Supporting Information for:

Synthesis and Characterization of Imidazolium Poly(azolyl)borate Ionic Liquids and Their Potential Application in SO_2 Absorption

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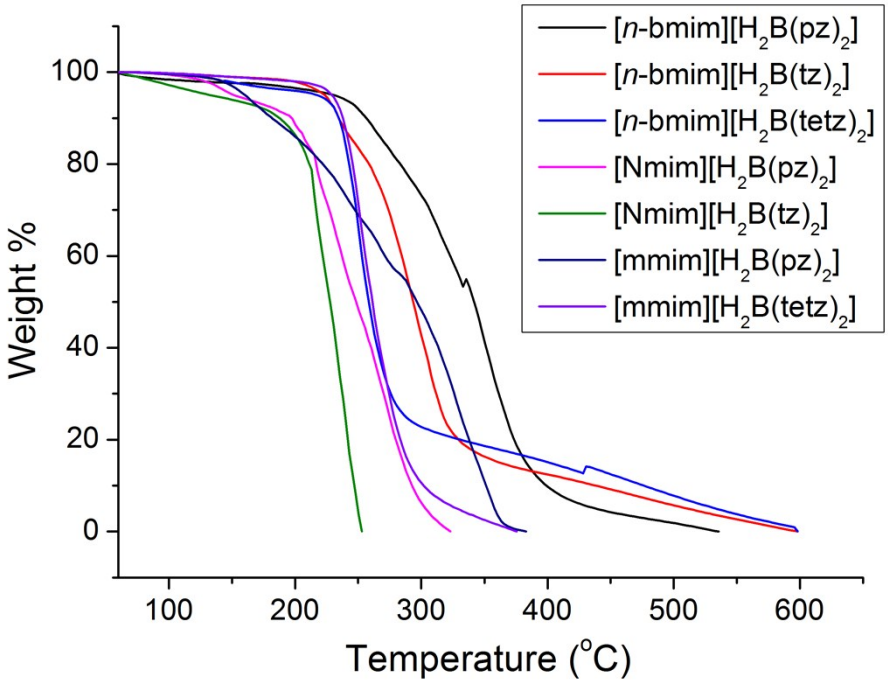
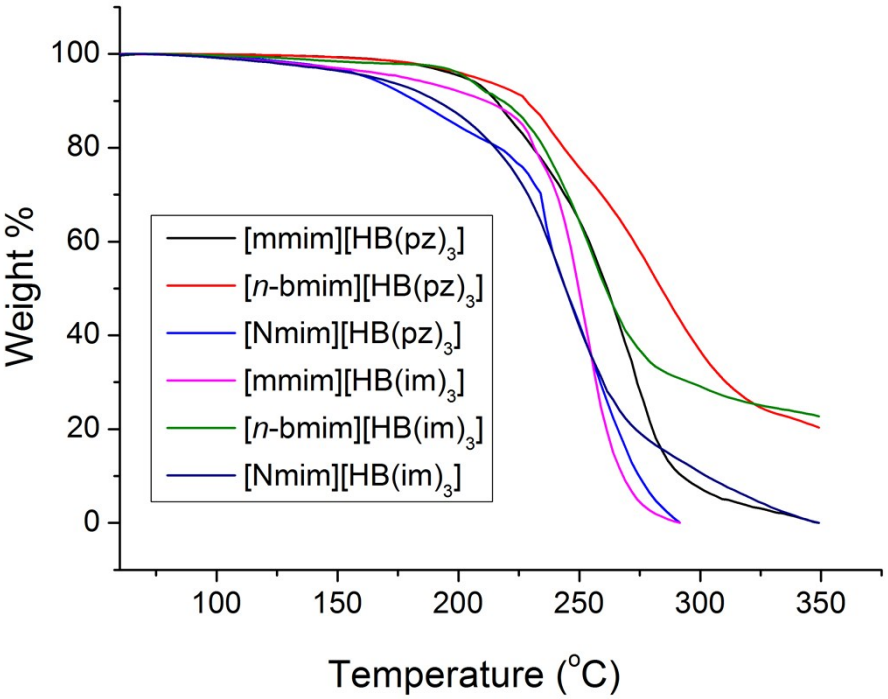


SFig 1. Thermogravimetric curves for imidazolium dihydrobis(azolyl)borates.



SFig 2. Thermogravimetric curves for imidazolium hydrotris(azolyl)borates.

3. X-Ray diffraction data for compound 9.

STable 1. Crystal data and structure refinement for 1.

Identification code	1
Empirical formula	C14 H19 B N8
Formula weight	310.18
Temperature	296 K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *p*
Unit cell dimensions	a = 8.7240 (14) Å alpha = 78.447 (2) deg. b = 8.8303 (15) Å beta = 74.927 (2) deg. c = 12.503 (2) Å gamma = 60.694 (2) deg.
Volume	807.9 (2) Å^3
Z, Calculated density	2, 1.275 Mg/m^3
Absorption coefficient	0.08 mm^-1
F(000)	328
Crystal size	0.27 x 0.19 x 0.14 mm
Theta range for data collection	2.6 to 27.6 deg.
Limiting indices	-11 <= h <= 11, -11 <= k <= 11, -16 <= l <= 16
Reflections collected / unique	3734 / 3309 [R_{int} = 0.012]
Completeness to theta = 27.6	99.0 %
Absorption correction	multi-scan
Max. and min. transmission	0.988 and 0.978
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3734 / 0 / 214
Goodness-of-fit on F^2	1.06
Final R indices [I>2sigma(I)]	R1 = 0.0621, wR2 = 0.1977
R indices (all data)	R1 = 0.0672, wR2 = 0.2037
Largest diff. peak and hole	0.65 and −0.66 e. Å^-3

STable 2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}
N3	0.39266(19)	0.19510(18)	0.28130(12)	0.0329(3)
N5	0.71929(19)	0.05440(19)	0.28742(13)	0.0340(3)
N7	0.5774(2)	-0.13098(19)	0.28216(13)	0.0342(3)
N4	0.3488(2)	0.3633(2)	0.23891(15)	0.0442(4)
N8	0.4764(3)	-0.1794(2)	0.24305(16)	0.0491(5)
N6	0.6939(3)	0.1392(3)	0.37462(16)	0.0502(5)
C11	0.8976(2)	-0.0388(2)	0.24655(17)	0.0369(4)
B1	0.5790(3)	0.0452(3)	0.23874(16)	0.0323(4)
C8	0.2598(2)	0.1883(3)	0.36277(16)	0.0405(4)
C14	0.6575(3)	-0.2500(3)	0.36169(17)	0.0423(4)
C12	0.4970(3)	-0.3299(3)	0.3012(2)	0.0508(5)
C6	0.1855(3)	0.4588(3)	0.2969(2)	0.0491(5)
C9	0.8602(3)	0.0993(3)	0.39166(18)	0.0473(5)
C10	0.9811(3)	-0.0109(3)	0.3099(2)	0.0528(6)
C7	0.1236(3)	0.3557(3)	0.3751(2)	0.00489(5)
C13	0.6094	-0.3810(3)	0.3763(2)	0.0516(5)
N1	0.8249(2)	0.2847(2)	0.00769(14)	0.0451(4)
N2	1.0619(3)	0.2628(2)	0.04766(15)	0.0466(4)
C5	0.9999(3)	0.2294(3)	-0.02619(17)	0.0441(5)
C4	0.7074(3)	0.2755(4)	-0.0528(2)	0.0593(6)
C2	0.9200(4)	0.3426(3)	0.13206(19)	0.576(6)
C1	1.2495(4)	0.2131(4)	0.0441(2)	0.0650(7)

STable 3. Bond lengths [Å] and angles [deg] for 1.

N3—C8	1.347 (2)	C8—C7	1.378 (3)
N3—N4	1.367 (2)	C14—C13	1.377 (3)
N3—B1	1.550 (2)	C12—C13	1.387 (3)
N5—N6	1.356 (2)	C6—C7	1.388 (3)
N5—C11	1.364 (2)	C9—C10	1.392 (3)
N5—B1	1.543 (2)	N1—C5	1.329 (3)
N7—C14	1.344 (2)	N1—C3	1.376 (3)
N7—N8	1.369 (2)	N1—C4	1.462 (3)
N7—B1	1.548 (2)	N2—C5	1.325 (3)

N4—C6	1.340 (3)	N2—C2	1.381 (3)
N8—C12	1.332 (3)	N2—C1	1.463 (3)
N6—C9	1.380 (3)	C3—C2	1.346 (4)
C11—C10	1.332 (3)		

C8—N3—N4	110.65 (15)	N7—C14—C13	108.24 (19)
C8—N3—B1	129.06 (15)	N8—C12—C13	112.07 (19)
N4—N3—B1	120.20 (14)	N4—C6—C7	111.85 (18)
N6—N5—C11	110.41 (15)	N6—C9—C10	104.63 (18)
N6—N5—B1	128.93 (15)	C11—C10—C9	111.60 (19)
C11—N5—B1	120.56 (15)	C8—C7—C6	104.43 (18)
C14—N7—N8	110.52 (16)	C14—C13—C12	104.28 (19)
C14—N7—B1	129.08 (15)	C5—N1—C3	108.67 (19)
N8—N7—B1	120.30 (15)	C5—N1—C4	125.47 (19)
C6—N4—N3	104.86 (16)	C3—N1—C4	125.8 (2)
C12—N8—N7	104.89 (17)	C5—N2—C2	108.0 (2)
N5—N6—C9	107.79 (18)	C5—N2—C1	125.9 (2)
C10—C11—N5	105.57 (17)	C2—N2—C1	126.0 (2)
N5—B1—N7	108.46 (14)	N2—C5—N1	108.98 (19)
N5—B1—N3	108.22 (14)	C2—C3—N1	106.7 (2)
N7—B1—N3	108.78 (14)	C3—C2—N2	107.6 (2)
N3—C8—C7	108.22 (18)		

Symmetry transformations used to generate equivalent atoms.

STable 4. Anisotropic displacement parameters (Å^2) for 1.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N3	0.0304 (7)	0.0299 (7)	0.0382 (8)	−0.0136 (6)	−0.0085 (6)	−0.0008 (6)
N5	0.0290 (7)	0.0334 (7)	0.0401 (8)	−0.0144 (6)	−0.0049 (6)	−0.0066 (6)
N7	0.0327 (7)	0.0318 (7)	0.0405 (8)	−0.0141 (6)	−0.0099 (6)	−0.0063 (6)
N4	0.0405 (9)	0.0312 (8)	0.0566 (10)	−0.0156 (7)	−0.0082 (7)	0.0011 (7)
N8	0.0523 (10)	0.0470 (10)	0.0625 (11)	−0.0277 (8)	−0.0224 (9)	−0.0069 (8)
N6	0.0564 (11)	0.0509 (10)	0.0488 (10)	−0.0280 (9)	−0.0108 (8)	−0.0055 (8)
C11	0.0221 (7)	0.0362 (9)	0.0516 (10)	−0.0097 (7)	−0.0034 (7)	−0.0168 (8)
B1	0.0309 (9)	0.0329 (9)	0.0337 (9)	−0.0147 (7)	−0.0063 (7)	−0.0041 (7)
C8	0.0356 (9)	0.0402 (10)	0.0445 (10)	−0.0188 (8)	−0.0037 (7)	−0.0026 (8)

C14	0.0424 (10)	0.0362 (9)	0.0475 (10)	−0.0159 (8)	−0.0145 (8)	0.0000 (8)
C12	0.0490 (11)	0.0420 (11)	0.0694 (14)	−0.0266 (9)	−0.0038 (10)	−0.0158 (10)
C6	0.0399 (10)	0.0326 (9)	0.0692 (14)	−0.0101 (8)	−0.0123 (9)	−0.0085 (9)
C9	0.0537 (12)	0.0501 (11)	0.0516 (11)	−0.0292 (10)	−0.0229 (9)	−0.0008 (9)
C10	0.0365 (10)	0.0486 (12)	0.0773 (15)	−0.0185 (9)	−0.0200 (10)	−0.0049 (10)
C7	0.0330 (9)	0.0478 (11)	0.0599 (13)	−0.0143 (9)	−0.0004 (8)	−0.0150 (10)
C13	0.0524 (12)	0.0337 (10)	0.0642 (14)	−0.0193 (9)	−0.0085 (10)	0.0003 (9)
N1	0.0429 (9)	0.0420 (9)	0.0419 (9)	−0.0155 (7)	−0.0086 (7)	0.0033 (7)
N2	0.0528 (10)	0.0457 (9)	0.0413 (9)	−0.0212 (8)	−0.0126 (7)	−0.0036 (7)
C5	0.0430 (10)	0.0440 (10)	0.0406 (10)	−0.0157 (8)	−0.0076 (8)	−0.0065 (8)
C3	0.0550 (13)	0.0540 (13)	0.0441 (11)	−0.0152 (11)	0.0007 (10)	−0.0050 (9)
C4	0.0521 (13)	0.0681 (15)	0.0620 (14)	−0.0334 (12)	−0.0218 (11)	0.0152 (12)
C2	0.0748 (16)	0.0530 (13)	0.0393 (11)	−0.0251 (12)	−0.0073 (10)	−0.0091 (9)
C1	0.0593 (14)	0.0782 (18)	0.0690 (16)	−0.0346 (13)	−0.0218 (12)	−0.0102 (13)

STable 5. Hydrogen coordinates and isotropic displacement parameters (Å^2) for 1.

	x	*y*	*z*	U_{iso}*/U_{eq}
H11	0.9499	-0.1075	0.1869	0.044*
H8	0.2600	0.0879	0.4036	0.049*
H14	0.7326	-0.2449	0.4002	0.051*
H12	0.4425	-0.3933	0.2924	0.061*
H6	0.1215	0.5795	0.2860	0.059*
H9	0.8858	0.1376	0.4457	0.057*
H10	1.1048	-0.0592	0.3007	0.063*
H7	0.0147	0.3916	0.4247	0.059*
H13	0.6443	-0.4809	0.4254	0.062*
H1	0.613(3)	0.052(3)	0.1475(17)	0.033(5)
H5	1.0680	0.1759	-0.0912	0.053*
H3	0.6570	0.4048	0.1493	0.069*
H4A	0.6156	0.2549	-0.0007	0.089*
H4B	0.7761	0.1820	-0.1003	0.089*
H4C	0.6533	0.3835	-0.0969	0.089*
H2	0.9255	0.3802	0.1947	0.069*
H1A	1.3025	0.1035	0.0872	0.097*
H1B	1.2563	0.3008	0.0744	0.097*
H1C	1.3129	0.2022	-0.0315	0.097*