## **Electronic Supplementary Information**

## Absorption and thermodynamic properties of CO<sub>2</sub> in amido-containing anion-functionalized ionic liquids

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## <sup>1</sup>H NMR, <sup>13</sup>C NMR and FT-IR data of the amido-based ILs



Numbering scheme for the positions in the amido-based anion-functionalized ILs

 $[P_{66614}][H-Suc]$ :<sup>1</sup>H NMR (DMSO-d<sub>6</sub>): 0.86 (m, 12H, 4×CH<sub>3</sub>), 1.236-1.469 (m, 48H, 24×CH<sub>2</sub>), 2.05(s, 4H, C3 and C4), 2.19 (m, 8H, 4×PCH<sub>2</sub>) ppm; <sup>13</sup>C NMR (DMSO-d<sub>6</sub>): 13.8, 13.8, 17.3, 17.6, 20.5, 20.6, 21.2, 21.8, 21.9, 22.1, 28.1, 28.7, 28.7, 29.0, 29.0, 29.1, 29.7, 29.8, 30.0, 30.4, 30.8, 31.3, 32.5 (C3 and C4), 34.5, 35.5, 177.0, 174.4, 194.2 (C2 and C5) ppm; IR: 2955, 2923, 2854, 1764, 1696, 1672, 1572, 1465, 1416, 1377, 1315, 1273, 1240, 1211, 1163, 1112, 1003, 987, 891, 857, 821, 720 cm<sup>-1</sup>.

 $[P_{66614}][Ph-Suc]:$ <sup>1</sup>H NMR(DMSO-d<sub>6</sub>): 0.86 (m, 12H, 4×CH<sub>3</sub>), 1.237-1.464 (m, 48H, 24×CH<sub>2</sub>), 2.18 (m, 8H, 4×PCH<sub>2</sub>), 7.30 - 7.36 (m, 4H, C4, C5, C6, and C7) ppm; <sup>13</sup>C NMR (DMSO-d<sub>6</sub>): 13.7, 13.8, 17.3, 17.6, 20.5, 20.6, 21.2, 21.8, 21.9, 22.1, 28.1, 28.7, 28.7, 29.0, 29.0, 29.1, 29.7, 29.8, 30.0, 30.4, 30.8, 31.3, 119.0 (C4 and C7), 125.8, 128.6, 129.3 (C5 and C6), 129.5, 129.9, 130.9, 139.6 (C3 and C8), 145.0, 169.4, 172.9, 185.0 (C2 and C9) ppm; IR: 2955, 2924, 2854, 1698, 1662, 1619, 1588, 1571, 1465, 1460, 1409, 1378, 1364, 1343, 1273, 1202, 1178, 1158, 1125, 1004, 861, 831, 814, 721 cm<sup>-1</sup>.

	Ι		
P <sub>CO2</sub> (100 kPa)	$n_{\rm CO2}$ (mol CO <sub>2</sub> mol <sup>-1</sup> IL)	P <sub>CO2</sub> (100 kPa)	$n_{\rm CO2}$ (mol CO <sub>2</sub> mol <sup>-1</sup> IL)
<i>T</i> = 308.15 K		<i>T</i> = 313.15 K	
0.025	0.36	0.025	0.16
0.05	0.50	0.05	0.26
0.075	0.57	0.075	0.35
0.10	0.61	0.10	0.43
0.15	0.70	0.15	0.52
0.20	0.76	0.20	0.57
0.25	0.82	0.25	0.64
0.30	0.86	0.30	0.68
0.50	0.92	0.50	0.73
0.70	0.94	0.70	0.74
1.00	0.95	1.00	0.76
<i>T</i> = 318.15 K		<i>T</i> = 323.15 K	
0.025	0.10	0.025	0.04
0.05	0.16	0.05	0.07
0.075	0.21	0.075	0.11
0.10	0.32	0.10	0.14
0.15	0.40	0.15	0.19
0.20	0.45	0.20	0.24
0.25	0.50	0.25	0.29
0.30	0.57	0.30	0.32
0.50	0.60	0.50	0.41
0.70	0.61	0.70	0.43
1.00	0.66	1.00	0.45

Table S1. Solubility ( $n_{CO2}$ ) of CO<sub>2</sub> in [P<sub>66614</sub>][H-Suc] at different temperatures (*T*) and

 $CO_2$  partial pressures ( $P_{CO2}$ ).

			1
P <sub>CO2</sub> (100 kPa)	$n_{\rm CO2}$ (mol CO <sub>2</sub> mol <sup>-1</sup> IL)	P <sub>CO2</sub> (100 kPa)	$n_{\rm CO2}$ (mol CO <sub>2</sub> mol <sup>-1</sup> IL)
<i>T</i> = 308.15 K		T = 313.15  K	
0.05	0.18	0.05	0.10
0.10	0.30	0.10	0.19
0.15	0.37	0.15	0.26
0.25	0.46	0.25	0.34
0.30	0.52	0.30	0.38
0.50	0.61	0.50	0.45
0.70	0.66	0.70	0.49
1.00	0.73	1.00	0.52
<i>T</i> = 318.15 K		<i>T</i> = 323.15 K	
0.05	0.06	0.05	0.04
0.10	0.13	0.10	0.09
0.15	0.19	0.15	0.13
0.25	0.25	0.25	0.19
0.30	0.28	0.30	0.22
0.50	0.35	0.50	0.27
0.70	0.41	0.70	0.31
1.00	0.47	1.00	0.38

Table S2. Solubility ( $n_{CO2}$ ) of CO<sub>2</sub> in [P<sub>66614</sub>][Ph-Suc] at different temperatures (*T*) and CO<sub>2</sub> partial pressures ( $P_{CO2}$ ).



Scheme S1. Possible mechanism of CO<sub>2</sub> absorption by [P<sub>66614</sub>][Ph-Suc].



Figure S1. <sup>1</sup>H NMR (a), <sup>13</sup>C NMR (b) and FT-IR (c) spectra of  $[P_{66614}]$ [Ph-Suc] before and after absorption of CO<sub>2</sub>.