Toward Modeling the Aromatic/aliphatic Separation by Extractive Distillation with Tricyanomethanide-based Ionic Liquids Using CPA EoS

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Supporting Information

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Table S1. Vapor-liquid and Vapor-liquid-liquid Equilibria[a] for Hydrocarbon (1) + $[C_2C_1im][TCM]$ (2)

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323		T/ K = 363		T/ K = 403	
***n*-hexane + $[C_2C_1im][TCM]$**					
6.2	0.0017	7.8	0.0007	8.7	0.0005
16.4	0.0067	22.2	0.0028	25.7	0.0017
33.7	0.0158	51.4	0.0063	49.2	0.0025
50.6	0.0273	83.3	0.0103	83.0	0.0053
52.3	0.0596	111.4	0.0151	112.9	0.0067
52.3	0.1624	168.2	0.0256	231.2	0.0168
54.0	0.2048	183.8	0.0518	291.0	0.0220
54.3	1.0000	185.7	0.1485	345.3	0.0314
		188.3	0.2286	402.0	0.0430
		187.9	1.0000	450.2	0.0470
				492.2	0.0581
				492.2	0.1095
				493.1	0.2140
				492.9	1.0000
***n*-octane + $[C_2C_1im][TCM]$**					
4.4	0.0061	8.1	0.0097	11.4	0.0008
5.9	0.0210	19.7	0.0239	26.9	0.0035
6.2	0.0513	31.7	0.0495	50.2	0.0067
6.3	0.0683	33.0	0.0790	75.5	0.0101
6.4	0.0792	32.9	0.1079	95.0	0.0240
6.6	0.1620	33.0	0.1747	105.8	0.0389
6.7	0.2146	33.1	0.2294	113.2	0.0866
6.7	1.0000	33.4	1.0000	113.9	0.1830
				113.8	0.2418
				114.0	0.3014
				114.1	0.3570
				114.1	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 S1. Continued

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323		T/ K = 363		T/ K = 403	
benzene + [C_2C_1im][TCM]					
0.9	0.0182	2.9	0.0172	6.3	0.0114
2.1	0.0428	6.7	0.0393	16.6	0.0298
4.1	0.0852	14.1	0.0782	34.4	0.0585
6.2	0.1294	22.3	0.1153	55.4	0.0851
8.0	0.1675	30.2	0.1507	75.3	0.1107
12.0	0.2501	45.8	0.2271	116.0	0.1843
15.9	0.3232	57.6	0.2951	159.8	0.2458
18.9	0.3885	70.5	0.3576	184.9	0.2890
21.8	0.4458	84.2	0.4129	227.8	0.3389
24.2	0.4936	95.3	0.4717	254.8	0.3940
27.4	0.5562	108.7	0.5234	290.5	0.4468
30.7	0.6058	120.0	0.5747	312.8	0.5028
33.1	0.6537	127.1	0.6242	343.4	0.5591
35.2	0.6927	132.7	0.6700	360.3	0.6128
35.5	0.7366	135.2	0.7172	377.3	0.6632
35.9	0.7766	135.7	0.7590	378.1	0.7147
36.0	0.8127	135.9	0.7994	378.4	0.7624
36.1	1.0000	136.0	1.0000	378.4	1.0000
***p*-xylene + [C_2C_1im][TCM]**					
0.2	0.0162	1.3	0.0137	4.2	0.0100
0.5	0.0369	3.1	0.0336	8.7	0.0267
1.0	0.0719	5.9	0.0666	17.8	0.0542
1.5	0.1054	8.4	0.0976	24.9	0.0830
1.9	0.1407	10.8	0.1310	30.2	0.1149
2.7	0.2125	14.3	0.2010	44.8	0.1803
3.3	0.2777	18.0	0.2575	57.9	0.2338
3.8	0.3353	20.8	0.3208	70.3	0.2885
4.3	0.3925	21.6	0.3799	79.5	0.3450
4.3	0.4429	22.5	0.4321	80.8	0.4052
4.3	0.4952	22.4	0.4896	80.8	0.4593
4.2	0.5471	22.5	0.5391	81.1	0.5151
4.2	0.5964	22.5	0.5898	80.6	0.5668
4.3	0.6417	22.5	0.6395	80.7	0.6182
4.3	1.0000	22.6	1.0000	80.8	0.6650
				80.8	0.7123
				80.6	0.7624
				80.6	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. Vapor-liquid and Vapor-liquid-liquid Equilibria[a] for Hydrocarbon (1) + [4-C_4C_1py][TCM] (2)

p/ kPa	x_1	p/ kPa	x_1	p/ kPa	x_1
T/ K = 323		T/ K = 363		T/ K = 403	
***n*-hexane + [4-C_4C_1py][TCM]**					
5.2	0.0028	6.7	0.0011	8.6	0.0002
13.7	0.0151	19.5	0.0035	24.7	0.0006
29.0	0.0315	46.0	0.0089	55.1	0.0018
39.8	0.0427	76.1	0.0134	85.9	0.0030
51.8	0.0684	108.7	0.0198	115.1	0.0038
53.5	0.1582	160.0	0.0322	165.0	0.0099
54.0	0.2122	180.1	0.0688	230.2	0.0125
54.3	1.0000	181.7	0.1887	290.1	0.0255
		187.9	1.0000	354.4	0.0285
				392.0	0.0434
				471.2	0.0711
				490.6	0.1739
				493.1	0.2453
				492.8	1.0000
***n*-octane + [4-C_4C_1py][TCM]**					
1.5	0.0026	5.8	0.0125	10.2	0.0082
4.5	0.0234	14.2	0.0307	23.4	0.0125
6.6	0.0580	27.6	0.0526	46.1	0.0198
6.7	0.0914	33.0	0.0778	66.2	0.0386
6.7	0.1238	33.3	0.1322	89.8	0.0461
6.7	0.1934	33.2	0.2053	103.2	0.0600
6.7	0.2565	33.3	0.2708	114.1	0.1000
6.7	1.0000	33.4	1.0000	114.1	0.1744
				114.2	0.2851
				114.2	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		T/ K = 363		T/ K = 403	
benzene + [4-C_4C_1py][TCM]					
0.6	0.0212	2.2	0.0212	6.5	0.0147
1.5	0.0541	5.2	0.0512	14.7	0.0412
3.0	0.1067	10.9	0.1010	39.5	0.0786
4.5	0.1548	16.8	0.1461	54.8	0.1126
6.0	0.2028	22.9	0.1905	75.9	0.1494
9.1	0.2958	36.3	0.2741	111.5	0.2126
11.3	0.3556	49.9	0.3512	164.1	0.3013
15.5	0.4395	63.0	0.4166	194.2	0.3550
17.5	0.5018	73.2	0.4665	227.2	0.4124
21.0	0.5602	87.1	0.5303	254.9	0.4648
24.2	0.6094	96.9	0.5811	284.0	0.5221
26.9	0.6497	105.5	0.6293	324.9	0.6188
31.2	0.7033	120.7	0.6942	340.4	0.6635
34.5	0.7361	125.2	0.7176	358.0	0.7112
35.9	0.7741	130.9	0.7565	368.4	0.7592
35.9	0.8099	134.7	0.7958	378.1	0.7973
36.0	0.8302	135.9	0.8309	378.4	0.8500
36.1	1.0000	136.0	1.0000	378.4	1.0000
***p*-xylene + [4-C_4C_1py][TCM]**					
0.1	0.0201	0.8	0.0179	2.4	0.0139
0.3	0.0459	1.9	0.0425	6.2	0.0369
0.6	0.0887	3.7	0.0847	12.3	0.0737
0.9	0.1284	5.4	0.1236	18.0	0.1080
1.1	0.1655	6.9	0.1620	24.2	0.1440
1.7	0.2517	10.6	0.2453	34.9	0.2164
2.2	0.3271	13.5	0.3113	46.6	0.2832
2.7	0.3828	16.1	0.3670	55.7	0.3447
3.1	0.4449	18.3	0.4337	61.7	0.4051
3.7	0.5001	20.4	0.4912	69.3	0.4569
4.3	0.5514	22.5	0.5430	75.5	0.5135
4.3	0.6036	22.5	0.5977	79.5	0.5670
4.3	0.6467	22.6	0.6391	80.7	0.6160
4.3	0.6886	22.7	0.6841	80.8	0.6694
4.3	0.7308	22.7	0.7263	80.7	0.7108
4.2	0.7690	22.8	0.7674	80.6	0.7487
4.3	0.8072	22.6	0.8063	80.6	0.7930
4.3	1.0000	22.6	1.0000	80.6	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. Vapor-liquid and Vapor-liquid-liquid Equilibria[a] for *n*-Hexane (1) + Benzene (2) + [C_2C_1im][TCM] (3) with S/F = 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_{21}
					T/K = 323.2						
8.9	0.0000	1.0000						0.0000	0.1963	0.8037	
26.2	0.6889	0.3111						0.0060	0.1775	0.8164	65.3
40.9	0.8207	0.1793						0.0142	0.1572	0.8286	50.7
51.0	0.8742	0.1258						0.0239	0.1414	0.8347	41.0
53.4	0.9032	0.0968	0.8412	0.1588	0.0160	0.1171	0.8669	0.0380	0.1182	0.8438	29.0
53.5	0.9205	0.0795	0.8766	0.1234	0.0171	0.0943	0.8886	0.0561	0.0956	0.8483	19.7
53.6	0.9348	0.0652	0.8982	0.1018	0.0175	0.0755	0.9070	0.0747	0.0772	0.8481	14.8
53.7	0.9513	0.0487	0.9260	0.0740	0.0171	0.0560	0.9269	0.0962	0.0575	0.8463	11.7
53.8	0.9686	0.0314	0.9532	0.0468	0.0170	0.0362	0.9468	0.1134	0.0373	0.8493	10.1
53.9	0.9823	0.0177	0.9741	0.0259	0.0163	0.0205	0.9632	0.1308	0.0211	0.8481	9.0
54.4	1.0000	0.0000	1.0000	0.0000	0.0171	0.0000	0.9829	0.1489	0.0000	0.8511	
					T/K = 363.2						
47.2	0.0000	1.0000						0.0000	0.1745	0.8255	
71.5	0.5059	0.4941						0.0020	0.1653	0.8327	84.6
86.9	0.6263	0.3737						0.0029	0.1437	0.8533	82.1
106.1	0.6925	0.3075						0.0036	0.1264	0.8700	78.9
130.7	0.7936	0.2064						0.0060	0.1094	0.8867	70.1
149.4	0.8765	0.1235						0.0111	0.0922	0.8967	58.9
161.5	0.9144	0.0856						0.0224	0.0772	0.9004	36.8
187.5	0.9466	0.0534	0.9293	0.0707	0.0157	0.0601	0.9242	0.0289	0.0609	0.9103	37.4
188.4	0.9642	0.0358	0.9531	0.0469	0.0156	0.0393	0.9451	0.0441	0.0400	0.9159	24.4
188.1	0.9847	0.0153	0.9848	0.0152	0.0158	0.0126	0.9716	0.0670	0.0190	0.9141	18.2
188.1	1.0000	0.0000	0.9995	0.0005	0.0167	0.0000	0.9833	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 S3. 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_{21}
					T/K = 403.2						
77.4	0.0000	1.0000						0.0000	0.1690	0.8310	
92.2	0.3615	0.6385						0.0017	0.1579	0.8403	52.0
103.7	0.6227	0.3773						0.0042	0.1460	0.8498	57.3
118.1	0.7523	0.2477						0.0074	0.1316	0.8610	53.9
137.7	0.8294	0.1706						0.0114	0.1128	0.8758	48.2
158.1	0.8860	0.1140						0.0174	0.0942	0.8884	42.1
173.5	0.9230	0.0770						0.0258	0.0768	0.8974	35.7
193.2	0.9481	0.0519						0.0318	0.0559	0.9122	32.1
209.7	0.9709	0.0291						0.0416	0.0375	0.9209	30.0
221.1	0.9850	0.0150						0.0494	0.0212	0.9295	28.2
233.3	1.0000	0.0000						0.0577	0.0000	0.9423	

[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. Vapor-liquid and Vapor-liquid-liquid Equilibria[a] for *n*-Hexane (1) + Benzene (2) + [4-C_4C_1py][TCM] (3) with S/F = 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_{21}
					T/K = 323.2						
9.1	0.0000	1.0000						0.0000	0.2319	0.7681	
17.0	0.6859	0.3141						0.0125	0.2117	0.7758	37.0
28.0	0.8382	0.1618						0.0237	0.1823	0.7939	39.8
40.9	0.8877	0.1123						0.0324	0.1626	0.8050	39.7
51.7	0.9270	0.0730						0.0444	0.1395	0.8161	39.9
53.6	0.9427	0.0573	0.8852	0.1148	0.0312	0.1140	0.8548	0.0652	0.1141	0.8207	28.8
53.7	0.9526	0.0474	0.9049	0.0951	0.0304	0.0921	0.8775	0.0880	0.0923	0.8198	21.1
53.9	0.9662	0.0338	0.9333	0.0667	0.0300	0.0669	0.9031	0.1085	0.0669	0.8245	17.6
54.0	0.9773	0.0227	0.9580	0.0420	0.0306	0.0440	0.9255	0.1303	0.0437	0.8260	14.5
54.0	0.9881	0.0119	0.9773	0.0227	0.0313	0.0242	0.9445	0.1441	0.0240	0.8319	13.8
54.4	1.0000	0.0000	1.0000	0.0000	0.0314	0.0000	0.9686	0.1609	0.0000	0.8391	
					T/K = 363.2						
25.8	0.0000	1.0000						0.0000	0.2075	0.7925	
45.5	0.5140	0.4860						0.0038	0.1915	0.8047	53.3
67.7	0.6460	0.3540						0.0066	0.1892	0.8222	52.1
89.0	0.7589	0.2411						0.0091	0.1495	0.8414	51.9
111.3	0.8283	0.1717						0.0114	0.1289	0.8597	54.7
138.4	0.8924	0.1076						0.0178	0.1120	0.8702	52.2
152.6	0.9275	0.0725						0.0215	0.0888	0.8898	52.9
174.9	0.9533	0.0467						0.0289	0.0689	0.9021	48.6
187.2	0.9726	0.0274	0.9730	0.0270	0.0274	0.0470	0.9256	0.0426	0.0474	0.9101	39.5
187.5	0.9886	0.0114	0.9886	0.0114	0.0282	0.0203	0.9515	0.0489	0.0205	0.9307	36.3
188.1	1.0000	0.0000	0.9995	0.0005	0.0286	0.0000	0.9714	0.0638	0.0000	0.9362	

[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_{21}
					T/K = 403.2						
66.0	0.0000	1.0000						0.0000	0.2009	0.7991	
85.4	0.3804	0.6196						0.0019	0.1857	0.8123	58.8
103.7	0.6047	0.3953						0.0052	0.1690	0.8258	49.7
118.7	0.7301	0.2699						0.0089	0.1527	0.8384	46.4
131.3	0.8151	0.1849						0.0130	0.1268	0.8602	42.9
157.0	0.8800	0.1200						0.0199	0.1100	0.8701	40.5
169.5	0.9145	0.0855						0.0237	0.0846	0.8917	38.3
181.4	0.9477	0.0523						0.0324	0.0623	0.9053	34.8
197.4	0.9710	0.0290						0.0448	0.0422	0.9131	31.5
208.0	0.9853	0.0147						0.0542	0.0240	0.9218	29.6
218.3	1.0000	0.0000						0.0595	0.0000	0.9405	

[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. Vapor-liquid and Vapor-liquid-liquid Equilibria[a] for *n*-Octane (1) + *p*-Xylene (2) + [C_2C_1im][TCM] (3) with S/F = 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_{21}
					T/K = 323.2						
1.9	0.0000	1.0000						0.0000	0.1598	0.8402	
5.6	0.6225	0.3775	0.5182	0.4818	0.0043	0.1431	0.8526	0.0131	0.1492	0.8377	18.8
5.9	0.6806	0.3194	0.5793	0.4207	0.0044	0.1207	0.8749	0.0286	0.1336	0.8378	9.9
6.0	0.7538	0.2462	0.6606	0.3394	0.0050	0.0974	0.8976	0.0436	0.1119	0.8445	7.9
6.2	0.7910	0.2090	0.7155	0.2845	0.0055	0.0821	0.9124	0.0579	0.0972	0.8449	6.4
6.3	0.8295	0.1705	0.7739	0.2261	0.0059	0.0667	0.9274	0.0721	0.0807	0.8472	5.4
6.5	0.8681	0.1319	0.8232	0.1768	0.0059	0.0525	0.9416	0.0874	0.0650	0.8475	4.9
6.4	0.9015	0.0985	0.8764	0.1236	0.0063	0.0393	0.9544	0.1026	0.0487	0.8487	4.3
6.6	0.9368	0.0632	0.9195	0.0805	0.0062	0.0251	0.9687	0.1175	0.0319	0.8506	4.0
6.7	0.9679	0.0321	0.9625	0.0375	0.0068	0.0128	0.9804	0.1326	0.0160	0.8514	3.6
6.7	1.0000	0.0000	1.0000	0.0000	0.0069	0.0000	0.9931	0.1465	0.0000	0.8535	
					T/K = 363.2						
12.6	0.0000	1.0000						0.0000	0.1749	0.8251	
27.2	0.5639	0.4361						0.0081	0.1605	0.8314	25.7
30.2	0.6869	0.3131	0.5579	0.4421	0.0055	0.1315	0.8630	0.0214	0.1405	0.8380	14.4
31.0	0.7363	0.2637	0.6307	0.3693	0.0061	0.1101	0.8838	0.0392	0.1239	0.8369	8.8
31.6	0.7959	0.2041	0.6979	0.3021	0.0067	0.0923	0.9010	0.0533	0.1065	0.8401	7.8
31.9	0.8145	0.1855	0.7502	0.2498	0.0070	0.0748	0.9182	0.0705	0.0898	0.8397	5.6
32.1	0.8554	0.1446	0.7994	0.2006	0.0068	0.0572	0.9360	0.0859	0.0715	0.8426	4.9
32.3	0.8945	0.1055	0.8560	0.1440	0.0069	0.0418	0.9513	0.1013	0.0532	0.8454	4.5
32.8	0.9335	0.0665	0.9078	0.0922	0.0075	0.0273	0.9652	0.1185	0.0353	0.8462	4.2
33.1	0.9666	0.0334	0.9540	0.0460	0.0074	0.0134	0.9792	0.1356	0.0178	0.8466	3.8
33.4	1.0000	0.0000	1.0000	0.0000	0.0077	0.0000	0.9923	0.1506	0.0000	0.8494	

[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_{21}
					T/K = 403.2						
38.9	0.0000	1.0000						0.0000	0.1435	0.8565	
63.0	0.3610	0.6390						0.0030	0.1322	0.8647	24.6
83.7	0.5545	0.4455						0.0058	0.1168	0.8774	25.2
100.2	0.6854	0.3146						0.0104	0.1018	0.8878	21.3
108.8	0.7602	0.2398						0.0180	0.0897	0.8923	15.8
110.5	0.8097	0.1903						0.0293	0.0746	0.8962	10.8
111.2	0.8522	0.1478						0.0424	0.0603	0.8973	8.2
112.9	0.8909	0.1091						0.0550	0.0452	0.8998	6.7
113.9	0.9301	0.0699						0.0678	0.0296	0.9026	5.8
114.4	0.9656	0.0344						0.0808	0.0149	0.9043	5.2
114.2	1.0000	0.0000						0.0937	0.0000	0.9063	

[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. Vapor-liquid and Vapor-liquid-liquid Equilibria[a] for *n*-Octane (1) + *p*-Xylene (2) + [4-C_4C_1py][TCM] (3) with S/F = 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_{21}
					T/K = 323.2						
1.0	0.0000	1.0000						0.0000	0.1855	0.8145	
4.5	0.7034	0.2966						0.0147	0.1709	0.8144	27.5
6.4	0.8260	0.1740	0.6238	0.3762	0.0080	0.1420	0.8500	0.0308	0.1510	0.8182	23.3
6.5	0.8537	0.1463	0.6946	0.3054	0.0087	0.1195	0.8718	0.0496	0.1308	0.8196	15.4
6.6	0.8653	0.1347	0.7497	0.2503	0.0092	0.1009	0.8899	0.0658	0.1125	0.8217	11.0
6.7	0.8937	0.1063	0.7977	0.2023	0.0099	0.0836	0.9066	0.0836	0.0948	0.8216	9.5
6.6	0.9182	0.0818	0.8428	0.1572	0.0104	0.0654	0.9242	0.1003	0.0755	0.8242	8.4
6.7	0.9395	0.0605	0.8848	0.1152	0.0108	0.0484	0.9408	0.1182	0.0567	0.8251	7.4
6.7	0.9603	0.0397	0.9242	0.0758	0.0104	0.0309	0.9587	0.1355	0.0371	0.8273	6.6
6.7	0.9796	0.0204	0.9626	0.0374	0.0105	0.0154	0.9740	0.1540	0.0188	0.8273	5.9
6.7	1.0000	0.0000	1.0000	0.0000	0.0107	0.0000	0.9894	0.1696	0.0000	0.8304	
					T/K = 363.2						
8.1	0.0000	1.0000						0.0000	0.2044	0.7956	
17.5	0.5856	0.4144						0.0122	0.1864	0.8013	21.5
27.3	0.7644	0.2356						0.0247	0.1666	0.8086	21.9
31.9	0.8341	0.1659	0.6787	0.3213	0.0087	0.1360	0.8553	0.0422	0.1453	0.8125	17.3
32.8	0.8712	0.1288	0.7316	0.2684	0.0091	0.1142	0.8767	0.0587	0.1249	0.8164	14.4
32.6	0.8822	0.1178	0.7848	0.2152	0.0097	0.0942	0.8961	0.0787	0.1050	0.8163	10.0
32.7	0.9117	0.0883	0.8295	0.1705	0.0100	0.0738	0.9162	0.0973	0.0841	0.8186	8.9
32.9	0.9265	0.0735	0.8726	0.1274	0.0101	0.0538	0.9362	0.1169	0.0629	0.8201	6.8
33.3	0.9591	0.0409	0.9180	0.0820	0.0108	0.0351	0.9541	0.1358	0.0415	0.8227	7.2
33.3	0.9778	0.0222	0.9611	0.0389	0.0105	0.0172	0.9722	0.1518	0.0204	0.8278	5.9
33.4	1.0000	0.0000	1.0000	0.0000	0.0107	0.0000	0.9893	0.1747	0.0000	0.8253	

[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_{21}
					T/K = 403.2						
26.8	0.0000	1.0000						0.0000	0.1728	0.8272	
44.0	0.4013	0.5987						0.0065	0.1581	0.8354	16.3
60.2	0.6001	0.3999						0.0129	0.1415	0.8456	16.5
79.3	0.7312	0.2688						0.0181	0.1230	0.8589	18.5
91.4	0.8023	0.1977						0.0251	0.1071	0.8678	17.3
102.6	0.8550	0.1450						0.0339	0.0906	0.8755	15.7
109.9	0.8986	0.1014						0.0451	0.0735	0.8814	14.5
110.4	0.9265	0.0735						0.0589	0.0542	0.8869	11.6
112.1	0.9516	0.0484						0.0769	0.0362	0.8868	9.3
113.2	0.9762	0.0238						0.0931	0.0182	0.8886	8.1
114.2	1.0000	0.0000						0.1098	0.0000	0.8902	

[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.