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Strategies Toward the Design of Energetic Ionic Liquids: Nitro- and Nitrile-substituted *N,N'*-Dialkylimidazolium Salts

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Table S1. Cation···Anion Close Contact Geometries

Hydrogen Type	D-H···A	D-H(Å)	H···A(Å)	-Δv dW	D···A(Å)	D-H···A (deg)	A symmetry code
3a							
Ring-*H*	C2-H2A···O5	0.94(3)	2.18(3)	-0.55	3.101(4)	167(2)	
	C5-H5A···O6	0.96(3)	2.26(3)	-0.46	3.048(4)	138(2)	0.5-x, 1.5+y, 0.5-z
N-*CH*$_3$	C7-H7C···O4	0.95(3)	2.44(3)	-0.29	3.170(4)	134(2)	-1+x, y, z
	C6-H6C···O6	1.00(3)	2.49(3)	-0.23	3.379(4)	147(2)	
	C6-H6B···O6	0.95(3)	2.55(3)	-0.18	3.384(4)	147(2)	-x, 1-y, -z
5a							
Ring-*H*	C2-H2A···O3	0.896(18)	2.201(19)	-0.52	3.076(2)	165.4(15)	
	C5-H5A···O4	0.921(19)	2.471(19)	-0.25	3.377(2)	168.0(15)	1+x, y, z
N-*CH*$_2$-CH$_3$	C6-H6B···O5	0.93(2)	2.43(2)	-0.29	3.302(2)	156.4(16)	1+x, y, z
7b							
Ring-*H*	C51-H51A···O31	0.88(3)	2.49(3)	-0.23	3.283(4)	149(2)	
	C52-H52A···O42	0.94(3)	2.57(3)	-0.15	3.478(4)	162(2)	
N-*CH*$_3$	C81-H81A···O51	0.89(4)	2.52(4)	-0.21	3.363(4)	157(3)	x, 1+y, z
	C61-H61B···O31	0.96(4)	2.60(4)	-0.11	3.485(5)	153(3)	
C-*CH*$_3$	C71-H71C···O62	0.98(4)	2.57(4)	-0.15	3.278(4)	130(3)	
	C71-H71A···O22	0.96(4)	2.58(4)	-0.15	3.510(4)	161(3)	1-x, 1-y, 1-z
	C72-H72B···O51	0.89(4)	2.59(4)	-0.12	3.281(5)	135(4)	
10a							
Ring-*H*	C4-H4A···O1	0.92(2)	2.59(2)	-0.14	3.243(3)	128.3(18)	-x, -0.5+y, 0.5-z
N-*CH*$_3$	C6-H6B···O5	1.00(3)	2.46(3)	-0.25	3.458(3)	175(2)	
	C7-H7C···O4	0.99(3)	2.53(3)	-0.20	3.282(3)	133(2)	1-x, 0.5+y, 0.5-z
	C7-H7A···O4	0.98(3)	2.58(3)	-0.14	3.549(3)	174(2)	-1+x, 0.5-y, 0.5+z
	C6-H6C···O1	0.98(3)	2.62(3)	-0.10	3.567(3)	161(2)	-x, 1-y, -z
	C6-H6A···O3	0.94(3)	2.63(3)	-0.10	3.330(3)	131.9(18)	1-x, 0.5+y, 0.5-z
13b							
Ring-*H*	C2-H2A···O2A	0.98(3)	2.20(3)	-0.52	2.888(6)	126(2)	
	C2-H2A···O3A	0.98(3)	2.33(3)	-0.39	3.144(6)	140(2)	1-x, -0.5+y, 1-z
	C2-H2A···O2	0.98(3)	2.47(3)	-0.25	2.931(6)	108.2(19)	
	C2-H2A···O1	0.98(3)	2.51(3)	-0.21	3.328(6)	141(2)	1-x, -0.5+y, 1-z
	C2-H2A···O3	0.98(3)	2.53(3)	-0.19	3.112(6)	118(2)	
N-*CH*$_3$	C6-H6C···O2	0.99(7)	2.17(8)	-0.55	3.020(8)	143(6)	
	C7-H7C···N5	0.96(5)	2.59(4)	-0.16	3.351(6)	136(3)	-x, 0.5+y, -z
	C6-H6B···O1A	0.94(5)	2.59(5)	-0.14	3.143(8)	118(4)	x, -1+y, z

Table S2. Bond Distances (Å) and Angles (deg) in the Imidazolium Rings

Bond lengths	3a	5a	7b	10a	13b
N(1)-C(2)	1.336(4)	1.328(2)	1.348(3)	1.335(3)	1.329(4)
C(2)-N(3)	1.328(3)	1.323(2)	1.342(4)	1.335(3)	1.315(4)
N(3)-C(4)	1.374(3)	1.378(2)	1.375(4)	1.366(3)	1.383(4)
C(4)-C(5)	1.353(4)	1.347(2)	1.341(4)	1.348(3)	1.353(4)
C(5)-N(1)	1.367(3)	1.360(2)	1.362(4)	1.372(3)	1.377(4)

Bond Angles	3a	5a	7b	10a	13b
C(2)-N(1)-C(5)	108.6(2)	108.77(14)	109.9(2)	106.81(18)	108.2(2)
C(2)-N(3)-C(4)	106.3(2)	106.50(13)	107.8(2)	106.84(18)	108.7(3)
N(3)-C(2)-N(1)	109.9(2)	109.81(14)	107.2(2)	110.42(18)	109.3(3)
C(5)-C(4)-N(3)	109.4(2)	108.69(14)	108.9(3)	108.2(2)	106.6(3)
C(4)-C(5)-N(1)	105.8(3)	106.22(14)	106.2(3)	107.7(2)	107.3(3)