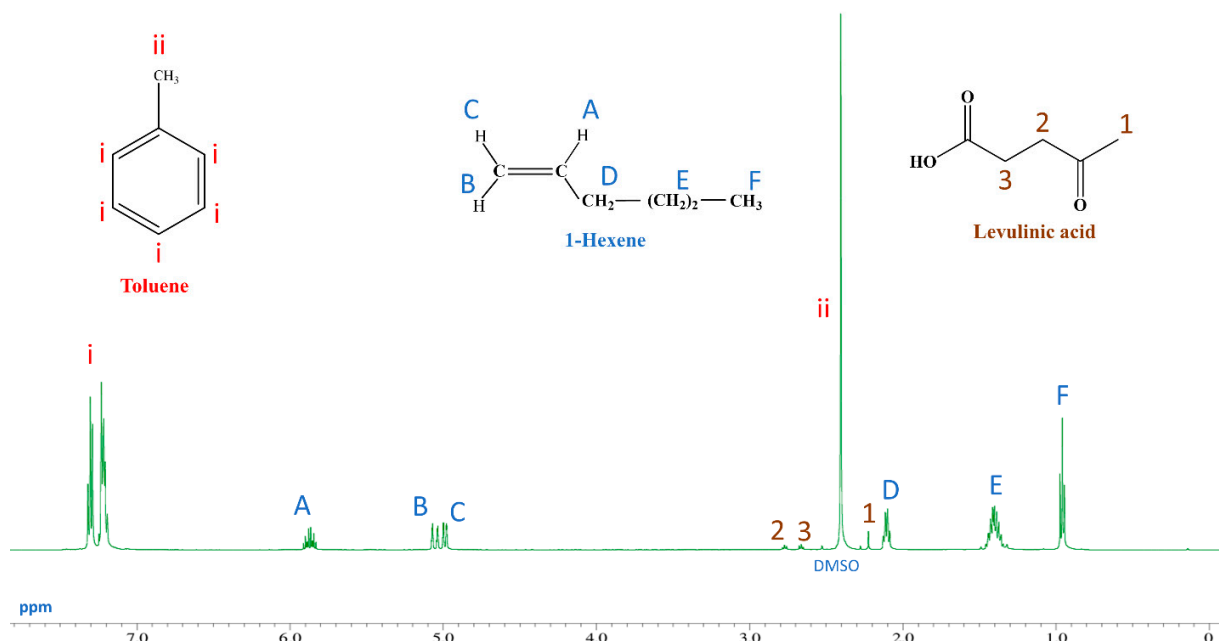


Figure S5:  $^1\text{H}$  NMR analysis of the raffinate phase using TBABr: LA (1:3) in DMSO.

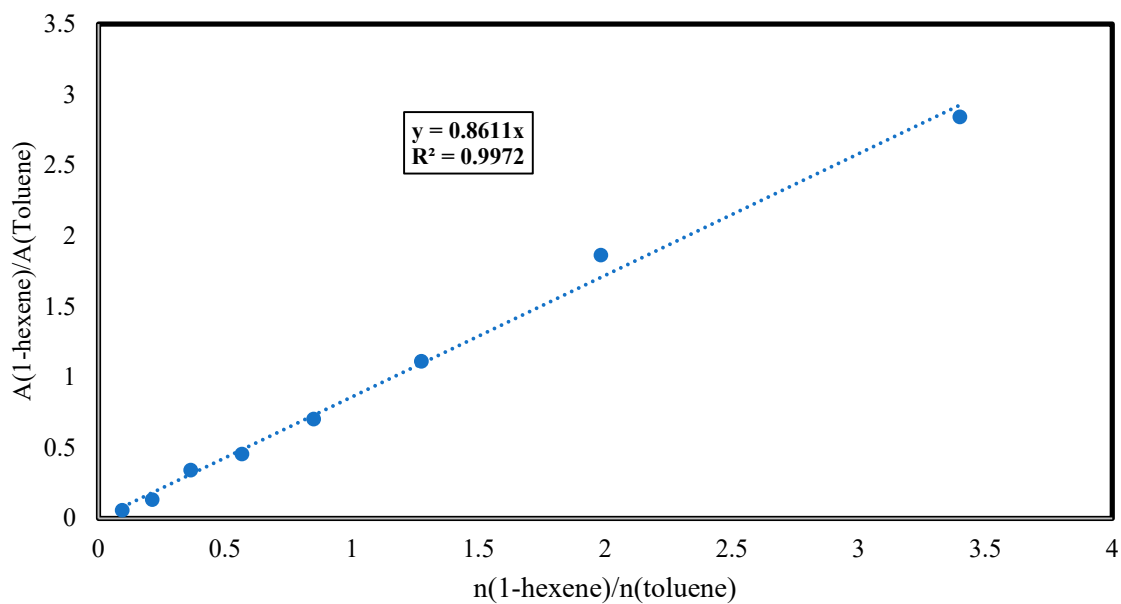


Figure S6. GC calibration curve of toluene/1-hexene.

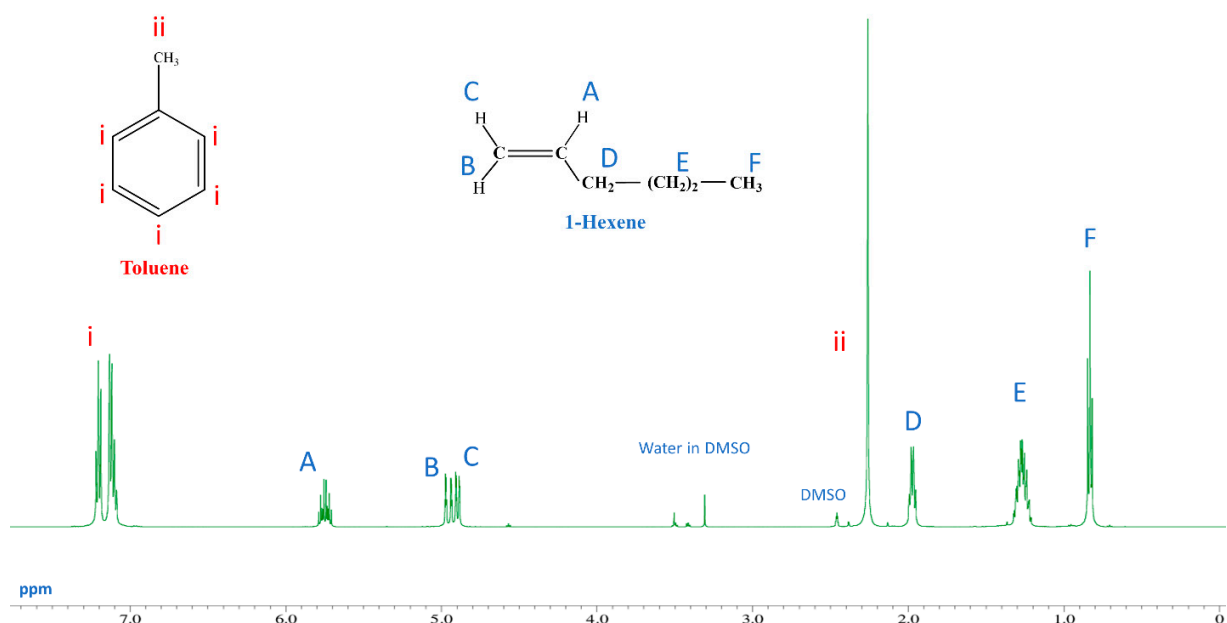


Figure S7:  $^1\text{H}$  NMR analysis of the raffinate phase using DES#1 in DMSO.

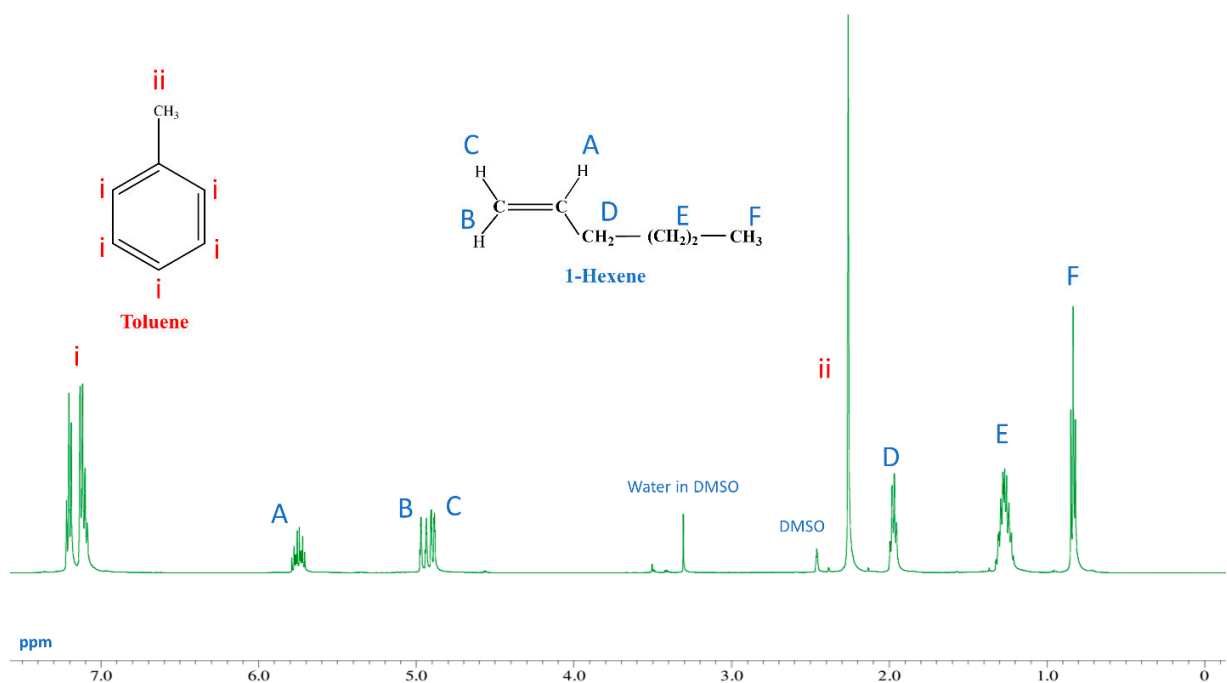


Figure S8:  $^1\text{H}$  NMR analysis of the raffinate phase using DES#2 in DMSO.

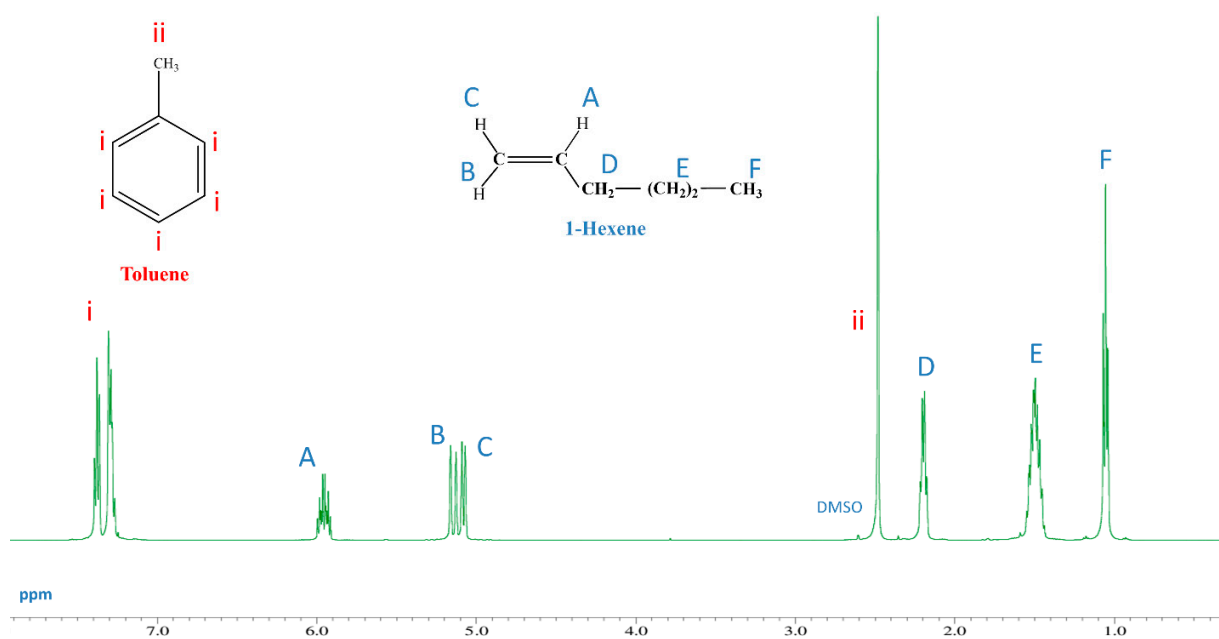


Figure S9:  $^1\text{H}$  NMR analysis of the raffinate phase using DES#3 in DMSO.

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