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

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

|  |  |  |
| --- | --- | --- |
| IL | **MCP,B | **MCH,B |
| S/F ratio | 1 | 5 | 10 | 1 | 5 | 10 |
| T/K = 323.2 K |
| [C2C1im][TCM] | 3.1 | 16.7 | 20.2 | 1.3 | 6.3 | 10.3 |
| [4-C4C1py][TCM] | 3.9 | 15.5 | 16.6 | 1.7 | 8.0 | 9.1 |
| [C2C1im][DCA] | 2.4 | 9.5 | 28.6 | 1.0 | 3.6 | 9.0 |
| [C2C1im][SCN] | 2.4 | 9.4 | 27.8 | 0.9 | 2.8 | 6.9 |
| [C4C1im]2[Co(SCN)4] | 2.4 | 5.9 | 21.1 | 1.0 | 2.3 | 6.8 |
| [C2C1im]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 |
| [C2C1im][TCM] | 2.5 | 14.0 | 17.3 | 1.2 | 7.4 | 8.2 |
| [4-C4C1py][TCM] | 3.3 | 13.0 | 13.0 | 1.5 | 5.8 | 6.6 |
| [C2C1im][DCA] | 2.0 | 15.9 | 34.5 | 0.9 | 4.5 | 11.9 |
| [C2C1im][SCN] | 1.9 | 10.2 | 30.0 | 0.9 | 3.4 | 19.7 |
| [C4C1im]2[Co(SCN)4] | 2.0 | 11.6 | 16.2 | 1.0 | 5.8 | 7.2 |
| [C2C1im]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 equilibriaa for hydrocarbon (1) + [C2C1im][SCN] (2)**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ***p*/ kPa** | ***x*1** | ***p*/ kPa** | ***x*1** | ***p*/ kPa** | ***x*1** |
| ***T*/ K** = 323 | ***T*/ K** = 363 | ***T*/ K** = 403 |
| **methylcyclopentane + [C2C1im][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 + [C2C1im][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 | ***T*/ K** = 363 | ***T*/ K** = 403 |
| **benzene + [C2C1im][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 equilibriaa for hydrocarbon (1) + [C2C1im][DCA] (2)**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| ***p*/ kPa** | ***x*1** | ***p*/ kPa** | ***x*1** | ***p*/ kPa** | ***x*1** |
| ***T*/ K** = 323 | ***T*/ K** = 363 | ***T*/ K** = 403 |
| **methylcyclopentane + [C2C1im][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 + [C2C1im][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 | ***T*/ K** = 363 | ***T*/ K** = 403 |
| **benzene + [C2C1im][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 equilibriaa for methylcyclopentane (1) + benzene (2) + [C2C1im][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** |  | ****12** |
| ** |
| 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 |  |   |
| ** |
| 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** |  | ****12** |
| ** |
| 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 equilibriaa for methylcyclohexane (1) + benzene (2) + [C2C1im][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** |  | ****12** |
| ** |
| 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 |  |   |
| ** |
| 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** |  | ****12** |
| ** |
| 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 equilibriaa for methylcyclopentane (1) + benzene (2) + [C2C1im][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** |  | ****12** |
| ** |
| 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 |  |   |
| ** |
| 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** |  | ****12** |
| ** |
| 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 equilibriaa for methylcyclohexane (1) + benzene (2) + [C2C1im][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** |  | ****12** |
| ** |
| 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 |  |   |
| ** |
| 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** |  | ****12** |
| ** |
| 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 equilibriaa for methylcyclopentane (1) + methylcyclohexane (2) + benzene (3) + [C2C1im][SCN] (4) with S/F mass ratio of 10**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *T*/ K |  | 323.2b |  | 343.2b |  | 363.2c |  | 383.2c |  | 403.2c |
| 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 |
| **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, ur(*P*) = 0.02, and u(*T*) = 0.1 K.

b VLLE data

c VLE data

**Table S9. Isothermal vapor-liquid and vapor-liquid-liquid equilibriaa for methylcyclopentane (1) + methylcyclohexane (2) + benzene (3) + [C2C1im][DCA] (4) with S/F mass ratio of 10**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| *T*/ K |  | 323.2b |  | 343.2b |  | 363.2c |  | 383.2c |  | 403.2c |
| 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 |
| **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, ur(*P*) = 0.02, and u(*T*) = 0.1 K.

b VLLE data

c VLE data

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