

Supporting Information for *Acta Phys. -Chim. Sin.* 2017, 33 (3), 513–519

doi: 10.3866/PKU.WHXB201610251

[C₂mim][Ala]丙氨酸离子液体水溶液粘滞流动的活化参数

佟 静* 刘 璐 张 朵 郑 煦 陈 霞 杨家振

(辽宁大学化学学院, 沈阳 110036)

Parameters of the Activation of Viscous Flow of Aqueous [C₂mim][Ala]

TONG Jing* LIU Lu ZHANG Duo ZHENG Xu CHEN Xia YANG

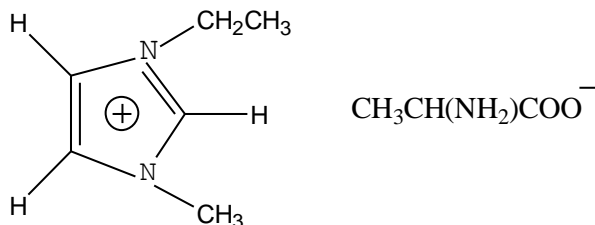
Jia-Zhen

(College of Chemistry, Liaoning University, Shenyang 110036, P. R. China)

*Corresponding author. Email: tongjinglnu@sina.com; Tel: +86-24-62207801.

表 S1 [C₂mim][Ala]离子液体的 ¹H NMR 表征

Table S1 ¹H NMR of IL [C₂mim][Ala]



| Chemical shift | Hydrogen number | Radical |
|-----------------|-----------------|--|
| 1.230-1.254 (d) | 3 | CH ₃ CH(NH ₂)COO ⁻ |
| 1.475-1.525 (t) | 3 | N-CH ₂ CH ₃ |
| 3.307-3.378 (m) | 1 | CH ₃ CH(NH ₂)COO ⁻ |
| 3.892 (s) | 3 | CH ₃ -N |
| 4.191-4.265 (m) | 2 | N-CH ₂ CH ₃ |
| 7.419-7.425 (d) | 1 | N-CH=CH-N |
| 7.487-7.493 (d) | 1 | N-CH=CH-N |

表 S2 288.15-328.15 K 不同浓度[C₂mim][Ala]溶液的平均摩尔体积(10⁵V_m)

Table S2 Values of the average molar volume (10⁵V_m) for aqueous [C₂mim][Ala] with various molalities

| <i>m</i> (/mol kg ⁻¹) | 10 ⁵ V _m /(m ³ mol ⁻¹) | | | | | | | | |
|--------------------------------------|---|----------|----------|----------|----------|----------|----------|----------|----------|
| | 288.15 K | 293.15 K | 298.15 K | 303.15 K | 308.15 K | 313.15 K | 318.15 K | 323.15 K | 328.15 K |
| 0.0163 | 1.8076 | 1.8093 | 1.8115 | 1.8140 | 1.8170 | 1.8203 | 1.8240 | 1.8280 | 1.8323 |
| 0.0220 | 1.8092 | 1.8109 | 1.8130 | 1.8156 | 1.8186 | 1.8219 | 1.8256 | 1.8296 | 1.8340 |
| 0.0278 | 1.8108 | 1.8125 | 1.8147 | 1.8173 | 1.8202 | 1.8236 | 1.8273 | 1.8313 | 1.8356 |
| 0.0556 | 1.8185 | 1.8203 | 1.8225 | 1.8251 | 1.8281 | 1.8315 | 1.8352 | 1.8393 | 1.8437 |
| 0.1670 | 1.8490 | 1.8510 | 1.8535 | 1.8563 | 1.8594 | 1.8629 | 1.8667 | 1.8709 | 1.8754 |
| 0.2789 | 1.8790 | 1.8813 | 1.8842 | 1.8872 | 1.8905 | 1.8941 | 1.8980 | 1.9022 | 1.9069 |
| 0.3914 | 1.9090 | 1.9115 | 1.9146 | 1.9177 | 1.9213 | 1.9250 | 1.9290 | 1.9332 | 1.9380 |
| 0.5040 | 1.9388 | 1.9416 | 1.9449 | 1.9482 | 1.9519 | 1.9556 | 1.9598 | 1.9643 | 1.9690 |
| 0.6173 | 1.9683 | 1.9714 | 1.9749 | 1.9785 | 1.9823 | 1.9862 | 1.9905 | 1.9951 | 1.9999 |
| 0.7312 | 1.9977 | 2.0010 | 2.0049 | 2.0087 | 2.0128 | 2.0166 | 2.0210 | 2.0257 | 2.0305 |
| 0.8452 | 2.0272 | 2.0303 | 2.0347 | 2.0387 | 2.0429 | 2.0469 | 2.0515 | 2.0562 | 2.0611 |
| 1.0079 | 2.0686 | 2.0721 | 2.0768 | 2.0810 | 2.0852 | 2.0896 | 2.0942 | 2.0992 | 2.1042 |

表 S3 288.15-328.15 K 不同浓度[C₂mim][Ala]溶液的表观摩尔体积(ϕV_B)
 Table S3 Values of apparent molar volume (ϕV_B) for aqueous [C₂mim][Ala] with various molalities

| $m/$ (mol kg ⁻¹) | $\phi V_B/(\text{cm}^3 \text{mol}^{-1})$ | | | | | | | | |
|---------------------------------|--|----------|----------|----------|----------|----------|----------|----------|----------|
| | 288.15 K | 293.15 K | 298.15 K | 303.15 K | 308.15 K | 313.15 K | 318.15 K | 323.15 K | 328.15 K |
| 0.0163 | 173.0 | 174.3 | 175.7 | 176.6 | 177.4 | 177.7 | 178.7 | 179.0 | 179.4 |
| 0.0220 | 172.9 | 174.0 | 175.5 | 176.2 | 177.3 | 177.6 | 178.4 | 178.7 | 179.1 |
| 0.0278 | 172.6 | 173.9 | 175.1 | 176.1 | 177.0 | 177.3 | 178.0 | 178.7 | 179.1 |
| 0.0556 | 172.1 | 173.4 | 174.8 | 175.8 | 176.6 | 177.2 | 177.7 | 178.2 | 178.8 |
| 0.1670 | 170.9 | 172.3 | 173.7 | 174.7 | 175.3 | 175.9 | 176.5 | 177.1 | 177.6 |
| 0.2789 | 169.9 | 171.3 | 172.9 | 173.8 | 174.5 | 175.0 | 175.7 | 176.1 | 176.9 |
| 0.3914 | 169.3 | 170.6 | 172.0 | 172.9 | 173.7 | 174.3 | 174.9 | 175.3 | 176.0 |
| 0.5040 | 168.8 | 170.2 | 171.5 | 172.4 | 173.2 | 173.7 | 174.4 | 174.9 | 175.5 |
| 0.6173 | 168.3 | 169.6 | 170.9 | 171.9 | 172.8 | 173.2 | 173.9 | 174.4 | 174.9 |
| 0.7312 | 167.7 | 169.0 | 170.4 | 171.4 | 172.3 | 172.8 | 173.4 | 173.9 | 174.4 |
| 0.8452 | 167.4 | 168.4 | 170.0 | 171.0 | 171.9 | 172.4 | 173.0 | 173.6 | 174.0 |
| 1.0079 | 166.9 | 168.0 | 169.5 | 170.4 | 171.1 | 171.8 | 172.4 | 173.0 | 173.4 |
| $a_0 =$ | 173.8 | 175.1 | 176.5 | 177.3 | 178.3 | 178.6 | 179.4 | 179.8 | 180.3 |
| a_1 | -7.043 | -7.116 | -7.065 | -6.887 | -7.044 | -6.818 | -6.973 | -6.881 | -6.821 |
| r^2 | 0.9980 | 0.9986 | 0.9982 | 0.9979 | 0.9988 | 0.9984 | 0.9979 | 0.9986 | 0.9981 |
| s | 0.1058 | 0.0880 | 0.1009 | 0.1059 | 0.0822 | 0.0920 | 0.1062 | 0.0878 | 0.0996 |

表 S4 用测定的溶液密度数据换算的物质的量浓度(c)
 Table S4 Values of concentration of substance (c) converted by the measured solution density

| m (mol kg ⁻¹) | $c/(\text{mol dm}^{-3})$ | | | | | | | | |
|--------------------------------|--------------------------|----------|----------|----------|----------|----------|----------|----------|----------|
| | 288.15 K | 293.15 K | 298.15 K | 303.15 K | 308.15 K | 313.15 K | 318.15 K | 323.15 K | 328.15 K |
| 0.0163 | 0.0163 | 0.0163 | 0.0162 | 0.0162 | 0.0162 | 0.0162 | 0.0161 | 0.0161 | 0.0160 |
| 0.0220 | 0.0219 | 0.0219 | 0.0218 | 0.0218 | 0.0218 | 0.0217 | 0.0217 | 0.0216 | 0.0216 |
| 0.0278 | 0.0276 | 0.0276 | 0.0276 | 0.0275 | 0.0275 | 0.0274 | 0.0274 | 0.0273 | 0.0273 |
| 0.0556 | 0.0550 | 0.0550 | 0.0549 | 0.0548 | 0.0547 | 0.0546 | 0.0545 | 0.0544 | 0.0543 |
| 0.1670 | 0.1623 | 0.1621 | 0.1619 | 0.1616 | 0.1613 | 0.1610 | 0.1607 | 0.1603 | 0.1600 |
| 0.2789 | 0.2661 | 0.2658 | 0.2654 | 0.2650 | 0.2645 | 0.2640 | 0.2634 | 0.2629 | 0.2622 |
| 0.3914 | 0.3668 | 0.3663 | 0.3657 | 0.3651 | 0.3644 | 0.3637 | 0.3630 | 0.3622 | 0.3613 |
| 0.5040 | 0.4641 | 0.4635 | 0.4627 | 0.4619 | 0.4610 | 0.4601 | 0.4591 | 0.4581 | 0.4570 |
| 0.6173 | 0.5588 | 0.5579 | 0.5569 | 0.5559 | 0.5548 | 0.5537 | 0.5525 | 0.5513 | 0.5499 |
| 0.7312 | 0.6509 | 0.6498 | 0.6485 | 0.6473 | 0.6460 | 0.6448 | 0.6433 | 0.6419 | 0.6403 |
| 0.8452 | 0.7398 | 0.7387 | 0.7371 | 0.7357 | 0.7342 | 0.7327 | 0.7311 | 0.7294 | 0.7277 |
| 1.0079 | 0.8621 | 0.8607 | 0.8587 | 0.8570 | 0.8553 | 0.8534 | 0.8516 | 0.8495 | 0.8475 |

表 S5 [C₂mim][Ala]水溶液的外推函数值(η')Table S5 Values of extrapolation function (η') for aqueous [C₂mim][Ala]

| m (mol kg ⁻¹) | $\eta'/(L^{1/2} \text{ mol}^{-1/2})$ | | | | | | | | |
|--------------------------------|--------------------------------------|----------|----------|----------|----------|----------|----------|----------|----------|
| | 288.15 K | 293.15 K | 298.15 K | 303.15 K | 308.15 K | 313.15 K | 318.15 K | 323.15 K | 328.15 K |
| 0.0163 | 0.1151 | 0.1082 | 0.1017 | 0.1012 | 0.0955 | 0.0927 | 0.0898 | 0.0870 | 0.0857 |
| 0.0220 | 0.1377 | 0.1316 | 0.1229 | 0.1225 | 0.1173 | 0.1143 | 0.1104 | 0.1065 | 0.1055 |
| 0.0278 | 0.1563 | 0.1523 | 0.1457 | 0.1432 | 0.1380 | 0.1320 | 0.1291 | 0.1250 | 0.1285 |
| 0.0556 | 0.2416 | 0.2332 | 0.2282 | 0.2169 | 0.2193 | 0.2107 | 0.2101 | 0.1959 | 0.2113 |
| 0.1670 | 0.4857 | 0.4846 | 0.4681 | 0.4375 | 0.4275 | 0.4072 | 0.3869 | 0.3767 | 0.3787 |
| 0.2789 | 0.6373 | 0.6273 | 0.5974 | 0.5576 | 0.5377 | 0.5227 | 0.5020 | 0.4925 | 0.4682 |
| 0.3914 | 0.7538 | 0.7338 | 0.7141 | 0.6648 | 0.6448 | 0.6150 | 0.5853 | 0.5756 | 0.5558 |
| 0.5040 | 0.8810 | 0.8414 | 0.7922 | 0.7577 | 0.7230 | 0.6933 | 0.6734 | 0.6341 | 0.6242 |
| 0.6173 | 0.9633 | 0.9308 | 0.8875 | 0.8458 | 0.8022 | 0.7727 | 0.7530 | 0.7030 | 0.7012 |
| 0.7312 | 1.0492 | 1.0133 | 0.9657 | 0.9066 | 0.8844 | 0.8346 | 0.8171 | 0.7792 | 0.7603 |
| 0.8452 | 1.1328 | 1.0927 | 1.0332 | 0.9882 | 0.9517 | 0.9054 | 0.8672 | 0.8154 | 0.8095 |
| 1.0079 | 1.2517 | 1.1927 | 1.1382 | 1.0916 | 1.0413 | 0.9999 | 0.9427 | 0.8967 | 0.8599 |

表 S6 用方程(9)预测[C₂mim][Ala]水溶液的粘度值(η_{pre})Table S6 Predicted values of viscosity (η_{pre}) for aqueous [C₂mim][Ala] by eq. (9)

| m /(mol kg ⁻¹) | $\eta_{pre}/(\mu\text{Pa s})$ | | | | | | | | |
|------------------------------|-------------------------------|----------|----------|----------|----------|----------|----------|----------|----------|
| | 288.15 K | 293.15 K | 298.15 K | 303.15 K | 308.15 K | 313.15 K | 318.15 K | 323.15 K | 328.15 K |
| 0.0167 | 1153.2 | 1014.7 | 900.8 | 808.7 | 727.3 | 660.6 | 603.3 | 553.7 | 510.5 |
| 0.0222 | 1160.3 | 1020.8 | 906.0 | 813.2 | 731.3 | 664.1 | 606.4 | 556.4 | 512.9 |
| 0.0278 | 1167.8 | 1027.2 | 911.5 | 818.0 | 735.4 | 667.7 | 609.6 | 559.2 | 515.4 |
| 0.0556 | 1205.1 | 1058.9 | 938.7 | 841.6 | 755.8 | 685.5 | 625.2 | 573.0 | 527.6 |
| 0.1670 | 1360.2 | 1190.4 | 1051.1 | 938.4 | 839.4 | 758.1 | 688.6 | 628.4 | 576.2 |
| 0.2789 | 1514.9 | 1321.4 | 1162.7 | 1034.5 | 922.1 | 829.9 | 751.0 | 682.9 | 623.8 |
| 0.3914 | 1666.7 | 1449.7 | 1272.0 | 1128.5 | 1002.9 | 899.9 | 812.0 | 736.0 | 670.2 |
| 0.5040 | 1814.5 | 1574.6 | 1378.3 | 1219.9 | 1081.4 | 968.0 | 871.1 | 787.5 | 715.1 |
| 0.6173 | 1958.8 | 1696.6 | 1482.1 | 1309.0 | 1158.0 | 1034.2 | 928.6 | 837.6 | 758.8 |
| 0.7312 | 2099.7 | 1815.6 | 1583.3 | 1395.9 | 1232.6 | 1098.8 | 984.7 | 886.4 | 801.4 |
| 0.8452 | 2236.2 | 1931.0 | 1681.3 | 1480.0 | 1304.8 | 1161.3 | 1039.0 | 933.6 | 842.6 |
| 1.0079 | 2424.3 | 2089.7 | 1816.2 | 1595.8 | 1404.3 | 1247.3 | 1113.6 | 998.5 | 899.2 |

表 S7 利用新 Eyring 半经验方法预测的[C₂mim][Ala]溶液粘度值(η_{pre})

Table S7 Predicted values of viscosity (η_{pre}) for aqueous [C₂mim][Ala] by the new Eyring' semi-empirical method

| $m/$ (mol kg ⁻¹) | $\eta_{pre}/(\mu\text{Pa s})$ | | | | | | | | |
|---------------------------------|-------------------------------|----------|----------|----------|----------|----------|----------|----------|----------|
| | 288.15 K | 293.15 K | 298.15 K | 303.15 K | 308.15 K | 313.15 K | 318.15 K | 323.15 K | 328.15 K |
| 0.0163 | 1157.1 | 1018.2 | 903.9 | 810.6 | 728.9 | 662.5 | 604.4 | 555.2 | 512.3 |
| 0.0220 | 1164.2 | 1024.4 | 909.1 | 815.0 | 732.8 | 665.8 | 607.3 | 557.8 | 514.6 |
| 0.0278 | 1171.5 | 1030.7 | 914.4 | 819.6 | 736.8 | 669.2 | 610.4 | 560.5 | 517.0 |
| 0.0556 | 1206.8 | 1061.0 | 940.2 | 841.4 | 755.9 | 685.6 | 625.1 | 573.4 | 528.6 |
| 0.1670 | 1352.0 | 1185.6 | 1045.9 | 930.7 | 833.8 | 752.7 | 685.0 | 625.8 | 575.5 |
| 0.2789 | 1503.1 | 1314.6 | 1154.9 | 1022.8 | 913.6 | 821.5 | 746.1 | 679.2 | 623.3 |
| 0.3914 | 1658.0 | 1446.1 | 1265.8 | 1116.7 | 994.4 | 891.5 | 807.9 | 733.0 | 671.4 |
| 0.5040 | 1813.7 | 1577.5 | 1376.4 | 1210.4 | 1074.4 | 961.5 | 869.2 | 786.1 | 719.1 |
| 0.6173 | 1968.4 | 1707.1 | 1485.3 | 1303.1 | 1152.9 | 1030.7 | 929.3 | 838.2 | 765.8 |
| 0.7312 | 2119.0 | 1832.3 | 1590.4 | 1393.2 | 1228.3 | 1098.3 | 987.5 | 888.6 | 811.1 |
| 0.8452 | 2261.0 | 1949.6 | 1688.7 | 1478.6 | 1298.9 | 1162.5 | 1042.2 | 935.8 | 853.8 |
| 1.0079 | 2443.6 | 2097.7 | 1813.6 | 1588.9 | 1388.6 | 1246.7 | 1112.6 | 996.6 | 909.0 |

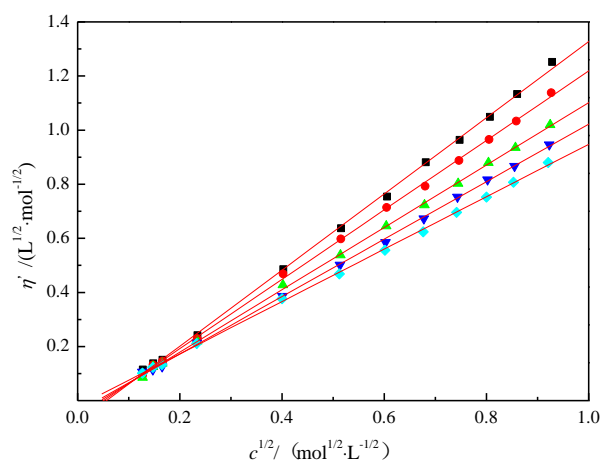


图 S1 288.15、298.15、308.15、318.15、328.15K 下外推函数 η' 对 $c^{1/2}$ 作图

Fig.S1 Plotting extrapolation function, η' vs $c^{1/2}$ at $T = (288.15, 298.15, 308.15, 318.15$ and $328.15)$ K

■ 288.15 K; ● 298.15 K; ▲ 308.15 K; ▼ 318.15 K; ◆ 328.15 K