Separation of benzene from methylcycloalkanes by extractive distillation with cyano-based ionic liquids: experimental and CPA EoS modelling

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Supporting Information

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Table S1. Methylcycloalkane/benzene relative volatility for methylcycloalkane (1) + benzene (2) + IL (3) systems regarding the experimental screening

IL	$\alpha_{MCP,B}$			$\alpha_{MCH,B}$		
S/F ratio	1	5	10	1	5	10
		T/K = 323.2 K				
$[C_2C_1im][TCM]$	3.1	16.7	20.2	1.3	6.3	10.3
$[4\text{-}C_4C_1py][TCM]$	3.9	15.5	16.6	1.7	8.0	9.1
$[C_2C_1im][DCA]$	2.4	9.5	28.6	1.0	3.6	9.0
$[C_2C_1im][SCN]$	2.4	9.4	27.8	0.9	2.8	6.9
$[C_4C_1im]_2[Co(SCN)_4]$	2.4	5.9	21.1	1.0	2.3	6.8
$[C_2C_1im]_2[Co(SCN)_4]$	2.5	7.6	27.1	1.1	2.9	8.0
without IL			*1.74*			*0.664*
		T/K = 363.2 K				
$[C_2C_1im][TCM]$	2.5	14.0	17.3	1.2	7.4	8.2
$[4\text{-}C_4C_1py][TCM]$	3.3	13.0	13.0	1.5	5.8	6.6
$[C_2C_1im][DCA]$	2.0	15.9	34.5	0.9	4.5	11.9
$[C_2C_1im][SCN]$	1.9	10.2	30.0	0.9	3.4	19.7
$[C_4C_1im]_2[Co(SCN)_4]$	2.0	11.6	16.2	1.0	5.8	7.2
$[C_2C_1im]_2[Co(SCN)_4]$	2.2	13.4	24.0	1.0	5.2	9.7
without IL			*1.58*			*0.649*

Table S2. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for hydrocarbon (1) + [C_2C_1im][SCN] (2)

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323.2		T/ K = 363.2		T/ K = 403.2	
methylcyclopentane + [C_2C_1im][SCN]					
5.9	0.0029	8.6	0.0013	10.0	0.0001
17.6	0.0082	25.7	0.0027	28.8	0.0003
38.6	0.0125	64.2	0.0057	62.9	0.0008
48.8	0.0353	102.5	0.0087	94.9	0.0016
49.9	0.0672	123.0	0.0156	120.0	0.0035
49.7	0.1490	158.5	0.0293	198.4	0.0045
49.1	1.0000	168.1	0.0502	292.6	0.0156
		171.4	0.1292	373.0	0.0303
		169.4	0.2214	423.5	0.0551
		171.8	1.0000	447.2	0.1254
				455.3	0.2103
				454.9	0.2666
				454.2	1.0000
methylcyclohexane + [C_2C_1im][SCN]					
6.8	0.0043	9.5	0.0035	14.8	0.0004
16.3	0.0087	25.0	0.0051	32.3	0.0011
18.0	0.0348	49.9	0.0087	64.4	0.0022
18.6	0.0640	68.6	0.0213	101.9	0.0032
18.6	0.0931	69.2	0.0512	126.1	0.0061
18.4	0.1629	70.1	0.1106	176.3	0.0238
18.5	0.2157	71.1	0.1757	200.0	0.0344
18.5	1.0000	72.2	0.2328	207.9	0.1285
		74.0	1.0000	210.1	0.2015
				211.8	0.2630
				215.3	1.0000

[a] Standard uncertainty (u) and relative standard uncertainty (u_r) are $u(x) = 0.0008$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K

Table S2. Continued

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323.2		T/ K = 363.2		T/ K = 403.2	
benzene + [C_2C_1im][SCN]					
1.5	0.0147	5.4	0.0144	8.9	0.0075
3.2	0.0331	10.3	0.0280	21.5	0.0213
6.4	0.0703	22.9	0.0570	51.9	0.0435
9.4	0.1053	35.6	0.0827	89.2	0.0558
12.4	0.1386	48.3	0.1100	118.8	0.0733
18.7	0.2105	74.4	0.1683	176.7	0.1236
24.2	0.2869	87.5	0.2290	229.5	0.1841
28.6	0.3460	102.3	0.2800	265.0	0.2441
30.1	0.3914	117.5	0.3524	304.9	0.2913
30.6	0.4471	124.1	0.4170	346.3	0.3501
32.4	0.5053	128.2	0.4715	366.2	0.4191
33.6	0.5576	131.7	0.5239	378.3	0.4775
34.8	0.6081	135.3	0.5792	377.9	0.5396
35.6	0.6504	135.5	0.6281	377.3	0.5972
36.0	0.6979	135.1	0.6759	376.7	0.6277
36.1	0.7398	136.4	0.7192	378.0	1.0000
36.1	0.7951	136.4	0.7619		
36.1	1.0000	136.0	1.0000		

[a] Standard uncertainty (u) and relative standard uncertainty (u_r) are $u(x) = 0.0008$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K

Table S3. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for hydrocarbon (1) + [C_2C_1im][DCA] (2)

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323.2		T/ K = 363.2		T/ K = 403.2	
methylcyclopentane + [C_2C_1im][DCA]					
5.1	0.0029	7.1	0.0009	11.9	0.0002
17.2	0.0081	22.6	0.0023	30.4	0.0005
36.8	0.0182	54.7	0.0072	64.5	0.0009
47.1	0.0381	88.2	0.0145	101.8	0.0020
48.5	0.0702	120.5	0.0254	159.1	0.0058
48.9	0.1303	164.0	0.0450	193.7	0.0077
49.1	1.0000	168.7	0.0606	254.9	0.0119
		169.5	0.0706	307.0	0.0151
		170.0	0.1084	379.3	0.0259
		170.0	1.0000	431.8	0.0435
				451.4	0.1187
				453.7	0.2041
				454.2	1.0000
methylcyclohexane + [C_2C_1im][DCA]					
5.8	0.0050	9.5	0.0037	18.4	0.0007
15.1	0.0126	23.4	0.0066	31.1	0.0011
17.2	0.0377	49.5	0.0116	62.5	0.0021
18.2	0.0691	69.3	0.0223	93.2	0.0046
18.3	0.0981	71.1	0.0519	119.4	0.0125
18.4	0.1612	71.5	0.1232	188.8	0.0205
18.5	1.0000	74.0	1.0000	206.6	0.0304
				213.9	0.1300
				215.1	0.2046
				215.0	1.0000

[a] Standard uncertainty (u) and relative standard uncertainty (u_r) are $u(x) = 0.0008$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K

Table S3. Continued

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323.2		T/ K = 363.2		T/ K = 403.2	
benzene + [C_2C_1im][DCA]					
1.0	0.0144	3.3	0.0122	9.9	0.0075
2.3	0.0347	8.4	0.0308	23.6	0.0195
4.9	0.0735	18.2	0.0624	47.0	0.0414
7.3	0.1110	28.3	0.0922	71.7	0.0665
9.9	0.1499	36.3	0.1245	86.7	0.0833
14.5	0.2201	56.4	0.1859	133.3	0.1251
19.4	0.2952	74.5	0.2469	171.5	0.1751
22.4	0.3449	89.6	0.3063	212.2	0.2389
26.6	0.4100	101.6	0.3648	244.6	0.2820
29.6	0.4875	116.1	0.4417	276.7	0.3317
33.0	0.5449	119.8	0.4808	309.5	0.3849
34.8	0.5937	128.8	0.5335	346.5	0.4474
35.8	0.6401	132.8	0.5899	372.8	0.5422
35.5	0.6854	135.7	0.6410	378.0	0.5934
35.4	0.7263	135.7	0.6891	378.4	0.6499
35.4	0.7683	135.9	0.7325	378.4	0.7104
35.4	0.8059	135.9	0.7727	378.4	0.7592
36.1	1.0000	136.0	1.0000	378.4	1.0000

[a] Standard uncertainty (u) and relative standard uncertainty (u_r) are $u(x) = 0.0008$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K

Table S4. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for methylcyclopentane (1) + benzene (2) + [C_2C_1im][SCN] (3) with S/F mass ratio of 10

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 323.2						
20.1	0.0000	1.0000						0.0000	0.1631	0.8369	
34.4	0.5402	0.4598						0.0067	0.1468	0.8464	25.6
48.4	0.7363	0.2637	0.6900	0.3100	0.0075	0.1311	0.8614	0.0149	0.1308	0.8543	24.5
48.5	0.7786	0.2214	0.7525	0.2475	0.0086	0.1116	0.8798	0.0298	0.1136	0.8566	13.4
48.9	0.8112	0.1888	0.8005	0.1995	0.0088	0.0945	0.8966	0.0436	0.0975	0.8589	9.6
49.2	0.8511	0.1489	0.8439	0.1561	0.0087	0.0779	0.9134	0.0577	0.0811	0.8612	8.0
49.2	0.9041	0.0959	0.8812	0.1188	0.0087	0.0597	0.9316	0.0720	0.0631	0.8650	8.3
49.5	0.9226	0.0774	0.9151	0.0849	0.0092	0.0442	0.9466	0.0873	0.0470	0.8658	6.4
49.4	0.9395	0.0605	0.9415	0.0585	0.0091	0.0306	0.9604	0.1027	0.0328	0.8646	5.0
49.6	0.9676	0.0324	0.9722	0.0278	0.0091	0.0145	0.9764	0.1191	0.0157	0.8653	3.9
49.2	1.0000	0.0000	1.0000	0.0000	0.0500	0.0000	0.9500	0.1323	0.0000	0.8677	
					T/K = 363.2						
64.7	0.0000	1.0000						0.0000	0.1383	0.8617	
90.8	0.3029	0.6971						0.0020	0.1334	0.8646	29.2
113.9	0.5130	0.4870						0.0037	0.1173	0.8790	33.0
133.9	0.6631	0.3369						0.0048	0.1033	0.8919	42.6
148.9	0.7480	0.2520						0.0101	0.0919	0.8980	27.1
160.8	0.8170	0.1830						0.0168	0.0781	0.9052	20.8
168.2	0.8687	0.1313						0.0278	0.0616	0.9106	14.7
174.7	0.9049	0.0951	0.9110	0.0890	0.0096	0.0438	0.9465	0.0374	0.0455	0.9170	11.6
175.2	0.9336	0.0664	0.9408	0.0592	0.0098	0.0302	0.9600	0.0504	0.0316	0.9179	8.8
174.5	0.9644	0.0356	0.9739	0.0261	0.0097	0.0140	0.9763	0.0651	0.0148	0.9201	6.2
172.0	1.0000	0.0000	1.0000	0.0000	0.0102	0.0000	0.9898	0.0683	0.0000	0.9317	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S4. Continued

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 403.2						
100.1	0.0000	1.0000						0.0000	0.1378	0.8622	
123.5	0.1892	0.8108						0.0016	0.1308	0.8676	19.1
149.5	0.3689	0.6311						0.0036	0.1182	0.8782	19.2
174.4	0.5125	0.4875						0.0061	0.1054	0.8885	18.2
193.3	0.6154	0.3846						0.0094	0.0900	0.9006	15.3
214.8	0.7191	0.2809						0.0135	0.0780	0.9085	14.8
235.9	0.8277	0.1723						0.0211	0.0635	0.9154	14.4
255.3	0.8753	0.1247						0.0239	0.0478	0.9283	14.1
275.2	0.9115	0.0885						0.0258	0.0333	0.9409	13.3
294.2	0.9593	0.0407						0.0338	0.0160	0.9502	11.2
300.2	1.0000	0.0000						0.0346	0.0000	0.9654	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S5. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for methylcyclohexane (1) + benzene (2) + [C_2C_1im][SCN] (3) with S/F mass ratio of 10

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 323.2						
20.1	0.0000	1.0000						0.0000	0.1652	0.8348	
27.3	0.4493	0.5507						0.0080	0.1580	0.8341	16.2
25.5	0.5303	0.4697	0.7354	0.2646	0.0068	0.1389	0.8543	0.0208	0.1396	0.8395	7.6
24.5	0.5907	0.4093	0.7611	0.2389	0.0066	0.1182	0.8752	0.0374	0.1228	0.8398	4.7
24.0	0.6226	0.3774	0.7925	0.2075	0.0065	0.0999	0.8936	0.0508	0.1056	0.8435	3.4
23.2	0.6812	0.3188	0.8342	0.1658	0.0065	0.0811	0.9124	0.0627	0.0866	0.8507	3.0
22.3	0.7377	0.2623	0.8698	0.1302	0.0064	0.0712	0.9224	0.0840	0.0763	0.8397	2.6
21.3	0.7940	0.2060	0.9108	0.0892	0.0067	0.0485	0.9448	0.0853	0.0519	0.8628	2.3
20.4	0.8520	0.1480	0.9366	0.0634	0.0070	0.0332	0.9598	0.1082	0.0364	0.8555	1.9
19.2	0.9434	0.0566	0.9747	0.0253	0.0075	0.0149	0.9776	0.1248	0.0161	0.8590	2.2
18.5	1.0000	0.0000	1.0000	0.0000	0.0075	0.0000	0.9925	0.1368	0.0000	0.8632	
					T/K = 363.2						
62.1	0.0000	1.0000						0.0000	0.1394	0.8606	
77.4	0.2569	0.7431						0.0035	0.1316	0.8649	13.0
94.5	0.4484	0.5516						0.0065	0.1199	0.8735	15.0
99.5	0.5638	0.4362	0.7738	0.2262	0.0066	0.1035	0.8899	0.0160	0.1043	0.8797	8.4
94.3	0.6251	0.3749	0.8059	0.1941	0.0066	0.0887	0.9047	0.0280	0.0909	0.8811	5.4
88.2	0.6837	0.3163	0.8447	0.1553	0.0070	0.0741	0.9189	0.0408	0.0769	0.8824	4.1
84.7	0.7446	0.2554	0.8787	0.1213	0.0072	0.0592	0.9336	0.0532	0.0620	0.8848	3.4
82.0	0.8023	0.1977	0.9120	0.0880	0.0071	0.0468	0.9461	0.0663	0.0491	0.8846	3.0
78.2	0.8719	0.1281	0.9451	0.0549	0.0069	0.0308	0.9623	0.0813	0.0324	0.8863	2.7
75.7	0.9426	0.0574	0.9767	0.0233	0.0070	0.0137	0.9793	0.0979	0.0145	0.8876	2.4
74.1	1.0000	0.0000	1.0000	0.0000	0.0071	0.0000	0.9929	0.1048	0.0000	0.8952	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S5. Continued

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 403.2						
100.1	0.0000	1.0000						0.0000	0.1378	0.8622	
115.6	0.1792	0.8208						0.0032	0.1292	0.8676	8.8
128.9	0.3587	0.6413						0.0081	0.1186	0.8733	8.2
147.4	0.5094	0.4906						0.0134	0.1059	0.8807	8.2
159.9	0.5908	0.4092						0.0169	0.0905	0.8926	7.7
165.9	0.6952	0.3048						0.0234	0.0782	0.8984	7.6
178.2	0.7525	0.2475						0.0281	0.0664	0.9055	7.2
184.2	0.8305	0.1695						0.0369	0.0513	0.9117	6.8
196.3	0.8925	0.1075						0.0486	0.0335	0.9179	5.7
203.4	0.9633	0.0367						0.0834	0.0154	0.9012	4.9
206.8	1.0000	0.0000						0.0857	0.0000	0.9143	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S6. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for methylcyclopentane (1) + benzene (2) + [C_2C_1im][DCA] (3) with S/F mass ratio of 10

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 323.2						
12.3	0.0000	1.0000						0.0000	0.1736	0.8264	
26.0	0.5463	0.4537						0.0089	0.1645	0.8266	22.3
49.0	0.7621	0.2379	0.7646	0.2354	0.0124	0.1437	0.8439	0.0161	0.1439	0.8400	28.6
48.9	0.8172	0.1828	0.8075	0.1925	0.0141	0.1179	0.8680	0.0287	0.1191	0.8522	18.5
48.9	0.8377	0.1623	0.8270	0.1730	0.0145	0.1040	0.8815	0.0460	0.1065	0.8475	11.9
48.9	0.8757	0.1243	0.8622	0.1378	0.0145	0.0839	0.9016	0.0594	0.0866	0.8539	10.3
48.8	0.9158	0.0842	0.8956	0.1044	0.0142	0.0657	0.9202	0.0766	0.0683	0.8551	9.7
48.8	0.9312	0.0688	0.9225	0.0775	0.0144	0.0482	0.9374	0.0926	0.0507	0.8567	7.4
48.7	0.9469	0.0531	0.9483	0.0517	0.0151	0.0336	0.9513	0.1084	0.0353	0.8562	5.8
48.7	0.9712	0.0288	0.9754	0.0246	0.0148	0.0155	0.9697	0.1220	0.0165	0.8615	4.6
48.7	1.0000	0.0000	1.0000	0.0000	0.0150	0.0000	0.9850	0.1402	0.0000	0.8598	
					T/K = 363.2						
50.8	0.0000	1.0000						0.0000	0.1470	0.8530	
72.3	0.3187	0.6813						0.0032	0.1361	0.8607	19.9
102.6	0.5474	0.4526						0.0047	0.1266	0.8687	32.3
121.2	0.6539	0.3461						0.0048	0.0982	0.8970	38.8
147.4	0.7913	0.2087						0.0077	0.0954	0.8969	64.7
160.0	0.8419	0.1581						0.0132	0.0819	0.9048	33.0
173.6	0.8895	0.1105	0.8947	0.1053	0.0192	0.0652	0.9156	0.0238	0.0660	0.9103	22.4
172.0	0.9179	0.0821	0.9253	0.0747	0.0191	0.0477	0.9332	0.0384	0.0487	0.9129	14.2
173.0	0.9422	0.0578	0.9473	0.0527	0.0193	0.0330	0.9477	0.0528	0.0340	0.9132	10.5
172.5	0.9705	0.0295	0.9762	0.0238	0.0195	0.0156	0.9649	0.0690	0.0162	0.9148	7.7
172.0	1.0000	0.0000	1.0000	0.0000	0.0201	0.0000	0.9799	0.0728	0.0000	0.9272	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S6. Continued

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 403.2						
94.6	0.0000	1.0000						0.0000	0.1437	0.8563	
116.9	0.1892	0.8108						0.0019	0.1377	0.8604	17.1
144.3	0.3903	0.6097						0.0037	0.1263	0.8700	21.9
169.3	0.5365	0.4635						0.0061	0.1117	0.8822	21.2
192.1	0.6394	0.3606						0.0103	0.0963	0.8934	16.6
213.2	0.7407	0.2593						0.0146	0.0838	0.9016	16.4
229.1	0.8343	0.1657						0.0219	0.0668	0.9113	15.4
247.9	0.8940	0.1060						0.0297	0.0517	0.9186	14.7
266.3	0.9201	0.0799						0.0349	0.0354	0.9297	11.7
277.0	0.9619	0.0381						0.0373	0.0172	0.9456	11.6
285.7	1.0000	0.0000						0.0606	0.0000	0.9394	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S7. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for methylcyclohexane (1) + benzene (2) + [C_2C_1im][DCA] (3) with S/F mass ratio of 10

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 323.2						
11.4	0.0000	1.0000						0.0000	0.1717	0.8283	
25.3	0.5039	0.4961						0.0070	0.1630	0.8299	23.5
24.2	0.5873	0.4127	0.7745	0.2255	0.0102	0.1443	0.8455	0.0203	0.1451	0.8346	10.2
23.4	0.6354	0.3646	0.7978	0.2022	0.0102	0.1233	0.8665	0.0370	0.1257	0.8373	5.9
23.1	0.6637	0.3363	0.8201	0.1799	0.0104	0.1071	0.8825	0.0519	0.1106	0.8375	4.2
21.8	0.7285	0.2715	0.8562	0.1438	0.0101	0.0900	0.8999	0.0663	0.0934	0.8403	3.8
21.6	0.7671	0.2329	0.8812	0.1188	0.0103	0.0715	0.9182	0.0811	0.0752	0.8437	3.1
20.7	0.8191	0.1809	0.9125	0.0875	0.0104	0.0554	0.9342	0.0947	0.0582	0.8471	2.8
20.2	0.8693	0.1307	0.9461	0.0539	0.0102	0.0363	0.9535	0.1117	0.0381	0.8502	2.3
18.9	0.9506	0.0494	0.9764	0.0236	0.0107	0.0159	0.9734	0.1291	0.0168	0.8541	2.5
18.5	1.0000	0.0000	1.0000	0.0000	0.0107	0.0000	0.9893	0.1405	0.0000	0.8595	
					T/K = 363.2						
50.8	0.0000	1.0000						0.0000	0.1470	0.8530	
65.8	0.2700	0.7300						0.0049	0.1430	0.8522	10.8
79.2	0.4610	0.5390						0.0095	0.1276	0.8629	11.5
92.4	0.6115	0.3885						0.0160	0.1111	0.8730	11.0
90.0	0.6712	0.3288	0.8346	0.1654	0.0127	0.0962	0.8911	0.0280	0.0969	0.8752	7.1
84.8	0.7244	0.2756	0.8654	0.1346	0.0137	0.0799	0.9064	0.0408	0.0811	0.8781	5.2
81.7	0.7775	0.2225	0.8972	0.1028	0.0146	0.0648	0.9207	0.0547	0.0661	0.8792	4.2
79.4	0.8302	0.1698	0.9253	0.0747	0.0143	0.0503	0.9354	0.0667	0.0514	0.8819	3.8
77.5	0.8895	0.1105	0.9521	0.0479	0.0153	0.0333	0.9514	0.0828	0.0341	0.8830	3.3
74.9	0.9504	0.0496	0.9789	0.0211	0.0155	0.0147	0.9698	0.0999	0.0151	0.8849	2.9
74.1	1.0000	0.0000	1.0000	0.0000	0.0162	0.0000	0.9838	0.1161	0.0000	0.8839	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S7. Continued

p/ kPa	y_1	y_2	$x_{1,I}$	$x_{2,I}$	$x_{1,II}$	$x_{2,II}$	$x_{3,II}$	x_1	x_2	x_3	α_{12}
					T/K = 403.2						
94.6	0.0000	1.0000						0.0000	0.1437	0.8563	
111.3	0.1888	0.8112						0.0037	0.1377	0.8586	8.7
125.3	0.3359	0.6641						0.0089	0.1225	0.8686	7.0
135.6	0.4665	0.5335						0.0137	0.1056	0.8807	6.7
148.3	0.5878	0.4122						0.0233	0.0940	0.8827	5.8
161.1	0.6871	0.3129						0.0342	0.0829	0.8829	5.3
175.0	0.7715	0.2285						0.0481	0.0692	0.8827	4.9
190.7	0.8463	0.1537						0.0633	0.0551	0.8816	4.8
197.5	0.9021	0.0979						0.0721	0.0363	0.8916	4.6
205.0	0.9663	0.0337						0.1071	0.0166	0.8763	4.5
209.0	1.0000	0.0000						0.0630	0.0000	0.9370	

[a] Standard uncertainty (u) are $u(y) = 0.001$, $u(x) = 0.001$, $u(x_I) = 0.02$, $u(x_{II}) = 0.002$, $u_r(P) = 0.02$, and $u(T) = 0.1$ K.

Table S8. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for methylcyclopentane (1) + methylcyclohexane (2) + benzene (3) + [C_2C_1im][SCN] (4) with S/F mass ratio of 10

T/ K	323.2[b]				343.2[b]				363.2[c]		383.2[c]		403.2[c]	
Compound	y	x	x_{II}	x_I	y	x	x_{II}	x_I	y	x	y	x	y	x
MCP	0.6988	0.0366	0.0085	0.753	0.6742	0.0209	0.0067	0.719	0.5828	0.0166	0.4959	0.0189	0.4277	0.0228
MCH	0.0373	0.0067	0.0008	0.056	0.0450	0.0054	0.0007	0.066	0.0469	0.0046	0.0419	0.0046	0.0374	0.0049
B	0.2638	0.1683	0.1088	0.191	0.2807	0.1644	0.1011	0.215	0.3703	0.1534	0.4621	0.1395	0.5348	0.1275
IL	-	0.7884	0.8819		-	0.8093	0.8915		-	0.8255	-	0.8370	-	0.8448
p/ kPa	39.2				83.3				116.7		145.1		166.4	
$\alpha_{MCA,B}$	10.7				15.7				12.1		6.8		4.0	

[a] Standard uncertainty (u) are u(y) = 0.001, u(x) = 0.001, u(x_I)= 0.01, u(x_{II}) = 0.002, $u_r(P)$ = 0.02, and u(T) = 0.1 K.

[b] VLLE data

[c] VLE data

Table S9. Isothermal vapor-liquid and vapor-liquid-liquid equilibria[a] for methylcyclopentane (1) + methylcyclohexane (2) + benzene (3) + [C_2C_1im][DCA] (4) with S/F mass ratio of 10

T/ K	323.2[b]				343.2[b]				363.2[c]		383.2[c]		403.2[c]	
Compound	y	x	x_{II}	x_I	y	x	x_{II}	x_I	y	x	y	x	y	x
MCP	0.7408	0.0340	0.0092	0.756	0.6958	0.0200	0.0071	0.721	0.6026	0.0169	0.5186	0.0180	0.4469	0.0223
MCH	0.0424	0.0064	0.0008	0.075	0.0506	0.0051	0.0006	0.072	0.0468	0.0047	0.0424	0.0046	0.0383	0.0049
B	0.2168	0.1658	0.1201	0.169	0.2536	0.1641	0.1266	0.207	0.3506	0.1538	0.4390	0.1418	0.5148	0.1307
IL	-	0.7938	0.8699		-	0.8108	0.8657		-	0.8246	-	0.8355	-	0.8421
p/ kPa	39.3				79.9				107.8		138.3		157.9	
$\alpha_{MCA,B}$	14.6				18.9				12.9		7.8		4.5	

[a] Standard uncertainty (u) are u(y) = 0.001, u(x) = 0.001, u(x_I)= 0.01, u(x_{II}) = 0.002, $u_r(P)$ = 0.02, and u(T) = 0.1 K.

[b] VLLE data

[c] VLE data