Supplementary Information for the paper titled "Invariom approach as a new tool in electron density studies of ionic liquids: a case of 1-butyl-2,3-dimethylimidazolium chloride BDMIM[Cl]"

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Supplementary Figures:

Figure S1. 3D-distribution of DED around the chloride anion in BDMIM[Cl] as obtained from the conventional multipole refinement; the chloride anion is in the center of the special cluster with a radius of 6 Å. Isosurface of DED equal to 0.55 eÅ^{-3} is shown by red; the negative isosurface (DED is –0.2 eÅ^{-3}) is shown by wireframe.

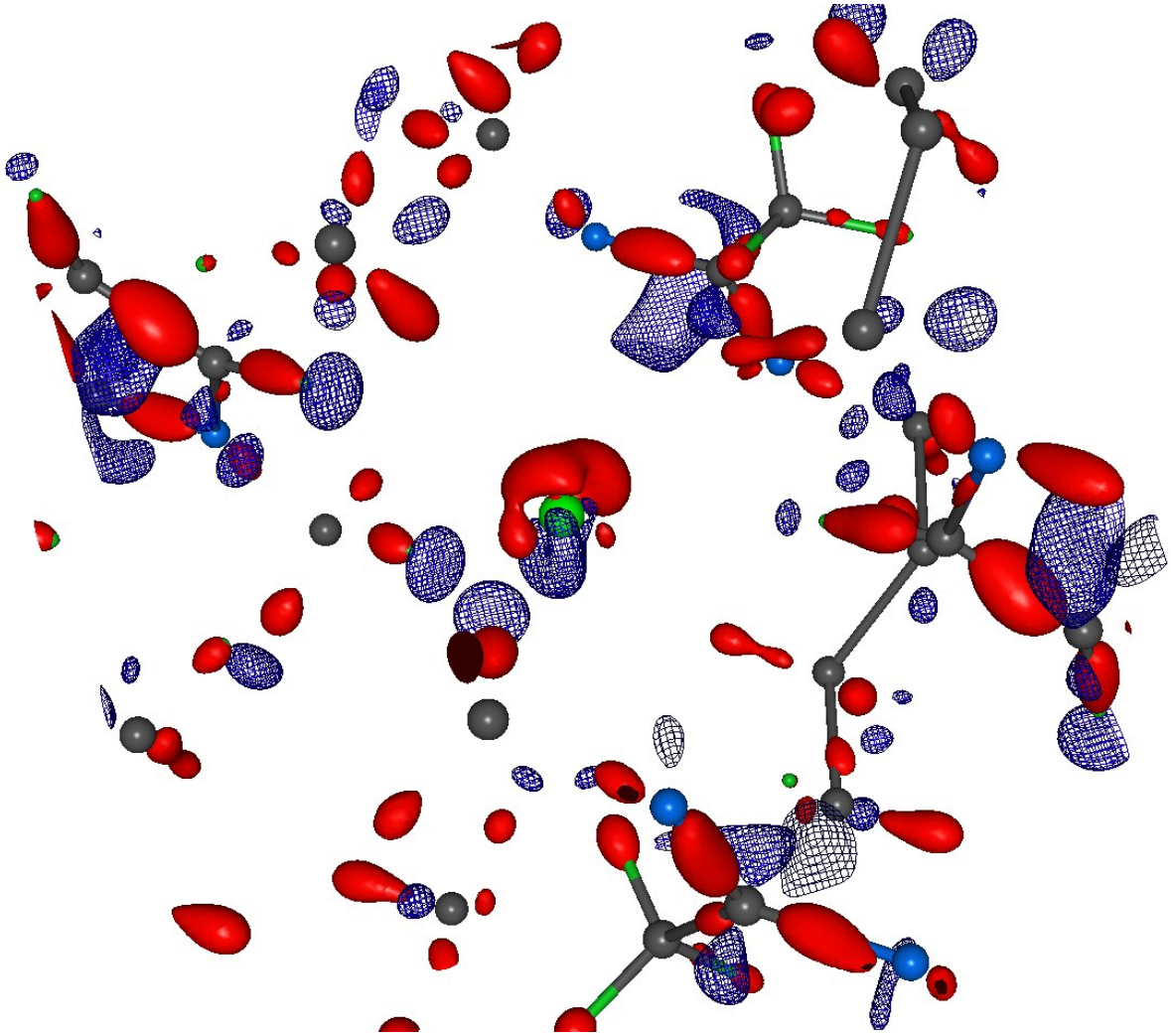


Figure S2. Distributions of the experimental DED in the plane of N(1)…C(4) bond paths from the conventional multipole refinement (**A**) and from the invariom approximation (**B**). Contours are drawn with 0.1 eÅ^{-3} step, negative ones are dashed. Stacking interactions are depicted as long black dashes, C-H…π contacts as short black dashes.

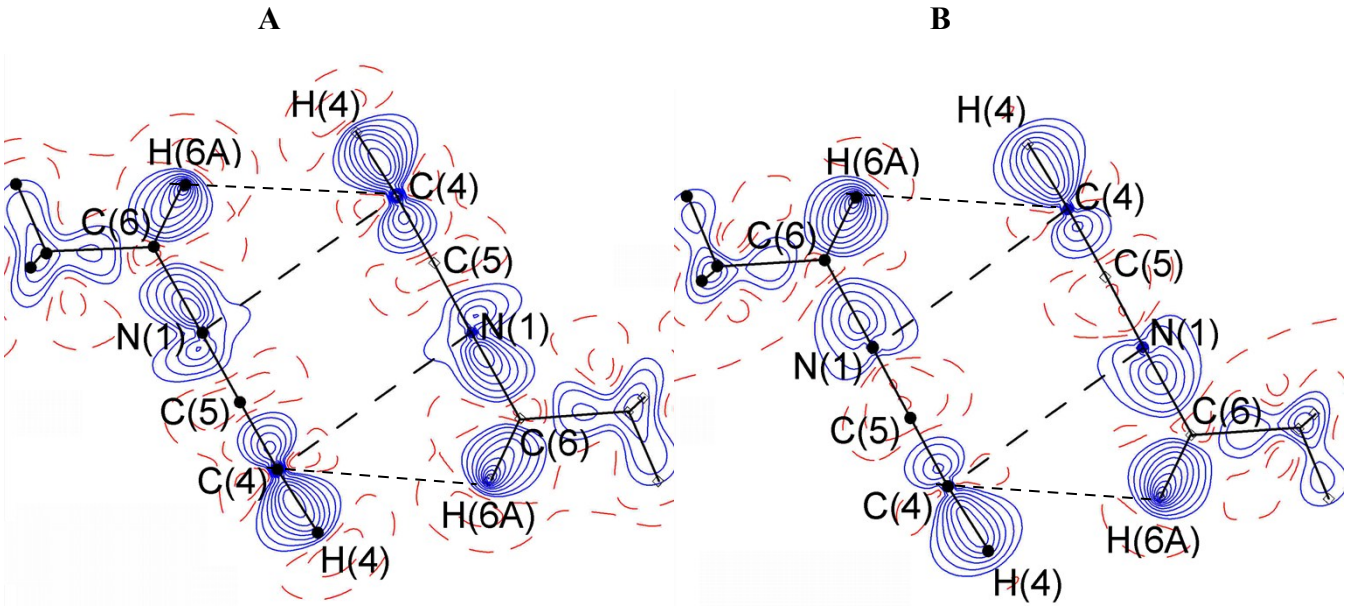


Figure S3. Distributions of the experimental DED in the plane of C-H…π contact in the ion-pair dimer with no stacking interaction from the conventional multipole refinement (**A**) and from the invariom approximation (**B**). Contours are drawn with 0.1 eÅ^{-3} step, negative ones are dashed.

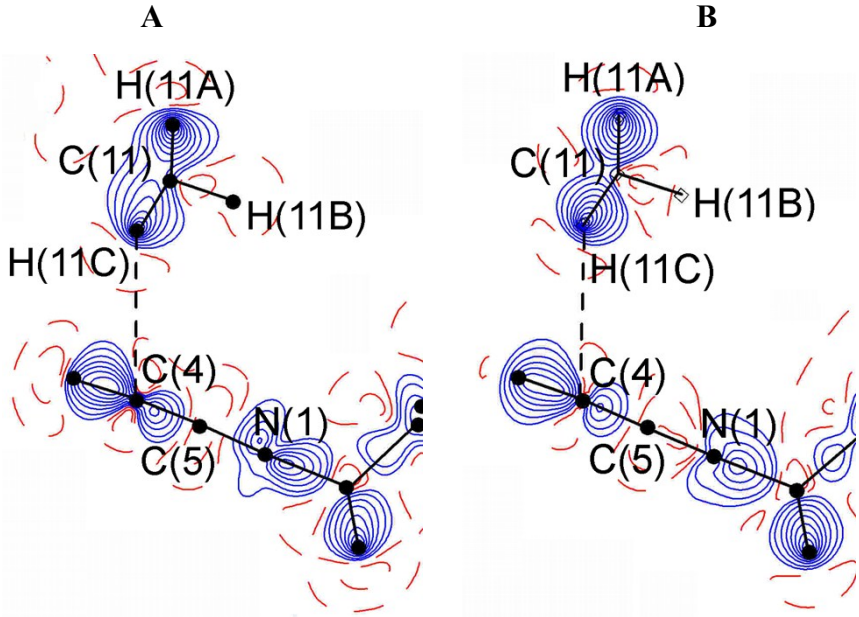
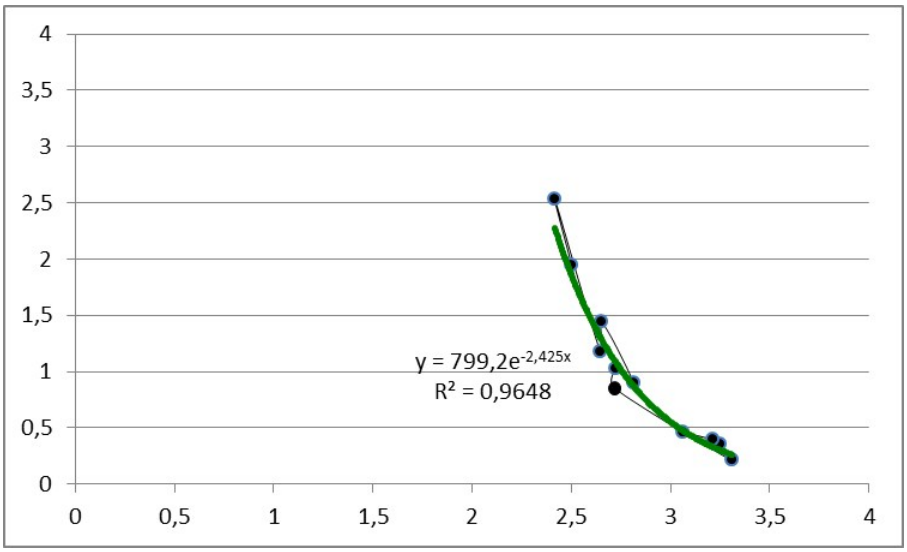
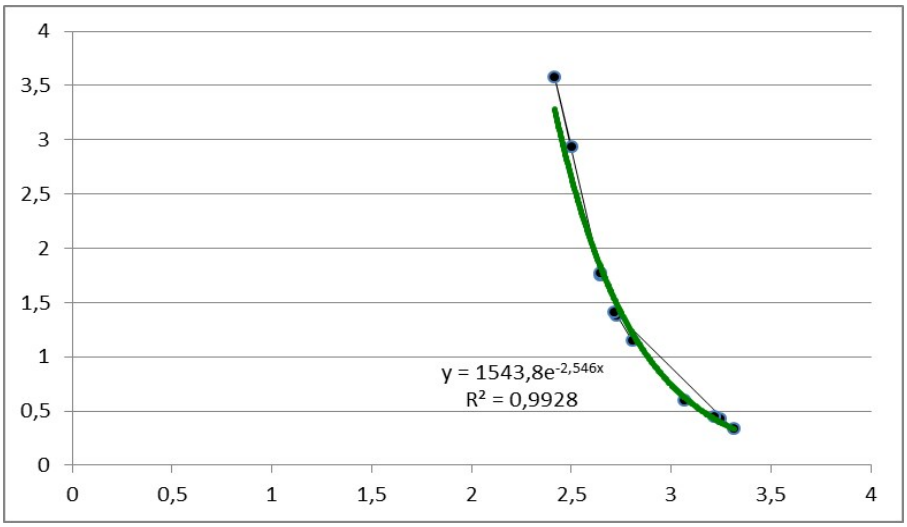


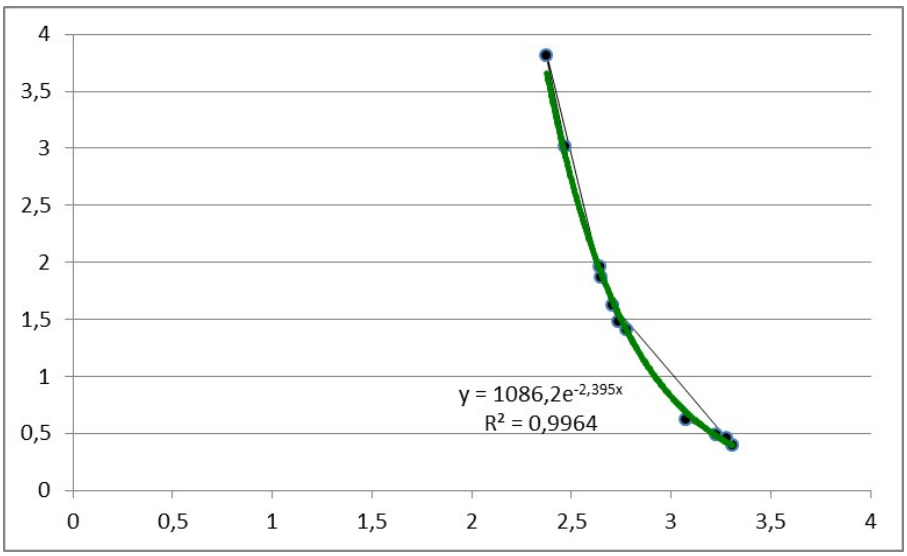
Figure S4. Interaction energies (kcal/mol) for H-bonds in BDMIM[Cl] plotted against H…Cl distance (Å), in black, from the conventional multipole refinement (**A**), the invariom approximation (**B**) and from periodic quantum chemistry (**C**).



A

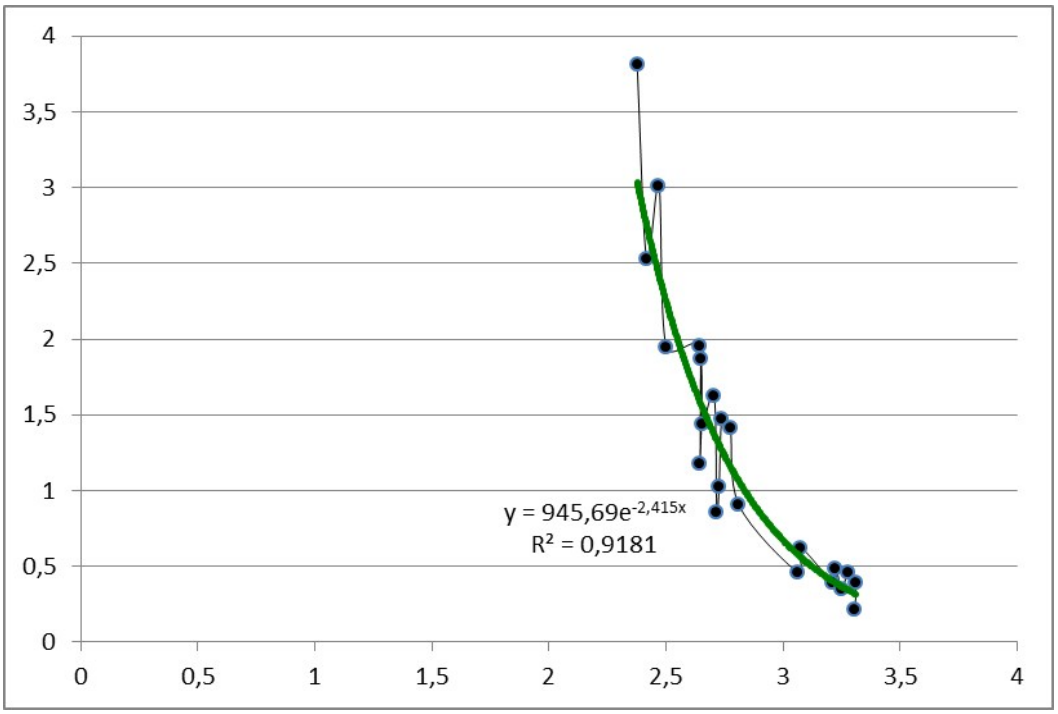


B

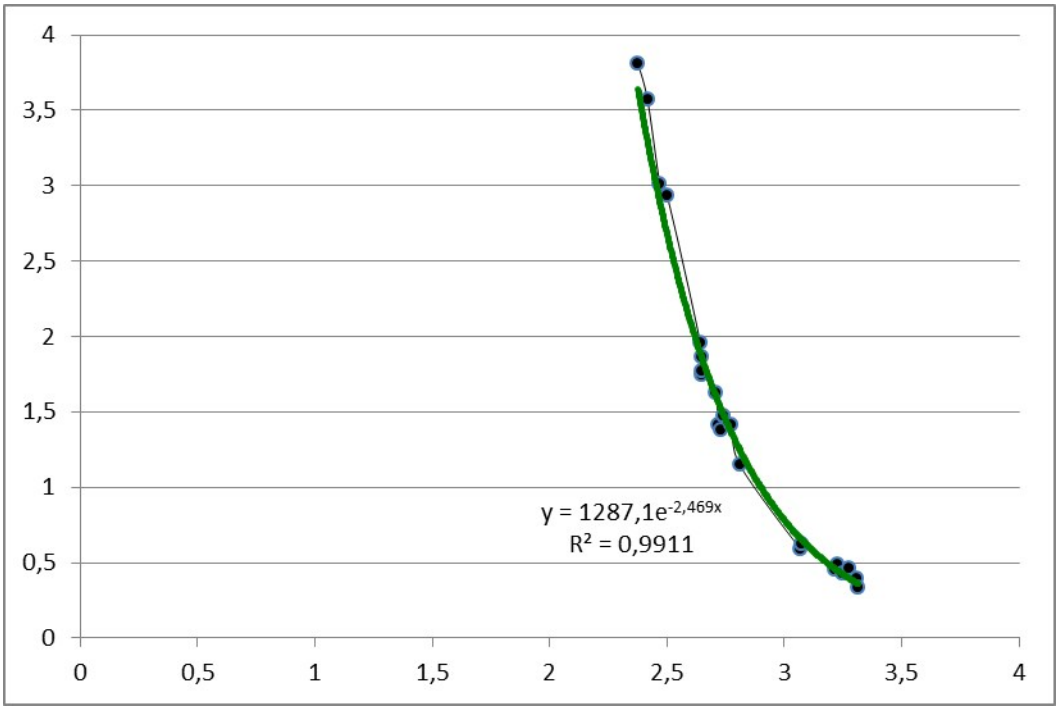


C

Figure S5. Interaction energies (kcal/mol) for H-bonds in BDMIM[Cl] plotted against H…Cl distance (Å), in black, from the conventional multipole refinement and periodic quantum chemistry (**A**) and from the invariom approximation and periodic quantum chemistry (**B**).



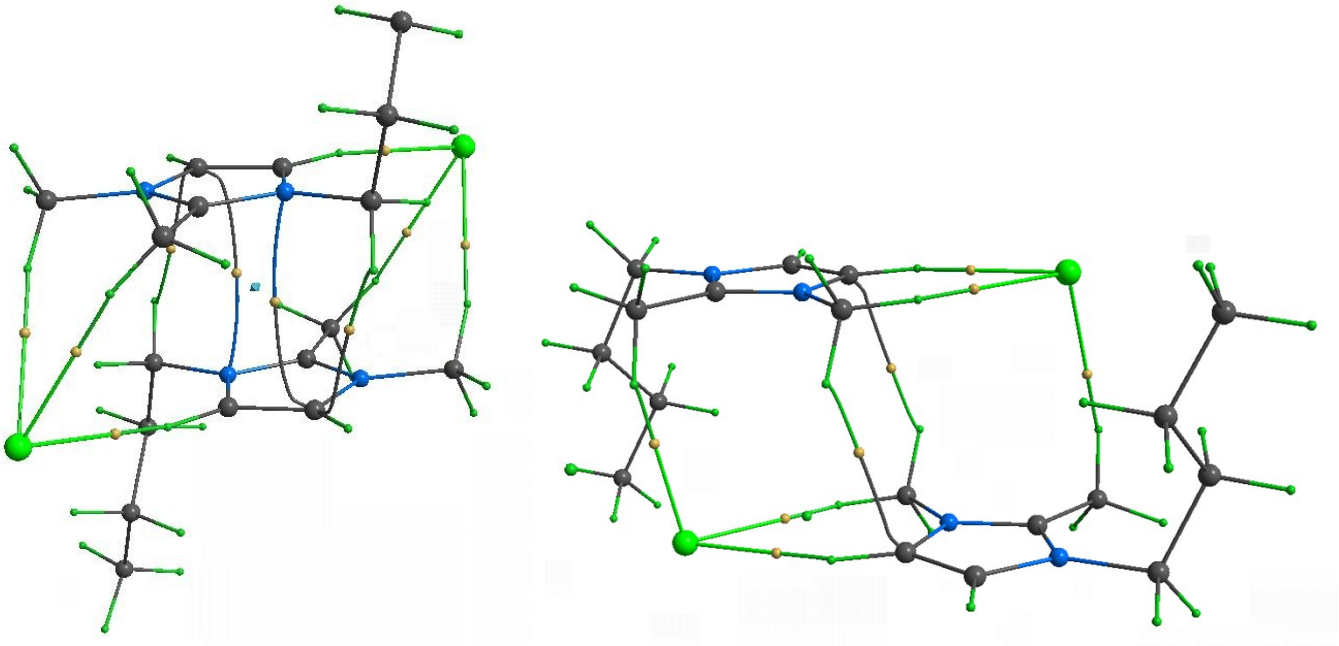
A



B

Figure S6. Molecular graph for the ion-pair dimer in BDMIM[Cl] that features stacking interaction (**A**) and the one that does not (**B**); bcp are shown as yellow spheres, rcp as a cyan rhomboid.

A **B**



Supplementary Tables:

Table S1. Topological parameters of ρ(**r**) in bcps for covalent bonds in BDMIM[Cl] from multipole and invariom (in parentheses) modeling of X-ray diffraction data and from periodic quantum chemistry (second entry).

Bond	d, Å [a)]	ρ(**r**), eÅ^{-3}	$-\nabla^2\rho(\mathbf{r})$, eÅ^{-5}	ε[b)]
N(1)-C(2)	1.3395(7) 1.350	2.52 (2.29) 2.28	25.87 (20.96) 23.73	0.19 (0.23) 0.27
C(2)-N(3)	1.3388(7) 1.348	2.54 (2.29) 2.30	26.80 (21.30) 24.13	0.21 (0.23) 0.21
N(3)-C(4)	1.3830(7) 1.385	2.25 (2.01) 2.05	20.88 (15.03) 18.49	0.14 (0.17) 0.19
C(4)-C(5)	1.3512(8) 1.366	2.45 (2.26) 2.25	25.41 (19.03) 23.57	0.27 (0.32) 0.29
C(5)-N(1)	1.3850(7) 1.387	2.22 (2.01) 2.05	19.90 (14.87) 18.26	0.10 (0.17) 0.16
N(1)-C(6)	1.4720(8) 1.469	1.87 (1.73) 1.70	13.88 (10.18) 13.64	0.06 (0.06) 0.02
N(3)-C(11)	1.4628(7) 1.460	1.86 (1.75) 1.72	13.45 (9.92) 13.80	0.05 (0.07) 0.07
C(2)-C(10)	1.4766(8) 1.472	1.86 (1.79) 1.81	14.24 (12.24) 17.27	0.05 (0.05) 0.06
C(4)-H(4)[a]	1.083 1.090	1.92 (1.88) 1.94	24.57 (19.57) 25.68	-
C(5)-H(5)	1.083 1.093	1.90 (1.88) 1.93	21.64 (19.57) 25.55	-
C(6)-C(7)	1.5212(10) 1.525	1.72 (1.69) 1.67	12.24 (11.57) 15.04	0.07 (0.03) 0.03
C(6)-H(6A)	1.091 1.099	1.73 (1.89) 1.92	14.83 (21.51) 23.85	-
C(6)-H(6B)	1.091 1.098	1.80 (1.90) 1.92	16.41 (21.51) 23.84	-
C(7)-C(8)	1.5198(8)	1.71 (1.66)	11.12 (11.12)	0.06 (0.02)

	1.526	1.66	14.85	0.015
C(7)-H(7A)	1.094 1.101	1.85 (1.86) 1.87	17.82 (20.28) 22.33	-
C(7)-H(7B)	1.094 1.101	1.85 (1.86) 1.86	17.9 (20.26) 22.15	-
C(8)-C(9)	1.5149(10) 1.525	1.75 (1.65) 1.65	12.31 (10.76) 14.77	0.11 (0.01) 0.01
C(8)-H(8A)	1.094 1.101	1.78 (1.86) 1.87	14.37 (20.28) 22.09	-
C(8)-H(8B)	1.094 1.101	1.72 (1.85) 1.86	12.7 (20.26) 21.94	-
C(9)-H(9A)	1.091 0.099	1.65 (1.85) 1.86	10.79 (20.20) 22.19	-
C(9)-H(9B)	1.091 1.100	1.62 (1.85) 1.86	7.43 (20.15) 22.06	-
C(9)-H(9C)	1.091 1.100	1.89 (1.85) 1.86	18.05 (20.18) 22.18	-
C(10)-H(10A)	1.089 1.094	1.77 (1.85) 1.88	15.00 (20.43) 22.67	-
C(10)-H(10B)	1.089 1.103	1.65 (1.85) 1.85	9.77 (20.37) 22.40	-
C(10)-H(10C)	1.089 1.101	1.82 (1.85) 1.86	16.43 (20.39) 22.75	-
C(11)-H(11A)	1.093 1.100	1.82 (1.88) 1.90	15.26 (21.50) 23.70	-
C(11)-H(11B)	1.093 1.097	1.87 (1.88) 1.92	20.29 (21.52) 24.26	-
C(11)-H(11C)	1.093 1.096	1.76 (1.88) 1.90	14.15 (21.49) 23.57	-

[a] In the multipole and the invariom refinements, the C-H distances were fixed at the values from the invariom database; [b] ε stands for the bond ellipticities that are given here for C-N and C-C bonds.

Table S2. Atomic charges (e) and volumes (Å^3) in BDMIM[Cl] from multipole and invariom (in parentheses) modeling of X-ray diffraction data and from periodic quantum chemistry (second entry).

Atom	Charge	Volume	Atom	Charge	Volume
Cl(1)	–0.85 (–1.01) –0.78	37.07 (34.40) 37.41	H(6B)	+0.22 (+0.09) +0.04	6.13 (6.76) 7.04
N(1)	–0.99 (–0.86) –2.17	10.11 (10.13) 12.53	H(7A)	+0.12 (+0.05) 0.00	6.27 (6.84) 7.33
N(3)	–0.94 (–0.85) –2.15	10.95 (11.02) 12.86	H(7B)	+0.09 (+0.05) 0.00	7.09 (7.31) 7.34
C(2)	+0.68 (+0.73) +1.83	7.53 (7.64) 5.55	H(8A)	+0.12 (+0.05) –0.02	7.50 (7.87) 8.10
C(4)	+0.01 (+0.21) +0.74	11.92 (10.80) 9.58	H(8B)	+0.08 (+0.05) –0.03	6.44 (6.86) 7.15
C(5)	+0.11 (+0.21) +0.74	12.67 (11.54) 10.23	H(9A)	+0.18 (+0.05) 0.00	6.65 (7.84) 7.68
C(6)	–0.01 (+0.24) +0.60	9.94 (8.06) 7.44	H(9B)	+0.22 (+0.05) –0.01	6.38 (6.81) 7.36
C(7)	–0.10 (–0.01) +0.05	8.74 (8.52) 8.24	H(9C)	+0.16 (+0.05) 0.00	5.73 (6.71) 6.70
C(8)	–0.18 (–0.01) +0.07	9.23 (8.51) 8.12	H(10A)	+0.23 (+0.08) +0.02	6.54 (7.63) 7.63
C(9)	–0.51 (–0.01) +0.02	13.67 (10.45) 10.25	H(10B)	+0.17 (+0.08) +0.08	5.33 (6.24) 6.03
C(10)	–0.37 (+0.06) +0.01	12.36 (9.93) 10.07	H(10C)	+0.18 (+0.08) +0.08	5.81 (6.56) 6.29
C(11)	+0.01 (+0.26) +0.55	12.27 (10.11) 9.16	H(11A)	+0.11 (+0.09) +0.07	6.14 (6.53) 6.60
H(4)	+0.35 (+0.02) +0.06	4.51 (6.62) 6.05	H(11B)	+0.25 (+0.08) +0.08	5.01 (6.91) 7.03
H(5)	+0.31 (+0.02) +0.08	4.68 (6.47) 5.68	H(11C)	+0.17 (+0.09) +0.03	37.07 (6.95) 7.41
H(6A)	+0.21 (+0.09) +0.04	6.15 (6.89) 7.17			

XD output from conventional multipole refinement of high-resolution X-ray diffraction data

Table M1. Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
CL(1)	7.883(15)	1.025	0.000	1.460	-0.883(15)
N(1)	5.025(17)	1.008	0.000	1.007	-0.024(17)
N(3)	4.949(17)	1.008	0.000	1.007	+0.051(17)
C(2)	4.158(20)	1.011	0.000	0.933	-0.158(20)
C(4)	4.208(27)	1.009	0.000	0.946	-0.208(27)
C(5)	4.170(26)	1.009	0.000	0.946	-0.169(26)
C(6)	4.190(28)	1.009	0.000	0.917	-0.190(28)
C(7)	4.099(29)	1.007	0.000	0.912	-0.098(29)
C(8)	4.202(28)	1.007	0.000	0.912	-0.202(28)
C(9)	4.393(34)	1.009	0.000	0.962	-0.392(34)
C(10)	4.243(32)	1.012	0.000	0.860	-0.242(32)
C(11)	4.144(32)	1.008	0.000	0.878	-0.143(32)
H(4)	0.735(14)	1.200	0.000	1.200	+0.265(14)
H(5)	0.758(14)	1.200	0.000	1.200	+0.242(14)
H(6A)	0.833(16)	1.200	0.000	1.200	+0.167(16)
H(6B)	0.799(17)	1.200	0.000	1.200	+0.200(17)
H(7A)	0.888(16)	1.200	0.000	1.200	+0.112(16)
H(7B)	0.902(16)	1.200	0.000	1.200	+0.098(16)
H(8A)	0.841(15)	1.200	0.000	1.200	+0.158(15)
H(8B)	0.953(16)	1.200	0.000	1.200	+0.046(16)
H(9A)	0.871(18)	1.200	0.000	1.200	+0.128(18)
H(9B)	0.774(18)	1.200	0.000	1.200	+0.225(18)
H(9C)	0.898(17)	1.200	0.000	1.200	+0.101(17)
H(10A)	0.793(18)	1.200	0.000	1.200	+0.207(18)
H(10B)	0.918(19)	1.200	0.000	1.200	+0.082(19)
H(10C)	0.832(19)	1.200	0.000	1.200	+0.168(19)
H(11A)	0.881(18)	1.200	0.000	1.200	+0.119(18)
H(11B)	0.821(16)	1.200	0.000	1.200	+0.179(16)
H(11C)	0.842(17)	1.200	0.000	1.200	+0.158(17)

Table M2. Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
CL(1)	-0.089(3)	0.231(3)	0.044(3)	1.460
N(1)	-0.020(7)	-0.011(7)	-0.012(6)	1.007
N(3)	0.058(7)	0.002(7)	0.001(6)	1.007
C(2)	-0.009(8)	-0.023(10)	-0.065(10)	0.933
C(4)	-0.015(9)	0.056(12)	0.004(8)	0.946
C(5)	-0.013(9)	-0.055(12)	-0.002(8)	0.946
C(6)	-0.081(9)	-0.050(11)	-0.087(13)	0.917
C(7)	-0.008(11)	-0.048(10)	-0.024(10)	0.912
C(8)	0.076(11)	0.033(10)	-0.035(10)	0.912
C(9)	-0.035(12)	-0.072(13)	-0.030(10)	0.962
C(10)	-0.111(15)	0.026(15)	-0.104(10)	0.860
C(11)	0.034(13)	0.083(13)	-0.060(8)	0.878
H(4)	0.000	0.000	0.178(9)	1.200
H(5)	0.000	0.000	0.151(9)	1.200
H(6A)	0.000	0.000	0.146(11)	1.200
H(6B)	0.000	0.000	0.101(10)	1.200
H(7A)	0.000	0.000	0.166(10)	1.200
H(7B)	0.000	0.000	0.124(10)	1.200
H(8A)	0.000	0.000	0.093(10)	1.200
H(8B)	0.000	0.000	0.143(10)	1.200
H(9A)	0.000	0.000	0.153(12)	1.200
H(9B)	0.000	0.000	0.066(11)	1.200
H(9C)	0.000	0.000	0.164(11)	1.200
H(10A)	0.000	0.000	0.117(10)	1.200
H(10B)	0.000	0.000	0.163(11)	1.200
H(10C)	0.000	0.000	0.169(11)	1.200
H(11A)	0.000	0.000	0.191(12)	1.200
H(11B)	0.000	0.000	0.222(9)	1.200
H(11C)	0.000	0.000	0.128(11)	1.200

Table M3. Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
CL(1)	-0.041(4)	-0.073(4)	0.020(4)	0.072(5)	0.015(5)	1.460
N(1)	-0.029(7)	-0.036(7)	0.023(7)	0.005(7)	-0.045(7)	1.007
N(3)	-0.043(6)	-0.016(6)	0.014(6)	-0.005(7)	-0.065(7)	1.007
C(2)	0.136(10)	-0.007(9)	-0.013(10)	-0.192(9)	-0.035(8)	0.933
C(4)	-0.207(9)	-0.012(8)	0.053(8)	-0.096(9)	-0.026(10)	0.946
C(5)	-0.182(9)	0.011(8)	0.060(8)	-0.086(10)	-0.002(10)	0.946
C(6)	0.017(9)	0.018(9)	0.022(11)	-0.062(9)	0.047(9)	0.917
C(7)	0.012(9)	-0.025(10)	0.045(10)	0.013(10)	-0.029(9)	0.912
C(8)	0.014(8)	-0.043(10)	-0.039(10)	0.026(10)	0.028(9)	0.912
C(9)	0.042(11)	0.060(10)	0.033(11)	0.096(9)	0.041(9)	0.962
C(10)	0.001(11)	0.027(10)	0.016(10)	0.021(11)	0.046(11)	0.860
C(11)	-0.090(9)	-0.015(9)	-0.025(9)	-0.013(10)	-0.006(10)	0.878
H(4)	0.075(11)	0.000	0.000	0.000	0.000	1.200
H(5)	0.054(12)	0.000	0.000	0.000	0.000	1.200
H(6A)	0.034(12)	0.000	0.000	0.000	0.000	1.200
H(6B)	0.037(12)	0.000	0.000	0.000	0.000	1.200
H(7A)	0.050(12)	0.000	0.000	0.000	0.000	1.200
H(7B)	0.074(13)	0.000	0.000	0.000	0.000	1.200
H(8A)	0.003(11)	0.000	0.000	0.000	0.000	1.200
H(8B)	0.049(12)	0.000	0.000	0.000	0.000	1.200
H(9A)	0.010(13)	0.000	0.000	0.000	0.000	1.200
H(9B)	-0.055(14)	0.000	0.000	0.000	0.000	1.200
H(9C)	0.069(13)	0.000	0.000	0.000	0.000	1.200
H(10A)	0.035(13)	0.000	0.000	0.000	0.000	1.200
H(10B)	0.045(13)	0.000	0.000	0.000	0.000	1.200
H(10C)	0.028(13)	0.000	0.000	0.000	0.000	1.200
H(11A)	-0.005(13)	0.000	0.000	0.000	0.000	1.200
H(11B)	0.099(12)	0.000	0.000	0.000	0.000	1.200
H(11C)	0.028(13)	0.000	0.000	0.000	0.000	1.200

Table M4. Octupole Population Parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
CL(1)	0.004(7)	-0.022(6)	-0.013(7)	0.023(6)	-0.048(6)	0.049(6)	-0.004(6)	1.460
N(1)	0.001(8)	0.022(8)	-0.029(8)	0.003(9)	0.007(9)	0.155(9)	0.046(10)	1.007
N(3)	0.003(8)	0.003(8)	-0.023(8)	0.033(8)	-0.007(9)	0.134(9)	0.053(10)	1.007
C(2)	0.300(14)	0.007(11)	-0.024(14)	0.239(12)	-0.011(11)	0.013(10)	0.021(10)	0.933
C(4)	0.012(10)	-0.045(10)	0.019(11)	-0.041(11)	-0.001(10)	0.337(13)	-0.130(12)	0.946
C(5)	0.006(10)	-0.039(10)	0.044(11)	-0.014(11)	0.003(11)	0.277(14)	-0.059(13)	0.946
C(6)	0.014(11)	-0.136(11)	-0.214(12)	0.037(12)	-0.010(13)	0.227(13)	-0.001(12)	0.917
C(7)	-0.027(12)	-0.013(10)	0.034(13)	-0.336(13)	-0.023(12)	0.047(13)	0.037(12)	0.912
C(8)	-0.017(12)	0.040(11)	-0.042(13)	-0.314(13)	0.042(12)	0.053(13)	0.038(11)	0.912
C(9)	0.244(14)	0.017(11)	0.017(12)	-0.026(13)	-0.012(13)	0.144(10)	0.013(8)	0.962
C(10)	0.284(14)	0.043(10)	0.019(10)	0.059(13)	-0.066(13)	-0.009(9)	-0.103(11)	0.860
C(11)	0.325(12)	0.014(9)	0.043(9)	-0.028(11)	0.013(10)	-0.095(8)	-0.105(11)	0.878
H(4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200

Table M5. Hexadecapole Population Parameters.

Atom	H40	H41+	H41-	H42+	H42-	H43+	H43-	H44+	H44-	Kappa'
CL(1)	-0.053(11)	0.052(10)	-0.027(10)	0.032(11)	-0.022(11)	-0.025(10)	0.086(10)	-0.016(9)	-0.038(9)	1.460
N(1)	0.024(10)	0.007(10)	0.014(10)	0.040(10)	-0.016(11)	-0.001(10)	0.000(13)	0.012(12)	-0.002(11)	1.007
N(3)	0.039(10)	-0.017(9)	0.028(9)	0.004(10)	-0.001(10)	-0.027(9)	-0.006(12)	0.025(11)	0.017(10)	1.007
C(2)	-0.003(17)	-0.014(12)	-0.003(16)	-0.082(16)	0.014(16)	0.023(12)	-0.022(14)	0.006(12)	-0.007(12)	0.933
C(4)	0.064(12)	-0.011(11)	-0.027(11)	-0.006(12)	-0.017(12)	-0.048(12)	-0.039(13)	0.091(14)	-0.037(14)	0.946
C(5)	0.041(13)	0.006(11)	-0.011(11)	-0.006(12)	-0.014(12)	-0.016(12)	-0.060(14)	0.064(15)	-0.009(15)	0.946
C(6)	0.155(13)	-0.077(12)	0.013(13)	-0.017(14)	0.007(15)	-0.025(14)	0.029(14)	0.075(14)	0.006(14)	0.917
C(7)	-0.048(14)	0.008(11)	0.028(15)	-0.009(13)	0.017(14)	0.030(13)	0.006(13)	0.025(13)	-0.033(12)	0.912
C(8)	-0.006(14)	-0.003(11)	-0.022(15)	-0.068(14)	0.024(14)	-0.024(13)	-0.017(13)	0.023(12)	-0.046(12)	0.912
C(9)	0.081(15)	0.037(14)	-0.058(15)	0.095(13)	-0.059(13)	0.062(14)	0.004(12)	0.017(11)	0.072(11)	0.962
C(10)	0.073(14)	-0.015(14)	0.042(13)	-0.026(12)	0.030(13)	-0.002(11)	-0.036(14)	0.087(12)	0.037(12)	0.860
C(11)	0.138(13)	0.017(12)	-0.007(13)	-0.006(12)	-0.004(12)	0.051(10)	0.002(13)	-0.019(10)	0.032(12)	0.878
H(4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200

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CL(1) N(1) X CL(1) N(3) Y

N(1) C(2) X N(1) C(6) Y

N(3) C(2) X N(3) C(11) Y

C(2) C(10) Z C(2) N(3) Y

C(4) N(3) X C(4) C(5) Y

C(5) N(1) X C(5) C(4) Y

C(6) N(1) X C(6) C(7) Y

C(7) DUM0 Z C(7) C(8) Y

C(8) DUM1 Z C(8) C(9) Y

C(9) C(8) Z C(9) H(9C) X

C(10) C(2) Z C(10) H(10C) Y

C(11) N(3) Z C(11) H(11C) Y

H(4) C(4) Z H(4) C(5) Y

H(5) C(5) Z H(5) C(4) Y

H(6A) C(6) Z H(6A) H(6B) Y

H(6B) C(6) Z H(6B) H(6A) Y

H(7A) C(7) Z H(7A) H(7B) Y

H(7B) C(7) Z H(7B) H(7A) Y

H(8A) C(8) Z H(8A) H(8B) Y

H(8B) C(8) Z H(8B) H(8A) Y

H(9A) C(9) Z H(9A) H(9B) Y

H(9B) C(9) Z H(9B) H(9A) Y

H(9C) C(9) Z H(9C) H(9A) Y

H(10A) C(10) Z H(10A) C(2) Y

H(10B) C(10) Z H(10B) C(2) Y

H(10C) C(10) Z H(10C) C(2) Y

H(11A) C(11) Z H(11A) H(11B) Y

H(11B) C(11) Z H(11B) H(11A) Y

H(11C) C(11) Z H(11C) H(11A) Y

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N(1)	0.609115	0.04399	0.353036	1	4	0.024
N(3)	0.762892	0.044268	0.517106	1	4	0.022
C(2)	0.687066	0.112	0.434268	1	4	0.023
C(4)	0.7333	-0.069035	0.487848	1	4	0.025
C(5)	0.636785	-0.069456	0.384672	1	4	0.026
C(6)	0.511028	0.083042	0.246203	1	4	0.032
C(7)	0.614306	0.125878	0.139047	1	4	0.028
C(8)	0.714677	0.032442	0.079718	1	4	0.029
C(9)	0.812669	0.078309	-0.028144	1	4	0.043
C(10)	0.692504	0.238461	0.435022	1	4	0.033
C(11)	0.860641	0.084972	0.622406	1	4	0.030
H(4)	0.777031	-0.138337	0.546286	1	4	0.036
H(5)	0.586866	-0.140845	0.332541	1	4	0.039
H(6A)	0.423289	0.145705	0.278014	1	4	0.043
H(6B)	0.439974	0.009666	0.215031	1	4	0.044
H(7A)	0.693165	0.193752	0.174469	1	4	0.044
H(7B)	0.533999	0.162654	0.068077	1	4	0.049
H(8A)	0.795222	-0.005219	0.149965	1	4	0.041
H(8B)	0.633932	-0.036604	0.050134	1	4	0.048
H(9A)	0.873705	0.009715	-0.077998	1	4	0.056
H(9B)	0.901485	0.140057	0.005781	1	4	0.053
H(9C)	0.733869	0.124248	-0.093143	1	4	0.060
H(10A)	0.597642	0.271277	0.373918	1	4	0.048
H(10B)	0.808332	0.265004	0.398619	1	4	0.048
H(10C)	0.673469	0.266513	0.53062	1	4	0.049
H(11A)	0.788936	0.144558	0.677264	1	4	0.049
H(11B)	0.898693	0.011247	0.678178	1	4	0.045
H(11C)	0.965579	0.128634	0.584666	1	4	0.045

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N(1) 0.022445 0.025669 0.024569 -0.000626 0.001094 -0.000013

N(3) 0.021891 0.02061 0.022947 -0.00106 0.002099 -0.001054

C(2) 0.023468 0.019686 0.024761 0.001237 0.002965 -0.000672

C(4) 0.027955 0.020089 0.026084 -0.001894 0.002526 0.000844

C(5) 0.028027 0.023284 0.027225 -0.005751 0.001977 -0.001463

C(6) 0.023839 0.042724 0.030427 0.004213 -0.002017 0.001266

C(7) 0.033015 0.024929 0.025278 0.004375 -0.003017 0.001035

C(8) 0.031436 0.027405 0.026927 0.004808 -0.001199 0.001432

C(9) 0.042534 0.058481 0.028481 0.009144 0.005248 0.008205

C(10) 0.043813 0.020224 0.033781 0.004774 0.005641 -0.001315

C(11) 0.028755 0.030423 0.029457 -0.001388 -0.002141 -0.004333

H(4) 0.035228 0.031249 0.040578 0.008122 -0.001162 -0.00093

H(5) 0.040162 0.030792 0.046129 -0.005197 -0.006471 -0.00598

H(6A) 0.045567 0.040521 0.041996 0.001473 0.002416 0.010218

H(6B) 0.048373 0.039846 0.043181 -0.002518 -0.00708 -0.006454

H(7A) 0.046993 0.038701 0.046255 -0.001011 0.003571 -0.002647

H(7B) 0.051023 0.056916 0.037666 0.008233 -0.003336 0.012419

H(8A) 0.046194 0.043313 0.034457 0.003702 -0.002128 0.005834

H(8B) 0.050952 0.048533 0.043454 -0.009046 -0.002209 -0.003383

H(9A) 0.073351 0.050713 0.045761 0.000241 0.015393 0.015889

H(9B) 0.061649 0.052296 0.046055 0.005469 0.005999 -0.005183

H(9C) 0.061158 0.074986 0.043927 0.019612 0.000356 0.020557

H(10A) 0.048265 0.038165 0.056978 0.00337 -0.01217 0.005303

H(10B) 0.040274 0.034252 0.068431 -0.000541 0.013275 -0.001768

H(10C) 0.064774 0.040305 0.040848 -0.008978 0.005582 0.002914

H(11A) 0.043713 0.054314 0.04765 -0.019102 0.000057 0.013302

H(11B) 0.051965 0.039223 0.043837 0.004018 -0.008262 0.002889

H(11C) 0.040917 0.049347 0.045788 -0.003761 0.004159 -0.013119

Differences of Mean-Squares Displacement Amplitudes (DMSDA) (1.E4 A**2) along the bonds

ATOM-->ATOM		/ DIST	DMSDA	ATOM	/ DIST	DMSDA	ATOM	/ DIST	DMSDA
N(1)	C(2)	1.3396	-1	C(5)	1.3859	5	C(6)	1.4699	7
N(3)	C(2)	1.3406	-2	C(4)	1.3811	4	C(11)	1.4619	16
C(2)	C(10)	1.4774	8						
C(4)	C(5)	1.3582	2						
C(6)	C(7)	1.5264	-8						
C(7)	C(8)	1.5179	1						
C(8)	C(9)	1.5196	7						

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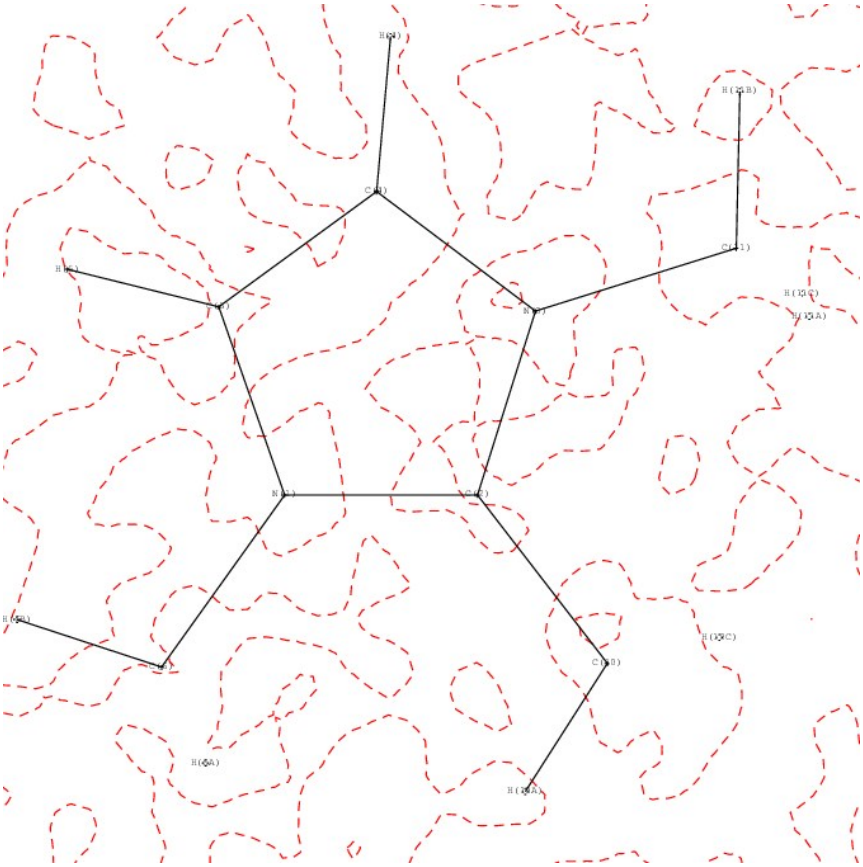

Figure M1. Residual electron density map in the plane of the imidazolium core of the cation. Contours are drawn with 0.1 eÅ^{-3} step, zero and negative ones are dashed.

XD output from invariom refinement of high-resolution X-ray diffraction data

Table I1. Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
CL(1)	8.000	1.011	0.000	1.000	-1.00000
N(1)	5.048	1.005	0.000	0.979	-0.04790
N(3)	5.048	1.005	0.000	0.979	-0.04790
C(2)	3.895	1.023	0.000	1.000	+0.10480
C(4)	3.959	1.019	0.000	1.000	+0.04090
C(5)	3.959	1.019	0.000	1.000	+0.04090
C(6)	3.874	1.014	0.000	1.000	+0.12590
C(7)	3.907	1.012	0.000	1.000	+0.09340
C(8)	3.907	1.012	0.000	1.000	+0.09340
C(9)	3.780	1.018	0.000	1.000	+0.22040
C(10)	3.709	1.026	0.000	1.000	+0.29120
C(11)	3.750	1.018	0.000	1.000	+0.25010
H(4)	1.092	1.082	0.000	1.200	-0.09200
H(5)	1.092	1.082	0.000	1.200	-0.09200
H(6A)	0.959	1.146	0.000	1.200	+0.04130
H(6B)	0.959	1.146	0.000	1.200	+0.04130
H(7A)	1.004	1.127	0.000	1.200	-0.00420
H(7B)	1.004	1.127	0.000	1.200	-0.00420
H(8A)	1.004	1.127	0.000	1.200	-0.00420
H(8B)	1.004	1.127	0.000	1.200	-0.00420
H(9A)	1.025	1.114	0.000	1.200	-0.02520
H(9B)	1.025	1.114	0.000	1.200	-0.02520
H(9C)	1.025	1.114	0.000	1.200	-0.02520
H(10A)	1.006	1.120	0.000	1.200	-0.00550
H(10B)	1.006	1.120	0.000	1.200	-0.00550
H(10C)	1.006	1.120	0.000	1.200	-0.00550
H(11A)	0.985	1.130	0.000	1.200	+0.01490
H(11B)	0.985	1.130	0.000	1.200	+0.01490
H(11C)	0.985	1.130	0.000	1.200	+0.01490

Table I2. Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
CL(1)	0.000	0.000	0.000	1.000
N(1)	0.027	0.022	0.000	0.979
N(3)	0.027	0.022	0.000	0.979
C(2)	0.000	0.000	0.023	1.000
C(4)	-0.032	0.058	0.000	1.000
C(5)	-0.032	0.058	0.000	1.000
C(6)	-0.042	0.003	0.000	1.000
C(7)	0.000	0.000	0.007	1.000
C(8)	0.000	0.000	0.007	1.000
C(9)	0.000	0.000	0.010	1.000
C(10)	0.000	0.000	0.004	1.000
C(11)	0.000	0.000	-0.033	1.000
H(4)	0.000	0.000	0.141	1.200
H(5)	0.000	0.000	0.141	1.200
H(6A)	0.000	0.000	0.146	1.200
H(6B)	0.000	0.000	0.146	1.200
H(7A)	0.000	0.000	0.144	1.200
H(7B)	0.000	0.000	0.144	1.200
H(8A)	0.000	0.000	0.144	1.200
H(8B)	0.000	0.000	0.144	1.200
H(9A)	0.000	0.000	0.151	1.200
H(9B)	0.000	0.000	0.151	1.200
H(9C)	0.000	0.000	0.151	1.200
H(10A)	0.000	0.000	0.158	1.200
H(10B)	0.000	0.000	0.158	1.200
H(10C)	0.000	0.000	0.158	1.200
H(11A)	0.000	0.000	0.154	1.200
H(11B)	0.000	0.000	0.154	1.200
H(11C)	0.000	0.000	0.154	1.200

Table I3. Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
CL(1)	0.000	0.000	0.000	0.000	0.000	1.000
N(1)	0.004	0.000	0.000	0.002	-0.007	0.979
N(3)	0.004	0.000	0.000	0.002	-0.007	0.979
C(2)	0.121	0.000	0.000	-0.091	0.000	1.000
C(4)	-0.104	0.000	0.000	-0.080	-0.003	1.000
C(5)	-0.104	0.000	0.000	-0.080	-0.003	1.000
C(6)	0.041	0.000	0.000	-0.053	-0.005	1.000
C(7)	-0.002	0.000	0.000	0.004	0.000	1.000
C(8)	-0.002	0.000	0.000	0.004	0.000	1.000
C(9)	-0.004	0.000	0.000	0.000	0.000	1.000
C(10)	-0.007	0.000	0.000	0.000	0.000	1.000
C(11)	-0.061	0.000	0.000	0.000	0.000	1.000
H(4)	0.046	0.000	0.000	0.000	0.000	1.200
H(5)	0.046	0.000	0.000	0.000	0.000	1.200
H(6A)	0.065	0.000	0.000	0.000	0.000	1.200
H(6B)	0.065	0.000	0.000	0.000	0.000	1.200
H(7A)	0.063	0.000	0.000	0.000	0.000	1.200
H(7B)	0.063	0.000	0.000	0.000	0.000	1.200
H(8A)	0.063	0.000	0.000	0.000	0.000	1.200
H(8B)	0.063	0.000	0.000	0.000	0.000	1.200
H(9A)	0.063	0.000	0.000	0.000	0.000	1.200
H(9B)	0.063	0.000	0.000	0.000	0.000	1.200
H(9C)	0.063	0.000	0.000	0.000	0.000	1.200
H(10A)	0.068	0.000	0.000	0.000	0.000	1.200
H(10B)	0.068	0.000	0.000	0.000	0.000	1.200
H(10C)	0.068	0.000	0.000	0.000	0.000	1.200
H(11A)	0.069	0.000	0.000	0.000	0.000	1.200
H(11B)	0.069	0.000	0.000	0.000	0.000	1.200
H(11C)	0.069	0.000	0.000	0.000	0.000	1.200

Table I4. Octupole Population Parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
CL(1)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000
N(1)	0.000	0.011	0.007	0.000	0.000	0.158	-0.063	0.979
N(3)	0.000	0.011	0.007	0.000	0.000	0.158	-0.063	0.979
C(2)	0.210	0.000	0.000	0.149	0.000	0.000	0.000	1.000
C(4)	0.000	-0.019	0.030	0.000	0.000	0.220	-0.067	1.000
C(5)	0.000	-0.019	0.030	0.000	0.000	0.220	-0.067	1.000
C(6)	0.000	-0.131	-0.193	0.000	0.000	0.189	-0.024	1.000
C(7)	-0.006	0.000	0.000	-0.281	0.000	0.000	0.000	1.000
C(8)	-0.006	0.000	0.000	-0.281	0.000	0.000	0.000	1.000
C(9)	0.217	0.000	0.000	0.000	0.000	0.168	0.000	1.000
C(10)	0.219	0.000	0.000	0.000	0.000	0.000	-0.165	1.000
C(11)	0.250	0.000	0.000	0.000	0.000	-0.005	-0.176	1.000
H(4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6A)	0.018	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6B)	0.018	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7A)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7B)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8A)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8B)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9A)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9B)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9C)	0.016	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10A)	0.017	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10B)	0.017	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10C)	0.017	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11A)	0.023	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11B)	0.023	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11C)	0.023	0.000	0.000	0.000	0.000	0.000	0.000	1.200

Table I5. Hexadecapole Population Parameters.

Atom	H40	H41+	H41-	H42+	H42-	H43+	H43-	H44+	H44-	Kappa'
CL(1)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000
N(1)	0.008	0.000	0.000	0.002	-0.010	0.000	0.000	0.016	-0.002	0.979
N(3)	0.008	0.000	0.000	0.002	-0.010	0.000	0.000	0.016	-0.002	0.979
C(2)	-0.010	0.000	0.000	-0.035	0.000	0.000	0.000	0.005	0.000	1.000
C(4)	0.024	0.000	0.000	-0.004	-0.022	0.000	0.000	0.031	-0.015	1.000
C(5)	0.024	0.000	0.000	-0.004	-0.022	0.000	0.000	0.031	-0.015	1.000
C(6)	0.017	0.000	0.000	-0.047	0.070	0.000	0.000	0.035	0.018	1.000
C(7)	-0.070	0.000	0.000	0.016	0.000	0.000	0.000	0.048	0.000	1.000
C(8)	-0.070	0.000	0.000	0.016	0.000	0.000	0.000	0.048	0.000	1.000
C(9)	0.026	0.000	0.000	0.000	0.000	-0.075	0.000	0.000	0.000	1.000
C(10)	0.033	0.000	0.000	0.000	0.000	0.000	0.068	0.000	0.000	1.000
C(11)	0.050	0.000	0.000	0.000	0.000	0.003	0.071	0.000	0.000	1.000
H(4)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(5)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(6B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(7B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(8B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9A)	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9B)	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(9C)	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10A)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10B)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(10C)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11A)	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11B)	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200
H(11C)	0.006	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.200

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N(1) C(2) X N(1) C(6) Y

N(3) C(2) X N(3) C(11) Y

C(2) C(10) Z C(2) N(3) Y

C(4) N(3) X C(4) C(5) Y

C(5) N(1) X C(5) C(4) Y

C(6) N(1) X C(6) C(7) Y

C(7) DUM0 Z C(7) C(8) Y

C(8) DUM1 Z C(8) C(9) Y

C(9) C(8) Z C(9) H(9C) X

C(10) C(2) Z C(10) H(10C) Y

C(11) N(3) Z C(11) H(11C) Y

H(4) C(4) Z H(4) C(5) Y

H(5) C(5) Z H(5) C(4) Y

H(6A) C(6) Z H(6A) H(6B) Y

H(6B) C(6) Z H(6B) H(6A) Y

H(7A) C(7) Z H(7A) H(7B) Y

H(7B) C(7) Z H(7B) H(7A) Y

H(8A) C(8) Z H(8A) H(8B) Y

H(8B) C(8) Z H(8B) H(8A) Y

H(9A) C(9) Z H(9A) H(9B) Y

H(9B) C(9) Z H(9B) H(9A) Y

H(9C) C(9) Z H(9C) H(9A) Y

H(10A) C(10) Z H(10A) C(2) Y

H(10B) C(10) Z H(10B) C(2) Y

H(10C) C(10) Z H(10C) C(2) Y

H(11A) C(11) Z H(11A) H(11B) Y

H(11B) C(11) Z H(11B) H(11A) Y

H(11C) C(11) Z H(11C) H(11A) Y

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_atom_site_fract_z

_atom_site_occupancy

_atom_site_symmetry_multiplicity

_atom_site_U_iso_or_equiv

CL(1)	0.065486(15)	0.208793(9)	0.269013(11)	1	4	0.033
N(1)	0.60919(4)	0.04373(3)	0.35300(3)	1	4	0.025
N(3)	0.76282(4)	0.04419(3)	0.51688(3)	1	4	0.022
C(2)	0.68702(5)	0.11187(3)	0.43419(4)	1	4	0.023
C(4)	0.73321(5)	-0.06890(3)	0.48774(4)	1	4	0.025
C(5)	0.63662(5)	-0.06923(3)	0.38456(4)	1	4	0.026
C(6)	0.51112(6)	0.08278(4)	0.24608(5)	1	4	0.033
C(7)	0.61409(6)	0.12604(4)	0.13927(4)	1	4	0.028
C(8)	0.71502(6)	0.03249(4)	0.07969(4)	1	4	0.029
C(9)	0.81275(7)	0.07840(5)	-0.02804(5)	1	4	0.043
C(10)	0.69197(6)	0.23852(4)	0.43508(5)	1	4	0.033
C(11)	0.86062(6)	0.08506(4)	0.62237(4)	1	4	0.030
H(4)	0.776944	-0.138202	0.546172	1	4	0.037
H(5)	0.586909	-0.140785	0.332585	1	4	0.041
H(6A)	0.423528	0.145535	0.277924	1	4	0.044
H(6B)	0.43982	0.009507	0.214958	1	4	0.045
H(7A)	0.693241	0.193818	0.174507	1	4	0.046
H(7B)	0.533985	0.162659	0.068069	1	4	0.050
H(8A)	0.795317	-0.005262	0.150045	1	4	0.044
H(8B)	0.634085	-0.036475	0.050186	1	4	0.050
H(9A)	0.873647	0.00978	-0.077949	1	4	0.061
H(9B)	0.901614	0.140147	0.005829	1	4	0.058
H(9C)	0.733914	0.124222	-0.093105	1	4	0.064
H(10A)	0.597375	0.271368	0.373746	1	4	0.050
H(10B)	0.807906	0.264906	0.398752	1	4	0.050
H(10C)	0.673444	0.266552	0.530752	1	4	0.051
H(11A)	0.788901	0.144586	0.677292	1	4	0.051
H(11B)	0.898656	0.011322	0.678123	1	4	0.047
H(11C)	0.965625	0.128652	0.584649	1	4	0.047

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N(1) 0.02278(16) 0.02613(15) 0.02478(17) -0.00070(11) 0.00176(12) -0.00013(12)

N(3) 0.02221(15) 0.02111(14) 0.02387(16) -0.00105(10) 0.00298(12) -0.00088(12)

C(2) 0.02411(18) 0.01971(15) 0.02546(18) 0.00105(12) 0.00382(13) -0.00068(13)

C(4) 0.0285(2) 0.02086(17) 0.02616(19) -0.00186(13) 0.00299(15) 0.00095(14)

C(5) 0.0283(2) 0.02389(18) 0.0272(2) -0.00558(13) 0.00266(16) -0.00186(14)

C(6) 0.0250(2) 0.0427(3) 0.0305(2) 0.00444(17) -0.00193(17) 0.00073(19)

C(7) 0.0333(2) 0.02553(19) 0.0257(2) 0.00407(14) -0.00276(17) 0.00107(15)

C(8) 0.0324(2) 0.0278(2) 0.0272(2) 0.00466(15) -0.00158(17) 0.00102(16)

C(9) 0.0445(3) 0.0557(3) 0.0282(2) 0.0080(2) 0.0047(2) 0.0064(2)

C(10) 0.0441(3) 0.02065(18) 0.0342(2) 0.00466(16) 0.0058(2) -0.00146(16)

C(11) 0.0295(2) 0.0313(2) 0.0293(2) -0.00167(15) -0.00255(17) -0.00395(17)

H(4) 0.036455 0.032985 0.042856 -0.001231 -0.001072 0.008663

H(5) 0.042193 0.031882 0.049019 -0.005965 -0.007066 -0.005171

H(6A) 0.047788 0.041119 0.043307 0.009697 0.002366 0.001479

H(6B) 0.050265 0.040493 0.044711 -0.006847 -0.006973 -0.002481

H(7A) 0.04914 0.041573 0.048065 -0.004241 0.002991 -0.000047

H(7B) 0.052865 0.059431 0.039099 0.010918 -0.003507 0.008819

H(8A) 0.048207 0.047743 0.035564 0.005828 -0.002039 0.003192

H(8B) 0.05305 0.052668 0.045031 -0.002967 -0.002385 -0.010096

H(9A) 0.075286 0.06284 0.046669 0.016715 0.015224 -0.000205

H(9B) 0.063305 0.062191 0.047385 -0.006556 0.005627 0.007446

H(9C) 0.062548 0.084529 0.045194 0.019458 0.000153 0.020779

H(10A) 0.051644 0.039365 0.05949 0.004876 -0.013715 0.003113

H(10B) 0.043531 0.035945 0.071211 -0.002729 0.011547 -0.000036

H(10C) 0.068493 0.042279 0.043423 0.003667 0.003789 -0.009953

H(11A) 0.046161 0.05726 0.049036 0.014414 -0.000124 -0.019827

H(11B) 0.053278 0.041408 0.04473 0.003043 -0.007504 0.004109

H(11C) 0.043217 0.050876 0.046979 -0.013294 0.004116 -0.003791

Differences of Mean-Squares Displacement Amplitudes (DMSDA) (1.E4 A**2) along the bonds

ATOM-->ATOM		/ DIST	DMSDA	ATOM	/ DIST	DMSDA	ATOM	/ DIST	DMSDA
N(1)	C(2)	1.3398	1	C(5)	1.3799	6	C(6)	1.4706	4
N(3)	C(2)	1.3391	-2	C(4)	1.3784	6	C(11)	1.4643	1
C(2)	C(10)	1.4795	11						
C(4)	C(5)	1.3586	3						
C(6)	C(7)	1.5237	-15						
C(7)	C(8)	1.5226	1						
C(8)	C(9)	1.5175	7						

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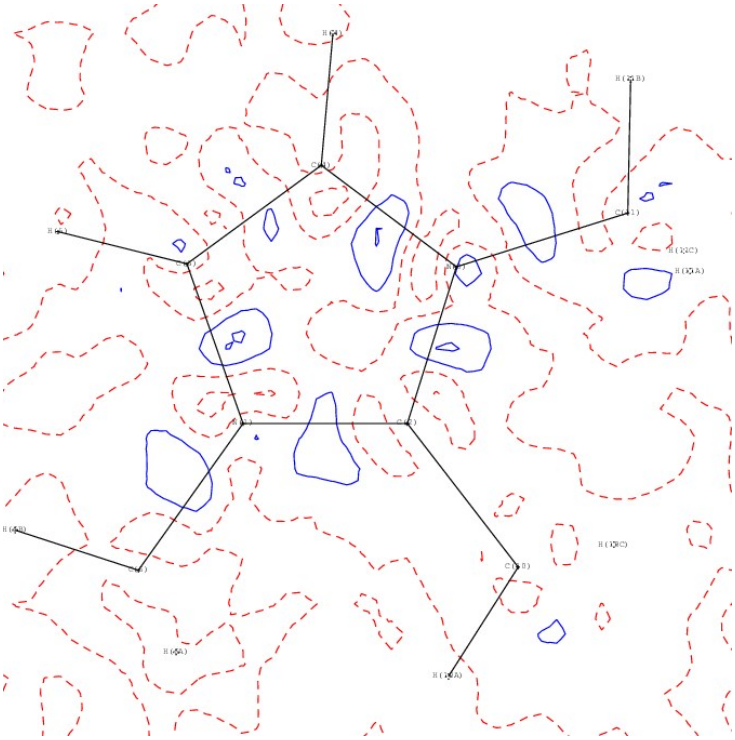

Figure I1. Residual electron density map in the plane of the imidazolium core of the cation. Contours are drawn with 0.1 eÅ^{-3} step, zero and negative ones are dashed.