Supporting Information

Understanding the effect of side groups in ionic liquids on carbon-capture properties: a combined experimental and theoretical effort

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Section S1

Tabulated data for Density, solubility and Diffusion Coefficients

Table S1-1: Density Data

Ionic Liquids	Experimental Density (g cm^{-3})	Simulation Density (g cm^{-3})	Simulation Density, bottom (g cm^{-3})	Simulation Density, up (g cm^{-3})
1-oct	1.311	1.348	1.345	1.351
1p	1.316	1.361	1.358	1.364
2p	1.338	1.369	1.366	1.372
1	1.355	1.39	1.387	1.393
2	1.377	1.403	1.4	1.406
3p	1.387	1.4	1.397	1.403
3	1.391	1.424	1.422	1.426

Note: the experiment error is within 0.3% (±0.0004 g/cm^3).

Table S1-2: Experimental Self-Diffusion Coefficients D_s

Ionic Liquid	Ionic Liquid Name		Temperature (K)	Self-Diffusion Coefficients (m^2/s)	
	Cation	Anion		Cation	Anion
1	1-hexyl-3-methyl-4-phenyl-1H-1,2,3-triazol-3-ium	Tf2N	333	2.32E-11	2.50E-11
			353	4.80E-11	5.18E-11
			373	8.50E-11	9.22E-11
1p	1-hexyl-3-methyl-4-propyl-1H-1,2,3-triazol-3-ium	Tf2N	333	5.97E-11	6.23E-11
			353	1.10E-10	1.13E-10
			373	1.87E-10	2.03E-10
1-oct	3-methyl-1-octyl-4-phenyl-1H-1,2,3-triazol-3-ium	Tf2N	333	1.95E-11	2.19E-11
			353	4.03E-11	4.56E-11
			373	7.19E-11	8.22E-11
2	3-methyl-4-phenyl-1-((trimethylsilyl)methyl)-1H-1,2,3-triazol-3-ium	Tf2N	333	9.76E-12	9.10E-12
			353	2.46E-11	2.25E-11
			373	5.11E-11	4.81E-11
2p	3-methyl-4-propyl-1-((trimethylsilyl)methyl)-1H-1,2,3-triazol-3-ium	Tf2N	333	4.74E-11	5.13E-11
			353	8.47E-11	9.49E-11
			373	1.38E-10	1.54E-10
3	1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3-methyl-4-phenyl-1H-1,2,3-triazol-3-ium	Tf2N	333	2.32E-11	2.86E-11
			353	4.98E-11	6.04E-11
			373	9.65E-11	1.12E-10

3p	1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3-methyl-4-propyl-1H-1,2,3-triazol-3-ium	Tf2N	333	4.33E-11	5.22E-11
			353	7.66E-11	9.03E-11
			373	1.30E-10	1.51E-10

Table S1-3: Simulation Self-Diffusion Coefficients D_s

Ionic Liquid	Ionic Liquid Name		Temperature (K)	Self-Diffusion Coefficients (m^2/s)	
	Cation	Anion		Cation	Anion
1	1-hexyl-3-methyl-4-phenyl-1H-1,2,3-triazol-3-ium	Tf2N	550	3.28E-10	3.58E-10
			500	1.61E-10	1.69E-10
			480	1.08E-10	1.28E-10
			450	5.65E-11	5.45E-11
			420	2.23E-11	2.77E-11
			333*	1.27E-12	9.38E-13
1p	1-hexyl-3-methyl-4-propyl-1H-1,2,3-triazol-3-ium	Tf2N	550	5.24E-10	5.63E-10
			510	3.19E-10	3.24E-10
			480	1.97E-10	2.17E-10
			450	1.14E-10	1.17E-10
			400	3.43E-11	3.52E-11
			333*	4.97E-12	4.80E-12
1-oct	3-methyl-1-octyl-4-phenyl-1H-1,2,3-triazol-3-ium	Tf2N	550	3.15E-10	3.64E-10
			510	1.87E-10	2.00E-10
			480	9.83E-11	1.12E-10
			450	5.16E-11	5.61E-11
			420	2.20E-11	2.45E-11
			333*	1.07E-12	9.82E-13
2	3-methyl-4-phenyl-1-((trimethylsilyl)methyl)-1H-1,2,3-triazol-3-ium	Tf2N	550	3.41E-10	3.82E-10
			520	2.30E-10	2.43E-10
			480	1.10E-10	1.15E-10
			450	5.85E-11	6.07E-11
			420	2.36E-11	2.48E-11
			333*	6.37E-13	6.11E-13
2p	3-methyl-4-propyl-1-((trimethylsilyl)methyl)-1H-1,2,3-triazol-3-ium	Tf2N	550	5.43E-10	4.76E-10
			510	3.01E-10	3.25E-10
			480	2.00E-10	2.08E-10
			450	1.16E-10	1.16E-10
			420	5.69E-11	5.90E-11
			333*	4.69E-12	4.31E-11
3	1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3-methyl-4-phenyl-1H-1,2,3-triazol-3-ium	Tf2N	550	4.40E-10	4.85E-10
			450	8.21E-11	8.98E-11
			420	3.81E-11	4.57E-11
			400	1.91E-11	2.11E-11
			390	1.01E-11	1.18E-11
			333*	1.61E-12	1.53E-12

3p	1-(2-(2-(2-methoxyethoxy)ethoxy)ethyl)-3-methyl-4-propyl-1H-1,2,3-triazol-3-ium	Tf2N	550	5.05E-10	6.07E-10
			510	3.40E-10	3.52E-10
			480	2.08E-10	2.40E-10
			450	1.29E-10	1.33E-10
			400	3.84E-11	4.09E-11
			333*	5.25E-12	4.52E-12

Note: 333* means at this temperature, D_s is calculated from the temperature dependence of Arrhenius relationship.

Table S1-4: Experimental and simulated self-diffusion activation energy E_a (kJ/mol)

Ionic Liquids	Experimental anion E_a	Experimetal cation E_a	Simulation anion E_a	Simulation cation E_a
1-oct	37.5	37.4	41.9	41.8
1p	30.3	30.1	33.5	33.5
2p	29.8	29.9	33.4	34.2
1	38.3	38.0	40.9	42.9
2	43.0	42.8	46.9	46.8
3p	32.9	33.2	33.8	34.1
3	40.4	41.0	41.7	40.8

Table S1-5: Solubility data for all ionic liquids

x, IL-1	P (bar), IL-1	x, IL-1p	P (bar), IL-1p	x, IL-1-oct	P (bar), IL-1-oct	x, IL-2	P (bar), IL-2
0.000	0.00	0.000	0.00	0.000	0.00	0.000	0.00
0.027	0.93	0.035	1.00	0.029	0.97	0.022	0.97
0.075	2.44	0.100	2.60	0.078	2.48	0.069	2.55
0.123	4.24	0.162	4.45	0.134	4.39	0.121	4.46
0.174	5.86	0.215	6.15	0.174	5.91	0.156	6.00
0.213	7.40	0.257	7.69	0.209	7.55	0.193	7.50
0.249	8.90	0.301	9.32	0.247	9.19	0.229	9.02
0.288	10.34	0.340	10.91	0.281	10.86	0.261	10.54
0.316	12.02	0.372	12.54	0.312	12.47	0.287	12.06

x, IL-2p	P (bar), IL-2p	x, IL-3	P (bar), IL_3	x, IL-3p	P (bar), IL-3p
0.000	0.00	0.000	0.00	0.000	0.00
0.024	0.96	0.025	0.98	0.030	0.99
0.072	2.44	0.077	2.57	0.083	2.51
0.123	4.21	0.127	4.32	0.142	4.36
0.167	5.78	0.167	5.87	0.187	6.01
0.207	7.44	0.202	7.47	0.228	7.48
0.236	9.02	0.237	9.04	0.269	9.21
0.274	10.46	0.282	10.70	0.305	10.87
0.306	12.10	0.311	12.37	0.341	12.51

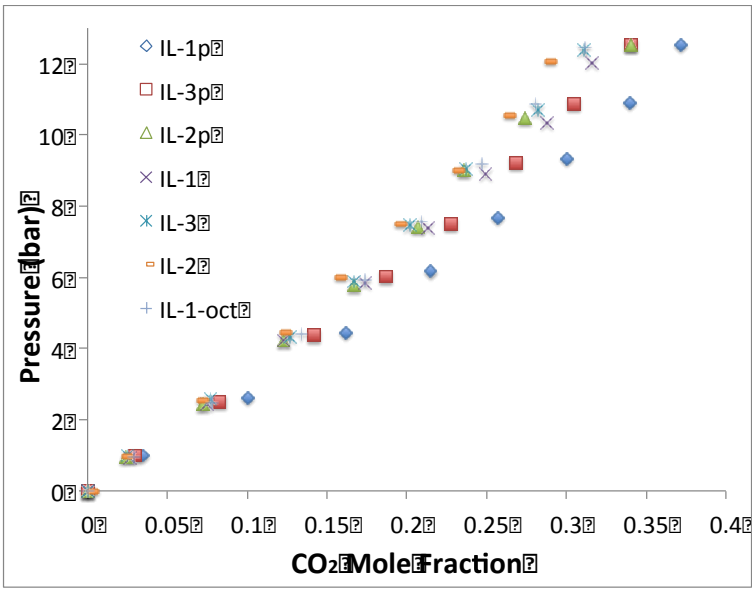


Fig. S1-1 Solubility of CO_2 in the ionic liquids considered in this paper as a function of the CO_2 pressure. Henry's Law coefficients were determined by creating a similar plot with fugacity on the y-axis and mole fraction on the x-axis. A second order polynomial of the form $f=ax^2+bx$ was fit to the data and the value of 'b' was taken as the Henry's Law coefficient. Fugacities were determined using the NIST Standard Reference Database 23.[1,2]

Table S1-6: Experimental and simulated Henry coefficient K_H

Ionic Liquids	Experimental K_H (bar)	Simulation K_H (bar)
1-oct	28.4	50.8
1p	23.2	52.7
2p	31.1	55.2
1	30.5	56.6
2	34.4	60.8
3p	27.2	54.2
3	31.6	58.1

Note: the experiment error is within ±1.5 bar.

Table S1-7: Simulated heat adsorption ΔH of CO_2 in ionic liquids and simulated molar volume V_m of these ionic liquids

Ionic Liquids	ΔH (kJ/mol)	V_m (cm^3/mol)
1-oct	-9.67	409.83
1p	-9.98	360.20
2p	-9.77	359.17
1	--9.87	377.16
2	-9.49	374.79
3p	-9.68	394.48
3	-9.55	411.72

Section S2

Experimental details of synthesis of different triazolium-based cations

Materials: Sodium azide and copper on charcoal (3 %w/w Cu) were purchased from Sigma Aldrich. 1-bromooctane, 1-iodomethane, acetonitrile and tetrahydrofuran were purchased from Acros. 1-phenyl acetylene was purchased from GFS Chemicals and lithium bis(trifluoromethylsulfonyl)imide, $LiTf_2N$, was purchased from TCI. All chemicals were used as received. FTIR was recorded on Nicolet IR100 Spectrometer (Thermo Scientific). Synthesis and characterization of **1**, **2**, **3**, **1p**, **2p** and **3p** have already been reported in literature.[3]

1-azidooctane: 1-bromooctane (100.0 mmol, 13.6 g) was mixed with sodium azide (150.0 mmol, 9.8 g) in 25 mL of DMF and stirred continuously at 60 °C overnight. The reaction mixture was cooled to ambient temperature and water was added to dissolve the excess sodium azide. The product was extracted with hexane, washed with water, dried over $MgSO_4$ and concentrated under *low vacuo* to obtain the product.
Yield: 95 %
ATIR (ν, cm^{-1}): 2090 ($C\text{-}N_3$)

1-octyl-4-phenyl-*1H*-1,2,3-triazole: Copper catalyzed click chemistry using Cu/C was employed to synthesize the triazole as reported in literature.[4] Briefly, triethylamine (58 mmol, 5.9 g) was dissolved in 50 mL of 1,4-dioxane in a 250 mL round bottom flask equipped with a magnetic stir bar. To this solution was added phenylacetylene (58 mmol, 5.9 g), 1-azidooctane (58 mmol, 9.0 g) and Cu/C (2.5 g). The mixture was stirred at 55 °C overnight. At the end of the reaction, the product was filtered from the catalyst and concentrated under *low vacuo*. Pure product was obtained by flash column chromatography using hexane-ethyl acetate (25:75)
Yield: 85 %. The product was used without further characterization.

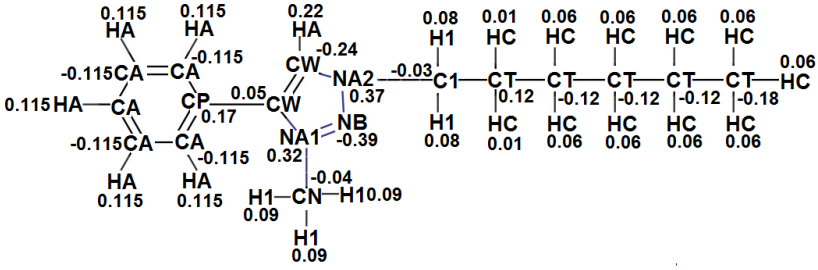
3-methyl-1-octyl-4-phenyl-*1H*-1,2,3-triazol-1,2,3-iumiodide:1-octyl-4-phenyl-*1H*-1,2,3-triazole (8g, 31.1 mmol) and methyl iodide (13.24 g, 93 mmol) were mixed and stirred at 60 °C overnight. Excess methyl iodide was removed under vacuum to yield a yellow liquid which was further washed with ethyl acetate. The product was dried under high vacuum to obtain a pale yellow solid.
Yield: 70 %
^{1}H NMR (700 MHz, chloroform-d, δ ppm): 0.84 (t, *J*=7.04 Hz, 3 H), 1.13-1.49 (m, 10 H), 2.07 (s, 2H), 4.33 (s, 3H), 4.76 (t, *J*=7.48 Hz, 2H), 7.50-7.59 (m, 3H), 7.72-7.80 (m, 2H), 9.47 (s, 1H)

3-methyl-1-octyl-4-phenyl-*1H*-1,2,3-triazol-1,2,3-ium-bis(trifluoromethylsulfonyl)imide:3-methyl-1-octyl-4-phenyl-*1H*-1,2,3-triazol-1,2,3-ium iodide (8.68 g, 21.74 mmol) and lithium bis(trifluoromethylsulfonyl)imide (7.18 g, 25 mmol) were mixed in 25 mL acetonitrile and refluxed overnight to give a yellow liquid. Acetonitrile was removed under *low vacuo* and the product was extracted from water with dichloromethane. The organic layer was dried over $MgSO_4$ and concentrated under vacuum.
Yield: 74 %
LCMS: calculated: 272 observed: 272 (cation)
calculated: 280 observed: 280 (anion)
^{1}H NMR (300 MHz, chloroform-d, δ ppm): 0.88 (m, *J*=13.19 Hz, 1H), 0.79-0.95 (m,1H), 1.16-1.48 (m,11H), 2.04 (qd, *J*=7.91, 6.78 Hz, 2H), 4.23 (s, 3H), 4.57 (t, *J*=7.54 Hz, 2H), 7.51-7.65 (m, 5H)
^{13}C NMR (75 MHz, chloroform-d, δ ppm): 14.06, 22.58, 26.16, 28.76, 28.92, 29.10, 31.65, 38.56, 54.42, 117.64, 121.90, 125.65, 126.16, 128.10, 128.85, 129.32, 129.74, 132.04, 143.57.

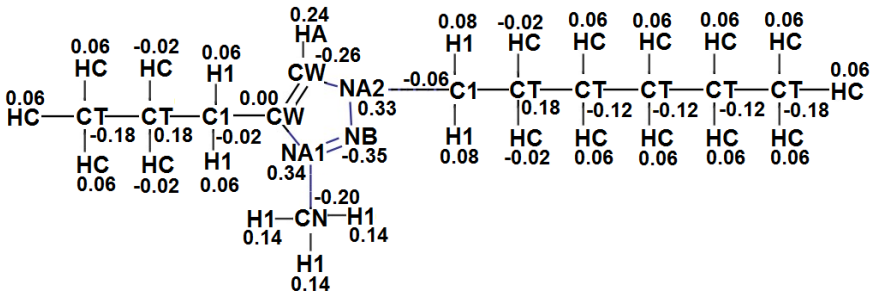
Section S3

Force Field parameters

All charges are obtained by using CHelpG[5] method at the level of MP2/cc-pVTZ(-f)//RHF/6-31G(d), except for the side chains when the carbon atom are 2 atom sites from the triazolium core, the OPLS[6] charges are used.



1 and 1-oct



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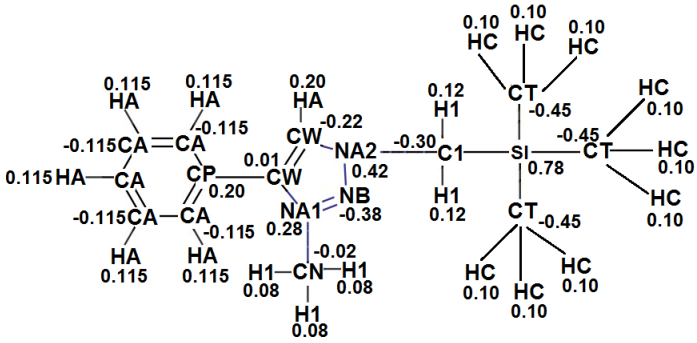

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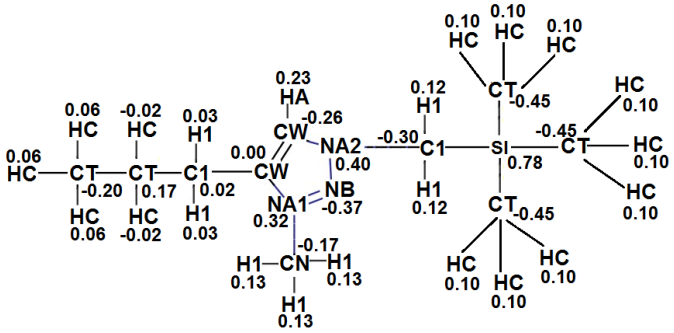

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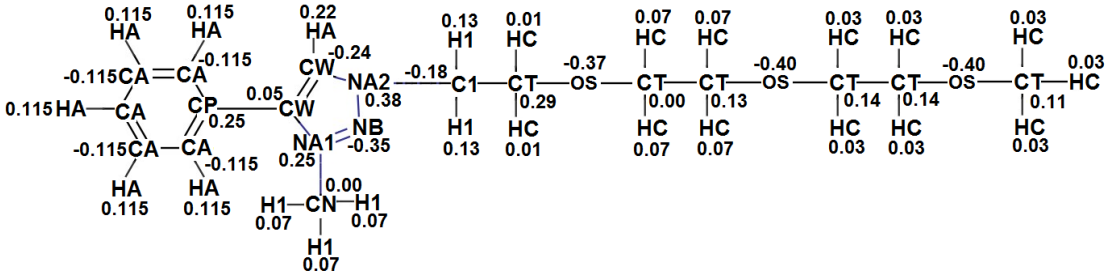

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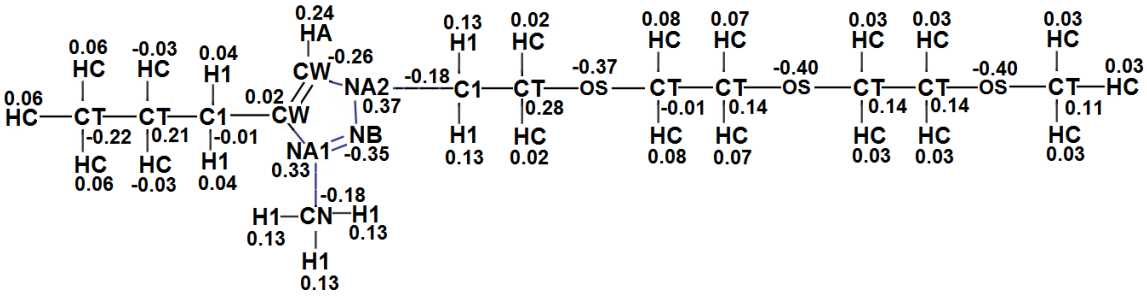

3p

Fig. S3-1 Charges and the atom types of all cations.

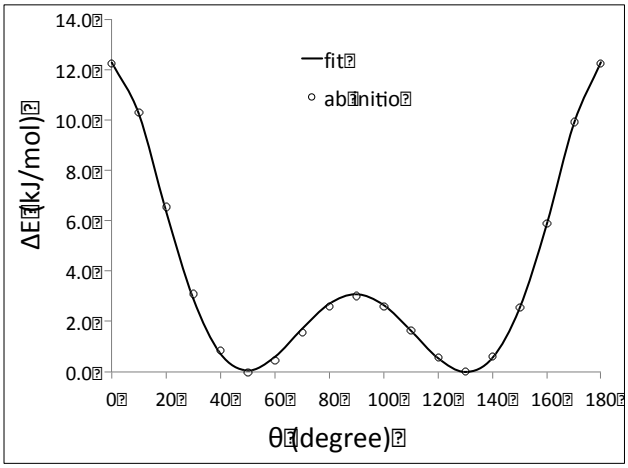

Fig. S3-2 *Ab-initio* dihedral angle scan and fitting for the dihedral angle CA-CP-CW-CW between the benzene group and triazolium core of 2, see Fig. S3-1 for the definition of this angle. ΔE is the energy difference between the scan energy and the global minimum energy.

Table S3-1. Lennard-Jones parameters for all cations.

Atom types	σ (Å)	ϵ(kJ mol^{-1})	Source
NA1	3.25	0.71128	OPLS
NB	3.25	0.71128	OPLS
NA2	3.25	0.71128	OPLS
CW	3.55	0.29288	OPLS
CN	3.50	0.27614	OPLS
C1	3.50	0.27614	OPLS
CA	3.55	0.29288	OPLS
CP	3.55	0.29288	OPLS
CT	3.50	0.27614	OPLS
OS	2.90	0.58576	OPLS
SI	4.00	0.41840	OPLS
H1	2.50	0.12252	OPLS
HC	2.50	0.12252	OPLS
HA	2.42	0.12252	OPLS

Table S3-2. Bond parameters.

Bonds	r_0 (Å)	K_r (kJ mol^{-1} Å^{-2})	Source
C1-H1	1.080	2845.100	OPLS, r_0 (this work)
CN-H1	1.080	2845.100	OPLS, r_0 (this work)
CT-HC	1.090	2845.100	OPLS, r_0 (this work)
CW-HA	1.070	3071.100	OPLS, r_0 (this work)
CN-NA1	1.468	2820.000	OPLS, r_0 (this work)
C1-NA2	1.476	2820.000	OPLS, r_0 (this work)
C1-CW	1.501	2652.700	OPLS, r_0 (this work)
CT-CT	1.529	2242.000	OPLS, r_0 (this work)
C1-CT	1.529	2242.000	OPLS, r_0 (this work)
CW-NA1	1.357	3573.100	OPLS, r_0 (this work)
CW-NA2	1.350	3573.100	OPLS, r_0 (this work)
CW-CW	1.362	4352.000	OPLS, r_0 (this work)
NB-NA1	1.287	4052.600	OPLS, r_0 (this work)
NB-NA2	1.277	4052.600	OPLS, r_0 (this work)
CA-HA	1.080	3071.100	OPLS, r_0 (this work)
CA-CA	1.400	3924.600	OPLS, r_0 (this work)
CA-CP	1.400	3924.600	OPLS, r_0 (this work)
CW-CP	1.478	3221.700	OPLS, r_0 (this work)
SI-C1	1.943	1565.000	OPLS, r_0 (this work)

SI-CT	1.943	1565.000	OPLS, r_0 (this work)
CT-OS	1.410	2677.800	OPLS, r_0 (this work)

Table S3-3. Angle parameters.

Angles	q_0 (deg)	k_q (kJ mol^{-1} rad^{-2})	Source
CA-CA-CA	120.000	527.200	OPLS
CA-CP-CA	120.000	527.200	OPLS
CA-CA-CP	120.000	527.200	OPLS
CW-CP-CA	120.000	527.200	OPLS
CA-CA-HA	120.000	292.900	OPLS
CP-CA-HA	120.000	292.900	OPLS
CT-CT-OS	109.500	418.400	OPLS
C1-CT-OS	109.500	418.400	OPLS
HC-CT-OS	109.500	292.900	OPLS
CT-OS-CT	109.500	502.100	OPLS
H1-C1-H1	107.800	276.100	Lopes, *et al.*[7]
HC-CT-HC	107.800	276.100	Lopes, *et al.*
CW-C1-CT	112.700	488.300	Lopes, *et al.*
C1-CT-CT	112.700	488.300	Lopes, *et al.*
CT-CT-CT	112.700	488.300	Lopes, *et al.*
NA2-C1-CT	112.700	488.300	Lopes, *et al.*
H1-CN-NA1	108.500	313.800	Lopes, *et al.*
H1-C1-NA2	106.000	313.800	Lopes, *et al.*
H1-C1-CW	110.700	313.800	Lopes, *et al.*
H1-C1-CT	110.700	313.800	Lopes, *et al.*
HC-CT-C1	110.700	313.800	Lopes, *et al.*
HC-CT-CT	110.700	313.800	Lopes, *et al.*
NA2-C1-SI	115.000	488.300	this work
HC-CT-SI	109.500	292.900	this work
H1-C1-SI	109.500	292.900	this work
CT-SI-CT	110.000	502.100	this work
H1-CN-H	110.000	334.700	this work
CN-NA1-CW	128.600	515.700	this work
C1-NA2-CW	128.100	516.800	this work
CN-NA1-NB	119.100	560.300	this work
C1-NA2-NB	120.200	557.400	this work
CP-CW-CW	130.900	523.900	this work
CP-CW-NA1	125.300	549.300	this work
C1-CW-CW	132.400	518.800	this work

C1-CW-NA1	123.900	547.900	this work
HA-CW-CW	131.200	395.000	this work
HA-CW-NA2	122.600	421.400	this work
NB-NA1-CW	112.300	605.500	this work
NB-NA2-CW	111.700	611.500	this work
NA1-NB-NA2	106.400	658.000	this work
NA2-CW-CW	105.860	627.600	this work
NA1-CW-CW	103.760	631.580	this work

Table S3-4. Dihedral angle parameters, the unit is in kJ mol^{-1}.

Dihedrals	V_1	V_2	V_3	V_4	Source
HA-CA-CA-HA	0.0000	30.3340	0.0000	0.0000	OPLS
CA-CA-CA-CA	0.0000	30.3340	0.0000	0.0000	OPLS
HA-CA-CA-CA	0.0000	30.3340	0.0000	0.0000	OPLS
HA-CA-CA-CP	0.0000	30.3340	0.0000	0.0000	OPLS
HA-CA-CP-CW	0.0000	30.3340	0.0000	0.0000	OPLS
HA-CA-CP-CA	0.0000	30.3340	0.0000	0.0000	OPLS
CA-CA-CP-CW	0.0000	30.3340	0.0000	0.0000	OPLS
CA-CA-CP-CA	0.0000	30.3340	0.0000	0.0000	OPLS
CA-CA-CA-CP	0.0000	30.3340	0.0000	0.0000	OPLS
CT-CT-OS-CT	2.7200	-1.0460	2.8030	0.0000	OPLS
CT-OS-CT-HC	0.0000	0.0000	3.1800	0.0000	OPLS
HC-CT-CT-OS	0.0000	0.0000	1.9580	0.0000	OPLS
H1-C1-CT-OS	0.0000	0.0000	1.9580	0.0000	OPLS
H1-CT-CT-OS	0.0000	0.0000	1.9580	0.0000	OPLS
OS-CT-CT-OS	-2.3010	0.0000	0.0000	0.0000	OPLS
C1-CT-OS-CT	2.2000	-3.3500	2.8030	0.0000	OPLS
CW-CW-NA1-NB	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
CW-CW-NA1-CN	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
C1-CW-NA1-NB	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
C1-CW-NA1-CN	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
NB-NA1-CW-CP	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
CN-NA1-CW-CP	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
HA-CW-CW-CP	0.0000	44.9800	0.0000	0.0000	Lopes, *et al.*
NA2-CW-CW-CP	0.0000	44.9800	0.0000	0.0000	Lopes, *et al.*
NA1-CW-CW-NA2	0.0000	44.9800	0.0000	0.0000	Lopes, *et al.*
NA1-CW-CW-HA	0.0000	44.9800	0.0000	0.0000	Lopes, *et al.*
NA2-CW-CW-C1	0.0000	44.9800	0.0000	0.0000	Lopes, *et al.*
C1-CW-CW-HA	0.0000	44.9800	0.0000	0.0000	Lopes, *et al.*

NB-NA2-CW-CW	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
NB-NA2-CW-HA	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
C1-NA2-CW-CW	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
C1-NA2-CW-HA	0.0000	12.5500	0.0000	0.0000	Lopes, *et al.*
HC-CT-CT-C1	0.0000	0.0000	1.5310	0.0000	Lopes, *et al.*
HC-CT-CT-HC	0.0000	0.0000	1.3310	0.0000	Lopes, *et al.*
HC-CT-C1-H1	0.0000	0.0000	1.3310	0.0000	Lopes, *et al.*
H1-C1-CT-CT	0.0000	0.0000	1.5310	0.0000	Lopes, *et al.*
CT-CT-CT-C1	0.7280	-0.6570	1.1670	0.0000	Lopes, *et al.*
CT-CT-CT-CT	0.7280	-0.6570	1.1670	0.0000	Lopes, *et al.*
HC-CT-CT-CT	0.0000	0.0000	1.5310	0.0000	Lopes, *et al.*
NA1-NB-NA2-CW	0.0000	40.1700	0.0000	0.0000	Alavi, *et al.*[8]
NA1-NB-NA2-C1	0.0000	40.1700	0.0000	0.0000	Alavi, *et al.*
CW-NA1-NB-NA2	0.0000	40.1700	0.0000	0.0000	Alavi, *et al.*
CN-NA1-NB-NA2	0.0000	40.1700	0.0000	0.0000	Alavi, *et al.*
CA-CP-CW-NA1	0.0000	2.7500	0.0000	-0.6250	this work
CA-CP-CW-CW	0.0000	2.7500	0.0000	-0.6250	this work
CT-CT-C1-CW	-3.0000	1.5000	1.8500	0.0000	this work
CT-SI-C1-NA2	0.0000	0.0000	-1.3500	0.0000	this work
H1-C1-NA2-NB	0.0000	0.0000	0.0000	0.0000	this work
H1-C1-NA2-CW	0.0000	0.0000	0.0000	0.0000	this work
H1-C1-CW-CW	0.0000	0.0000	0.0000	0.0000	this work
H1-C1-CW-NA1	0.0000	0.0000	0.0000	0.0000	this work
HC-CT-C1-CW	0.0000	0.0000	0.0000	0.0000	this work
HC-CT-C1-NA2	0.0000	0.0000	0.0000	0.0000	this work
HC-CT-SI-CT	0.0000	0.0000	0.7531	0.0000	this work
HC-CT-SI-C1	0.0000	0.0000	0.7531	0.0000	this work
H1-C1-SI-CT	0.0000	0.0000	0.7531	0.0000	this work
CT-C1-CW-NA1[1]	5. 0000	0.0000	0.0000	0.0000	this work
CT-C1-CW-CW[1]	0.1000	-2.3500	-2.7000	0.0000	this work
CT-CT-C1-NA2[1]	-5.4000	0.5000	3.8000	0.0000	this work
CT-C1-NA2-CW[1]	-5.7500	-2.0000	0.0000	0.0000	this work
CT-C1-NA2-NB[1]	-4.0000	0.0000	0.0000	0.0000	this work

SI-C1-NA2-NB^{2}	-4.8000	0.0000	0.0000	0.0000	this work
SI-C1-NA2-CW^{2}	-3.0000	-3.5000	0.8000	0.0000	this work
OS-CT-C1-NA2^{3}	-8.8500	-5.0000	2.0000	0.0000	this work
CT-C1-NA2-CW^{3}	-4.2000	-3.0000	0.0000	0.0000	this work
CT-C1-NA2-NB^{3}	-4.5000	0.0000	0.0000	0.0000	this work
CT-C1-CW-NA1^{1p}	4. 5000	0.0000	0.0000	0.0000	this work
CT-C1-CW-CW^{1p}	-5.0000	2.0000	0.0000	0.0000	this work
CT-CT-C1-NA2^{1p}	-6.2500	0.2000	3.0000	0.0000	this work
CT-C1-NA2-CW^{1p}	-3.2500	-1.8000	-0.2500	0.0000	this work
CT-C1-NA2-NB^{1p}	-3.0000	0.0000	0.0000	0.0000	this work
SI-C1-NA2-NB^{2p}	-4.5500	0.0000	0.0000	0.0000	this work
SI-C1-NA2-CW^{2p}	-3.0000	-2.3000	0.8000	0.0000	this work
OS-CT-C1-NA2^{3p}	-10.0000	-3.5000	3.0000	0.0000	this work
CT-C1-NA2-CW^{3p}	-4.5000	-2.8000	0.0000	0.0000	this work
CT-C1-NA2-NB^{3p}	-4.2500	0.0000	0.0000	0.0000	this work

Note: V_0 is equal to zero for all cases. Some dihedral angles from different cations have different force constants, For example, CT-C1-CW-NA1^{1} is for cation 1 and CT-C1-CW-NA1^{1p} is for cation 1p.

Table S3-5. Improper dihedral angle parameters

Dihedrals	n	ϕ_s (deg)	k_ϕ (kJ mol^{-1})	Source
--NA1-*	2.0	180.0	4.185	OPLS
--NA2-*	2.0	180.0	4.185	OPLS
--CW-*	2.0	180.0	4.602	OPLS
--CP-*	2.0	180.0	4.602	OPLS
--CA-*	2.0	180.0	4.602	OPLS

Section S4

Radial distribution function of CO_2 with different ionic liquids at 303 K and 5 bar

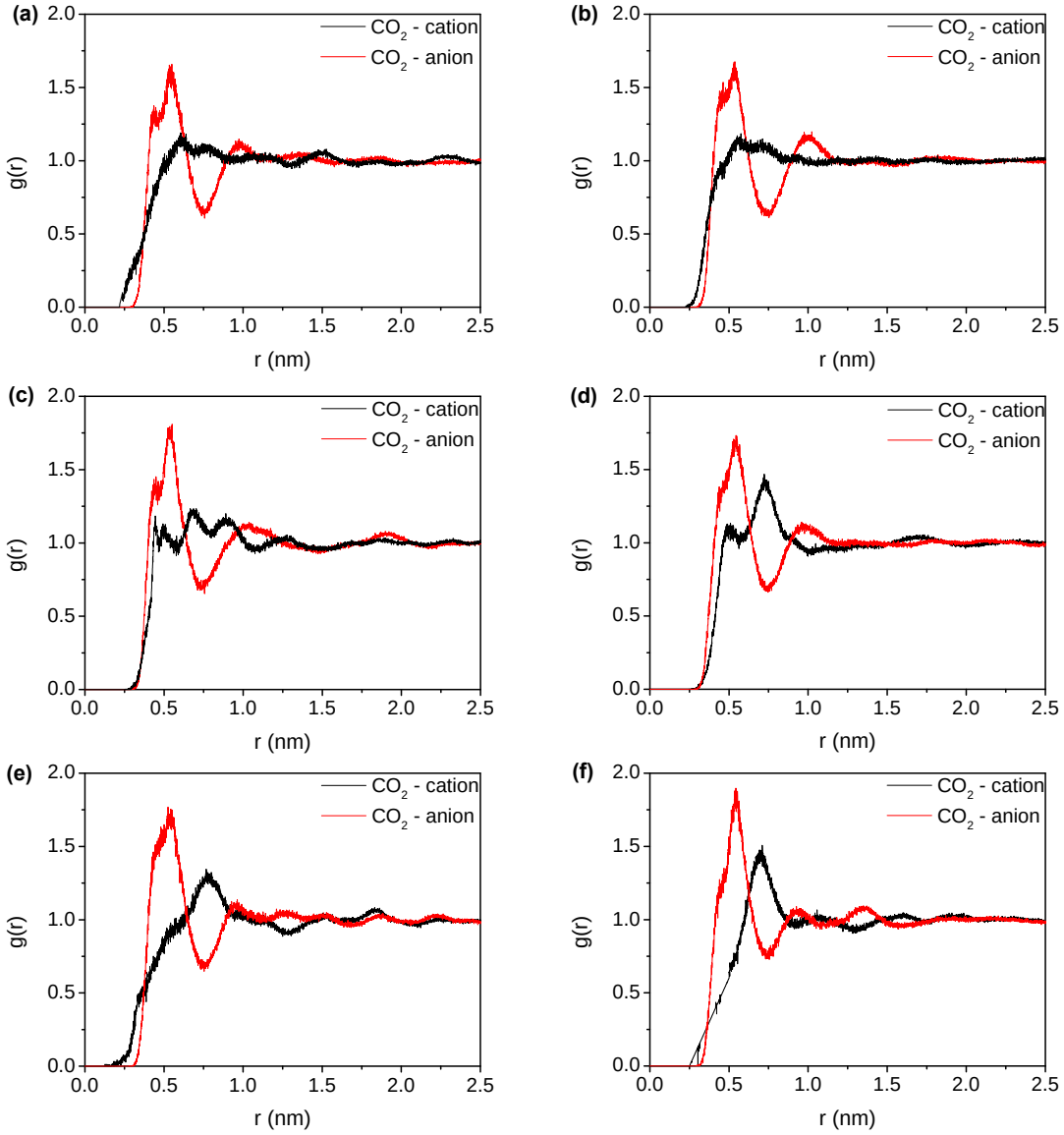

Fig. S4-1 Radial distribution functions of CO_2-anion and CO_2-cation of ionic liquids (a) 1-oct. (b) 1p. (c) 2. (d) 2p. (e) 3. (f) 3p.

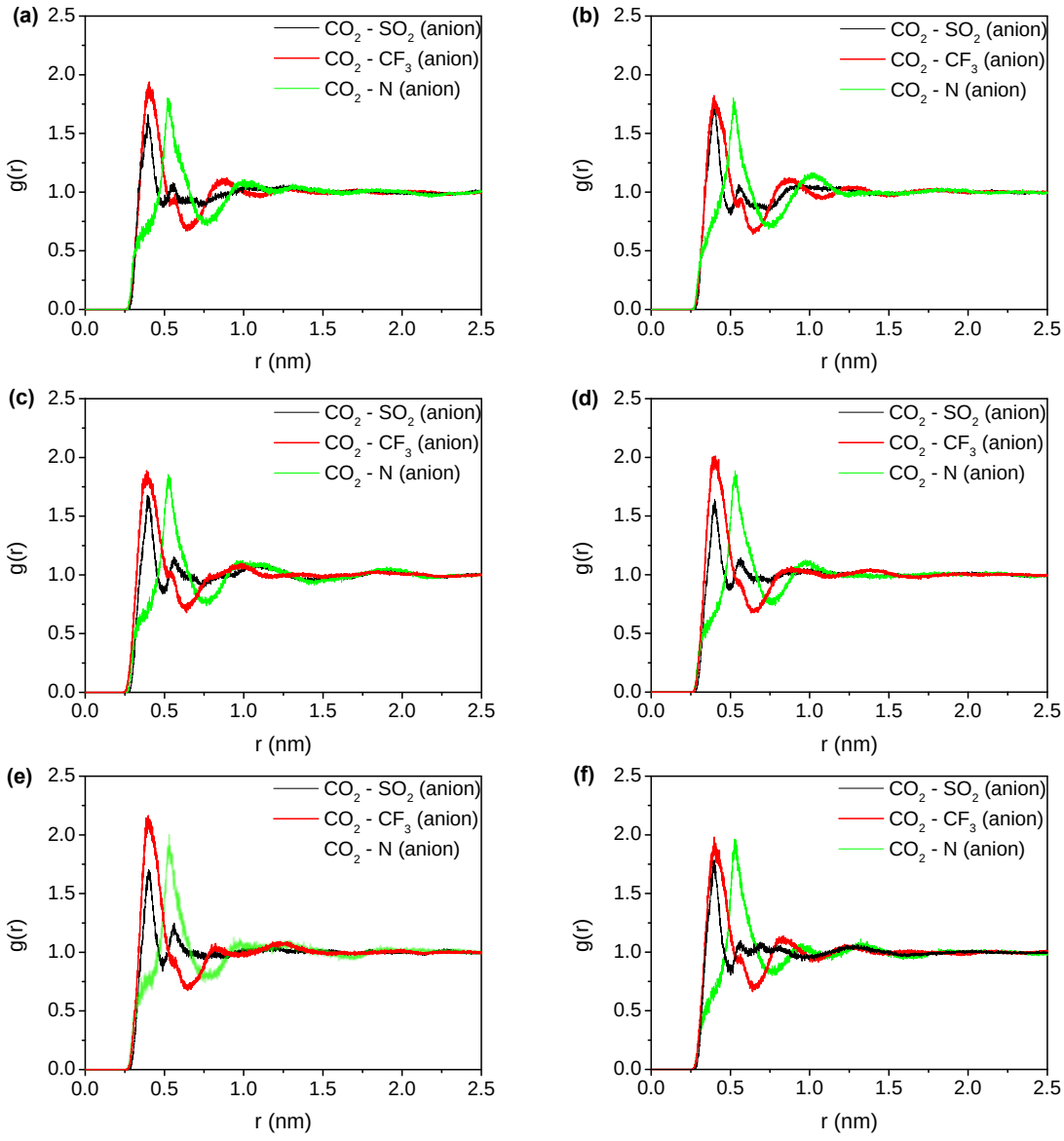

Fig. S4-2 RDFs of CO_2 with CF_3, N and SO_2 of anion TF_2N^- of ionic liquids (a) 1-oct. (b) 1p. (c) 2. (d) 2p. (e) 3. (f) 3p.

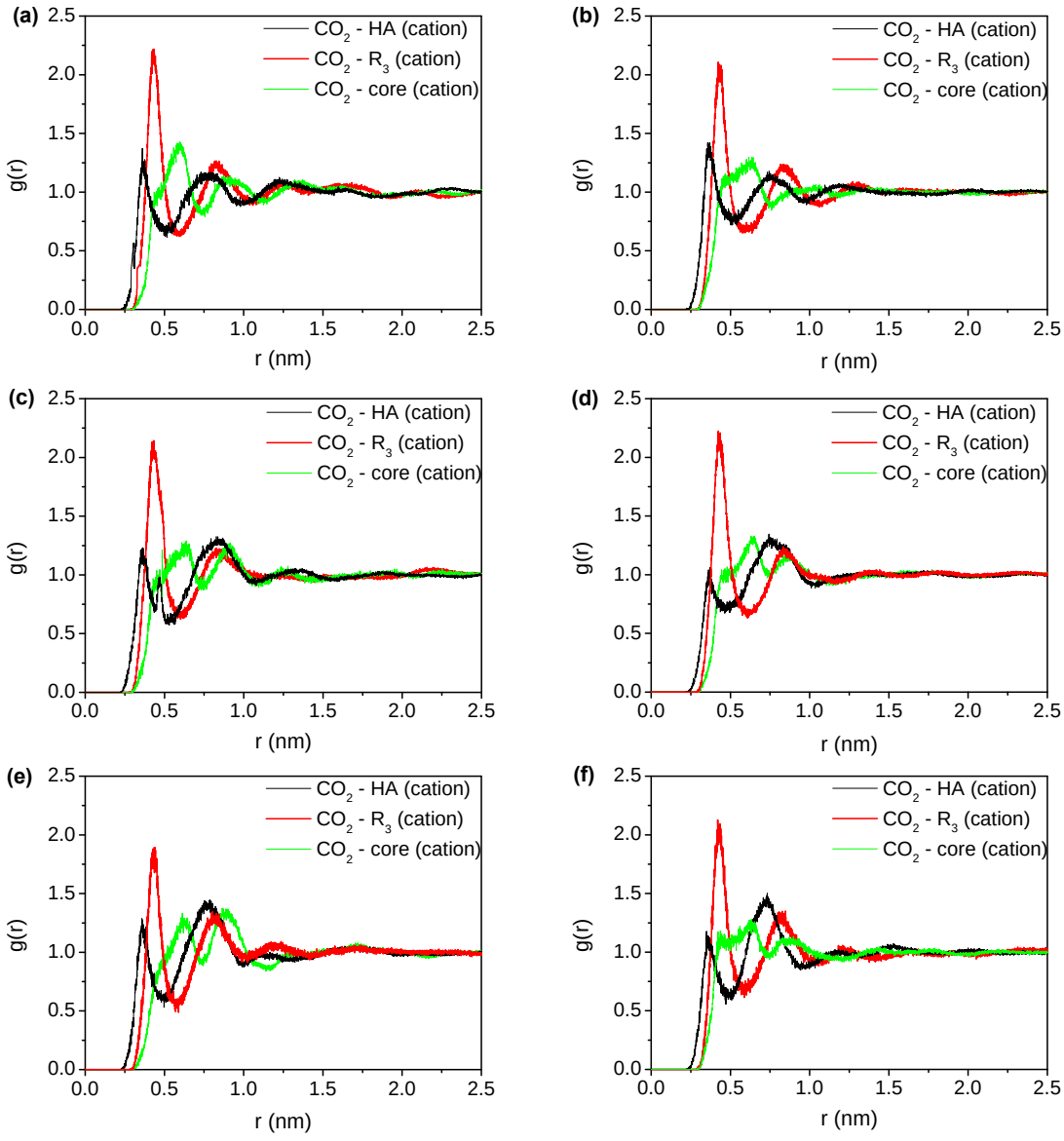

Fig. S4-3 RDFs of CO_2 with R_3, HA, and core of cations of ionic liquids (a) 1-oct. (b) 1p. (c) 2. (d) 2p. (e) 3. (f) 3p.

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