Electronic Supplementary Information

Improving SO₂ capture by basic ionic liquids in acid gas mixture (10% vol SO₂) through tethering formyl group to the anions

Fengtao Zhang, Guokai Cui, Ning Zhao, Yanjie Huang, Yuling Zhao, and Jianji Wang*

Henan Key Laboratory of Green Chemistry, Collaborative Innovation Center of Henan Province for Green Manufacturing of Fine Chemicals, Key Laboratory of Green Chemical Media and Reactions, Ministry of Education, School of Chemistry and Chemical Engineering, Henan Normal University, Xinxiang, Henan 453007, China.

E-mail: jwang@htu.cn
NMR and IR data of the formyl-containing anion-functionalized ILs

\[ \text{[P}_{66614}\text{][3-CHO-Indo]}: \] \( ^1H \) NMR (DMSO-d6): 0.85-0.91 (m, 12H, CH\(_3\)), 1.22-1.45 (m, 48H, CH\(_2\)), 2.03-2.10 (m, 8H, PCH\(_2\)), 6.89 (m, 2H, C6 and C7), 7.36 (d, 1H, C5), 7.90 (d, 1H, C8), 7.91 (s, 1H, C2), 9.61 (s, 1H, CHO) ppm; \( ^{13}C \) NMR (DMSO-d6): 14.3, 14.4, 17.7, 17.8, 18.1, 18.2, 21.0, 21.0, 21.1, 22.3, 22.6, 28.6, 29.1, 29.2, 29.5, 29.5, 30.1, 30.2, 30.3, 30.4, 30.9, 31.8, 117.1 (C5), 118.2 (C6 and C7), 119.9 (C4), 128.8 (C5), 149.5 (C9), 150.4 (C2), 179.9 (CHO) ppm; IR: 2955, 2924, 2854, 2758, 2700, 2656, 1654, 1612, 1596, 1479, 1465, 1371, 1339, 1294, 1262, 1243, 1213, 1172, 1143, 1112, 1081, 1004, 926, 875, 811, 790, 769, 744, 721, 637 cm\(^{-1}\).

\[ \text{[P}_{66614}\text{][2-CHO-Pyro]}: \] \( ^1H \) NMR (DMSO-d6): 0.84-0.90 (m, 12H, CH\(_3\)), 1.21-1.50 (m, 48H, CH\(_2\)), 2.13-2.20 (m, 8H, PCH\(_2\)), 5.99 (s, 1H, C4), 6.72 (d, 1H, C5), 7.02 (d, 1H, C3), 9.33 (s, 1H, CHO) ppm; \( ^{13}C \) NMR (DMSO-d6): 14.3, 14.4, 17.7, 17.8, 18.0, 18.1, 21.0, 21.1, 21.1, 22.3, 22.6, 28.6, 29.2, 29.5, 29.5, 29.6, 30.2, 30.3, 30.4, 30.5, 30.9, 31.8, 110.9 (C4), 126.5 (C5), 133.6 (C3), 155.7 (C2), 180.9
(CHO) ppm; IR: 2956, 2924, 2854, 2734, 2696, 1660, 1620, 1466, 1404, 1378, 1352, 1332, 1278, 1255, 1214, 1178, 1159, 1087, 1063, 1024, 986, 960, 882, 862, 812, 773, 745, 721 cm\(^{-1}\).

\([P_{66614}]_{[4-CHO-PhO]}\): \(^1\)H NMR (CDCl\(_3\)): 0.75-0.82 (m, 12H, CH\(_3\)), 1.13-1.40 (m, 48H, CH\(_2\)), 2.01-2.11 (m, 8H, PCH\(_2\)), 6.35 (d, 2H, C2 and C6), 7.40 (d, 2H, C3 and C5), 9.31 (s, 1H, CHO) ppm; \(^{13}\)C NMR (CDCl\(_3\)): 13.8, 13.8, 14.0, 14.0, 18.6, 18.6, 18.9, 18.9, 21.6, 21.6, 21.6, 22.2, 22.6, 28.8, 29.2, 29.4, 29.5, 29.5, 29.6, 30.2, 30.3, 30.6, 30.7, 30.9, 31.8, 119.9 (C2 and C6), 120.2 (C3 and C5), 133.1 (C4), 178.5 (C1), 187.9 (CHO) ppm; IR: 2955, 2924, 2854, 2709, 1646, 1572, 1513, 1454, 1375, 1302, 1239, 1226, 1137, 1112, 1089, 979, 844, 720, 637 cm\(^{-1}\).

\([P_{66614}]_{[4-CHO-PhCOO]}\): \(^1\)H NMR (DMSO-d6): 0.82-0.89 (m, 12H, CH\(_3\)), 1.20-1.50 (m, 48H, CH\(_2\)), 2.14-2.24 (m, 8H, PCH\(_2\)), 7.80 (d, 2H, C2 and C6), 7.99 (d, 2H, C3 and C5), 10.01 (s, 1H, CHO) ppm; \(^{13}\)C NMR (DMSO-d6): 14.3, 14.4, 17.6, 17.7, 18.1, 18.2, 19.1, 20.1, 21.0, 21.0, 21.1, 22.3, 22.6, 28.6, 29.2, 29.2, 29.5, 29.6, 30.2, 30.4, 30.4, 30.6, 30.9, 31.8, 129.1 (C2 and C6), 129.8 (C3 and C5), 136.5 (C4), 147.2 (C1), 167.5 (COO), 193.5 (CHO) ppm; IR: 2955, 2924, 2854, 2720, 1703, 1602, 1562, 1554, 1465, 1410, 1350, 1263, 1202, 1162, 1111, 1088, 1014, 968, 867, 797, 776, 755, 721 cm\(^{-1}\).
**Figure S1** Optimized structures of different formyl-containing anions and anion–SO$_2$ complexes at B3LYP/6-31++G(d,p) level.