

Supporting information for:

A Dime a Dozen: Common Structural Attributes of 1,2-dimethylimidazolium Halide Ionic Liquids

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Table S1. Crystallographic details for the two crystal structures.

Compound	DimeBr	DimeI
Chemical formula	Br·C ₇ H ₁₃ N ₂	I·C ₇ H ₁₃ N ₂
M_r	205.10	252.09
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/c$
Temperature (K)	150	150
a, b, c (Å)	6.8003 (4), 17.1874 (9), 7.9486 (4)	9.0499 (4), 7.8198 (3), 13.5789 (5)
β (°)	101.531 (2)	95.844 (1)
V (Å ³)	910.28 (9)	955.96 (7)
Z	4	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	4.45	3.29
Crystal size (mm)	0.28 × 0.12 × 0.08	0.36 × 0.08 × 0.05
Data collection		
Diffractometer	Bruker AXS D8 Quest Eco diffractometer with PhotonII charge-integrating pixel array detector (CPAD)	Bruker AXS D8 Quest Eco diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.0855 before and 0.0424 after correction. The Ratio of minimum to maximum transmission is 0.6344. The $\lambda/2$ correction factor is Not present.	Multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.0710 before and 0.0435 after correction. The Ratio of minimum to maximum transmission is 0.7318. The $\lambda/2$ correction factor is Not present.
T_{min}, T_{max}	0.473, 0.746	0.546, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11610, 2167, 1837	19287, 2932, 2731
R_{int}	0.030	0.024
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.659	0.716
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.025, 0.060, 1.09	0.022, 0.044, 1.20
No. of reflections	2167	2932
No. of parameters	94	95
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.45, -0.39	0.66, -0.85

Table S2. Torsion angle data used in the analysis of the ethyl group geometries.

CSD Entry	C2-N1-C6-C7 Torsion	Absolute Value
1053981	143.50	143.50
1053983	147.11	147.11
1053984	146.34	146.34
1056065	85.40	85.40
1175742	-82.34	82.34
1179274	82.60	82.60
1179276	104.30	104.30
1284386	98.65	98.65
1284387	99.89	99.89
1284388	143.87	143.87
1414151	142.94	142.94
1472569a	-95.58	95.58
1472569b	-80.16	80.16
1472569c	-84.51	84.51
1472570a	83.73	83.73
1472570b	95.14	95.14
1472570c	81.00	81.00
1472571a	91.81	91.81
1472571b	-82.86	82.86
1472571c	-84.84	84.84
1485858	83.12	83.12
1485859	79.15	79.15
1485860a	-77.65	77.65
1485860b	79.83	79.83
1514187	-93.33	93.33
1537072	114.02	114.02
1537073a	78.07	78.07
1537073b	101.94	101.94
1537082a	84.93	84.93
1537082b	93.62	93.62
1579534	83.65	83.65
1579535	-85.99	85.99
1579536	85.86	85.86
1579537	88.27	88.27
1579538	-89.10	89.10
1579539	-88.90	88.90
1579540	-133.00	133.00
169678a	-83.37	83.37
169678b	-104.00	104.00
1960297a	89.12	89.12

1960297b	-100.79	100.79
2044903	-83.70	83.70
2044904	-79.44	79.44
2052351	86.43	86.43
2052354	174.38	174.38
2068820a	-97.59	97.59
2068820b	95.27	95.27
2068824a	87.53	87.53
2068824b	-100.91	100.91
2112307	91.00	91.00
2120110	-144.31	144.31
274594	-93.07	93.07
653109	90.31	90.31
794465	110.31	110.31
841379	73.84	73.84
854947	-174.96	174.96
920917	-143.16	143.16
973145	98.38	98.38
975938	79.22	79.22