Electronic Supplementary Information

Improving SO_2 capture by basic ionic liquids in acid gas mixture (10% vol SO_2) through tethering formyl group to the anions

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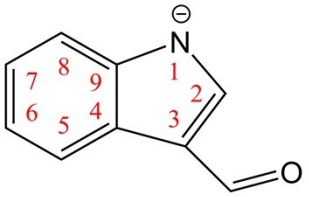
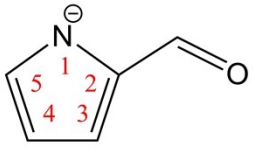
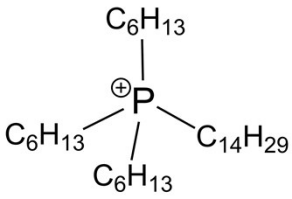
NMR and IR data of the formyl-containing anion-functionalized ILs



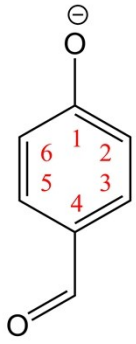
[3-CHO-Indo]



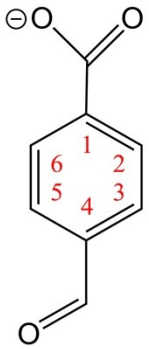
[2-CHO-Pyro]



[P_{66614}]



[4-CHO-PhO]



[4-CHO-PhCOO]

[P_{66614}][3-CHO-Indo]: ^{1}H 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, 29.6, 30.1, 30.2, 30.3, 30.4, 30.9, 31.8, 117.1 (C5), 118.2 (C3), 119.2 (C8), 119.9(C6 and C7), 128.8 (C4), 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}.

[P_{66614}][2-CHO-Pyro]: ^{1}H 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, 29.2, 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}.

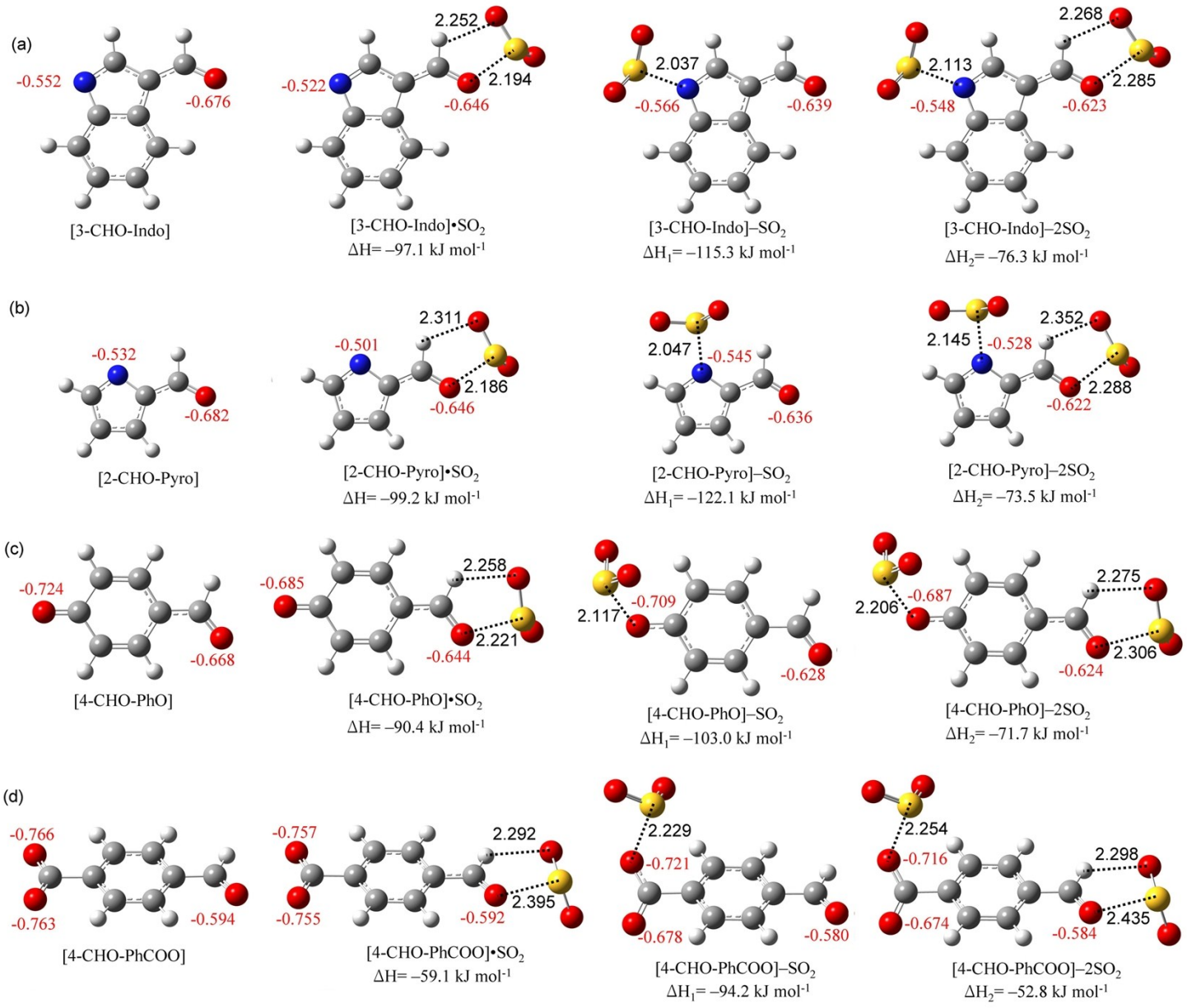


Figure S1 Optimized structures of different formyl-containing anions and anion–SO_2 complexes at B3LYP/6-31++G(d,p) level.