Supporting Information

Physicochemical Properties and Electrochemical Behavior of Systematically Functionalized Aryltrifluoroborate-Based Room-Temperature Ionic Liquids

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Table S1. Fitted parameters for the densities of the [C_4mim][$ArBF_3$] RTILs

RTILs	a / g·cm^{-3}	$b \times 10^4$/ g·cm^{-3}·K^{-1}	$\|R\|$
[C_4mim][BF_4]	1.413	−7.113	> 0.9999
[C_4mim][$PhBF_3$]	1.339	−6.510	> 0.9999
[C_4mim][*o*-$OMeC_6H_4BF_3$]	1.387	−6.891	> 0.9999
[C_4mim][*m*-$OMeC_6H_4BF_3$]	1.366	−6.683	> 0.9999
[C_4mim][*p*-$OMeC_6H_4BF_3$]	1.370	−6.714	> 0.9999
[C_4mim][*o*-$FC_6H_4BF_3$]	1.405	−6.875	> 0.9999
[C_4mim][*m*-$FC_6H_4BF_3$]	1.393	−6.880	> 0.9999
[C_4mim][*p*-$FC_6H_4BF_3$]	1.400	−6.985	> 0.9999
[C_4mim][*m*-$CF_3C_6H_4BF_3$]	1.472	−7.710	> 0.9999
[C_4mim][*p*-$CF_3C_6H_4BF_3$]	1.478	−7.844	> 0.9999
[C_4mim][*m*-$CNC_6H_4BF_3$]	1.365	−6.887	> 0.9999
[C_4mim][*p*-$CNC_6H_4BF_3$]	1.366	−6.855	> 0.9999

Table S2. Fitted parameters for the VTF equations of viscosity and equivalent conductivity for the $[C_4mim][ArBF_3]$ RTILs

RTILs	derived from viscosity				derived from equivalent conductivity			
	T_0 / K	k_η / K	ln A_η	$\|R\|$	T_0 / K	k_Λ / K	ln A_Λ	$\|R\|$
$[C_4mim][BF_4]$	171	8.71×10^2	5.08	0.9999	148	2.70×10^3	13.2	0.9999
$[C_4mim][PhBF_3]$	168	9.61×10^2	5.48	0.9999	152	1.04×10^3	9.21	0.9999
$[C_4mim][o\text{-}OMeC_6H_4BF_3]$	205	9.54×10^2	5.56	0.9999	176	1.44×10^3	11.3	0.9999
$[C_4mim][m\text{-}OMeC_6H_4BF_3]$	179	9.82×10^2	5.53	0.9999	160	1.25×10^3	10.4	0.9999
$[C_4mim][p\text{-}OMeC_6H_4BF_3]$	187	9.53×10^2	5.52	0.9999	166	1.27×10^3	10.6	0.9999
$[C_4mim][o\text{-}FC_6H_4BF_3]$	180	8.83×10^2	5.19	0.9999	136	1.47×10^3	10.9	0.9999
$[C_4mim][m\text{-}FC_6H_4BF_3]$	187	7.29×10^2	4.80	0.9999	158	1.04×10^3	9.62	0.9999
$[C_4mim][p\text{-}FC_6H_4BF_3]$	180	8.66×10^2	5.35	0.9999	127	1.59×10^3	11.2	0.9999
$[C_4mim][m\text{-}CF_3C_6H_4BF_3]$	181	8.50×10^2	5.14	0.9999	137	1.40×10^3	10.5	0.9999
$[C_4mim][p\text{-}CF_3C_6H_4BF_3]$	182	8.98×10^2	5.46	0.9999	137	1.43×10^3	10.5	0.9999
$[C_4mim][m\text{-}CNC_6H_4BF_3]$	192	8.81×10^2	5.45	0.9999	171	1.12×10^3	10.1	0.9999
$[C_4mim][p\text{-}CNC_6H_4BF_3]$	195	8.72×10^2	5.38	0.9999	177	1.13×10^3	10.3	0.9999

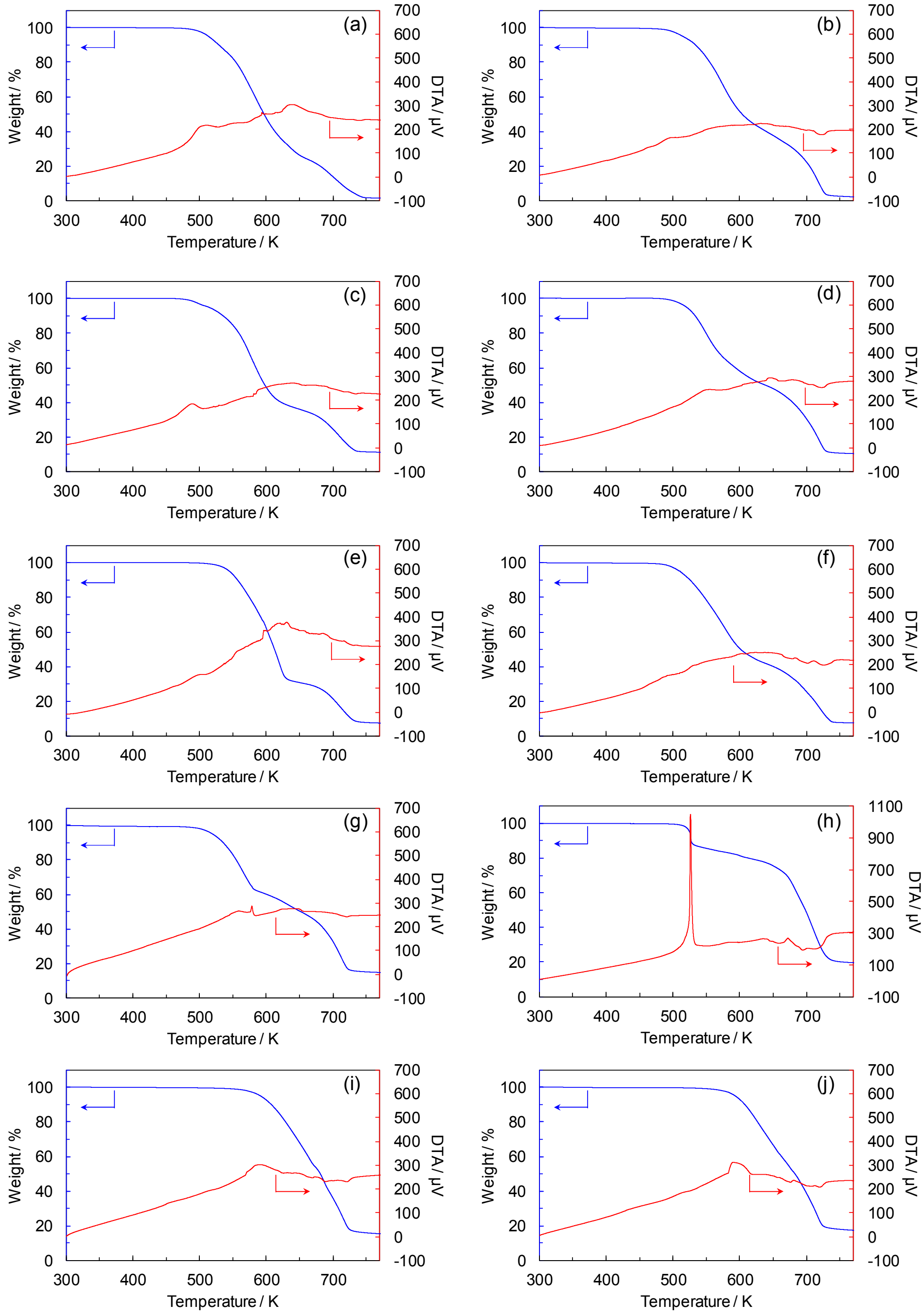


Figure S1. TG-DTA measurement results of (a) [C_4mim][*o*-OMe$C_6H_4BF_3$], (b) [C_4mim][*m*-OMe$C_6H_4BF_3$], (c) [C_4mim][*p*-OMe$C_6H_4BF_3$], (d) [C_4mim][*o*-F$C_6H_4BF_3$], (e) [C_4mim][*m*-F$C_6H_4BF_3$], (f) [C_4mim][*p*-F$C_6H_4BF_3$], (g) [C_4mim][*m*-$CF_3C_6H_4BF_3$], (h) [C_4mim][*p*-$CF_3C_6H_4BF_3$], (i) [C_4mim][*m*-CN$C_6H_4BF_3$], and (j) [C_4mim][*p*-CN$C_6H_4BF_3$]. The measurements were conducted at 5 $K \cdot min^{-1}$.

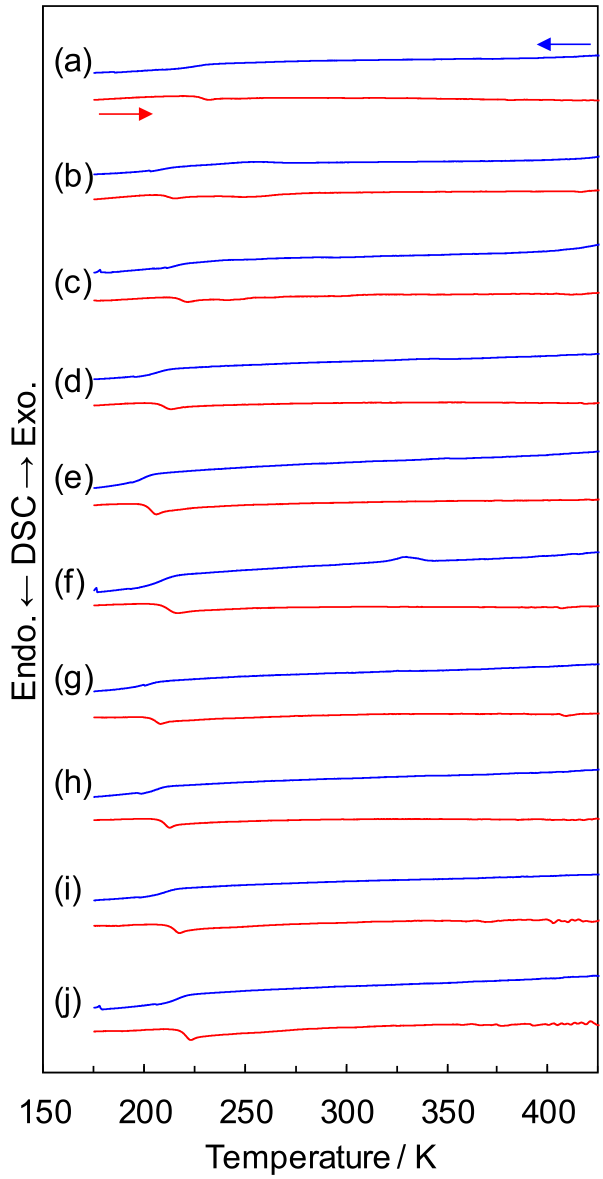


Figure S2. DSC curves of (a) [C_4mim][*o*-OMe$C_6H_4BF_3$], (b) [C_4mim][*m*-OMe$C_6H_4BF_3$], (c) [C_4mim][*p*-OMe$C_6H_4BF_3$], (d) [C_4mim][*o*-F$C_6H_4BF_3$], (e) [C_4mim][*m*-F$C_6H_4BF_3$], (f) [C_4mim][*p*-F$C_6H_4BF_3$], (g) [C_4mim][*m*-$CF_3C_6H_4BF_3$], (h) [C_4mim][*p*-$CF_3C_6H_4BF_3$], (i) [C_4mim][*m*-CN$C_6H_4BF_3$], and (j) [C_4mim][*p*-CN$C_6H_4BF_3$]. The measurements were conducted at 5 $K \cdot min^{-1}$.

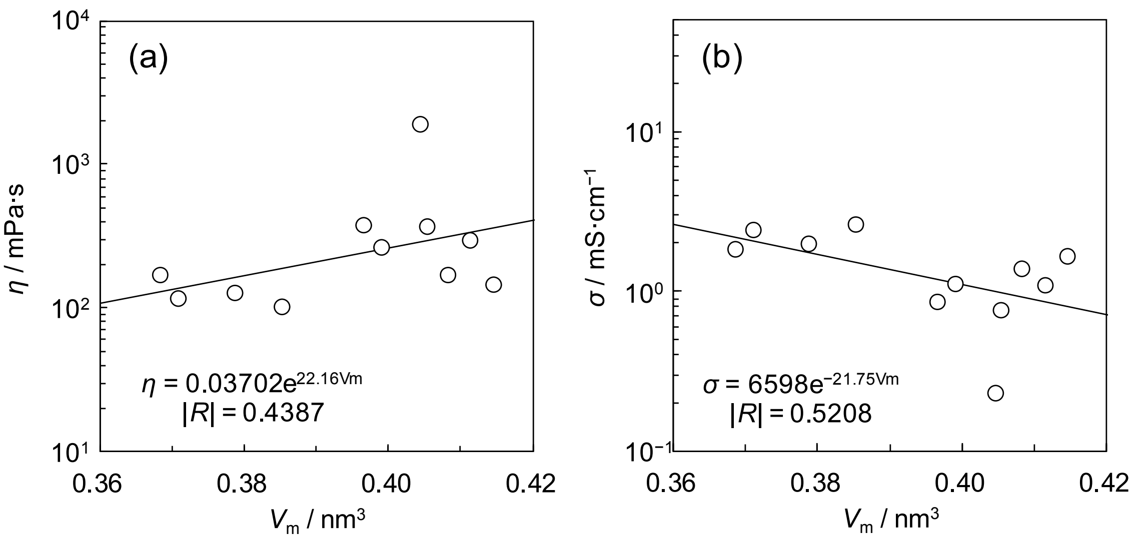


Figure S3. Correlation between the (a) ionic pair volume and viscosity at 298 K and the (b) ionic pair volume and ionic conductivity at 303 K. V_m is the sum of V_a and V_c. In this study, V_c, as the volume of $[C_4mim]^+$ is 0.207 nm^3, which is calculated by the Gaussian 09 program at the B3LYP/6-31G+(d) level. The original data are given in Table 1.

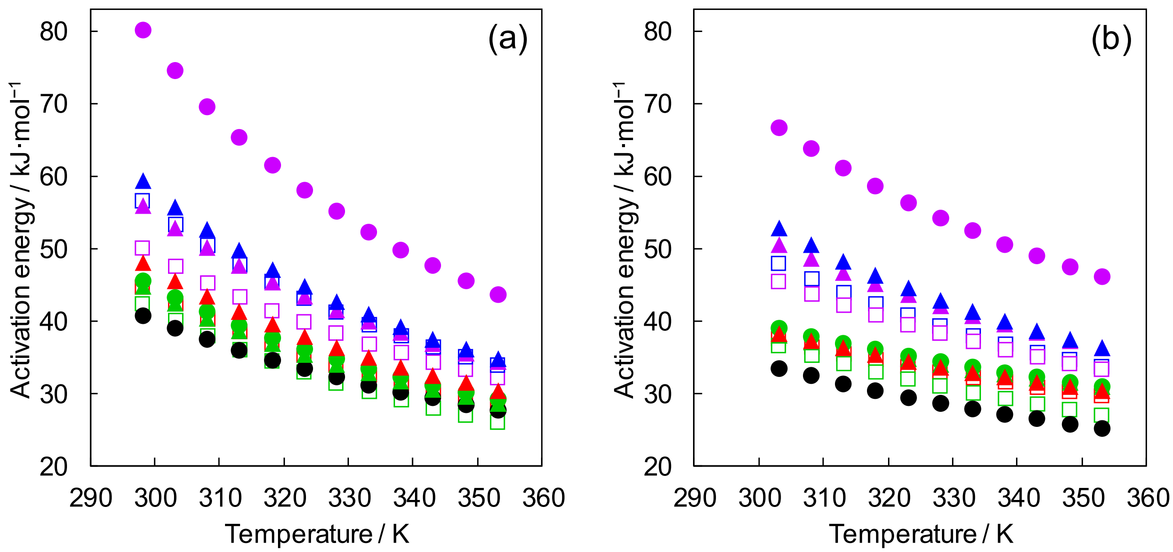
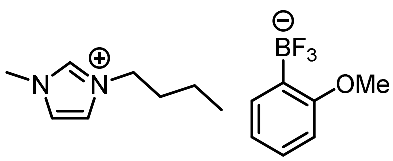


Figure S4. Temperature dependences of the activation energies derived from (a) the viscosities and (b) the ionic conductivities for (●) [C_4mim][*o*-OMe$C_6H_4BF_3$], (□) [C_4mim][*m*-OMe$C_6H_4BF_3$], (▲) [C_4mim][*p*-OMe$C_6H_4BF_3$], (●) [C_4mim][*o*-F$C_6H_4BF_3$], (□) [C_4mim][*m*-F$C_6H_4BF_3$], (▲) [C_4mim][*p*-F$C_6H_4BF_3$], (□) [C_4mim][*m*-$CF_3C_6H_4BF_3$], (▲) [C_4mim][*p*-$CF_3C_6H_4BF_3$], (□) [C_4mim][*m*-CN$C_6H_4BF_3$], (▲) [C_4mim][*p*-CN$C_6H_4BF_3$], and (●) [C_4mim][PhBF_3].

Characterization of aryltrifluoroborate-based room-temperature ionic liquids

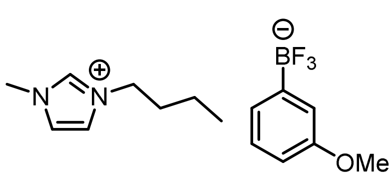
^{1}H, ^{13}C, ^{19}F, and ^{11}B NMR spectra were recorded on a JEOL JNM-ECS400 spectrometer operating at 400, 100, 376, and 128 MHz, respectively. $CDCl_3$ was used as the solvent for the samples in this study. ^{1}H and ^{13}C NMR spectra were referenced to the residual solvent signal as the internal standard: $CDCl_3$ $\delta = 7.26$ ppm (^{1}H) and $\delta = 77.0$ ppm (^{13}C). Chemical shift values in ^{19}F and ^{11}B NMR were reported relative to the external references of $C_6H_5CF_3$ $\delta = -63.7$ ppm (^{19}F) and $BF_3{\cdot}OEt_2$ $\delta = 0.0$ ppm (^{11}B). The signal of ^{13}C bound to the ^{11}B atom was too broad due to the quadrupolar relaxation mechanism of the ^{11}B nucleus.[1] High-resolution mass spectrometry (HRMS) was operated on a JEOL JMS-700 MStation mass spectrometer using fast atom bombardment (FAB) ionization. HRMS and elemental analysis (C, H, and N) were performed at the Analytical Instrumentation Facility, Graduate School of Engineering, Osaka University.

1-butyl-3-methylimidazolium (ortho-methoxyphenyl)trifluoroborate ([C$_4$mim][*o*-OMeC$_6$H$_4$BF$_3$])



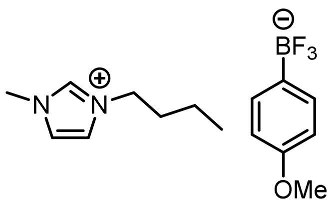
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.899 (t, 3H, $^{3}J_{HH} = 7.4$ Hz), 1.27 (m, 2H, $^{3}J_{HH} =$ 7.7 Hz), 1.72 (m, 2H, $^{3}J_{HH} = 7.8$ Hz), 3.75 (s, 3H), 3.84 (s, 3H), 4.02 (t, 2H, $^{3}J_{HH} = 7.6$ Hz), 6.77 (d, 1H, $^{3}J_{HH} = 8.0$ Hz), 6.84 (t, 1H, $^{3}J_{HH} = 7.2$ Hz), 7.11 (d, 1H, $^{3}J_{HH} = 1.6$ Hz), 7.15 (dt, 1H, $^{3}J_{HH}$ = 1.6 Hz, 7.7 Hz), 7.20 (d, 1H, $^{3}J_{HH} = 1.6$ Hz), 7.54 (d, 1H, $^{1}J_{HH} = 6.8$ Hz), 9.09 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.3 (s), 19.3 (s), 31.9 (s), 36.3 (s), 49.8 (s), 55.1 (s), 109.9 (s), 113.8 (s), 120.6 (s), 121.9 (s), 123.5 (s), 129.4 (s), 136.8 (s), 159.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −139.2 (s, 3F, BF_3). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.49 (s, BF$_3$). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{37}N_4OBF_3^+$ 453.3007 [M + [C$_4$mim]]$^+$; found 453.3017. Elemental analysis calcd. for $C_{15}H_{22}N_2OBF_3$: C, 57.35; H, 7.06; N, 8.92; found: C, 56.61; H, 7.27; N, 8.75.

1-butyl-3-methylimidazolium (meta-methoxyphenyl)trifluoroborate ([C$_4$mim][*m*-OMeC$_6$H$_4$BF$_3$])



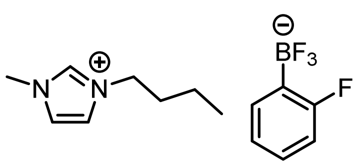
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.910 (t, 3H, $^{3}J_{HH} = 7.4$ Hz), 1.27 (m, 2H, $^{3}J_{HH} =$ 7.7 Hz), 1.71 (m, 2H, $^{3}J_{HH} = 7.7$ Hz), 3.77 (s, 3H), 3.78 (s, 3H), 3.97 (t, 2H, $^{3}J_{HH} = 7.4$ Hz), 6.68–6.72 (m, 1H), 7.07 (t, 1H, $^{3}J_{HH} = 1.8$ Hz), 7.12–7.15 (m, 4H), 8.77 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.3 (s), 19.3 (s), 31.9 (s), 36.2 (s), 49.7 (s), 55.1 (s), 113.8 (s), 120.6 (s), 122.0 (s), 123.6 (s), 129.4 (s), 136.4 (s), 159.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −141.5 (s, 3F, B*F*$_3$). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.47 (s, *B*F_3). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{37}N_4OBF_3^+$ 453.3007 [M + [C_4mim]]$^+$; found 453.3012. Elemental analysis calcd. for $C_{15}H_{22}N_2OBF_3$: C, 57.35; H, 7.06; N, 8.92; found: C, 56.59; H, 7.17; N, 8.78.

1-butyl-3-methylimidazolium (para-methoxyphenyl)trifluoroborate ([C_4mim][*p*-OMe$C_6H_4BF_3$])



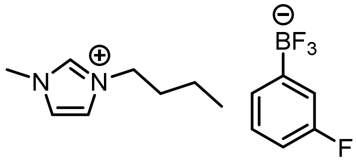
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.911 (t, 3H, $^3J_{HH}$ = 7.2 Hz), 1.27 (m, 2H, $^3J_{HH}$ = 7.7 Hz), 1.71 (m, 2H, $^3J_{HH}$ = 7.7 Hz), 3.76 (s, 3H), 3.79 (s, 3H), 3.98 (t, 2H, $^3J_{HH}$ = 7.4 Hz), 6.78 (d, 2H, $^3J_{HH}$ = 8.4 Hz), 7.08 (t, 1H, $^3J_{HH}$ = 1.8 Hz), 7.13 (t, 1H, $^3J_{HH}$ = 1.8 Hz), 7.49 (d, 2H, $^3J_{HH}$ = 8.4 Hz), 8.85 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.3 (s), 19.3 (s), 31.9 (s), 36.2 (s), 49.7 (s), 55.0 (s), 113.8 (s), 122.1 (s), 123.6 (s), 129.4 (s), 136.5 (s), 159.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −140.6 (s, 3F, B*F*$_3$). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.71 (s, *B*F_3). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{37}N_4OBF_3^+$ 453.3007 [M + [C_4mim]]$^+$; found 453.3013. Elemental analysis calcd. for $C_{15}H_{22}N_2OBF_3$: C, 57.35; H, 7.06; N, 8.92; found: C, 56.47; H, 7.12; N, 8.87.

1-butyl-3-methylimidazolium (ortho-fluorophenyl)trifluoroborate ([C_4mim][*o*-F$C_6H_4BF_3$])



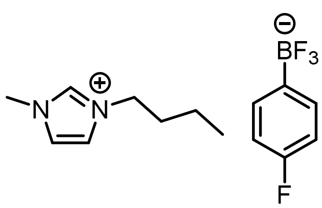
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.854 (t, 3H, $^3J_{HH}$ = 7.3 Hz), 1.22 (m, 2H, $^3J_{HH}$ = 7.6 Hz), 1.69 (m, 2H, $^3J_{HH}$ = 7.5 Hz), 3.79 (s, 3H), 4.00 (t, 2H, $^3J_{HH}$ = 7.6 Hz), 6.80 (t, 1H, $^3J_{HH}$ = 8.7 Hz), 6.97 (t, 1H, $^3J_{HH}$ = 7.1 Hz), 7.08–7.14 (m, 1H), 7.18 (t, 1H, $^3J_{HH}$ = 1.8 Hz), 7.23 (t, 1H, $^3J_{HH}$ = 1.6 Hz), 7.51 (t, 1H, $^3J_{HH}$ = 6.9 Hz), 8.83 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.2 (s), 31.8 (s), 36.0 (s), 49.5 (s), 114.0 (d, $^2J_{CF}$ = 24.8 Hz), 121.9 (s), 123.0 (s), 123.5 (s), 128.0 (d, $^3J_{CF}$ = 7.6 Hz), 134.1 (d, $^3J_{CF}$ = 12.4 Hz), 136.4 (s), 166.0 (d, $^1J_{CF}$ = 237.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): σ −139.4 (s, 3F, B*F*$_3$), −109.7 (s, 1F, *o*-*F*C_6H_4). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.02 (s, *B*F_3). HRMS (FAB), *m*/*z*: calcd. for $C_{22}H_{34}N_4BF_4^+$ 441.2807 [M + [C_4mim]]$^+$; found 441.2819. Elemental analysis calcd. for $C_{14}H_{19}N_2BF_4$: C, 55.66; H, 6.34; N, 9.27; found: C, 55.21; H, 6.43; N, 9.15.

1-butyl-3-methylimidazolium (meta-fluorophenyl)trifluoroborate ([C_4mim][*m*-$FC_6H_4BF_3$])



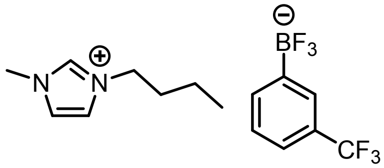
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.926 (t, 3H, $^3J_{HH}$ = 7.6 Hz), 1.30 (m, 2H, $^3J_{HH}$ = 7.7 Hz), 1.76 (m, 2H, $^3J_{HH}$ = 7.6 Hz), 3.85 (s, 3H), 4.04 (t, 2H, $^3J_{HH}$ = 7.4 Hz), 6.79–6.84 (m, 1H), 7.10 (t, 1H, $^3J_{HH}$ = 2.0 Hz), 7.14 (t, 1H, $^3J_{HH}$ = 1.8 Hz), 7.16–7.21 (m, 2H), 7.33 (d, 1H, $^3J_{HH}$ = 6.8 Hz), 8.95 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.2 (s), 31.7 (s), 36.0 (s), 49.5 (s), 112.6 (d, $^2J_{CF}$ = 21.0 Hz), 117.3 (d, $^2J_{CF}$ = 17.1 Hz), 121.9 (s), 123.4 (s), 126.8 (s), 128.6 (d, $^3J_{CF}$ = 6.7 Hz), 136.1 (s), 162.6 (d, $^1J_{CF}$ = 242.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): σ −142.0 (s, 3F, B*F₃*), −116.9 (s, 1F, *m*-*F*C_6H_4). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.31 (s, *B*F_3). HRMS (FAB), *m*/*z*: calcd. for $C_{22}H_{34}N_4BF_4^+$ 441.2807 [M + [C_4mim]]$^+$; found 441.2815. Elemental analysis calcd. for $C_{14}H_{19}N_2BF_4$: C, 55.66; H, 6.34; N, 9.27; found: C, 55.04; H, 6.39; N, 9.15.

1-butyl-3-methylimidazolium (para-fluorophenyl)trifluoroborate ([C_4mim][*p*-$FC_6H_4BF_3$])



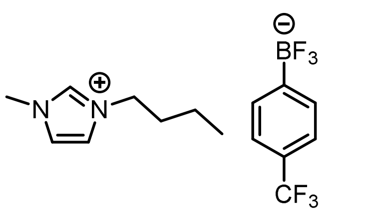
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.849 (t, 3H, $^3J_{HH}$ = 7.2 Hz), 1.19 (m, 2H, $^3J_{HH}$ = 7.7 Hz), 1.63 (m, 2H, $^3J_{HH}$ = 7.6 Hz), 3.69 (s, 3H), 3.89 (t, 2H, $^3J_{HH}$ = 7.6 Hz), 6.85 (t, 2H, $^3J_{HH}$ = 9.2 Hz), 7.08 (t, 1H, $^3J_{HH}$ = 1.8 Hz), 7.12 (t, 1H, $^3J_{HH}$ = 2.0 Hz), 7.46 (t, 2H, $^3J_{HH}$ = 7.2 Hz), 8.62 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.2 (s), 31.7 (s), 35.9 (s), 49.4 (s), 113.5 (d, $^2J_{CF}$ = 19.2 Hz), 121.9 (s), 123.4 (s), 132.8 (d, $^3J_{CF}$ = 5.7 Hz), 136.1 (s), 161.9 (d, $^1J_{CF}$ = 242.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): σ −141.1 (s, 3F, B*F₃*), −118.5 (s, 1F, *p*-*F*C_6H_4). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.68 (s, *B*F_3). HRMS (FAB), *m*/*z*: calcd. for $C_{22}H_{34}N_4BF_4^+$ 441.2807 [M + [C_4mim]]$^+$; found 441.2811. Elemental analysis calcd. for $C_{14}H_{19}N_2BF_4$: C, 55.66; H, 6.34; N, 9.27; found: C, 54.99; H, 6.36; N, 9.13.

1-butyl-3-methylimidazolium (meta-trifluoromethylphenyl)trifluoroborate ($[C_4mim][m\text{-}CF_3C_6H_4BF_3]$)



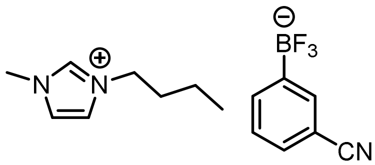
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.874 (t, 3H, $^3J_{HH}$ = 7.6 Hz), 1.24 (m, 2H, $^3J_{HH}$ = 7.7 Hz), 1.70 (m, 2H, $^3J_{HH}$ = 7.5 Hz), 3.80 (s, 3H), 3.99 (t, 2H, $^3J_{HH}$ = 7.6 Hz), 7.11 (t, 1H, $^3J_{HH}$ = 1.6 Hz), 7.15 (t, 1H, $^3J_{HH}$ = 1.8 Hz), 7.31 (t, 1H, $^3J_{HH}$ = 7.4 Hz), 7.39 (d, 1H, $^3J_{HH}$ = 7.6 Hz), 7.72–7.75 (m, 2H), 8.84 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.2 (s), 31.7 (s), 36.1 (s), 49.7 (s), 121.8 (s), 122.7 (s), 123.3 (s), 125.0 (q, $^1J_{CF}$ = 270.8 Hz, CF_3), 127.2 (s), 127.7 (s), 128.7 (q, $^2J_{CF}$ = 30.5 Hz), 134.9 (s), 136.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −142.2 (s, 3F, BF_3), −63.1 (s, 3F, CF_3). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.31 (s, BF_3). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{34}N_4BF_6^+$ 491.2775 [M + $[C_4mim]]^+$; found 491.2782. Elemental analysis calcd. for $C_{15}H_{19}N_2BF_6$: C, 51.16; H, 5.44; N, 7.96; found: C, 50.40; H, 5.62; N, 7.88.

1-butyl-3-methylimidazolium (para-trifluoromethylphenyl)trifluoroborate ($[C_4mim][p\text{-}CF_3C_6H_4BF_3]$)



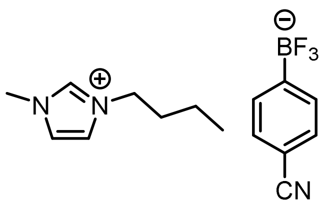
Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$): σ 0.871 (t, 3H, $^3J_{HH}$ = 7.4 Hz), 1.18–1.28 (m, 2H), 1.64–1.73 (m, 2H), 3.79 (m, 3H), 3.95–3.99 (m, 2H), 7.09 (d, 1H, $^3J_{HH}$ = 1.2 Hz), 7.13 (d, 1H, $^3J_{HH}$ = 1.6 Hz), 7.44 (d, 2H, $^3J_{HH}$ = 8.0 Hz), 7.64 (d, 2H, $^3J_{HH}$ = 8.0 Hz), 8.82 (d, 1H, $^3J_{HH}$ = 6.0 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.2 (s), 31.7 (s), 36.1 (s), 49.6 (s), 121.8 (s), 123.3 (s), 123.5 (s), 124.8 (q, $^1J_{CF}$ = 270.3 Hz), 128.0 (q, $^2J_{CF}$ = 31.5 Hz), 131.5 (s), 136.3 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −142.3 (s, 3F, BF_3), −63.1 (s, 3F, CF_3). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.44 (s, BF_3). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{34}N_4BF_6^+$ 491.2775 [M + $[C_4mim]]^+$; found 491.2783. Elemental analysis calcd. for $C_{15}H_{19}N_2BF_6$: C, 51.16; H, 5.44; N, 7.96; found: C, 50.58; H, 5.53; N, 7.93.

1-butyl-3-methylimidazolium (meta-cyanophenyl)trifluoroborate ($[C_4mim][m\text{-}CNC_6H_4BF_3]$)



Colorless liquid. ^1H NMR (400 MHz, $CDCl_3$): σ 0.889 (t, 3H, $^3J_{HH}$ = 7.3 Hz), 1.27 (m, 2H, $^3J_{HH}$ = 7.6 Hz), 1.74 (m, 2H, $^3J_{HH}$ = 7.6 Hz), 3.86 (s, 3H), 4.06 (t, 2H, $^3J_{HH}$ = 7.3 Hz), 7.21 (m, 1H), 7.24 (m, 1H), 7.30 (t, 1H, $^3J_{HH}$ = 7.8 Hz), 7.42 (d, 1H, $^3J_{HH}$ = 7.3 Hz), 7.77−7.79 (m, 2H), 8.91 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.3 (s), 31.8 (s), 36.2 (s), 49.8 (s), 110.3 (s), 120.4 (s), 121.9 (s), 123.4 (s), 127.6 (s), 129.7 (s), 135.1 (s), 136.0 (s), 136.4 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −142.5 (s, 3F, BF_3). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.27 (s, BF_3). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{34}N_5BF_3^+$ 448.2854 [M + $[C_4mim]]^+$; found 448.2843. Elemental analysis calcd. for $C_{15}H_{19}N_3BF_3$: C, 58.28; H, 6.20; N, 13.59; found: C, 57.53; H, 6.42; N, 13.49.

1-butyl-3-methylimidazolium (para-cyanolphenyl)trifluoroborate ($[C_4mim][p\text{-}CNC_6H_4BF_3]$)



Colorless liquid. ^1H NMR (400 MHz, $CDCl_3$): σ 0.890 (t, 3H, $^3J_{HH}$ = 7.3 Hz), 1.27 (m, 2H, $^3J_{HH}$ = 7.1 Hz), 1.74 (m, 2H, $^3J_{HH}$ = 7.3 Hz), 3.85 (s, 3H), 4.03−4.09 (m, 2H), 7.18 (s, 1H), 7.21 (s, 1H), 7.48 (d, 2H, $^3J_{HH}$ = 7.8 Hz), 7.64 (d, 2H, $^3J_{HH}$ = 7.8 Hz), 8.92 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): σ 13.2 (s), 19.2 (s), 31.7 (s), 36.1 (s), 49.6 (s), 109.1 (s), 120.1 (s), 122.0 (s), 123.4 (s), 130.5 (s), 131.9 (s), 136.2 (s). ^{19}F NMR (376 MHz, $CDCl_3$): σ −142.6 (s, 3F, BF_3). ^{11}B NMR (128 MHz, $CDCl_3$): σ 3.25 (s, BF_3). HRMS (FAB), *m*/*z*: calcd. for $C_{23}H_{34}N_5BF_3^+$ 448.2854 [M + $[C_4mim]]^+$; found 448.2855. Elemental analysis calcd. for $C_{15}H_{19}N_3BF_3$: C, 58.28; H, 6.20; N, 13.59; found: C, 57.40; H, 6.38; N, 13.49.

REFERENCE

(1) Oliveira, R. A.; Silva, R. O.; Molander, G. A.; Menezes, P. H. ^1H, ^{13}C, ^{19}F and ^{11}B NMR Spectral Reference Data of Some Potassium Organotrifluoroborates. *Magn. Reson. Chem.* **2009**, *47*, 873–878.