Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary Information I

Rapid, Comprehensive Screening of Ionic liquids towards Sustainable Applications

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Table S1 Summary of the ionic liquid property data obtained from literature. "C" and "A" indicate the number of different cations and anions. N_{data} is the total number of data points for a given property. For properties such as viscosity (η), density (ρ), heat capacity (C_p) and CO_2 solubility (x_{CO2}) temperature and pressure ranges are indicated.

Property	N_{data}	Range	T [°C]	P [MPa]	# C/A
T_m	2212	-96 – 359			1369/141
T_g	654	-117 – 160			327/109
T_d	1288	43 – 487			538/192
$\log_{10}(\eta)$ [mPa·s]	8652	-0.13 – 6.85	-20 – 300	0.10 – 300	847/227
ρ [kg/m^3]	16956	$1\cdot10^{-4}$ – 1853	-82 – 298	0.10 – 200	333/120
C_p [J/K/mol]	9083	0.401 – 9160	-268 – 390	0.10 – 60	115/48
γ [N/m]	2980	0.0155 – 0.0671	-10 – 471		131/68
n_D	3102	1.355 – 1.659	10 – 298		237/85
x_{CO2}	10923	0.0024 – 0.92	-2 – 180	$1\cdot10^{-5}$ – 105	78/74
$\mathrm{Log}_{10}(EC_{50})$	227	-0.42 – 4.58			114/25

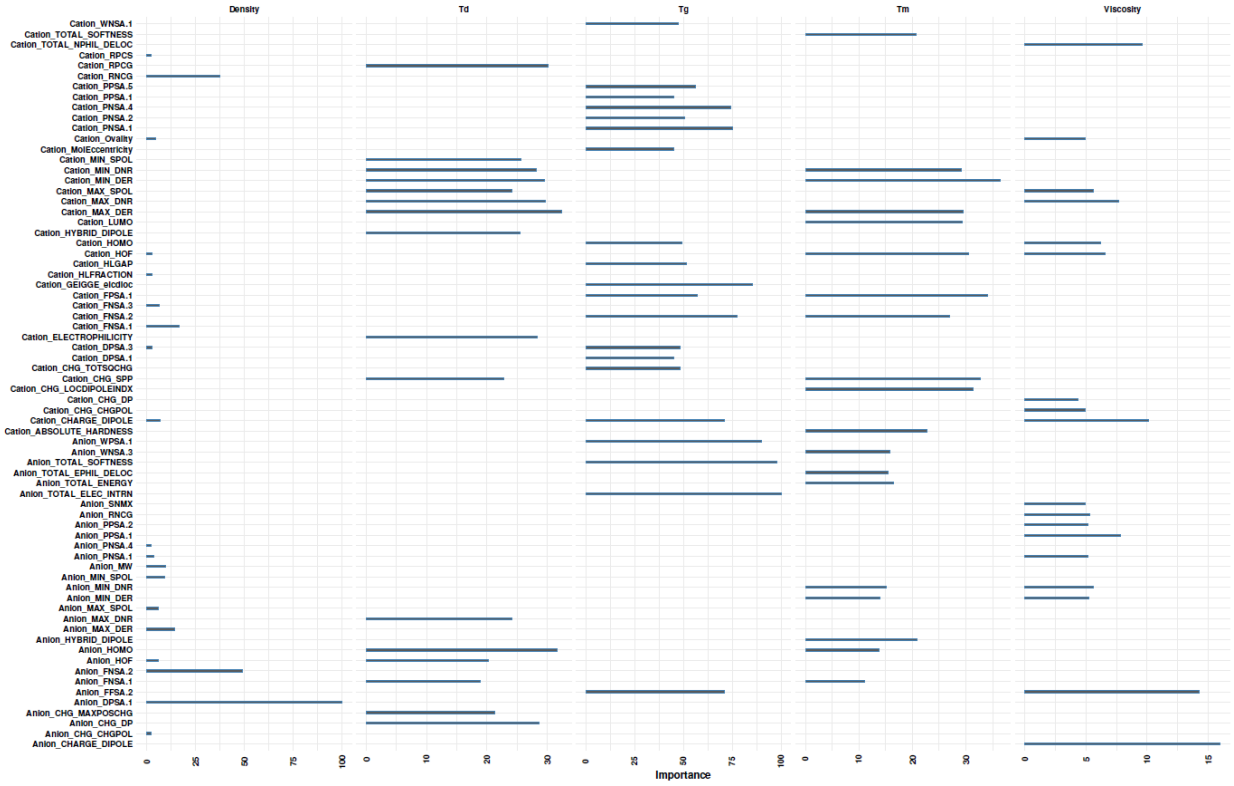


Fig S1 Variable importance plots for T_m, T_g, T_d, η, and ρ.

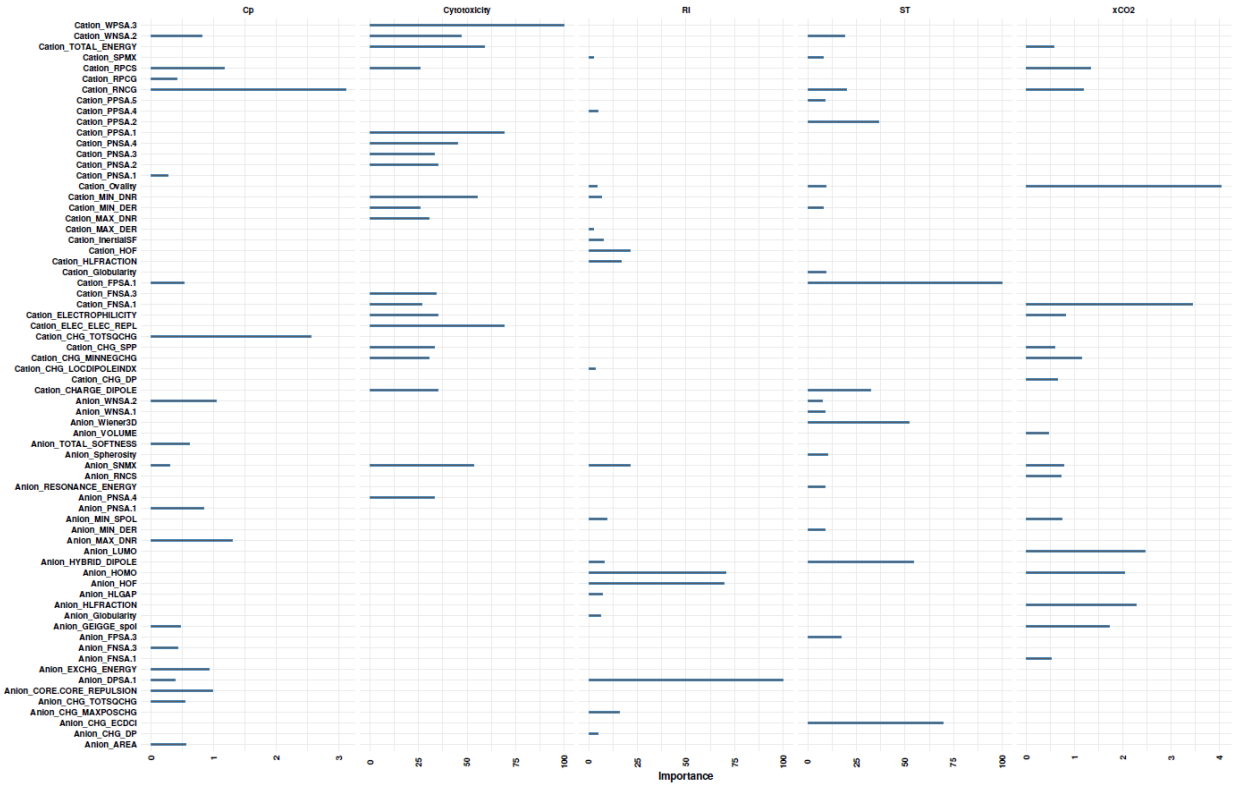
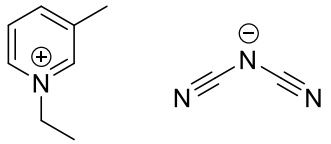


Fig S2 Variable importance plot for C_p, γ, n_D, cytotoxicity and x_{CO2}.

Experimental Information

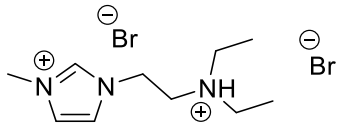
^{1}H and ^{13}C NMR spectroscopy was measured using Bruker Avance 400 MHz spectrometer. IR spectra were recorded using a Bruker Alpha FTIR spectrometer.

1-Ethyl-3-methylpyridinium dicyanamide IL-1



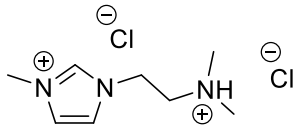
1-Ethyl-3-methylpyridinium bromide (12.22 g, 100 mmol, 1 eq.) and sodium dicyanamide (8.94 g, 100 mmol) were dissolved in acetone (40 mL) and stirred for 24 h. The formed precipitate was filtered off, and the remaining solution was placed in a fridge for 24 h. The chilled solution was filtered and the solvent was removed under vacou at 50 °C for 48 h. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.01 (s, 1H), 8.93 (d, 1H, J = 6.0 Hz), 8.44 (d, 1H, J = 8.0 Hz), 8.05 (dd, 1H, J = 6.0, 8.0 Hz), 4.58 (q, 2H, J = 7.3 Hz), 2.50 (s, 3H), 1.55 (t, 3H, J = 7.3 Hz); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 146.0, 144.0, 141.5, 140.4, 128.1, 119.9, 57.6, 18.8, 16.9; IR (thin film cm^{-1}) 3052, 2259, 2124, 1739, 1636, 1505, 1456, 1304, 1248, 1205, 1160, 981, 902, 807, 684.

1-(2-(Diethylamine)ethyl)-3-methylimidazolium bromide hydrobromide



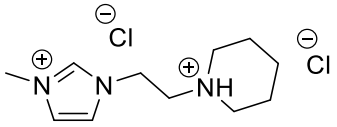
1-Methylimidazole (8.21 g, 100 mmol, 1 eq.) and 2-bromo-*N*,*N*-diethylethanamine hydrobromide (26.1 g, 100 mmol, 1 eq.) were dissolved in ACN (50 mL) and stirred at 50 °C for 72 h. The solvent was removed and the solid residue was washed with diethyl ether (3x50 mL) to afford the 3-(2-(diethylamino)ethyl)-1-methylimidazolium bromide hydrobromide in 85% yield (32.6 g) as a white solid. ^{1}H NMR (400 MHz, CD_3OD) δ (ppm) 9.16 (s, 1H), 7.82 (t, 1H, J = 1.7 Hz), 7.67 (s, 1H, J = 1.7 Hz), 4.74 (m, 2H), 3.98 (s, 3H), 3.70 (m, 2H), 3.32 (m, 4H), 1.37 (t, 6H, J = 6.1 Hz).

1-(2-(Dimethylamine)ethyl)-3-methylimidazolium chloride hydrochloride



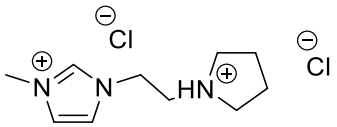
1-Methylimidazole (9.41 g, 115 mmol, 1 eq.) and 2-chloro-*N*,*N*-dimethylethanamine hydrochloride (16.5 g, 115 mmol, 1 eq.) were dissolved in ACN (50 mL) and stirred at 50 °C for 72 h. The solvent was removed and the solid residue was washed with diethyl ether (3x50 mL) to afford the 3-(2-(dimethylamino)ethyl)-1-methylimidazolium bromide hydrobromide in 67% yield (17.3 g) as a white solid. ^{1}H NMR (400 MHz, CD_3OD) δ (ppm) 9.18 (t, 1H), 7.82 (s, 1H, J = 1.8 Hz), 7.68 (s, 1H, J = 1.8 Hz), 4.77 (t, 2H, J = 6.6 Hz), 3.98 (s, 3H), 3.79 (t, 2H, J = 6.6 Hz), 3.01 (s, 6H).

1-(2-(3-Methylimidazolium-1-yl)ethyl)piperidine chloride hydrochloride



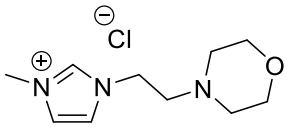
1-Methylimidazole (8.20 g, 100 mmol, 1 eq.) and 1-(2-chloroethyl)piperidine hydrochloride (18.4 g, 100 mmol, 1 eq.) were dissolved in ACN (50 mL) and stirred at 70 °C for 72 h. The solvent was removed and the solid residue was washed with diethyl ether (3x50 mL) to afford the 1-methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium chloride hydrochloride in 78% yield (20.8 g) as a white solid. ^{1}H NMR (400 MHz, CD_3OD) δ (ppm) 9.14 (s, 1H), 7.79 (s, 1H), 7.66 (s, 1H), 4.76 (t, 2H, J = 6.6 Hz), 3.98 (s, 3H), 3.66 (t, 2H, J = 6.2 Hz), 3.33 (m, 4H), 1.94 (quintet, 4H, J = 5.7 Hz), 1.71 (m, 2H).

3-Methyl-1-(2-(pyrrolidin-1-yl)ethyl)imidazolium chloride hydrochloride



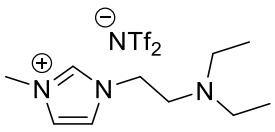
1-Methylimidazole (8.29 g, 101 mmol, 1 eq.) and 1-(2-chloroethyl)pyrrolidine hydrochloride (17.25 g, 101 mmol, 1 eq.) were dissolved in ACN (50 mL) and stirred at 70 °C for 72 h. The solvent was removed and the solid residue was washed with diethyl ether (3x50 mL) to afford the 3-methyl-1-(2-(pyrrolidinium-1-yl)ethyl)imidazolium chloride hydrochloride in 79% yield (19.8 g) as a brown solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.79 (s, 1H), 7.45 (t, 1H, J = 1.7 Hz), 7.27 (t, 1H, J = 1.7 Hz), 4.24 (m, 2H), 3.93 (s, 3H), 2.90 (m, 2H), 2.57 (m, 4H), 1.78 (m, 4H).

3-Methyl-1-(2-morpholinonethyl)imidazolium chloride



1-Methylimidazole (8.23 g, 100 mmol, 1 eq.) and 4-(2-chloroethyl)morpholine hydrochloride (18.64 g, 100 mmol, 1 eq.) were dissolved in ACN (50 mL). K_2CO_3 (15.2 g, 110 mmol, 1.1 eq.) was added and the slurry was stirred at 70 °C for 72 h. The solvent was removed and the solid residue was extracted with DCM (3x50 mL) to afford the 3-methyl-1-(2-morpholinonethyl)imidazolium chloride in 88% yield (23.5 g) as a yellow solid. ^{1}H NMR (400 MHz, CD_3OD) δ (ppm) 10.33 (s, 1H), 7.73 (s, 1H), 7.62 (s, 1H), 4.51 (m, 2H), 3.68 (m, 4H), 2.82 (m, 2H), 2.55 (m, 4H).

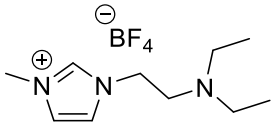
3-(2-(Diethylamino)ethyl)-1-methylimidazolium bis((trifluoromethyl)sulfonyl)amide IL-02



3-(2-(Diethylamino)ethyl)-1-methylimidazolium bromide hydrobromide (15.1 g, 44 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (7.08 g, 66 mmol, 1.5 eq.) and $LiNTf_2$ (13.8 g, 48 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 3-(2-(diethylamino)ethyl)-1-methylimidazolium bis((trifluoromethyl)sulfonyl)amide in 82% yield (18.6 g) as a colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.69 (s, 1H), 7.45 (t, 1H, J = 1.7 Hz), 7.27 (t, 1H, J = 1.7 Hz), 4.17 (m, 2H), 3.93 (s, 3H), 2.77

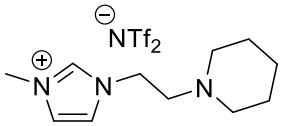
(m, 2H), 2.53 (q, 4H, J = 7.1 Hz), 0.91 (t, 6H, J = 7.1 Hz); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.3, 123.1, 122.9, 119.8 ($^1J_{CF}$ = 321 Hz), 52.4, 48.4, 46.7, 36.2, 11.5; IR (thin film, cm^{-1}) 3157, 3122, 2973, 2821, 1571, 1460, 1347, 1330, 1176, 1133, 1051, 789, 739, 653, 614.

3-(2-(Diethylamino)ethyl)-1-methylimidazolium tetrafluoroborate IL-03



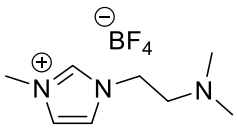
3-(2-(Diethylamino)ethyl)-1-methylimidazolium bromide hydrobromide (6.86 g, 20 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (2.23 g, 21 mmol, 1.05 eq.) and $NaBF_4$ (2.20 g, 20 mmol, 1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 3-(2-(diethylamino)ethyl)-1-methylimidazolium tetrafluoroborate in 77% yield (4.14 g) as a colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.78 (s, 1H), 7.48 (t, 1H, J = 1.7 Hz), 7.35 (t, 1H, J = 1.7 Hz), 4.20 (m, 2H), 3.94 (s, 3H), 2.78 (m, 2H), 2.53 (q, 2H, J = 7.1 Hz), 0.91 (t, 3H, J = 7.1 Hz); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.9, 122.9, 122.7, 52.5, 48.3, 46.8, 36.2, 11.6; IR (thin film cm^{-1}) 3159, 3122, 2970, 2876, 2815, 1572, 1460, 1386, 1342, 1286, 1173, 1032, 911, 845, 744, 653, 522, 520.

1-Methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium bis((trifluoromethyl)sulfonyl)amide IL-04



1-Methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium chloride hydrochloride (7.99 g, 30 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (4.86 g, 45 mmol, 1.5 eq.) and $LiNTf_2$ (9.47 g, 33 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 1-methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium bis((trifluoromethyl)sulfonyl)amide in 80% yield (12.8 g) as a colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.76 (s, 1H), 7.17 (t, 1H, J = 1.7 Hz), 7.23 (t, 1H, J = 1.6 Hz), 4.22 (t, 2H, J = 5.5 Hz), 3.94 (s, 3H), 2.70 (t, 2H, J = 5.5 Hz), 2.43 (t, 4H, J = 4.3 Hz), 1.56 (quintet, 4H, J = 5.3 Hz), 1.45 (quintet, 2H, J = 5.2 Hz); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.4, 123.1, 122.8, 119.8 ($^1J_{CF}$ = 321 Hz), 57.5, 54.3, 47.0, 36.3, 25.9, 24.0; IR (thin film, cm^{-1}) 3156, 3122, 2939, 2856, 2805, 1571, 1458, 1347, 1330, 1178, 1133, 1052, 739, 614.

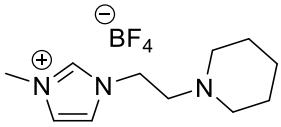
1-(2-(Dimethylamino)ethyl)-3-methylimidazolium tetrafluoroborate IL-05



3-(2-(Dimethylamino)ethyl)-1-methylimidazolium chloride hydrochloride (9.05 g, 40 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (4.48 g, 42 mmol, 1.05 eq.) and $NaBF_4$ (4.83 g, 44 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 3-(2-(dimethylamino)ethyl)-1-methylimidazolium tetrafluoroborate in 40% yield (2.89 g) as a colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.82 (s, 1H), 7.47 (t, 1H, J = 1.8 Hz), 7.31 (t, 1H, J = 1.8 Hz), 4.26 (m, 2H), 3.95 (s, 3H), 2.72 (m, 2H), 2.28 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.7, 123.0, 122.9, 58.0, 47.2, 45.0, 36.2; IR (thin

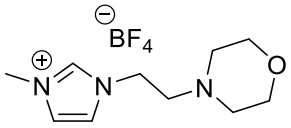
film cm^{-1}) 3161, 3121, 2951, 2868, 2829, 2777, 1738, 1573, 1462, 1357, 1285, 1234, 1173, 1016, 941, 846, 780, 755, 703, 654, 623.

1-Methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium tetrafluoroborate IL-06



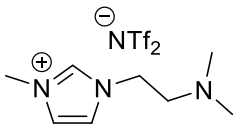
1-Methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium chloride hydrochloride (8.23 g, 31 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (3.45 g, 33 mmol, 1.05 eq.) and $NaBF_4$ (3.74 g, 34 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 1-methyl-3-(2-(piperidin-1-yl)ethyl)-imidazolium tetrafluoroborate in 82% yield (7.15 g) as a colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.73 (s, 1H), 7.50 (t, 1H, J = 1.6 Hz), 7.38 (t, 1H, J = 1.6 Hz), 4.23 (m, 2H), 3.94 (s, 3H), 2.69 (m, 2H), 2.41 (m, 4H), 1.53 (quintet, 4H, J = 5.4 Hz), 1.42 (quintet, 2H, J = 5.4 Hz); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.4, 123.0, 123.0, 57.5, 54.2, 46.8, 36.0, 25.8, 24.1; IR (thin film cm^{-1}) 3160, 3122, 2935, 2857, 2804, 1739, 1572, 1467, 1354, 1285, 1171, 1031, 924, 847, 757, 653, 623.

3-Methyl-1-(2-morpholinoethyl)imidazolium tetrafluoroborate IL-07



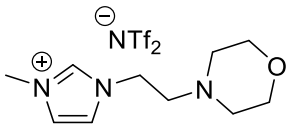
3-Methyl-1-(2-morpholinonethyl)imidazolium chloride (9.27 g, 40 mmol, 1 eq.) was dissolved in water (30 mL) with $NaBF_4$ (4.83 g, 44 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 3-methyl-1-(2-morpholinonethyl)imidazolium tetrafluoroborate in 88% yield (9.96 g) as a yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.87 (s, 1H), 7.47 (t, 1H, J = 1.8 Hz), 7.29 (t, 1H, J = 1.8 Hz), 4.29 (m, 2H), 3.97 (s, 3H), 3.70 (m, 4H), 2.79 (m, 2H), 2.53 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.9, 122.9, 122.9, 66.8, 57.3, 53.2, 46.4, 36.3; IR (thin film cm^{-1}) 3160, 3121, 2957, 2855, 2816, 1738, 1574, 1456, 1358, 1299, 1146, 1015, 930, 912, 853, 764, 652, 622, 520.

1-(2-(Dimethylamino)ethyl)-3-methylimidazolium bis((trifluoromethyl)sulfonyl)amide IL-08



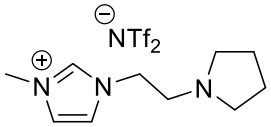
3-(2-(Dimethylamino)ethyl)-1-methylimidazolium chloride hydrochloride (5.73 g, 25 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (3.20 g, 30 mmol, 1.2 eq.) and $LiNTf_2$ (8.02 g, 2.8 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 3-(2-(dimethylamino)ethyl)-1-methylimidazolium bis((trifluoromethyl)sulfonyl)amide in 55% yield (5.93 g) as a colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.79 (s, 1H), 7.45 (t, 1H, J = 1.8 Hz), 7.26 (t, 1H, J = 1.8 Hz), 4.23 (m, 2H), 3.95 (s, 3H), 2.71 (m, 2H), 2.28 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.2, 123.0, 123.0, 119.8 ($^1J_{CF}$ = 321 Hz), 57.9, 47.3, 44.9, 36.2; IR (thin film cm^{-1}) 3157, 3122, 2954, 2832, 2781, 1569, 1462, 1347, 1175, 1132, 1051, 942, 840, 788, 740, 653, 612.

3-Methyl-1-(2-morpholinoethyl)imidazolium bis((trifluoromethyl)sulfonyl)amide IL-09



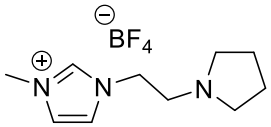
3-Methyl-1-(2-morpholinonethyl)imidazolium chloride (9.30 g, 40 mmol, 1 eq.) was dissolved in water (30 mL) with $LiNTf_2$ (12.3 g, 44 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removedunder vacou at 50 °C for 48 h to afford 3-methyl-1-(2-morpholinonethyl)imidazolium bis((trifluoromethyl)sulfonyl)amide in 92% yield (17.5 g) as a yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.73 (s, 1H), 7.45 (t, 1H, J = 1.8 Hz), 7.27 (t, 1H, J = 1.8 Hz), 4.24 (m, 2H), 3.93 (s, 3H), 3.67 (m, 4H), 2.75 (m, 2H), 2.50 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.1, 123.1, 123.1, 119.7 ($^1J_{CF}$ = 321 Hz), 66.7, 57.2, 53.2, 46.4, 36.2; IR (thin film cm^{-1}) 3158, 3121, 2964, 2858, 2819, 1573, 1457, 1176, 1134, 1114, 1051, 930, 912, 855, 789, 762, 739, 703, 652, 611.

3-Methyl-1-(2-(pyrrolidin-1-yl)ethyl)imidazolium bis((trifluoromethyl)sulfonyl)amide IL-10



1-Methyl-3-(2-(pyrrolidin-1-yl)ethyl)-imidazolium chloride hydrochloride (5.12 g, 20 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (2.20 g, 2.1 mmol, 1.05 eq.) and $LiNTf_2$ (5.83 g, 20 mmol, 1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 1-methyl-3-(2-(pyrrolidin-1-yl)ethyl)-imidazolium bis((trifluoromethyl)sulfonyl)amide in 85% yield (7.82 g) as a dark yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.77 (s, 1H), 7.44 (t, 1H, J = 1.6 Hz), 7.26 (t, 1H, J = 1.6 Hz), 4.24 (m, 2H), 3.93 (s, 3H), 2.89 (m, 2H), 2.56 (m, 4H), 1.79 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.0, 123.1, 123.1, 119.8 ($^1J_{CF}$ = 321 Hz), 54.7, 53.7, 36.3, 23.6; IR (thin film cm^{-1}) 3157, 2970, 2805, 1739, 1572, 1461, 1347, 1330, 1176, 1132, 1051, 842, 789, 739, 653, 612.

3-Methyl-1-(2-(pyrrolidin-1-yl)ethyl)imidazolium tetrafluoroborate IL-11

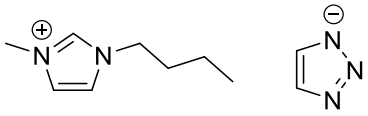


1-Methyl-3-(2-(pyrrolidin-1-yl)ethyl)-imidazolium chloride hydrochloride (9.09 g, 36 mmol, 1 eq.) was dissolved in water (30 mL) with Na_2CO_3 (3.95 g, 37 mmol, 1.03 eq.) and $NaBF_4$ (4.51 g, 4.1 mmol, 1.1 eq.) and stirred for 2 h. The aqueous phase was washed with DCM (3x30 mL) and the combined organic phases were washed with water (30 mL), dried over $MgSO_4$, filtered and the solvent removed under vacou at 50 °C for 48 h to afford 1-methyl-3-(2-(pyrrolidin-1-yl)ethyl)-imidazolium bis((trifluoromethyl)sulfonyl)amide in 80% yield (7.69 g) as a dark yellow liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.74 (s, 1H), 7.48 (t, 1H, J = 1.6 Hz), 7.37 (t, 1H, J = 1.6 Hz), 4.26 (m, 2H), 3.93 (s, 3H), 2.89 (m, 2H), 2.55 (m, 4H), 1.76 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 136.5, 123.1, 122.9, 54.8, 53.7, 48.4, 36.1, 23.6; IR (thin film cm^{-1}) 3160, 3122, 2967, 2879, 2799, 1710, 1573, 1460, 1353, 1285, 1171, 1032, 847, 733, 702, 653, 623.

Preparation of triazolate ionic liquids

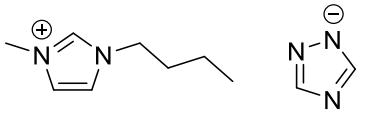
Ion exchange to hydroxide was performed on the corresponding imidazolium or pyrrolidine bromide using an Amberlite® IRN78 hydroxide resin to form the imidazolium or pyrrolidinium hydroxide. The salt was washed through the resin three times and halide exchange was checked with $AgNO_3$ and HNO_3. Hydroxide and triazolate were mixed 1:1 in water and the aqueous phase was washed with EtOAc thrice. The solvent was removed under vacou at 50 °C for 48 h.

1-Butyl-3-methylimidazolium 1,2,3-triazolate IL-12



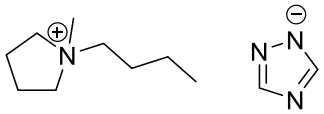
^{1}H NMR (400 MHz, CD_3OD) δ (ppm) 7.61 (s, 1H), 7.56 (s, 2H), 7.54 (s, 1H), 4.18 (t, 2H, J = 7.2 Hz), 3.90 (s, 3H), 1.86 (quintet, 2H, J = 7.4 Hz), 1.38 (sextet, 2H, J = 7.4 Hz), 1.00, (t, 3H, J = 7.3 Hz); ^{13}C NMR (101 MHz, MeOD) δ (ppm) 129.4, 123.5, 122.2, 49.1, 35.0, 31.6, 19.0, 12.3; IR (thin film, cm^{-1}) 3071, 2959, 2935, 2873, 1567, 1463, 1428, 1383, 1169, 1124, 1036, 953, 782, 653, 622.[1]

1-Butyl-3-methylimidazolium 1,2,4-triazolate IL-13



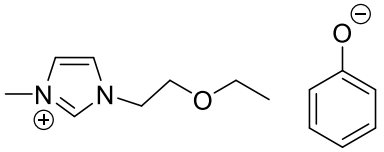
^{1}H NMR (400 MHz, CD_3OD) δ (ppm) 8.00 (s, 2H), 7.61 (s, 1H), 7.54 (s, 1H), 4.19 (t, 2H, J = 7.2 Hz), 3.91 (s, 3H), 1.86 (quintet, 2H, J = 7.4 Hz), 1.38 (sextet, 2H, J = 7.4 Hz), 0.99 (t, 3H, J = 7.2 Hz); ^{13}C NMR (101 MHz, MeOD) δ (ppm) 148.2, 123.5, 122.2, 49.2, 35.0, 31.6, 19.0, 12.3; IR (thin film, cm^{-1}) 3071, 2959, 2934, 2873, 1568, 1471, 1383, 1239, 1170, 1142, 962, 849, 753, 682, 653, 623.[2]

1-Butyl-1-methylpyrrolidine 1,2,4-triazolate IL-14



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.07 (s, 2H), 3.50 (m, 4H), 3.30 (m, 2H), 3.00 (s, 3H), 2.16 (m, 4H), 1.65 (m, 2H), 1.38 (m, 2H), 0.97 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 149.1, 64.1, 64.0, 48.1, 25.8, 21.5, 19.7, 13.6; IR (thin film, cm^{-1}) 2961, 2875, 1582, 1470, 1378, 1270, 1238, 1141, 1005, 961, 929, 849, 739, 683, 641.

Synthesis of 1-(2-ethoxyethyl)-3-methylimidazolium phenolate IL-15



To a solution of 1-(2-ethoxyethyl)-3-methylimidazolium bromide (2.5 g, 10.63 mmol) in dichloromethane (50 mL), sodium phenolate(1.35 g, 11.63 mmol) was added and stirred at room temperature for 24 hrs. The precipitate formed was filtered off and the clear solution was kept in the fridge for 12 hrs. The precipitated NaBr was filtered of and the cooling procedure is repeated until there is no precipitation of NaBr. The solvent was removed under vacuum and the ionic liquids obtained was further dried in Schlenk line for 24 hrs at 50 ºC. 1-(2-ethoxyethyl)-3-methylimidazolium phenolate obtained as a pale yellow liquid. Yield: 2.2 g (83%). ^{1}H NMR (400 MHz, DMSO(d6), δ (ppm): 9.42 (d, 1H, J=## Hz), 7.82 (d, 2H, J= ## Hz), 7.31 (m, 2H, J= ## Hz), 7.10 (m, 2H), 7.01(t, 1H, J =## Hz), 4.38 (t, 2H, J= 7.3 Hz),

3.89 (s, 3H), 3.72 (t, 2H, J= 7.3 Hz), 3.45 (m, 2H), 1.06 (t, 3H, J= 7.3 Hz). ^{13}C NMR (101 MHz, DMSO (d6)) δ (ppm)= 15.32, 36.17, 48.84, 65.94, 68.01, 116.09, 122.63, 123.09, 130.08, 130.35, 137.40, 159.35.

Differential scanning calorimetry

A Netzch DSC 214 Polyma was used to measure the glass transition temperatures (T_g) at a scan rate of 10 K/min. The samples were twice heated under nitrogen atmosphere from 133.15 K to 373.15 K at a rate of 10 K/min.

Thermogravimetric analysis

A Netzxch TG 209 Libra was used to measure decomposition temperatures (T_d). Ionic liquid samples were heated from 303 K to 773 K at a heating rate of 20 K/min under nitrogen atmosphere. Cellulose samples were heated from 303 K to 873 K at a rate of 10 K/min under nitrogen atmosphere.

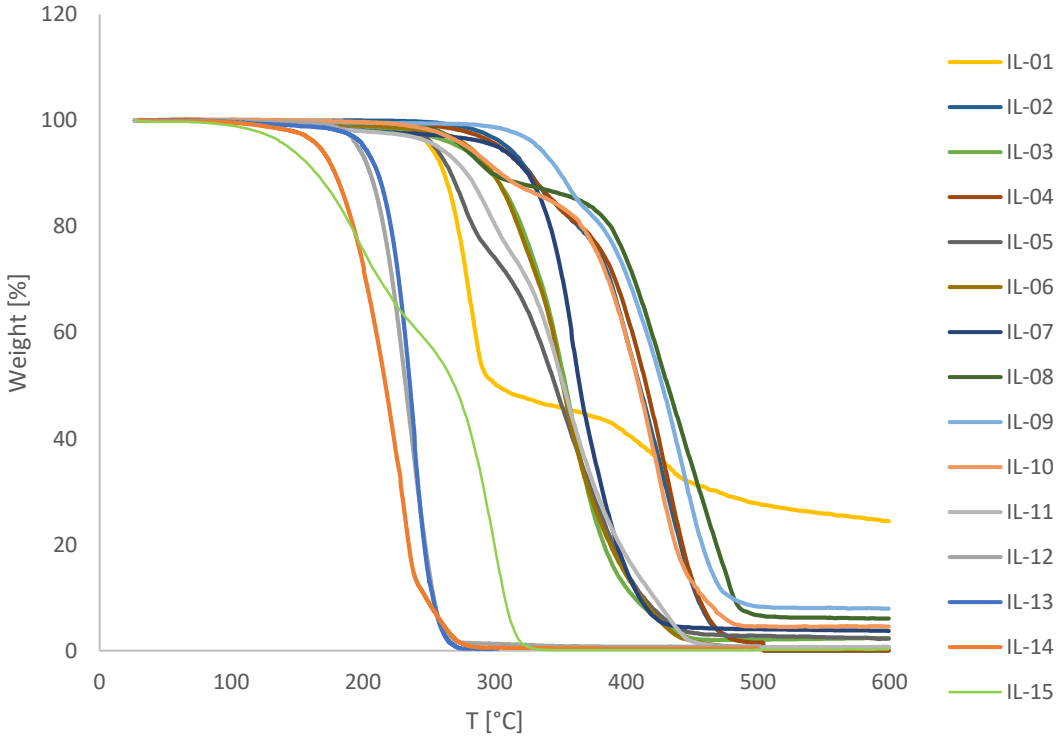


Fig S3 Thermal gravimetric analysis (TGA) of IL-01-IL-15.

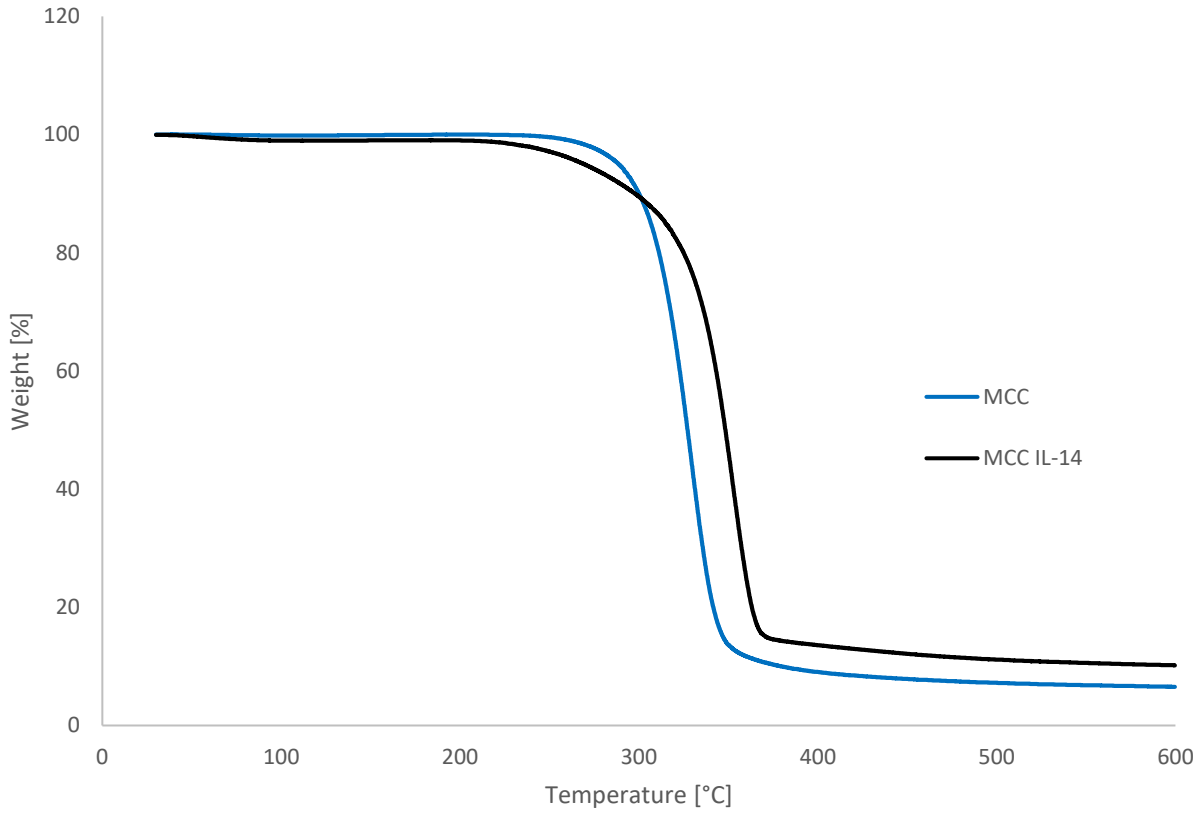


Figure S4 Thermal gravimetric analysis (TGA) of microcrystalline cellulose (MCC) before and after dissolution in IL-14.

Refractive index

Refractive indices were measured at 276.5±0.5 K using a PAL-RI refractometer from Atago, with an uncertainty of ±0.0003 (water at 273 K).

Heat capacity

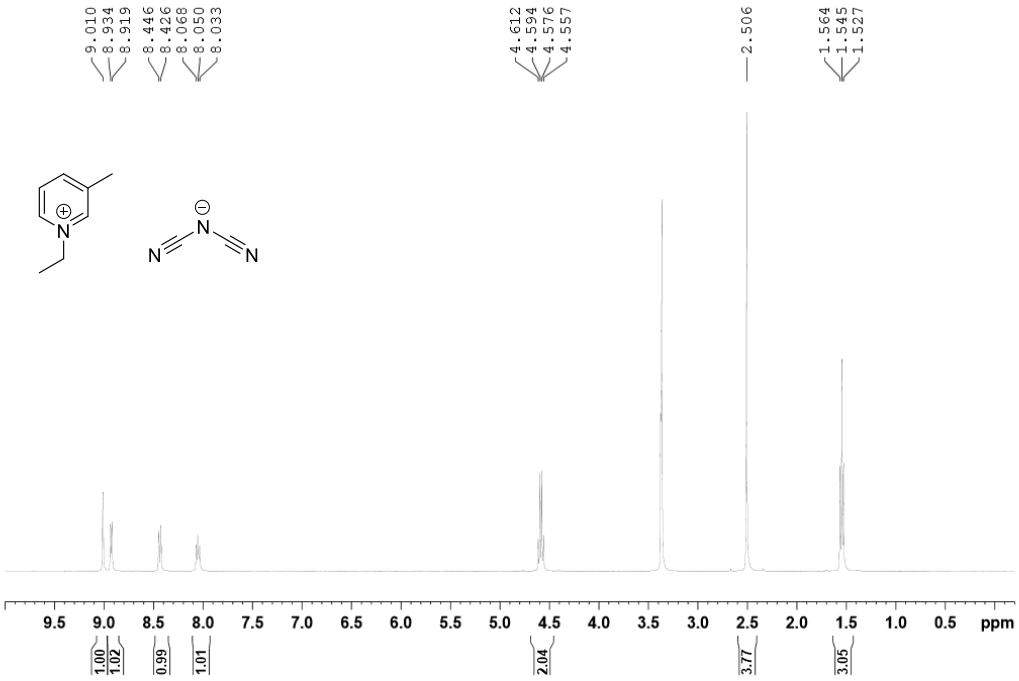
The specific heat capacity (Cp) and glass transition temperature (Tg) were measured using Differential Scanning Calorimetry (DSC), Perkin-Elmer (model Pyris1, USA). The measurements were performed with a heating rate of 10 °C·min^{-1} under helium flow. The sapphire method was used to calculate the specific heat capacity.

Surface tension

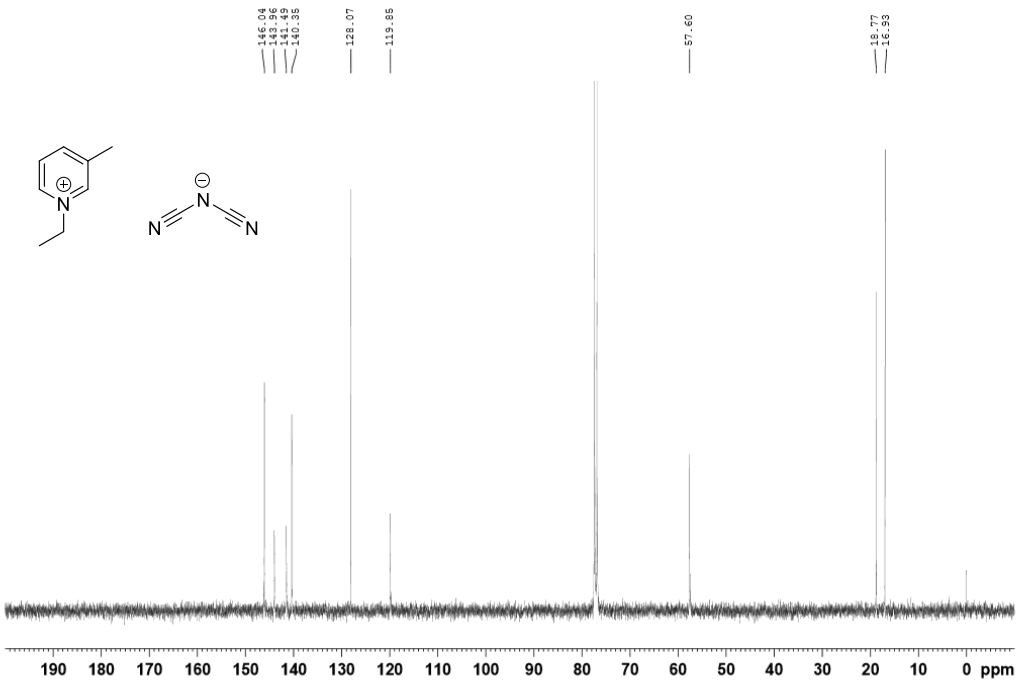
Surface tension was measured using the pendant drop method. The temperature range was from 293.15 to 353.15 K with uncertainty of u(σ) = ± 0.04 mN·m^{-1} and u(T) = ± 0.01 K. A commercial tensiometer (Krüss GmbH, Germany) has been used. An axially symmetrical pendant drop is formed by a steel needle in a homogeneous gravitation field.

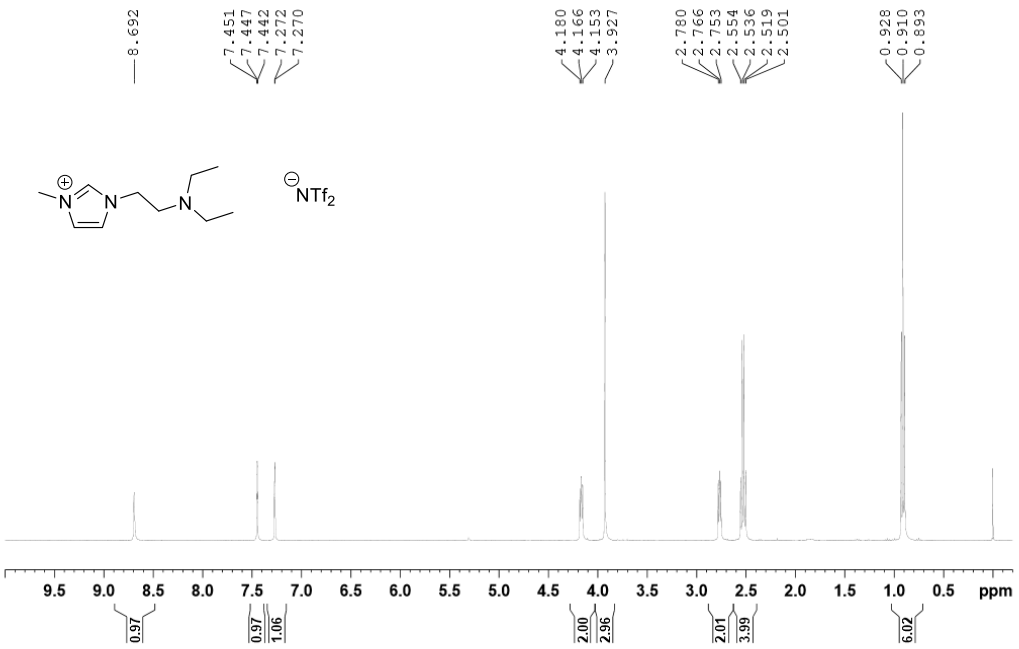
CO_2 solubility

CO_2 solubility measurements were measured in a Rubotherm from TA Instruments by differentials in sample weight. CO_2 pressures during experiments were 1, 2, 5 or 10 bar, and temperatures 25, 40 or 50 °C. Before measurements the equipment and sample were evacuated for 24 h at 50 °C. The weight of the empty sample holder at each condition was used as weight zero point. Effects of buoyancy was included in calculations of weight.

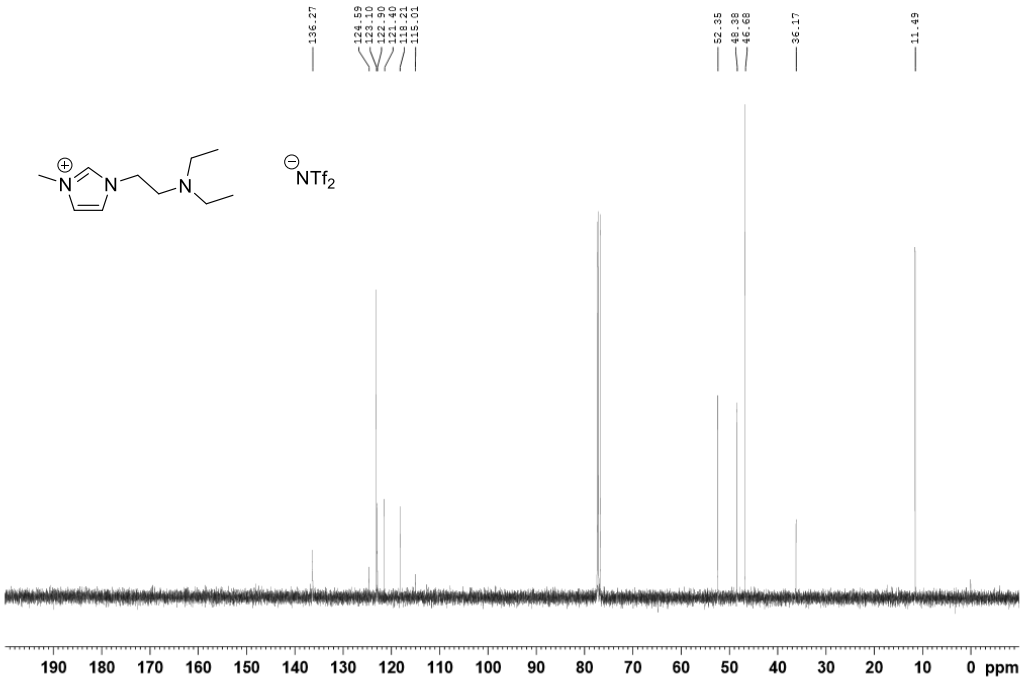

9.010
8.934
8.919
8.446
8.426
8.068
8.050
8.033
4.612
4.594
4.576
4.557
2.506
1.564
1.545
1.527
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.02
0.99
1.01
2.04
3.77
3.05

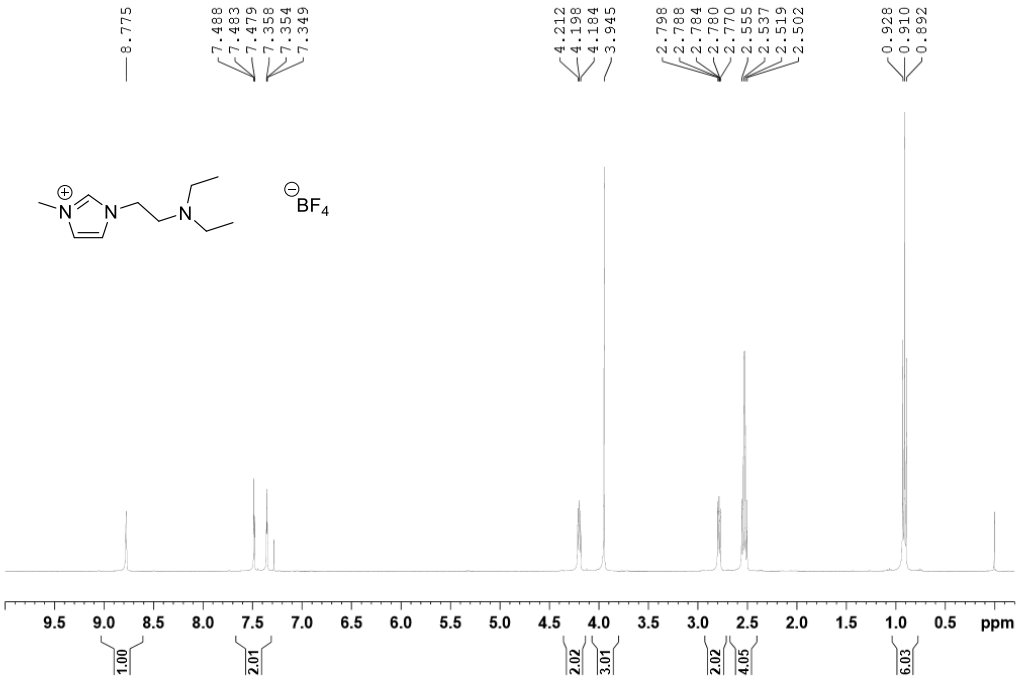
IL-01


146.04
143.66
141.49
140.36
128.07
119.86
57.60
18.77
16.33
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.692
7.451
7.447
7.442
7.272
7.270
4.180
4.166
4.153
3.927
2.780
2.766
2.753
2.554
2.536
2.519
2.501
0.928
0.910
0.893
NTf2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.97
0.97
1.06
2.00
2.96
2.01
3.99
6.02

IL-02


136.27
124.59
123.10
122.90
121.40
118.21
115.01
52.35
48.38
46.68
36.17
11.49
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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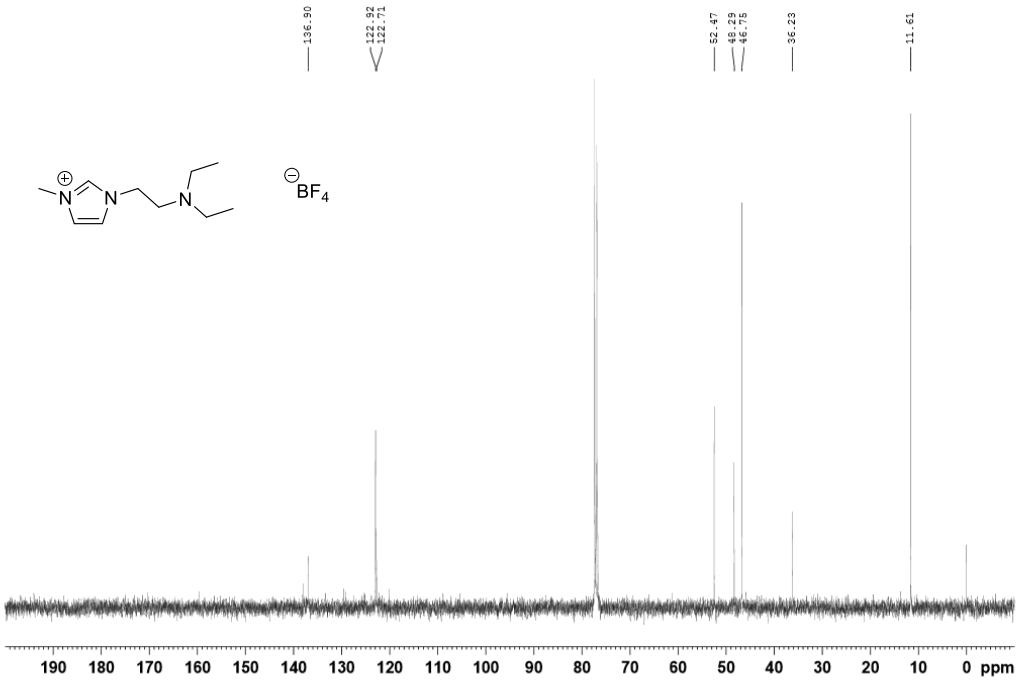
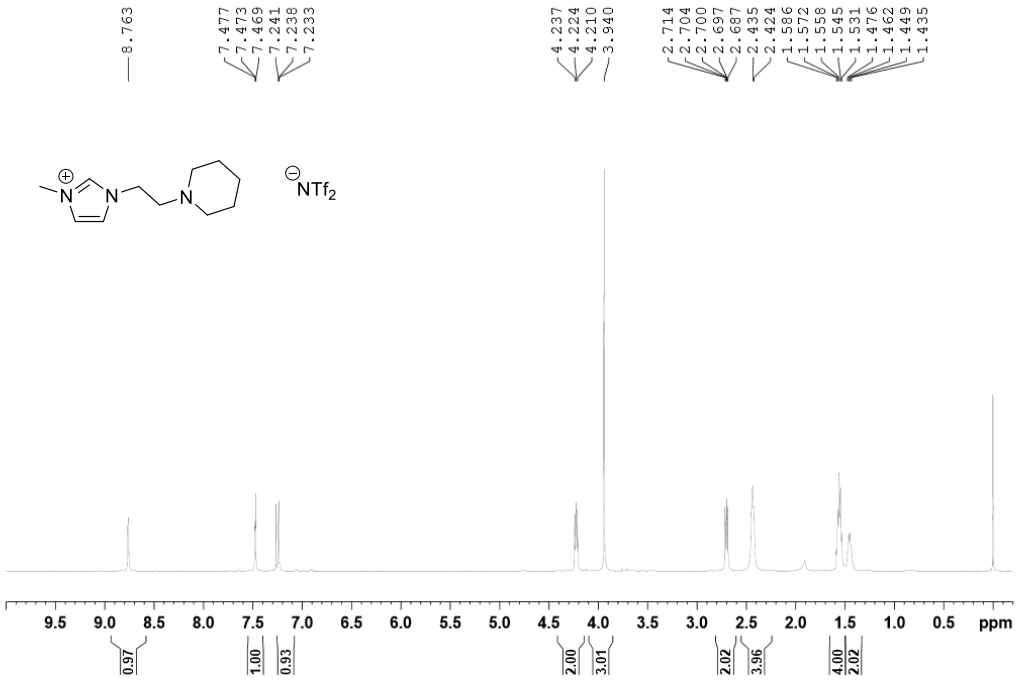
7.488
7.483
7.479
7.358
7.354
7.349
4.212
4.198
4.184
3.945
2.798
2.788
2.784
2.780
2.770
2.555
2.537
2.519
2.502
0.928
0.910
0.892
BF4
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.01
2.02
3.01
2.02
4.05
6.03

IL-03


136.90
122.82
122.71
52.47
48.29
46.75
36.23
11.61
BF4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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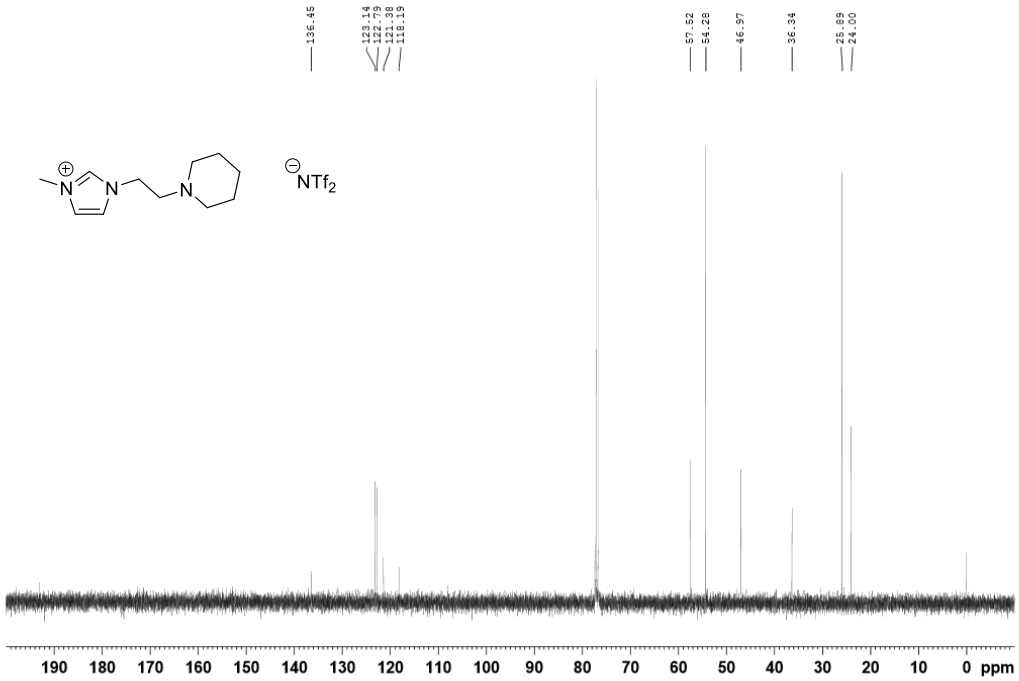
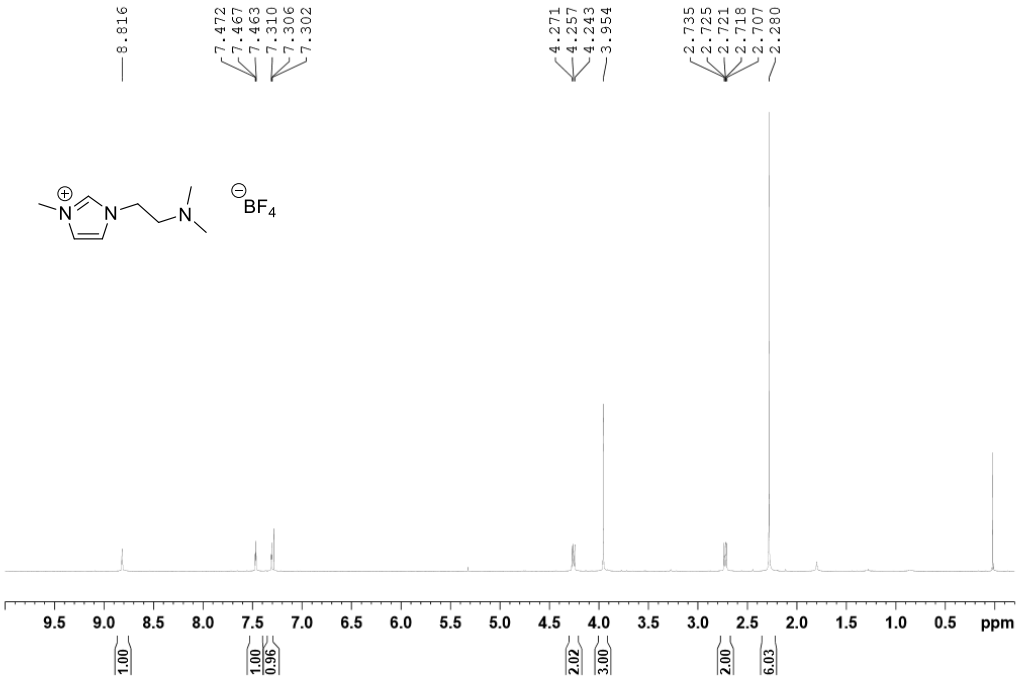
7.473
7.469
7.241
7.238
7.233
4.237
4.224
4.210
3.940
2.714
2.704
2.700
2.697
2.687
2.435
2.424
1.586
1.572
1.558
1.545
1.531
1.476
1.462
1.449
1.435
NTf2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
0.97
1.00
0.93
2.00
3.01
2.02
3.96
4.00
2.02

IL-04


136.45
123.14
122.79
121.38
118.19
57.52
54.28
46.97
36.34
25.89
24.00
NTf2
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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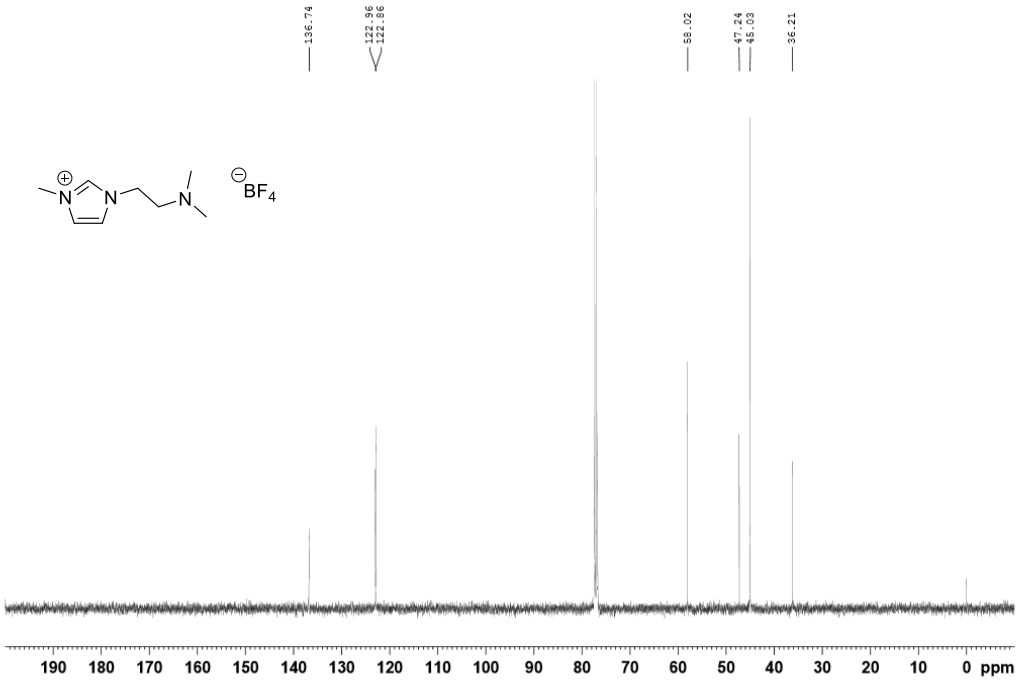
7.472
7.467
7.463
7.310
7.306
7.302
4.271
4.257
4.243
3.954
2.735
2.725
2.721
2.718
2.707
2.280
BF4
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.00
0.96
2.02
3.00
2.00
6.03

IL-05


136.74
122.96
122.86
58.02
47.24
45.03
36.21
BF4
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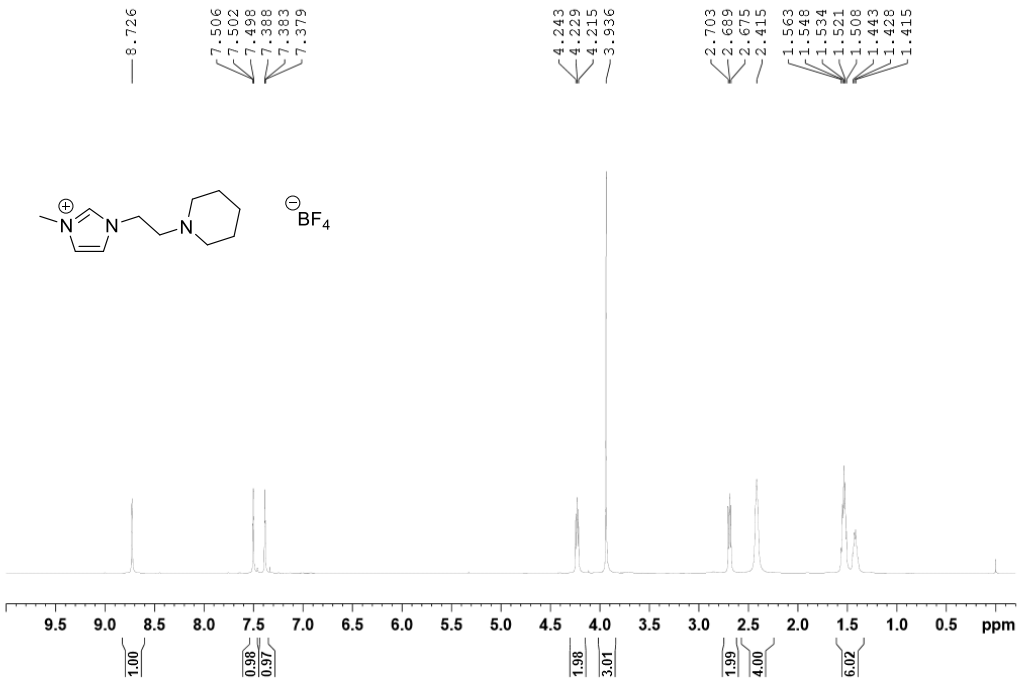
8.726
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7.498
7.388
7.383
7.379
4.243
4.229
4.215
3.936
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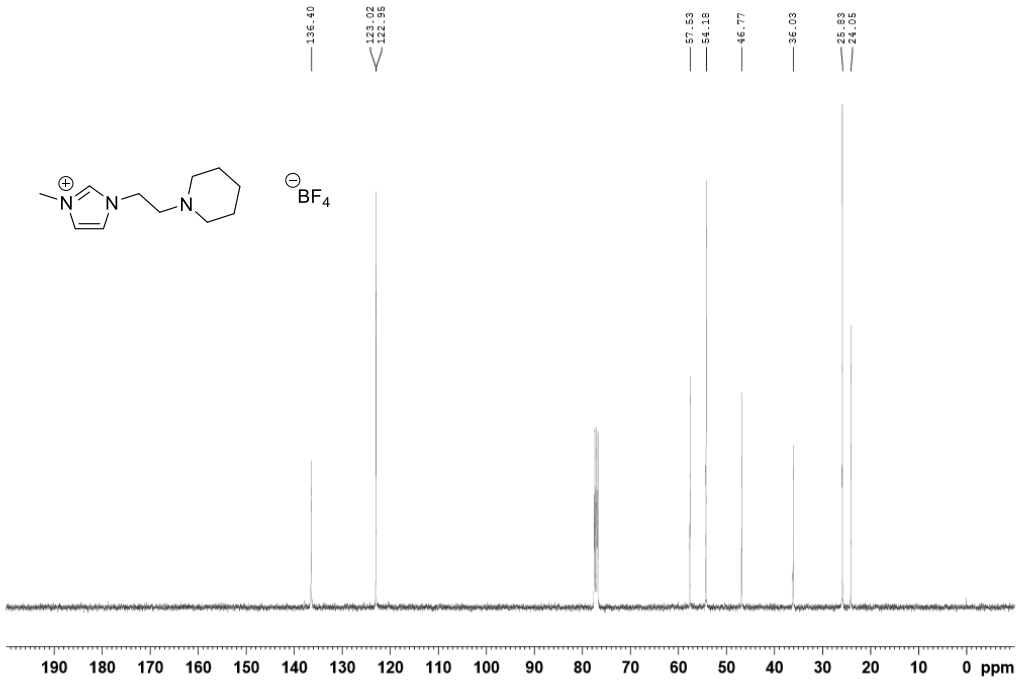
2.675
2.415
1.563
1.548
1.534
1.521
1.508
1.443
1.428
1.415
BF4
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
0.98
0.97
1.98
3.01
1.99
4.00
6.02

IL-06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57.53
54.18
46.77
36.03
25.83
24.05
BF4
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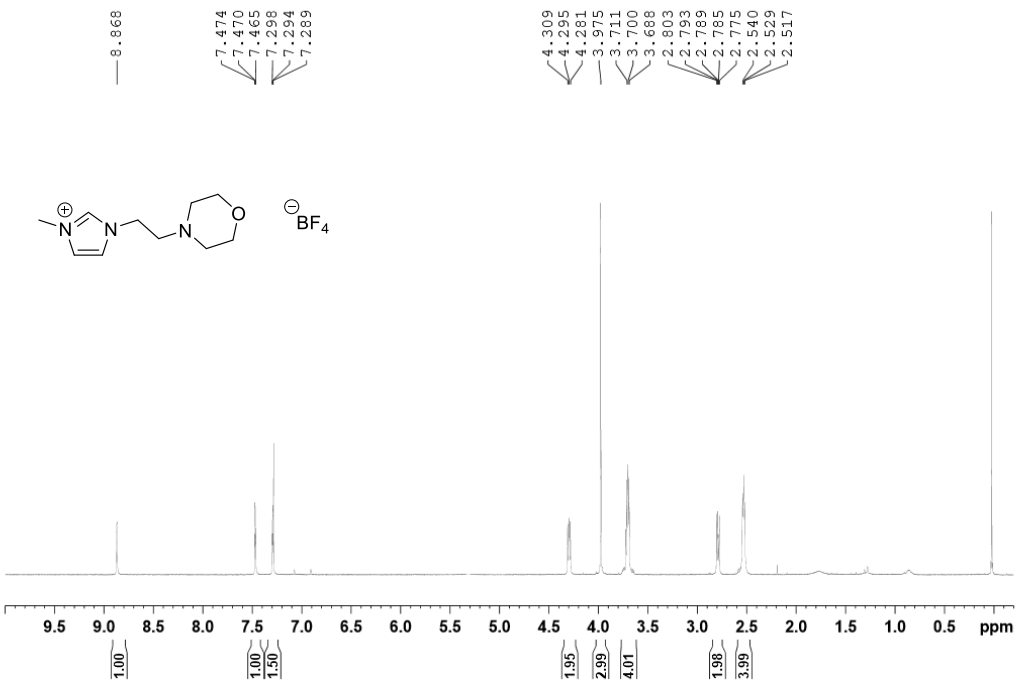
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7.294
7.289
4.309
4.295
4.281
3.975
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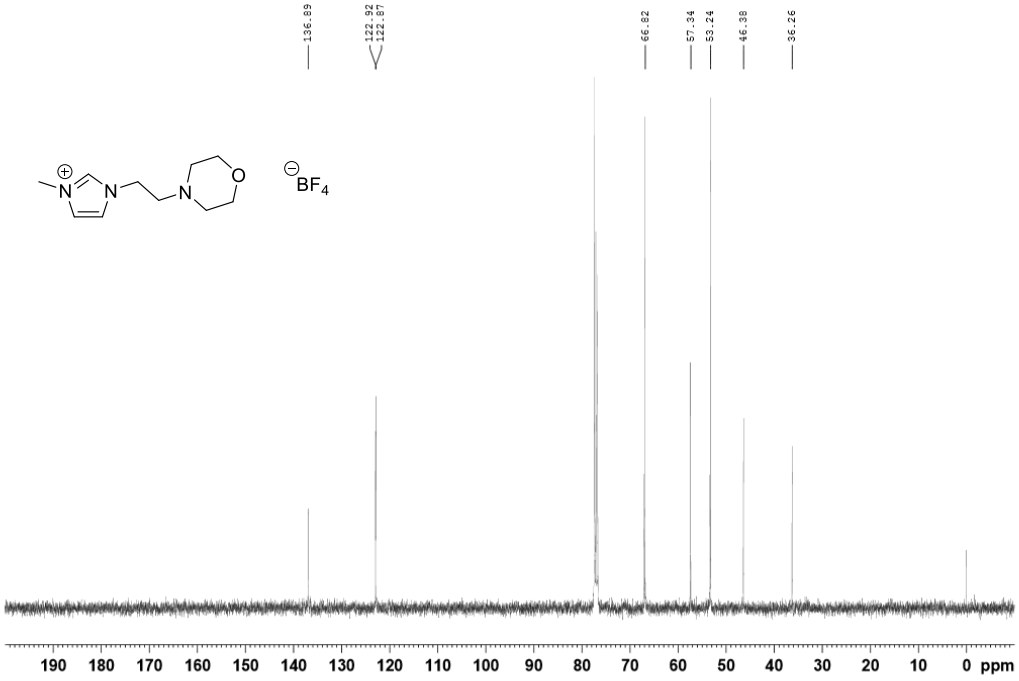
3.688
2.803
2.793
2.789
2.785
2.775
2.540
2.529
2.517
BF4
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.00
1.50
1.95
2.99
4.01
1.98
3.99

IL-07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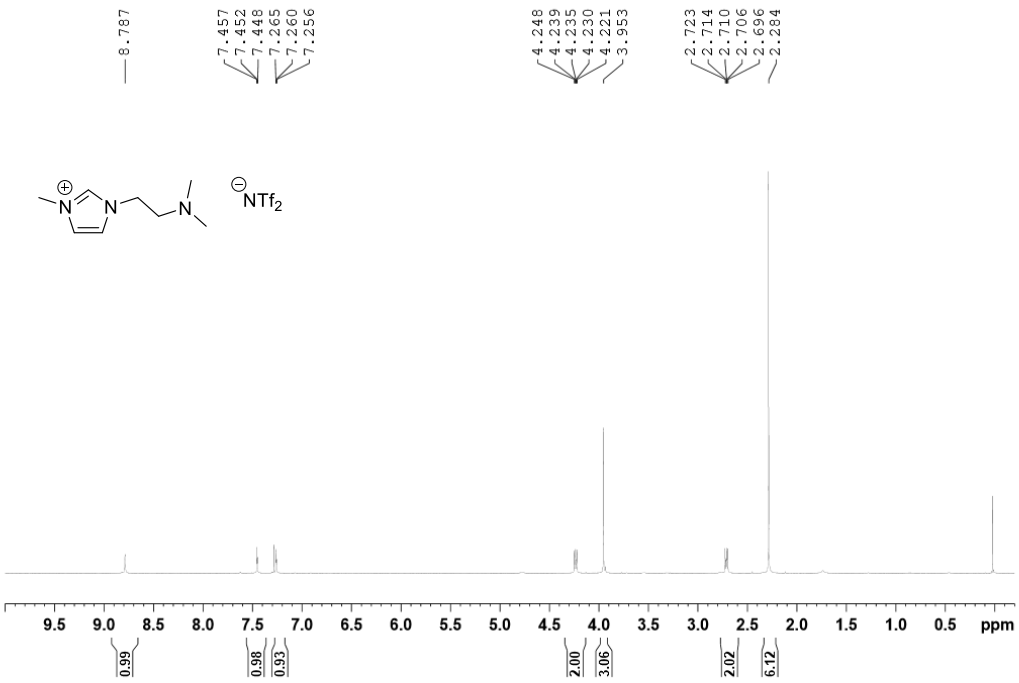
57.34
53.24
46.38
36.26
BF4
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.452
7.448
7.265
7.260
7.256
4.248
4.239
4.235
4.230
4.221
3.953
2.723
2.714
2.710
2.706
2.696
2.284
NTf2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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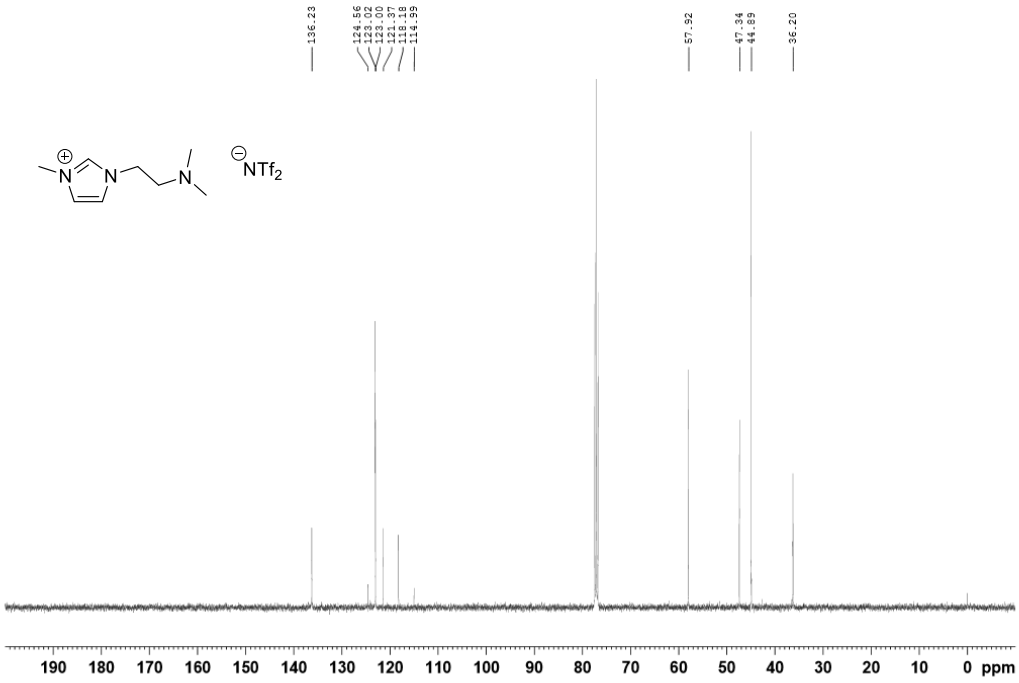
0.98
0.93
2.00
3.06
2.02
6.12

IL-08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123.02
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121.37
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57.92
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44.89
36.20
NTf2
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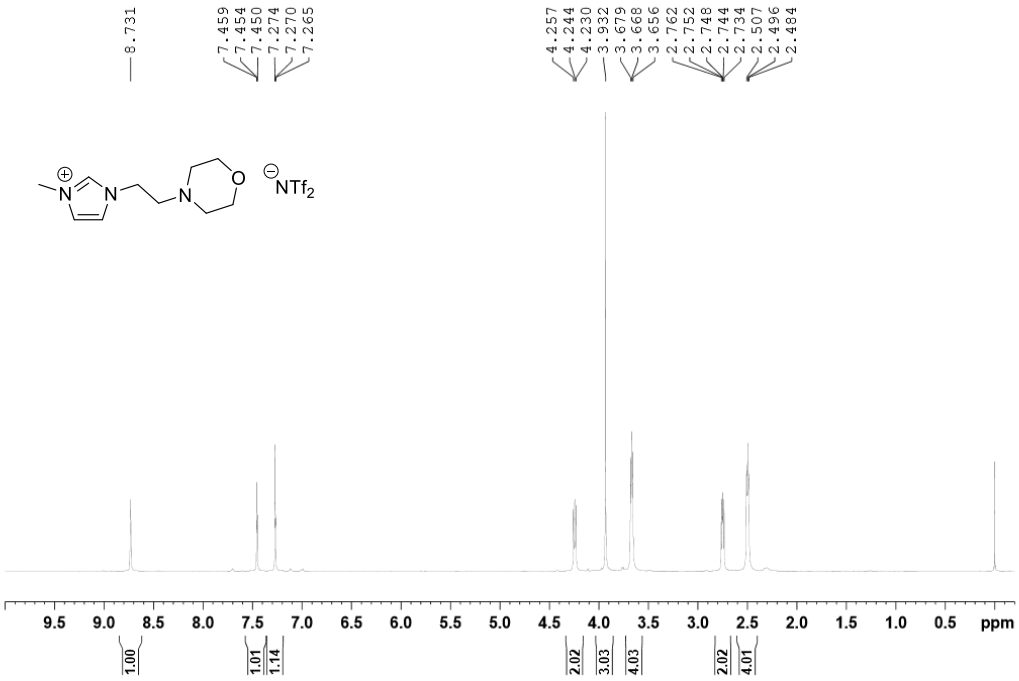
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3.668
3.656
2.762
2.752
2.748
2.744
2.734
2.507
2.496
2.484
NTf2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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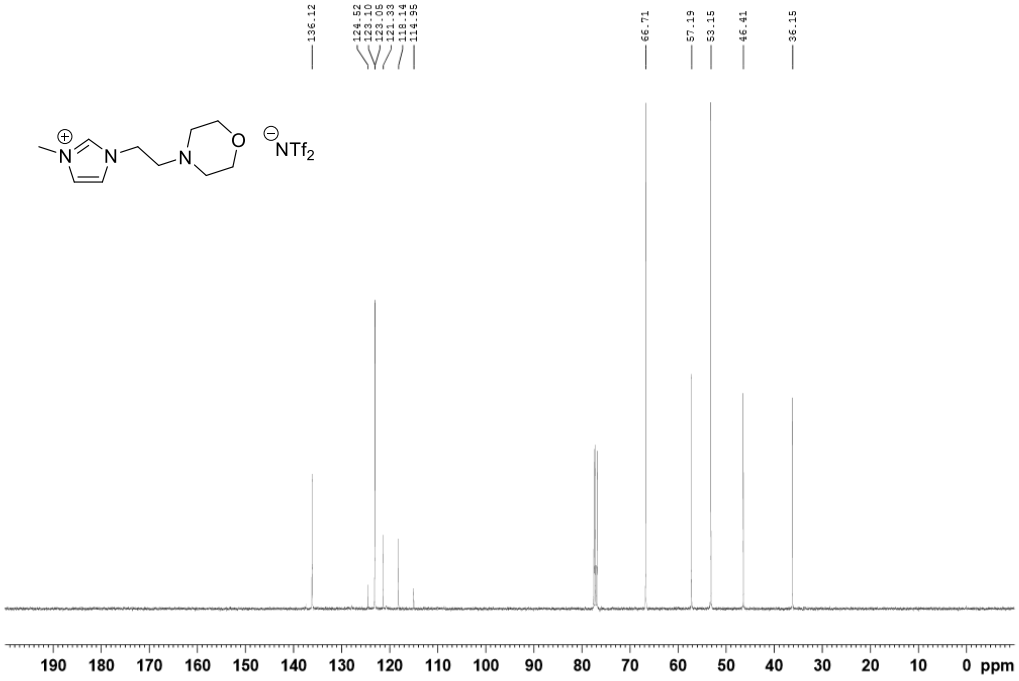
1.14
2.02
3.03
4.03
2.02
4.01

IL-09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124.52
123.10
123.05
121.33
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114.95
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57.19
53.15
46.41
36.15
NTf2
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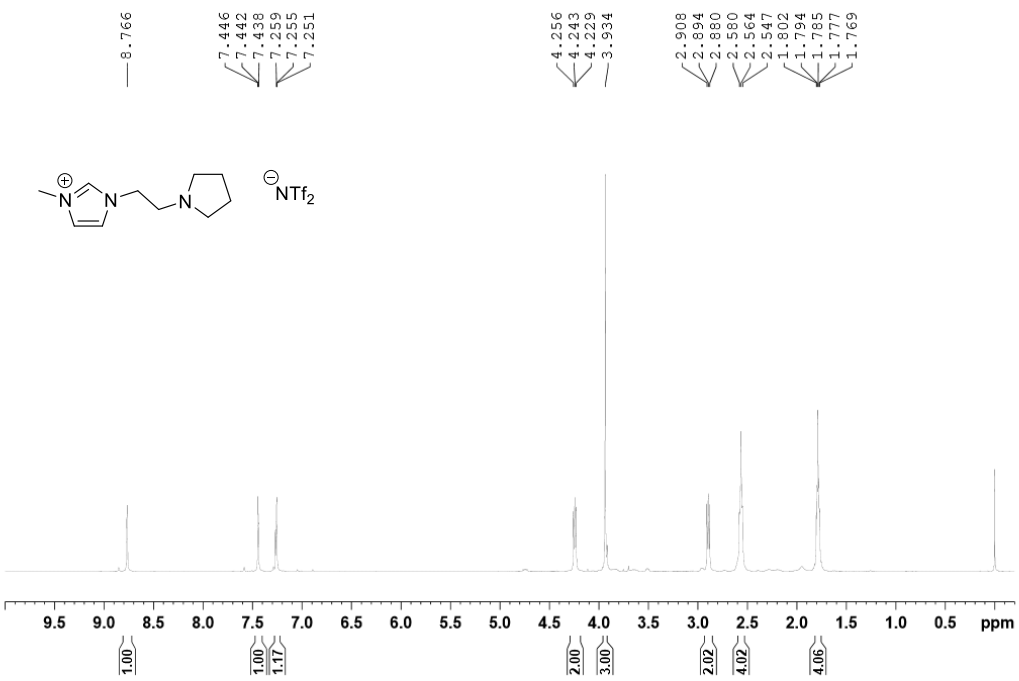
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7.442
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7.259
7.255
7.251
4.256
4.243
4.229
3.934
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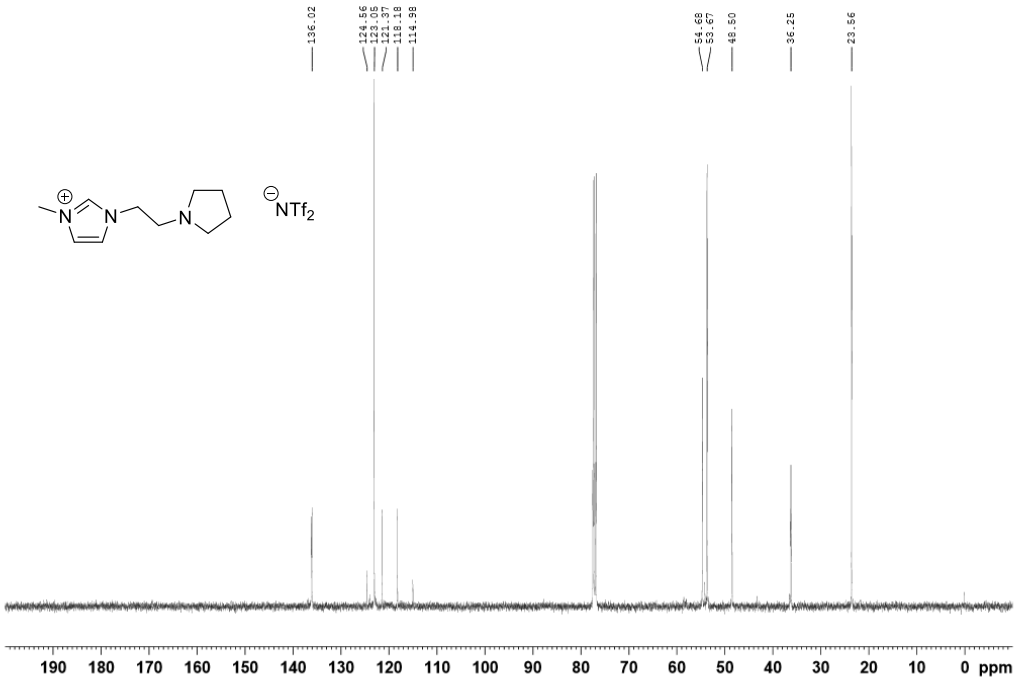
2.894
2.880
2.580
2.564
2.547
1.802
1.794
1.785
1.777
1.769
NTf2
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.00
1.17
2.00
3.00
2.02
4.02
4.06

IL-10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123.05
121.37
118.18
114.98
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53.67
48.50
36.25
23.56
NTf2
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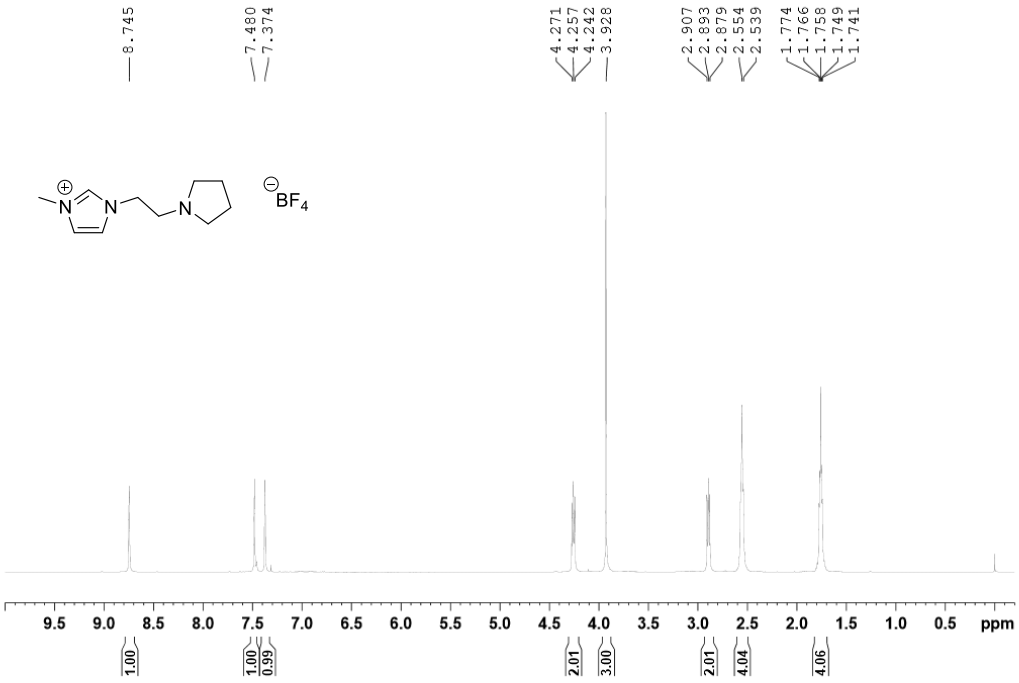
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2.907
2.893
2.879
2.554
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1.774
1.766
1.758
1.749
1.741
BF4
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
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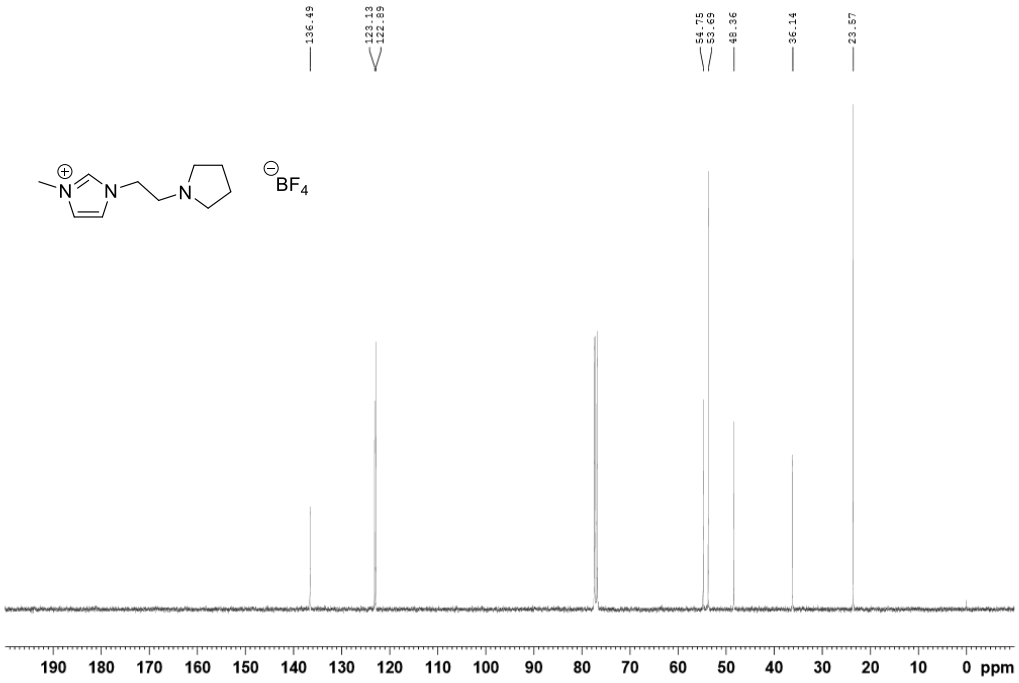
1.00
0.99
2.01
3.00
2.01
4.04
4.06

IL-11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123.13
122.89
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53.69
48.36
36.14
23.57
BF4
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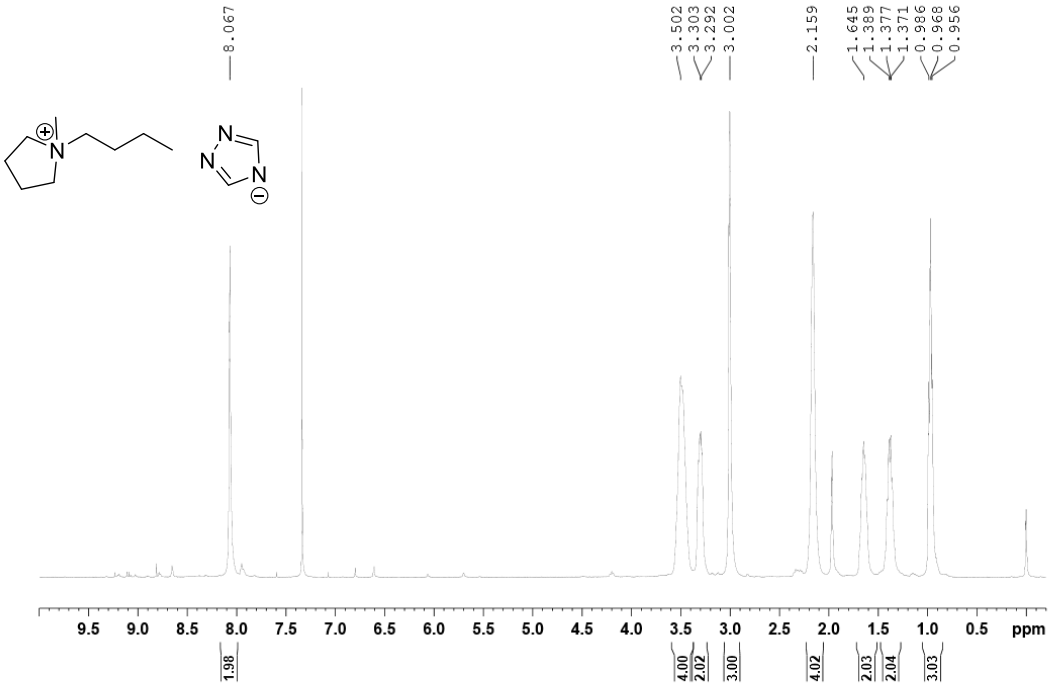
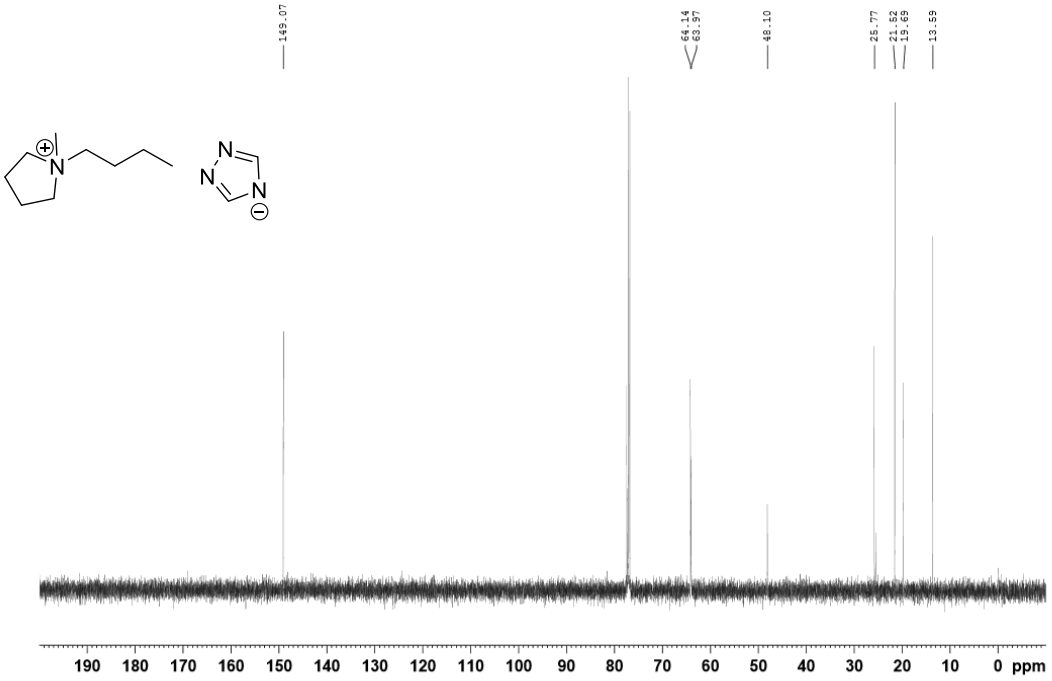
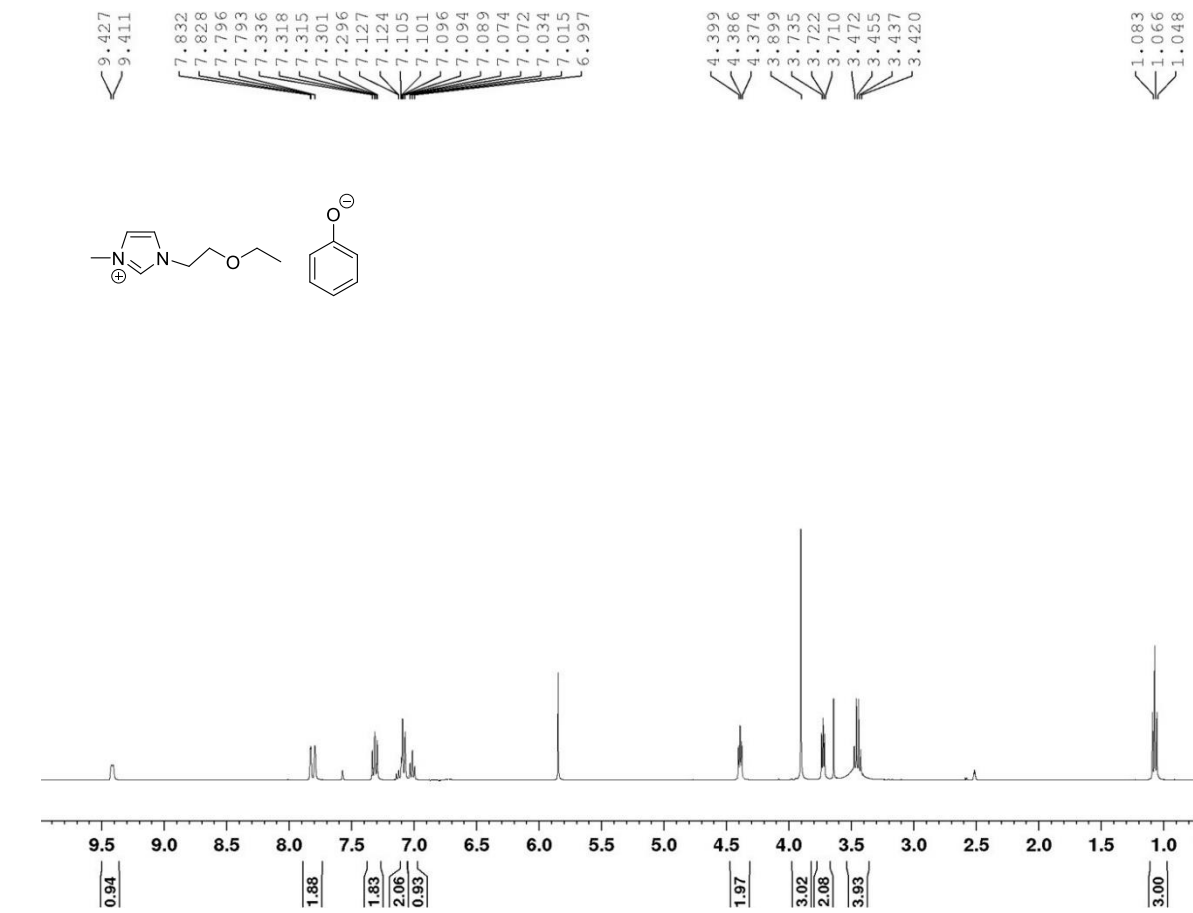

8.067
3.502
3.303
3.292
3.002
2.159
1.645
1.389
1.377
1.371
0.986
0.968
0.956
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.98
4.00
2.02
3.00
4.02
2.03
2.04
3.03

IL-14


149.07
64.14
63.97
48.10
25.77
21.52
19.69
13.59
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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9.411
7.832
7.828
7.796
7.793
7.336
7.318
7.315
7.301
7.296
7.127
7.124
7.105
7.101
7.096
7.094
7.089
7.074
7.072
7.034
7.015
6.997
4.399
4.386
4.374
3.899
3.735
3.722
3.710
3.472
3.455
3.437
3.420
1.083
1.066
1.048
O
N
N
O
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.94
1.88
1.83
2.06
0.93
1.97
3.02
2.08
3.93
3.00

IL-15

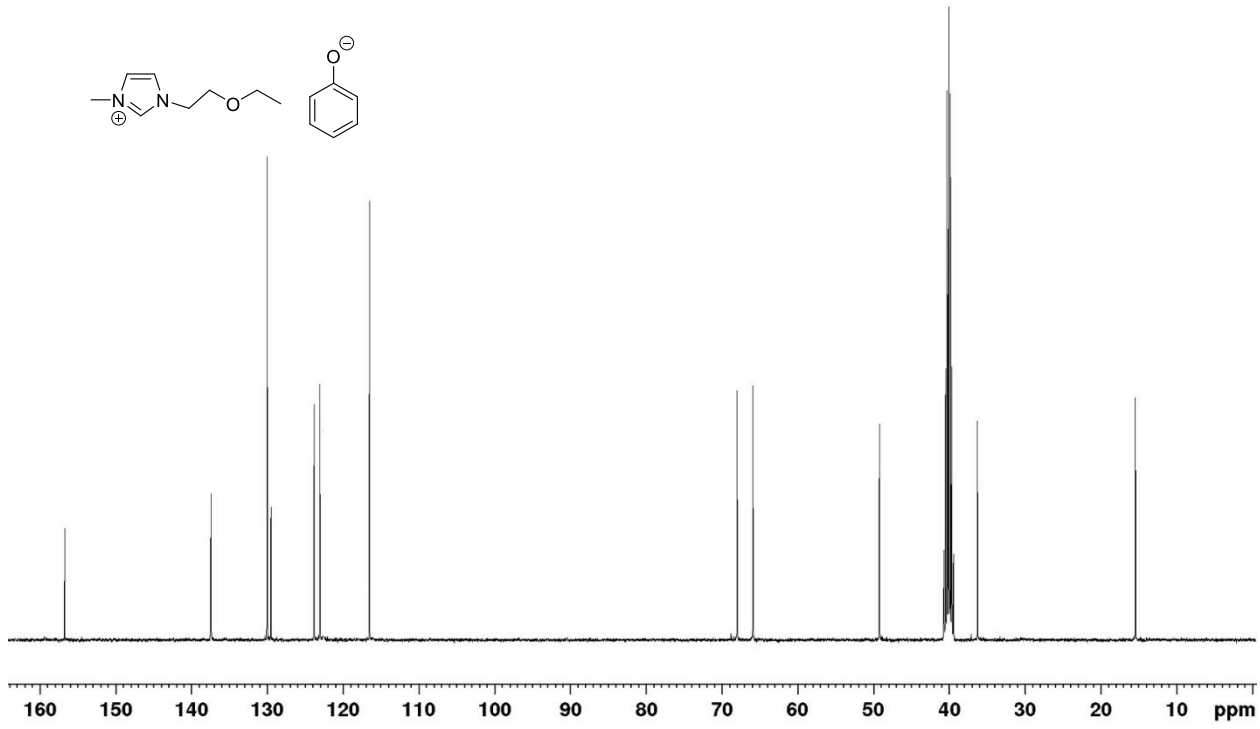
O
N
N
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Table S2 Comparison of experimental densities with COSMO-RS and ML predictions.

		ρ [g/cm3]					ρ [g/cm3]					ρ [g/cm3]]		
IL	[°C]	Experimental	COSMO	ML	IL	[°C]	Experimental	COSMO	ML	IL	[°C]	Experimental	COSMO	ML
IL-12	10	1.1011	1.0664	1.1012	IL-02	10	1.3894	1.3925	1.4213	IL-04	55	1.3779	1.3777	1.3184
IL-12	15	1.0979	1.0633	1.0962	IL-02	15	1.3847	1.3878	1.4173	IL-04	60	1.3734	1.3730	1.3172
IL-12	20	1.0948	1.0602	1.0944	IL-02	20	1.3800	1.3831	1.4107	IL-04	65	1.3689	1.3684	1.3112
IL-12	25	1.0917	1.0571	1.0787	IL-02	25	1.3753	1.3784	1.4057	IL-04	70	1.3645	1.3637	1.3102
IL-12	30	1.0885	1.0541	1.0773	IL-02	30	1.3707	1.3738	1.4026	IL-04	75	1.3600	1.3591	1.3071
IL-12	35	1.0854	1.0510	1.0721	IL-02	35	1.3660	1.3691	1.3975	IL-04	80	1.3556	1.3545	1.3011
IL-12	40	1.0823	1.0479	1.0707	IL-02	40	1.3615	1.3645	1.3953	IL-15	20	1.1327	1.0814	1.2008
IL-12	45	1.0792	1.0449	1.0669	IL-02	45	1.3569	1.3599	1.3893	IL-15	30	1.1259	1.0750	1.2074
IL-12	50	1.0761	1.0419	1.0649	IL-02	50	1.3523	1.3553	1.3837	IL-15	40	1.1189	1.0685	1.2063
IL-12	55	1.0731	1.0388	1.0602	IL-02	55	1.3478	1.3507	1.3778	IL-01	20	1.1414	1.0674	1.0883
IL-12	60	1.0700	1.0358	1.0580	IL-02	60	1.3433	1.3461	1.3760	IL-01	30	1.1348	1.0613	1.0825
IL-12	65	1.0670	1.0328	1.0554	IL-02	65	1.3388	1.3416	1.3686	IL-01	40	1.1283	1.0554	1.0780
IL-12	70	1.0640	1.0298	1.0543	IL-02	70	1.3343	1.3370	1.3676	IL-06	20	1.2029	1.1912	1.2195
IL-12	75	1.0610	1.0268	1.0500	IL-02	75	1.3298	1.3325	1.3646	IL-06	30	1.1957	1.1839	1.2107
IL-12	80	1.0580	1.0238	1.0506	IL-02	80	1.3253	1.3280	1.3580	IL-06	40	1.1885	1.1766	1.1969
IL-13	10	1.0890	1.0638	1.0464	IL-03	10	1.1743	1.1556	1.1834	IL-09	20	1.4567	1.4482	1.4149
IL-13	20	1.0828	1.0576	1.0423	IL-03	15	1.1707	1.1521	1.1805	IL-09	30	1.4475	1.4384	1.4135
IL-13	30	1.0766	1.0515	1.0255	IL-03	20	1.1672	1.1486	1.1744	IL-09	40	1.4386	1.4288	1.4032
IL-13	40	1.0705	1.0454	1.0197	IL-03	25	1.1637	1.1450	1.1702					
IL-13	50	1.0645	1.0393	1.0146	IL-03	30	1.1602	1.1415	1.1681					
IL-13	60	1.0585	1.0333	1.0088	IL-03	35	1.1567	1.1380	1.1614					
IL-13	70	1.0525	1.0273	1.0049	IL-03	40	1.1532	1.1346	1.1597					
IL-13	80	1.0466	1.0213	1.0008	IL-03	45	1.1497	1.1311	1.1550					
IL-14	10	1.0664	1.0131	1.0735	IL-03	50	1.1463	1.1276	1.1529					
IL-14	15	1.0634	1.0101	1.0687	IL-03	55	1.1428	1.1241	1.1502					
IL-14	20	1.0604	1.0071	1.0663	IL-03	60	1.1394	1.1207	1.1459					
IL-14	25	1.0574	1.0041	1.0526	IL-03	65	1.1360	1.1173	1.1409					
IL-14	30	1.0545	1.0012	1.0507	IL-03	70	1.1326	1.1138	1.1399					
IL-14	35	1.0516	0.9982	1.0456	IL-03	75	1.1292	1.1104	1.1362					
IL-14	40	1.0486	0.9953	1.0446	IL-03	80	1.1259	1.1070	1.1339					
IL-14	45	1.0457	0.9923	1.0420	IL-04	15	1.4148	1.4156	1.3791					
IL-14	50	1.0428	0.9894	1.0399	IL-04	20	1.4101	1.4108	1.3733					
IL-14	55	1.0399	0.9865	1.0347	IL-04	25	1.4055	1.4061	1.3671					
IL-14	60	1.0370	0.9836	1.0326	IL-04	30	1.4008	1.4013	1.3642					
IL-14	65	1.0341	0.9807	1.0300	IL-04	35	1.3962	1.3965	1.3570					
IL-14	70	1.0312	0.9778	1.0289	IL-04	40	1.3916	1.3918	1.3535					
IL-14	75	1.0284	0.9749	1.0255	IL-04	45	1.3870	1.3871	1.3420					
IL-14	80	1.0255	0.9720	1.0260	IL-04	50	1.3824	1.3824	1.3364					

Table S3 Comparison of experimental heat capacities, C_p, with ML predictions.

IL	[°C]	C_p [J/K/mol]	
		Experimental	ML
IL-01	0	297.21	338.66
IL-01	10	310.38	351.15
IL-01	20	317.90	377.27
IL-01	30	321.66	367.94
IL-01	40	325.42	394.83
IL-01	50	329.19	400.14
IL-01	60	332.95	407.83
IL-01	70	340.47	414.18
IL-01	80	344.23	423.67
IL-15	0	306.72	192.08
IL-15	10	332.47	249.55
IL-15	20	341.84	314.62
IL-15	30	346.52	299.63
IL-15	40	351.21	308.18
IL-15	50	355.89	318.50
IL-15	60	362.91	327.50
IL-15	70	367.60	327.50
IL-15	80	372.28	312.31
IL-09	0	571.27	595.78
IL-09	10	585.56	632.06
IL-09	20	595.08	656.26
IL-09	30	604.60	685.69
IL-09	40	614.12	691.62
IL-09	50	623.64	686.23
IL-09	60	633.16	714.84
IL-09	70	647.44	721.04
IL-09	80	656.97	693.72
IL-06	0	362.71	404.32
IL-06	10	393.64	421.77
IL-06	20	404.88	497.03
IL-06	30	413.32	514.55
IL-06	40	418.94	530.92
IL-06	50	421.75	531.28
IL-06	60	424.57	540.48
IL-06	70	427.38	545.17
IL-06	80	430.19	608.93

Table S4 Comparison of experimental surface tensions, γ, with ML predictions.

IL	[°C]	γ [N/m]	
		Experimental	ML
IL-01	20	0.042	0.054
IL-01	30	0.040	0.053
IL-01	40	0.039	0.051
IL-15	20	0.036	0.033
IL-15	30	0.034	0.034
IL-15	40	0.033	0.033
IL-09	20	0.026	0.037
IL-09	30	0.025	0.035
IL-09	40	0.022	0.034
IL-06	20	0.035	0.042
IL-06	30	0.034	0.040
IL-06	40	0.034	0.039

Table S5 Comparison of experimental refractive indices, n_D, with ML predictions at 25 °C.

IL	RI	
	Experimental	ML
IL-01	>1.53	1.5150
IL-02	1.4363	1.4502
IL-03	1.4403	1.4487
IL-04	1.4490	1.4638
IL-05	1.4353	1.4527
IL-06	1.4565	1.4651
IL-07	1.4575	1.4597
IL-08	1.4347	1.4519
IL-09	1.4512	1.4584
IL-10	1.4485	1.451
IL-11	1.4551	1.4523
IL-12	1.5206	1.5007
IL-13	1.5214	1.5210
IL-14	1.5063	1.4934
IL-15	>1.53	1.5498

Table S6 Comparison of experimental glass transition state temperatures, T_g, with ML predictions.

IL	[°C]	
	T_g	ML
IL-01	-87	-80
IL-02	-84	-77
IL-03	-76	-77
IL-04	-68	-74
IL-05	-64	-71
IL-06	-52	-77
IL-07	-46	-73
IL-08	-76	-66
IL-09	-61	-68
IL-10	-68	-66
IL-11	-57	-71
IL-12	-68	-95
IL-13	-70	-93
IL-14	-68	-98
IL-15	-59	-53

Table S7 Comparison of experimental thermal degradation temperatures, T_d, with ML predictions.

IL	[°C]	
	T_d	ML
IL-01	251	233
IL-02	328	300
IL-03	299	290
IL-04	327	308
IL-05	267	305
IL-06	280	302
IL-07	325	294
IL-08	298	320
IL-09	333	316
IL-10	350	312
IL-11	279	304
IL-12	205	249
IL-13	211	253
IL-14	179	217
IL-15	165	209

Table S8 Comparison of experimental viscosities, η, with COSMO-RS and ML predictions.

IL	[°C]	η [mPa·s]			IL	[°C]	η [mPa·s]		
		Experimental	COSMO	ML			Experimental	COSMO	ML
IL-01	20	43.32	35.79	37.40	IL-02	30	81.26	79.62	79.76
IL-01	30	28.53	21.57	25.06	IL-02	40	54.40	52.18	52.99
IL-01	40	20.02	13.68	11.89	IL-02	50	37.38	35.65	33.03
IL-15	20	925.88	291.11	56.11	IL-02	60	28.24	25.26	22.09
IL-15	30	760.71	165.07	40.23	IL-02	70	21.75	18.48	15.44
IL-15	40	320.36	99.12	25.50	IL-02	80	16.79	13.91	10.64
IL-09	20	193.64	221.07	265.49	IL-14	10	1486.00	354.51	418.14
IL-09	30	110.00	134.77	209.23	IL-14	15	923.40	256.83	309.29
IL-09	40	67.91	86.37	92.59	IL-14	20	595.50	189.35	212.79
IL-06	20	1848.40	412.17	803.30	IL-14	25	397.50	141.89	123.46
IL-06	30	630.66	243.56	511.77	IL-14	30	274.10	107.96	102.66
IL-06	40	176.65	151.79	232.82	IL-14	35	194.90	83.31	70.06
IL-04	10	397.10	219.48	1156.00	IL-14	40	142.90	65.15	44.70
IL-04	15	266.00	167.63	789.27	IL-14	45	107.40	51.58	42.88
IL-04	20	194.10	129.92	574.45	IL-14	50	82.41	41.31	36.99
IL-04	25	142.60	102.07	487.56	IL-14	55	64.32	33.45	34.19
IL-04	30	109.60	81.22	397.65	IL-14	60	51.08	27.37	31.87
IL-04	35	83.90	65.40	356.04	IL-14	65	41.43	22.60	29.07
IL-04	40	66.02	53.24	222.20	IL-13	10	440.30	445.88	499.89
IL-04	45	52.69	43.80	156.44	IL-13	20	240.50	234.21	252.85
IL-04	50	43.45	36.38	116.74	IL-13	30	108.90	131.55	130.73
IL-04	55	35.62	30.50	97.10	IL-13	40	62.69	78.33	57.56
IL-04	60	28.72	25.78	77.58	IL-13	50	39.18	49.07	43.22
IL-04	70	20.79	18.87	48.09	IL-13	60	26.20	32.15	35.42
IL-04	80	17.92	14.20	31.31	IL-13	70	19.23	21.91	30.41
IL-03	10	884.00	724.11	371.77	IL-13	80	16.49	15.46	18.04
IL-03	15	594.90	535.43	255.50	IL-12	10	531.30	341.01	403.54
IL-03	20	391.70	402.45	188.41	IL-12	30	119.50	181.27	124.15
IL-03	25	273.00	307.15	152.35					
IL-03	30	194.10	237.77	126.30					
IL-03	35	143.20	186.52	102.36					
IL-03	40	108.40	148.15	73.18					
IL-03	45	83.57	119.05	60.82					
IL-03	50	66.17	96.70	51.48					
IL-03	55	52.99	79.36	44.05					
IL-03	60	43.30	65.75	36.52					
IL-03	65	35.64	54.97	28.19					
IL-03	70	30.27	46.34	21.45					
IL-03	80	22.40	33.72	14.77					
IL-02	10	241.15	215.24	224.08					
IL-02	20	130.85	127.39	108.52					

Table S9 Comparison of experimental CO_2 mole fractions, x_{CO2}, with COSMO-RS and ML predictions.

IL	*P* [bar]	[°C]	x_{CO2}		
			Experimental	**COSMO**	**ML**
IL-05	1	25	0.0172	0.0359	0.2297
IL-05	2	25	0.0338	0.07	0.2358
IL-05	5	25	0.0792	0.163	0.262
IL-05	10	25	0.1449	0.2923	0.3191
IL-05	1	40	0.0123	0.0253	0.1978
IL-05	2	40	0.0245	0.0497	0.2038
IL-05	5	40	0.0588	0.1182	0.2357
IL-05	10	40	0.1094	0.2186	0.2822
IL-05	1	50	0.0097	0.0204	0.1931
IL-05	2	50	0.0194	0.0403	0.1991
IL-05	5	50	0.049	0.0968	0.231
IL-05	10	50	0.0912	0.1817	0.2638
IL-03	1	25	0.0185	0.0411	0.1445
IL-03	2	25	0.0385	0.0799	0.1563
IL-03	5	25	0.0937	0.1844	0.1762
IL-03	10	25	0.1743	0.3268	0.2087
IL-03	1	40	0.0114	0.0292	0.1038
IL-03	2	40	0.0232	0.0573	0.1156
IL-03	5	40	0.0549	0.1353	0.1384
IL-03	10	40	0.1087	0.2477	0.1728
IL-03	1	50	0.0083	0.0237	0.1018
IL-03	2	50	0.016	0.0467	0.1136
IL-03	5	50	0.0421	0.1115	0.1364
IL-03	10	50	0.0858	0.2074	0.1604
IL-10	1	25	0.0328	0.0596	0.2677
IL-10	2	25	0.0646	0.1141	0.2873
IL-10	5	25	0.1486	0.2524	0.3124
IL-10	10	25	0.2598	0.4227	0.4459
IL-10	1	40	0.0259	0.0422	0.2491
IL-10	2	40	0.0508	0.0818	0.2632
IL-10	5	40	0.1183	0.1872	0.2961
IL-10	10	40	0.2111	0.3281	0.419
IL-10	1	50	0.0214	0.0341	0.2356
IL-10	2	50	0.0421	0.0665	0.2497
IL-10	5	50	0.0984	0.1548	0.2826
IL-10	10	50	0.1816	0.2776	0.3903
IL-11	1	25	0.0144	0.0394	0.2478
IL-11	2	25	0.0292	0.0766	0.2539
IL-11	5	25	0.0693	0.1772	0.2823
IL-11	10	25	0.1296	0.3151	0.3428
IL-11	1	40	0.0096	0.0278	0.2136

Table S9 Cont.

IL	*P* [bar]	[°C]	x_{CO2}		
			Experimental	**COSMO**	**ML**
IL-11	2	40	0.0188	0.0546	0.2196
IL-11	5	40	0.0455	0.1292	0.2538
IL-11	10	40	0.087	0.2372	0.3037
IL-11	1	50	0.0063	0.0225	0.2044
IL-11	2	50	0.0133	0.0443	0.2105
IL-11	5	50	0.0324	0.1061	0.2446
IL-11	10	50	0.0627	0.1979	0.2793
IL-09	1	25	0.0321	0.0555	0.1476
IL-09	2	25	0.0618	0.1066	0.1755
IL-09	5	25	0.1428	0.2382	0.2444
IL-09	10	25	0.2487	0.4042	0.3861
IL-09	1	40	0.0225	0.0393	0.1218
IL-09	2	40	0.0445	0.0764	0.1442
IL-09	5	40	0.108	0.1762	0.2181
IL-09	10	40	0.1951	0.3119	0.3492
IL-09	1	50	0.0178	0.0318	0.1173
IL-09	2	50	0.0346	0.0622	0.1397
IL-09	5	50	0.0851	0.1456	0.2137
IL-09	10	50	0.1683	0.2632	0.3311
IL-12	1	25	0.503	0.0524	0.3705
IL-13	1	25	0.494	0.0532	0.3699
IL-14	1	25	0.488	0.071	0.362

Table S10. Performance comaparison of COSMO-RS and ML predictions with experimental data

Model	R2	RMSE	MAE	AARD
		Density (ρ)		
COSMO-RS	0.99	0.03	0.02	2.22
ML	0.94	0.03	0.02	2.04
		Heat Capacity (Cp)		
ML	0.83	76.45	69.06	17.13
		Surface tension (γ)		
ML	0.51	0.008	0.007	24.11
		Refractive Index		
ML	0.92	0.01	0.009	0.67
		Glass transition temperature (T_g)		
ML	0.05	16.49	13.26	21.54
		Thermal decomposition temperature (T_d)		
ML	0.78	30.94	29	11.84
		Viscosity (η)		
COSMO-RS	0.52	273.45	112.54	32.64
ML	0.27	296.62	159.33	67.63
		x_{CO2}		
COSMO-RS	0.46	0.16	0.15	515.62
ML	0.16	0.12	0.08	112.34

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