Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supplementary Information

X-ray crystallographic analysis

X-ray crystallographic analysis reveals that half of the structures crystallise in monoclinic lattices, the [C4mpyr] salts and [C2mim][NTf_2] crystallise in orthorhombic systems. All have one discrete ion pair as the asymmetric unit, except [C2mim][NTf_2] which displays two. All structures, with numbering scheme and thermal ellipsoids, are shown in Figure 1.

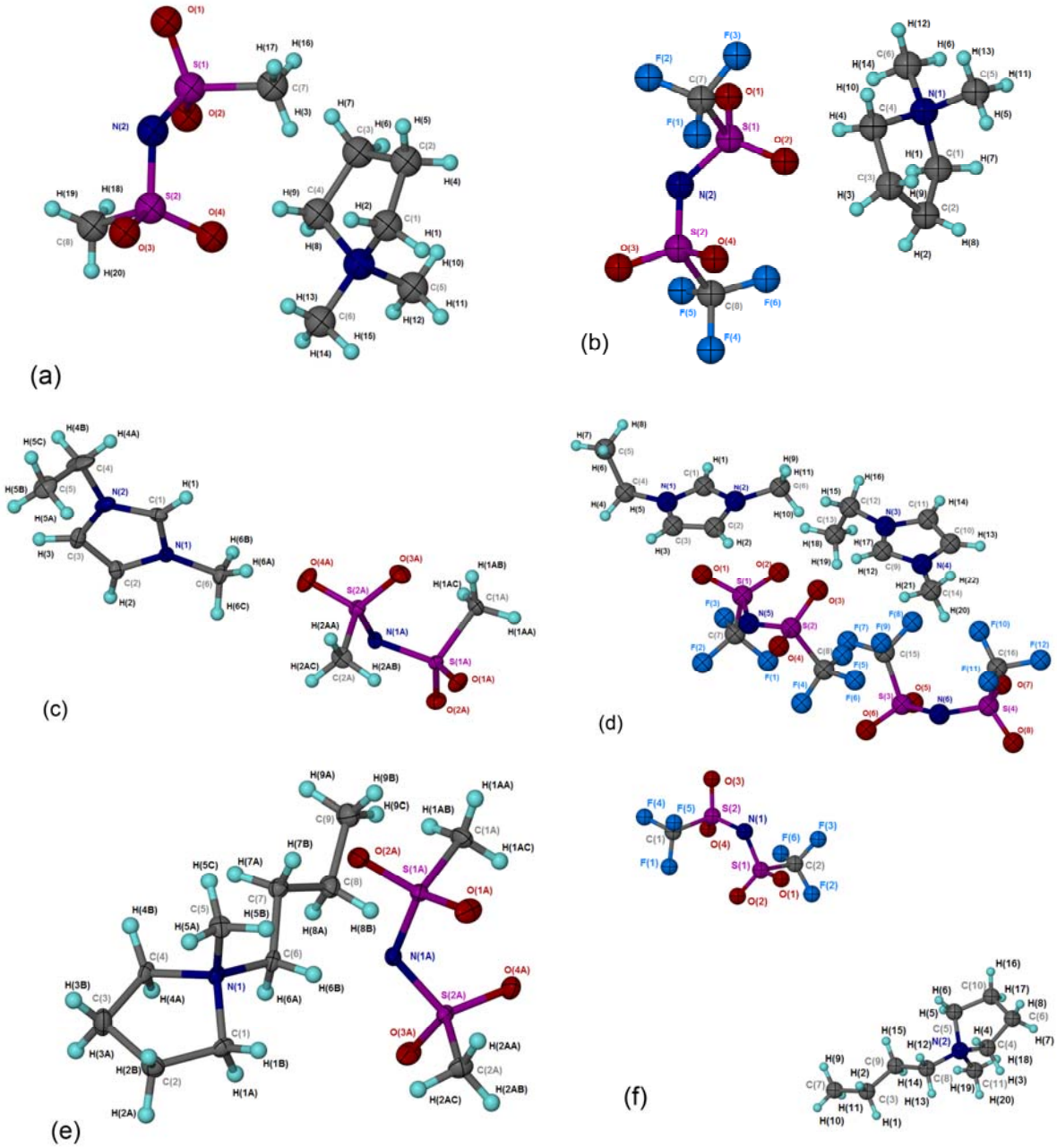


Figure 1. The asymmetric unit of (a) [C1mpyr][$NMes_2$], (b) [C1mpyr][NTf_2], (c) [C2mim][$NMes_2$], (d) [C2mim][NTf_2], (e) [C4mpyr][$NMes_2$] and (f) [C4mpyr][NTf_2] shown with spherical atoms and hydrogen atoms as spheres of arbitrary size. [C2mim][$NMes_2$] and [C4mpyr][$NMes_2$] are shown with 50% thermal ellipsoids.

Low data collection temperatures were used (-150 °C), excepting, once again, [C2mim][NTf_2] where collection took place at -43 °C. The bond distances and angles of the pyrrolidinium cations are all similar, with the alkyl substituents adopting the energetically preferred *anti* conformation and the rings adopting the envelope (C_s) conformation. Similarly, the dimensions of the carbon-nitrogen imidazolium skeleton do not vary significantly. The imidazolium aromatic ring is planar with the β-carbon of the ethyl substituent lying out of the plane of the ring. All of the NTf_2 anions display similar bond distances and angles to each other, as with the $NMes_2$ anionic set. The NTf_2 S-CF_3 groups are orientated *trans* to each other (torsion angles C-S-S-C (°) [C1mpyr], -173.4(1); [C4mpyr], 161.7 (2) °; except [C2mim] which displays the higher energy *cisoid* conformation of 26.8 (12) ° and 27.0 (11) °. The $NMes_2$ anionic set adopts the energetically preferred *transoid* conformation, with C-S-S-C torsion angles of; [C4mpyr], 141.4 (1) °; [C1mpyr], -147.4 (1) and [C2mim] -148.2 (2) °. Overall the $NMes_2$ anions have lower torsion angles due to less steric demand from the CH_3 groups and display shorter S-C bond lengths which are an indication of the difference of electronegativity of fluorine versus hydrogen atoms.

The extended packing diagrams of all of the salts show distinct alternating two-dimensional sheets of anions and cations, all noticeably parallel to or at an approximate 45 degree angle to each one of the planes. The $NMes_2$ salts show shorter cation-anion N···N interaction distances (the centres of nominal charge) than the NTf_2 salts (Table 1), indicating a greater charge concentration on the N atom of the anion due to less electron withdrawing nature of CH_3 groups versus CF_3 groups.

Table 1. Comparison of the shortest cation-anion N···N interaction distances of the $NMes_2$ and NTf_2 ionic liquids.

	$NMes_2$	NTf_2[10,12,13]
	Distance /Å	Distance /Å
[C1mpyr]	4.021(2)[i]	4.543(1)[ii]
[C4mpyr]	3.817(3)	4.233(2)[iii]
[C2mim]	3.718(3)[iv]	3.965(3)

Symmetry operations: (i) 1+x,y,z; (ii) x-1,y,z; (iii) ½-x,1-y,z-½; (iv) x,y,z-1

The extended structure packs in layers of groups of anions and cations which are interconnected by an extended network of weak close contacts identified as C-H···H, C-H···O, C-H···N, C-F···F, C-F···H and C-H···π, of which the most predominant is the C-H···O contact. Each cation is surrounded by several anions and each anion is surrounded by the equivalent amount of cations and a number of anions in all structures. No classical hydrogen bonding is observed in all structures, all non-classical hydrogen bonds and C-H···π interactions are listed in Tables 2 and 3.

Analysis of molecular conformations and other structural parameters was performed using PLATON (Spek, A.L. PLATON, A multipurpose crystallographic tool, Version 10500, © **1980-2000**).

Table 2. Non-classical hydrogen bond data for the bisamide salts.

Compound	X_{donor}---H···$X_{acceptor}$ [Symmetry code]	X_{donor}---H /Å	H··$X_{acceptor}$ /Å	X_{donor}···$X_{acceptor}$ /Å	Angle /° (X_d---H···X_a)
[C1mpyr][NTf_2]	C(1) -- H(1) .. O(2)$^{[x,1/2-y,-1/2+z]}$	0.93(2)	2.31(3)	3.199(2)	161(2)
	C(6) -- H(6) .. O(3)$^{[1+x,1/2-y,-1/2+z]}$	0.944(19)	2.417(18)	3.324(3)	161.0(17)
[C1mpyr][$NMes_2$]	C(1) -- H(2) .. O(1)$^{[1/2-x,-1/2+y,1/2-z]}$	0.989(16)	2.564(15)	3.0618(19)	111.0(10)
	C(7) -- H(3) .. O(1)$^{[1/2-x,-1/2+y,1/2-z]}$	0.954(18)	2.578(18)	3.1214(19)	116.4(13)
	C(4) -- H(8) .. N(2)$^{[1+x,y,z]}$	0.953(16)	2.503(16)	3.4224(19)	162.0(13)
	C(5) -- H(10) .. O(2)$^{[-1/2-x,-1/2+y,1/2-z]}$	0.939(17)	2.363(17)	3.2317(19)	153.7(14)
	C(6) -- H(13) .. O(4)$^{[x,y,z]}$	0.906(17)	2.563(17)	3.450(2)	166.5(15)
	C(6) -- H(14) .. O(3)$^{[1+x,y,z]}$	0.940(17)	2.576(17)	3.465(2)	158.1(14)
[C4mpyr][NTf_2]	C(4) -- H(4) .. O(3)$^{[1/2-x,1-y,1/2+z]}$	0.99	2.58	3.483(5)	151
	C(5) -- H(5) .. O(2)$^{[1/2+x,3/2-y,1-z]}$	0.99	2.59	3.529(6)	158
	C(8) -- H(12) .. O(3)$^{[1/2-x,1-y,1/2+z]}$	0.99	2.55	3.479(6)	156
	C(9) -- H(14) .. O(3)$^{[3/2+x,3/2-y,1-z]}$	0.99	2.52	3.439(6)	155
	C(10) -- H(16) .. O(1)$^{[1/2-x,1-y,1/2+z]}$	0.99	2.60	3.537(5)	159
	C(11) -- H(19) .. O(3)$^{[3/2+x,3/2-y,1-z]}$	0.98	2.53	3.344(5)	140
[C4mpyr][$NMes_2$]	C1 -- H1A .. O3A$^{[-x,1-y,-z]}$	0.97(2)	2.51(2)	3.296(2)	137.9(18)
	C1 -- H1B .. O4A$^{[1/2-x,-1/2+y,z]}$	0.95(2)	2.52(2)	3.271(2)	135.5(17)
	C2 -- H2B .. O1A$^{[1/2-x,-1/2+y,z]}$	0.94(2)	2.53(2)	3.444(3)	165(2)
	C4 -- H4A .. O3A$^{[-x,1-y,-z]}$	0.95(2)	2.41(2)	3.205(2)	140.5(18)
	C5 -- H5B .. N1A$^{[x,y,z]}$	0.96(3)	2.54(2)	3.455(2)	159.2(19)
	C5 -- H5C .. O1A$^{[-1/2+x,y,1/2-z]}$	0.97(2)	2.59(2)	3.556(2)	174.2(18)
	C6 -- H6A .. O3A$^{[-x,1-y,-z]}$	0.96(2)	2.57(2)	3.415(2)	146.2(17)
	C6 -- H6B .. O3A$^{[x,y,z]}$	0.94(2)	2.53(2)	3.416(2)	156.6(19)
[C2mim][NTf_2]	C(1) -- H(1) .. O(5)$^{[2-x,-y,-1/2+z]}$	0.93	2.47	3.26(3)	143
	C(1) -- H(1) .. O(7)$^{[2-x,-y,-1/2+z]}$	0.93	2.49	3.29(2)	144
	C(2) -- H(2) .. O(6)$^{[3/2-x,y,-1/2+z]}$	0.93	2.25	3.16(2)	163
	C(3) -- H(3) .. O(8)$^{[3/2-x,-1+y,-1/2+z]}$	0.93	2.50	3.42(3)	175
	C(6) -- H(9) .. O(5)$^{[2-x,-y,-1/2+z]}$	0.96	2.60	3.46(2)	151
	C(6) -- H(10) .. O(3)$^{[x,y,z]}$	0.96	2.52	3.43(3)	156
	C(9) -- H(12) .. O(2)$^{[x,y,z]}$	0.93	2.53	3.29(2)	139
	C(9) -- H(12) .. O(3)$^{[x,y,z]}$	0.93	2.46	3.30(3)	149
	C(10) -- H(13) .. O(4)$^{[1/2+x,1-y,z]}$	0.93	2.37	3.26(3)	159
	C(11) -- H(14) .. O(1)$^{[1/2+x,-y,z]}$	0.93	2.60	3.53(3)	177
	C(14) -- H(22) .. O(5)$^{[2-x,1-y,-1/2+z]}$	0.96	2.48	3.43(2)	169
[C2mim][$NMes_2$]	C1 -- H1 .. O4A$^{[x,y,1+z]}$	0.95	2.55	3.193(2)	125
	C3 -- H3 .. O2A$^{[-x,1/2+y,1-z]}$	0.95	2.59	3.457(2)	151
	C2A -- H2AA .. O2A$^{[-x,1/2+y,1-z]}$	0.98	2.50	3.4465(19)	163
	C6 -- H6A .. O2A$^{[x,y,1+z]}$	0.98	2.56	3.431(2)	149
	C6 -- H6C .. O3A$^{[-1+x,y,z]}$	0.98	2.30	3.198(2)	153

Table 3. X--H···π ring interactions

Compound	X_{donor}-H-> Cg1	Symmetry Code	*d* H···Cg(J) /Å	*d* X···Cg(J) /Å	Angle /° (X-H···Cg(J))
[C2mim][$NMes_2$]	C1A -H1AC -> Cg1	[1+X,Y,-1+Z]	2.6051	3.438(2)	143.00

Where: Cg1 is the centre of gravity for the imidazolium ring.

Selected bond distances and angles for the above identified close contacts for the anions are listed in Table 4. These distances are contacts less than the sum of the van der Waals Radii as those given by A.Bondi, J.Phys.Chem. (1964), 68, 441.

Table 4. Close contact bond distances and angles for the bisamide anions.

Compound	$X_{donor}\cdots X_{acceptor}$	Symmetry code	$X_{donor}\cdots X_{acceptor}$ /Å	Angle /° (X_d---H$\cdots X_a$)
[C1mpyr][NTf_2]	F(4) .... H(10)	[2-x,-1/2+y,3/2-z]	2.58(2)	131.0(5)
	F(1) .... F(5)	[x,1/2-y,1/2+z]	2.9840(17)	
	F(2) .... F(4)	[1-x,1/2+y,3/2-z]	3.0859(19)	169.93(13)
	F(3) .... F(6)	[2-x,1/2+y,3/2-z]	3.0104(19)	150.79(14)
	F(4) .... F(2)	[1-x,-1/2+y,3/2-z]	3.0859(19)	
	F(4) .... H(2)	[2-x,-y,1-z]	2.79(3)	
	F(5) .... H(8)	[-1+x,y,z]	2.63(3)	128.2(6)
	F(5) .... F(1)	[x,1/2-y,1/2+z]	2.9840(17)	108.03(10)
	F(6) .... H(3)	[x,y,z]	2.64(3)	158.0(6)
	F(6) .... F(3)	[2-x,-1/2+y,3/2-z]	3.0104(19)	127.49(11)
	O(1) .... H(12)	[2-x,1-y,1-z]	2.64(2)	164.3(5)
	O(2) .... H(1)	[x,1/2-y,1/2+z]	2.31(3)	156.8(6)
	O(3) .... H(6)	[-1+x,1/2-y,1/2+z]	2.417(18	153.7(5)
[C1mpyr][$NMes_2$]	O(1) .... H(3)	[1/2-x,1/2+y,1/2-z]	2.578(18)	116.9(4)
	N(2) .... H(8)	[1+x,y,z]	2.503(16)	120.6(3)
	O(1) .... H(2)	[1/2-x,1/2+y,1/2-z]	2.564(15)	159.0(3)
	O(1) .... H(15)	[1/2+x,1/2-y,-1/2+z]	2.699(16)	142.8(4)
	O(2) .... H(10)	[-1/2-x,1/2+y,1/2-z]	2.363(17)	112.5(4)
	O(4) .... H(15)	[-x,-y,1-z]	2.725(18)	125.6(4)
	H(19) .... O(3)	[1-x,1-y,1-z]	2.748(18)	170.2(14)
	O(3) .... H(16)	[1/2+x,1/2-y,1/2+z]	2.678(19)	152.3(4)
	H(3) .... O(1)	[1/2-x,-1/2+y,1/2-z]	2.578(18)	116.4(13)
	H(16) .... O(3)	[-1/2+x,1/2-y,-1/2+z]	2.678(19)	170.7(15)
[C4mpyr][NTf_2]	O(1) .... H(3)	[3/2-x,1-y,-1/2+z]	2.6229	110.53
	F(1) .... F(2)	[1/2-x,1-y,-1/2+z]	3.046(4)	116.3(2)
	O(2) .... H(5)	[-1/2+x,3/2-y,1-z]	2.5912	134.35
	F(2) .... H(2)	[-1+x,y,z]	2.7979	
	F(2) .... F(1)	[1/2-x,1-y,1/2+z]	3.046(4)	140.6(2)
	O(3) .... H(12)	[1/2-x,1-y,-1/2+z]	2.5507	139.65
	O(1) .... H(7)	[1-x,-1/2+y,3/2-z]	2.6523	165.11
	F(5) .... F(6)	[-x,-1/2+y,1/2-z]	2.928(5)	154.4(3)
	F(6) .... F(5)	[-x,1/2+y,1/2-z]	2.928(5)	162.4(3)
	O(3) .... H(14)	[-3/2+x,3/2-y,1-z]	2.5169	118.95
[C4mpyr][$NMes_2$]	O3A H6B	[x,y,z]	2.53(2)	102.1(5)
	O4A H1B	[1/2-x,1/2+y,z]	2.52(2)	146.8(5)
	O2A H3B	[-x,1/2+y,1/2-z]	2.68(3)	114.3(7)
	O2A H9A	[-x,-1/2+y,1/2-z]	2.75(3)	162.1(5)
	H2AC O4A	[1/2-x,-1/2+y,z]	2.63(2)	164(2)
	O3A H4A	[-x,1-y,-z]	2.41(2)	127.3(5)
	O4A H8A	[1/2+x,3/2-y,-z]	2.85(2)	107.7(5)
	O4A H2AC	[1/2-x,1/2+y,z]	2.63(2)	117.2(5)
[C2mim][NTf_2]	F(1) .... C(2)	[3/2-x,y,1/2+z]	3.33(2)	124.9(13)
(N5)	F(3) .... F(11)	[x,-1+y,z]	2.79(2)	141.6(14)
	F(3) .... H(20)	[x,-1+y,z]	2.7659	126.84
	F(4) .... H(8)	[3/2-x,1+y,1/2+z]	2.7812	106.22
	F(4) .... F(12)	[-1/2+x,1-y,z]	2.80(2)	157.0(16)
	F(5) .... F(9)	[x,y,z]	2.99(2)	165.7(14)
	F(6) .... O(1)	[x,1+y,z]	3.157(18)	154.1(15)
	O(3) .... H(10)	[x,y,z]	2.5219	130.84
	O(1) .... H(14)	[-1/2+x,-y,z]	2.5994	116.33
	O(3) .... H(12)	[x,y,z]	2.4618	128.09
	O(3) .... H(5)	[x,1+y,z]	2.7377	114.79
	O(4) .... H(13)	[-1/2+x,1-y,z]	2.3736	144.20
	O(4) .... O(6)	[3/2-x,y,-1/2+z]	3.22(2)	121.1(8)
[C2mim][NTf_2]	F(7) .... F(12)	[x,-1+y,z]	2.911(18)	141.2(15)
(N6)	F(9) .... F(5)	[x,y,z]	2.99(2)	152.3(14)

	F(9) .... H(19)	[x,y,z]	2.8323	
	F(11) .... F(3)	[x,1+y,z]	2.79(2)	167.9(13)
	F(12) .... F(7)	[x,1+y,z]	2.911(18)	105.9(12)
	F(12) .... C(13)	[x,1+y,z]	3.34(2)	108.5(11)
	F(12) .... H(11)	[2-x,1-y,1/2+z]	2.6410	139.66
	F(12) .... F(4)	[1/2+x,1-y,z]	2.80(2)	120.9(11)
	O(5) .... H(1)	[2-x,-y,1/2+z]	2.4743	126.93
	O(5) .... H(15)	[2-x,-y,1/2+z]	2.7908	118.23
	O(5) .... H(22)	[2-x,1-y,1/2+z]	2.4837	123.33
	O(6) .... O(4)	[3/2-x,y,1/2+z]	3.22(2)	119.7(8)
	O(6) .... H(2)	[3/2-x,y,1/2+z]	2.2540	153.76
	O(8) .... H(3)	[3/2-x,1+y,1/2+z]	2.4958	119.09
[C2mim][$NMes_2$]	O4A H1	[x,y,-1+z]	2.5508	103.32
	O1A H6B	[1-x,-1/2+y,1-z]	2.7096	150.72
	O2A H3	[-x,-1/2+y,1-z]	2.5942	
	O2A H2AA	[x,y,-1+z]	2.4993	152.25
	O3A H6C	[1+x,y,z]	2.2964	161.50
	O4A H6B	[x,y,z]	2.6591	123.09
	H2AA O2A	[x,y,1+z]	2.4993	162.60

It is immediately apparent that, although useful, these meticulous tables are tedious and time consuming to prepare. The Hirshfeld Surface and its associated fingerprint plot are effective and efficient whereby the basic close contact information relayed in these tables are immediately apparent in a visual manner. Additionally the fingerprint plots' elucidates information of the entire lattice and not only close atom-atom contacts. It is highly recommended to utilise these two techniques, standard crystallographic analysis and the Hirshfeld analysis, in unison to fully understand the intermolecular interactions occurring in a crystal.

Table 5. Comparison of the mean *dnorm* of the $NMes_2$ and NTf_2 Hirshfeld surfaces.

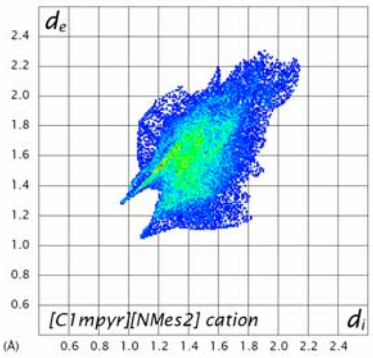
	Cation	Anion
[C1mpyr][$NMes_2$]	0.3421	0.3564
[C1mpyr][NTf_2]	0.4212	0.3875
[C4mpyr][$NMes_2$]	0.4082	0.3786
[C4mpyr][NTf_2]	0.4618	0.4360
[C2mim][$NMes_2$]	0.3623	0.3259
[C2mim][NTf_2]	0.4515 *(N1)*/ 0.4454 (*(N3)*	0.4280 *(N5)*/ 0.4132 *(N6)*

Hirshfeld Analysis

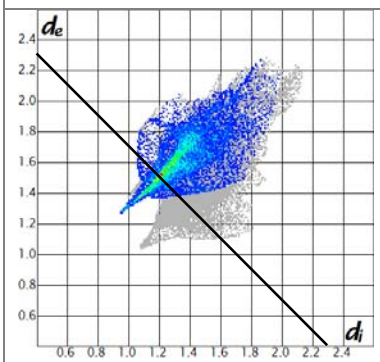
Legend:
Close Contacts X···Y
Where: X=atom inside the surface
Y=atom outside the surface

[C1mpyr][NMes2]

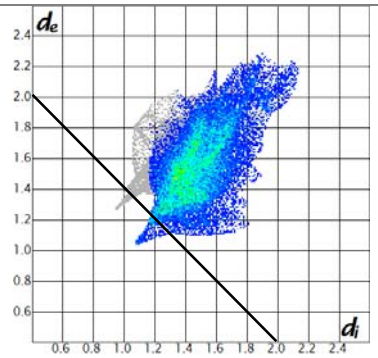
Cation: Full Plot



Cation-anion close contacts



H···O 28.6 %



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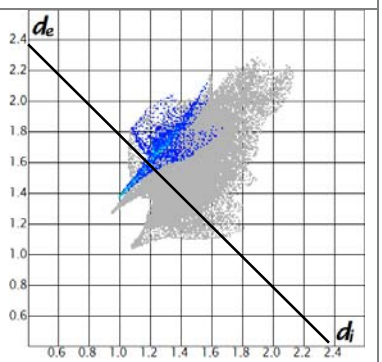

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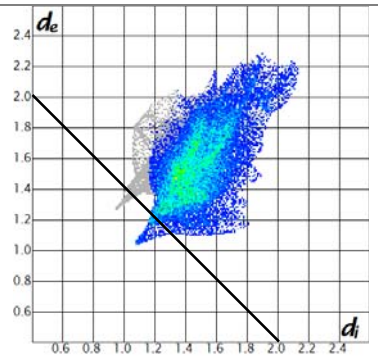
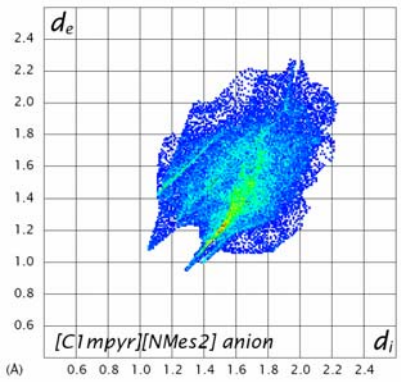
Cation-cation close contacts

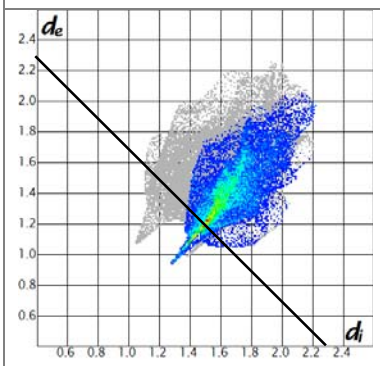


H···H 66.9 %

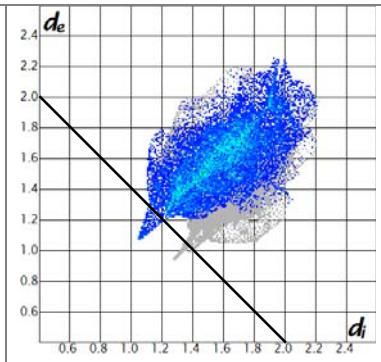
Anion: Full Plot



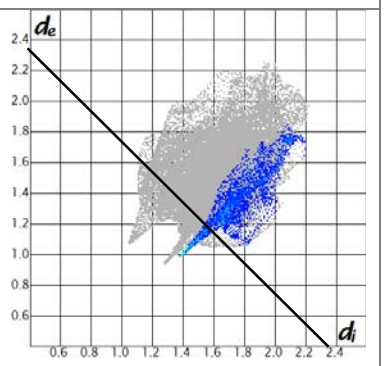
Cation-anion close contacts



O···H 43.1 %

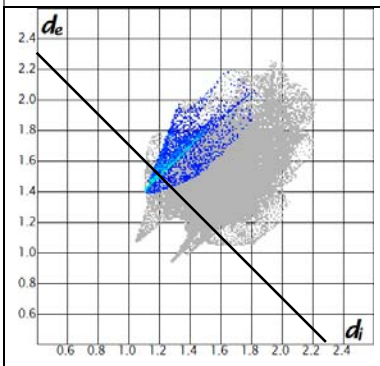


H···H 43.1 %



N···H 6.1 %

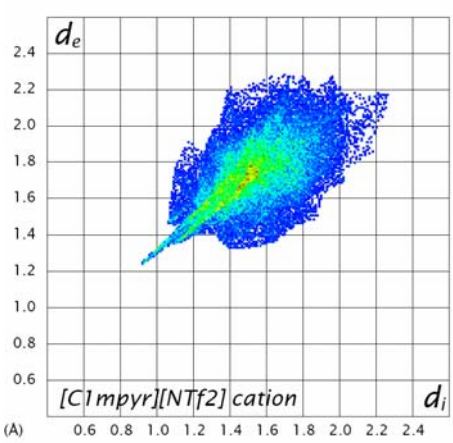
Anion-anion close contacts



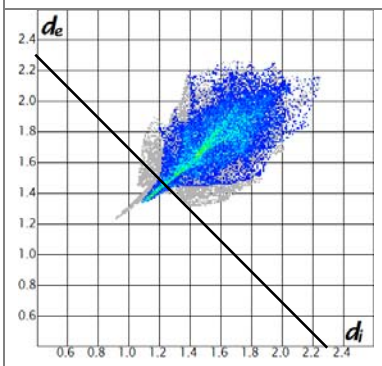
H···O 7.1 %

[C1mpyr][NTf2]

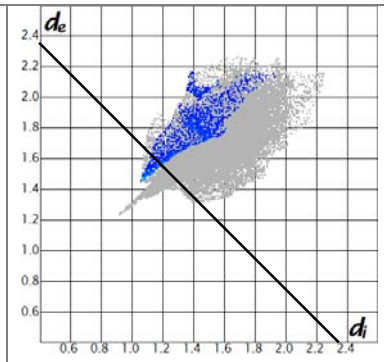
Cation: Full Plot



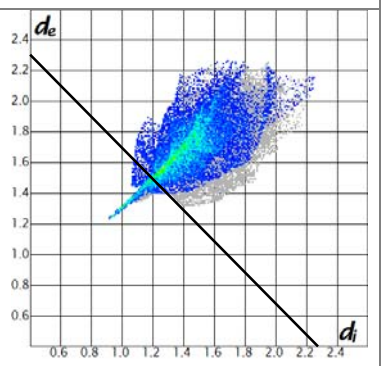
Cation-anion close contacts



H···F 36.6 %

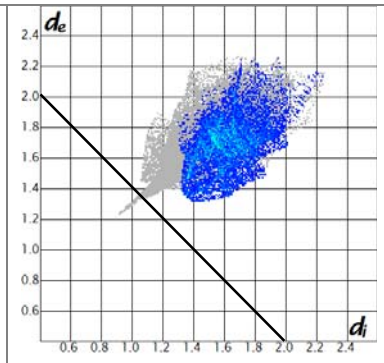


H···N 4.1 %



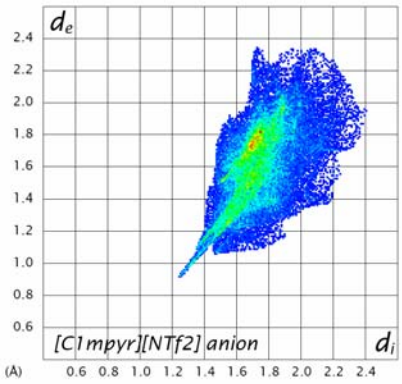
H···O 37.8 %

Cation-cation close contacts

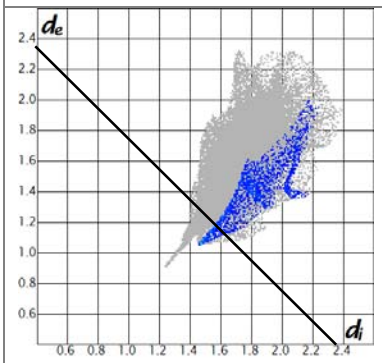


H···H 21.6 %

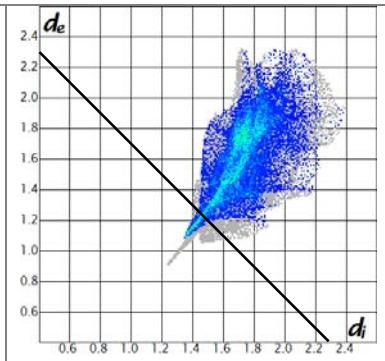
Anion: Full Plot



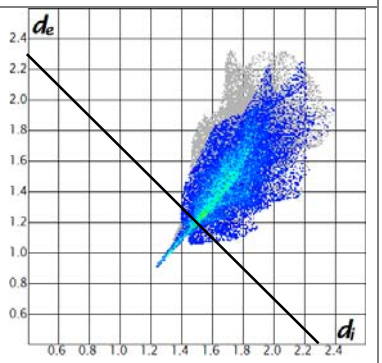
Cation-anion close contacts



N···H 3.7 %

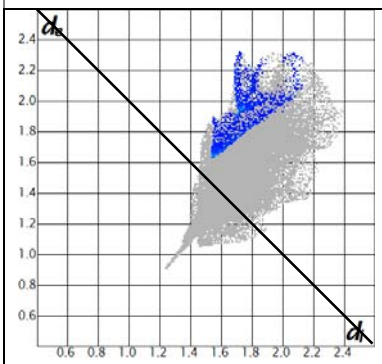


F···H 33.4 %

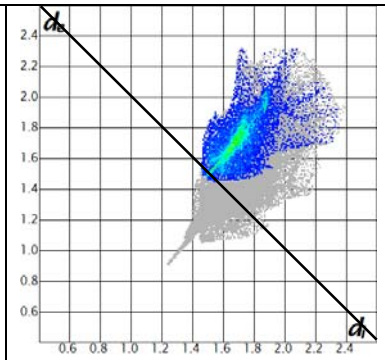


O···H 33.9 %

Anion-anion close contacts



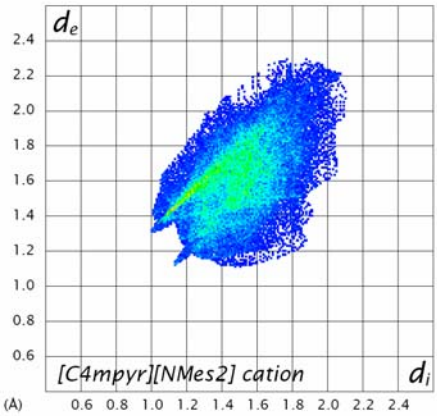
F···O 2.9 %



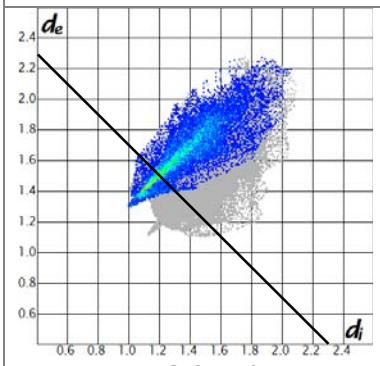
F···F 21.8 %

[C4mpyr][NMes2]

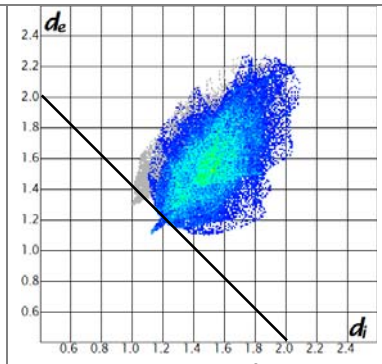
Cation: Full Plot



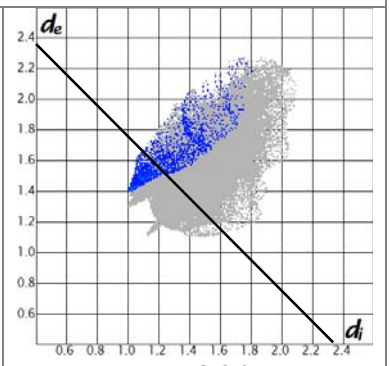
Cation-anion close contacts



H···O 25.5 %

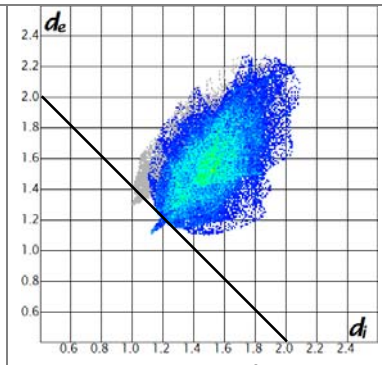


H···H 71.5 %



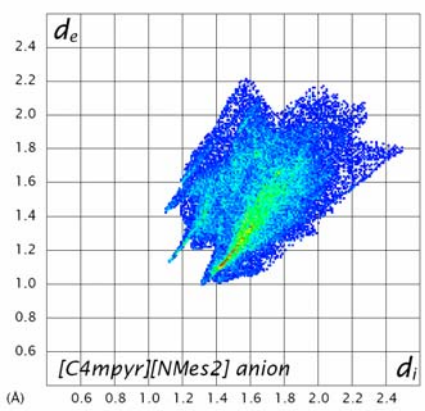
H···N 3.0 %

Cation-cation close contacts

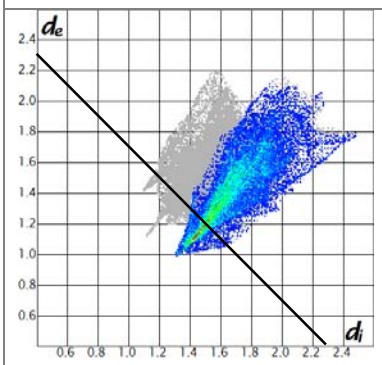


H···H 71.5 %

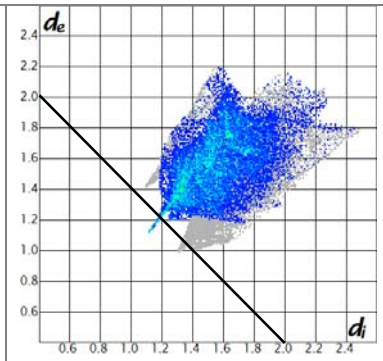
Anion: Full Plot



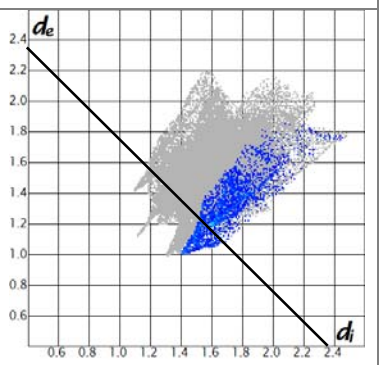
Cation-anion close contacts



O···H 44.7 %

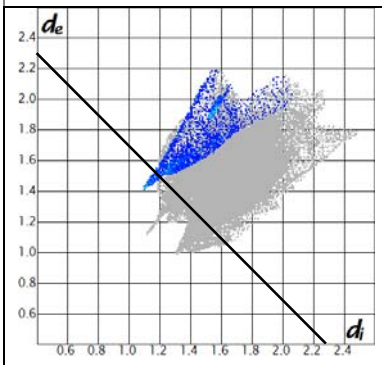


H···H 43.1 %



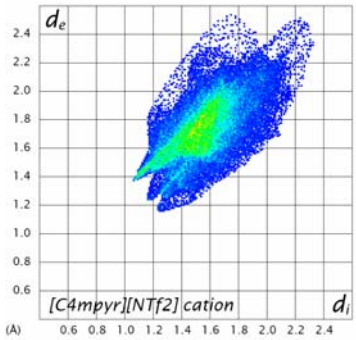
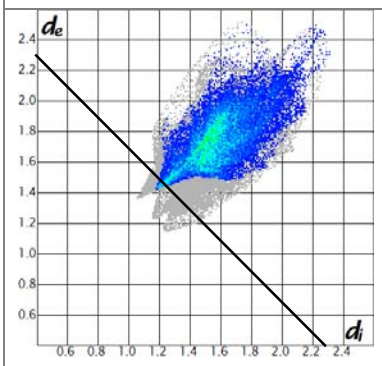
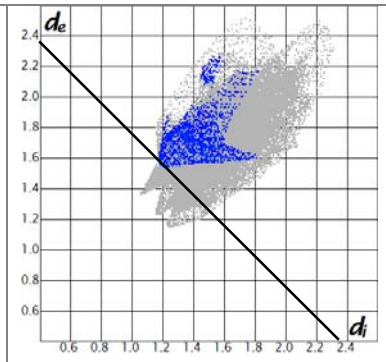
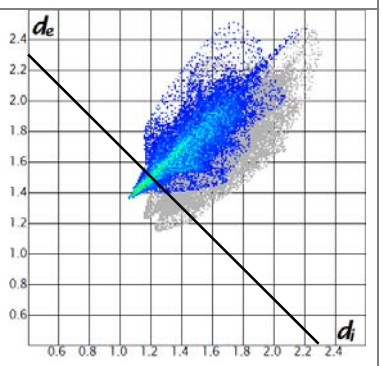
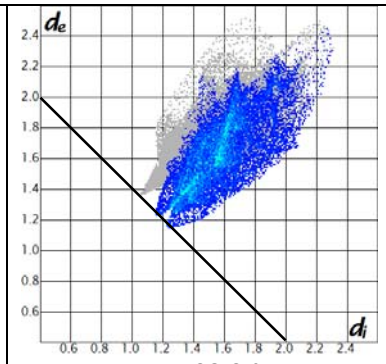
N···H 6.0 %

Anion-anion close contacts

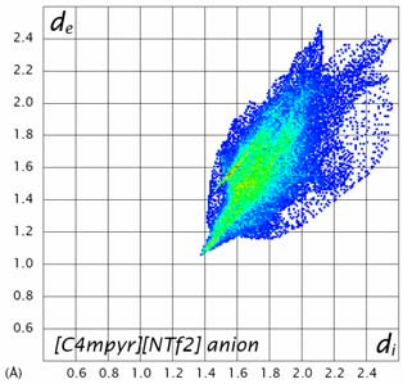


H···O 4.9 %

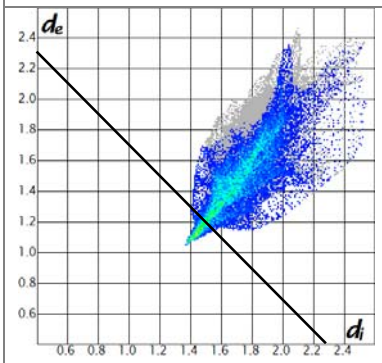
[C4mpyr][NTf2]

Cation: Full Plot

Cation-anion close contacts
 *H···F 38.7 %*  *H···N 3.2 %*  *H···O 29.8 %*
Cation-cation close contacts
 *H···H 28.2 %*

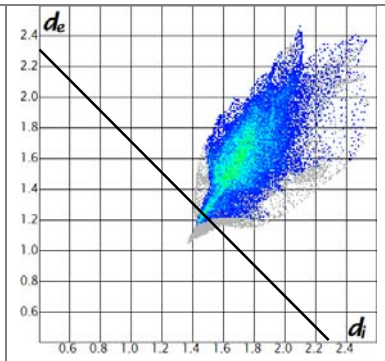
Anion: Full Plot



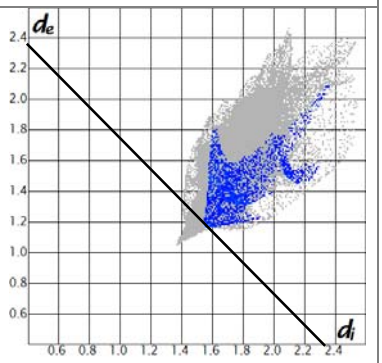
Cation-anion close contacts



O···H 37.7 %

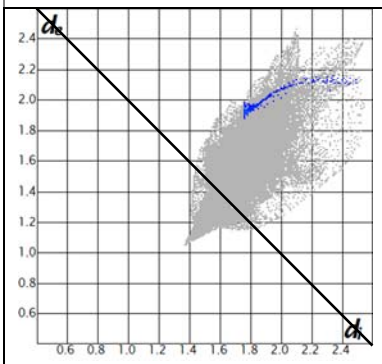


F···H 48.0 %

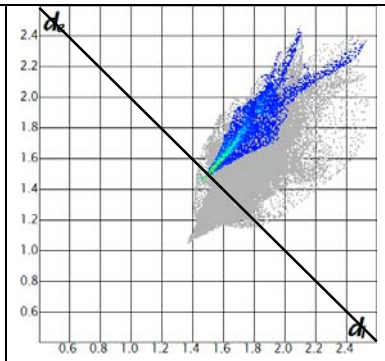


N···H 4.0 %

Anion-anion close contacts



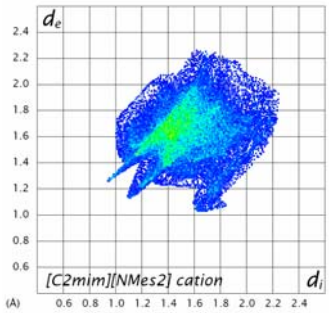
F···O 0.4 %



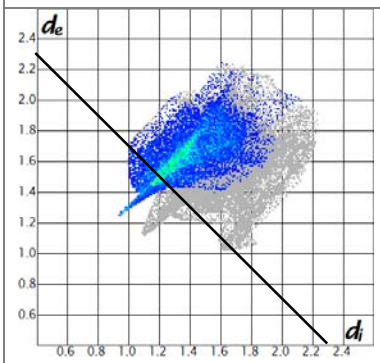
F···F 9.2 %

[C2mim][NMes2]

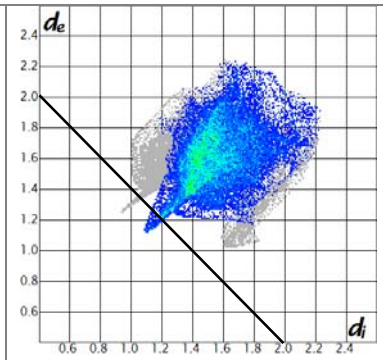
Cation: Full Plot



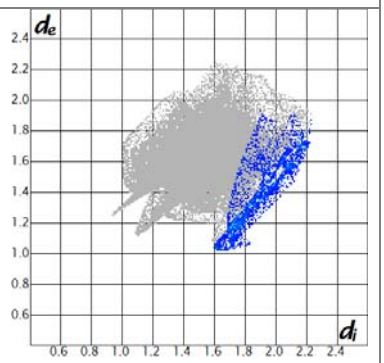
Cation-anion close contacts



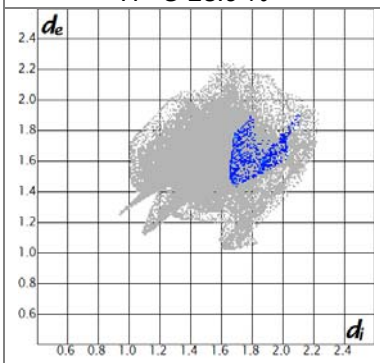
H···O 28.9 %



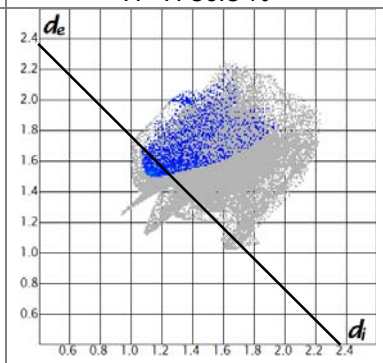
H···H 56.5 %



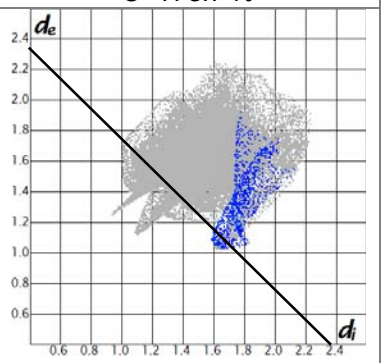
C···H 5.7 %



C···O 1.7 %

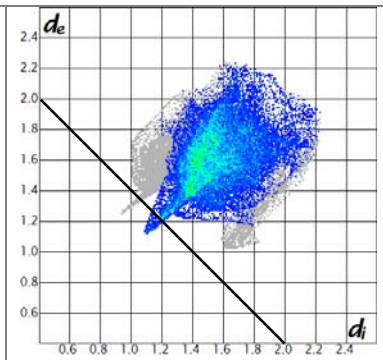


H···N 3.5 %



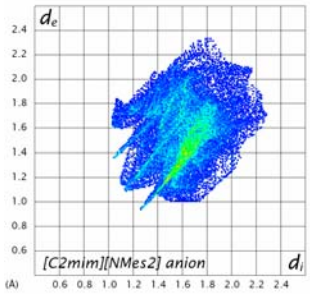
N···H 2.4 %

Cation-cation close contacts

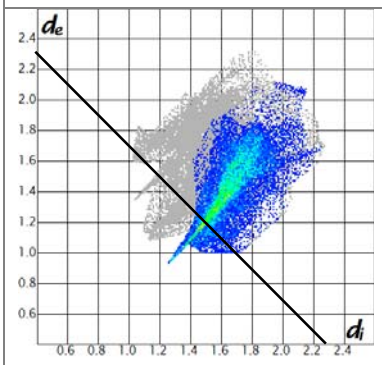


H···H 56.5 %

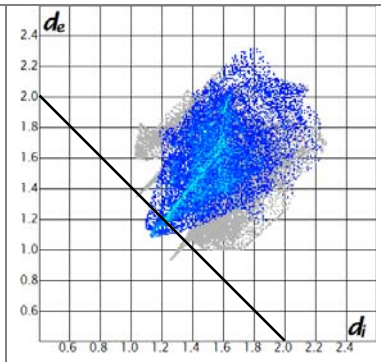
Anion: Full Plot



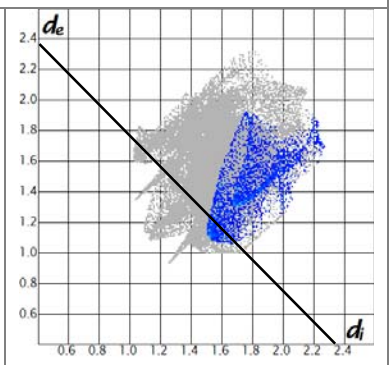
Cation-anion close contacts



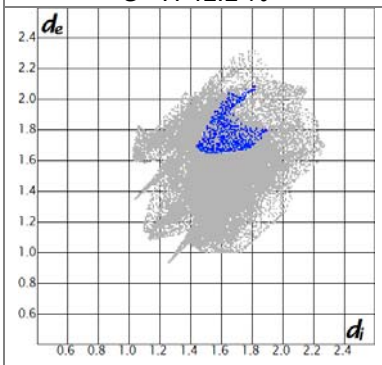
O···H 41.1 %



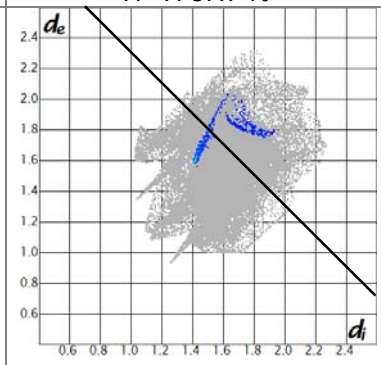
H···H 37.7 %



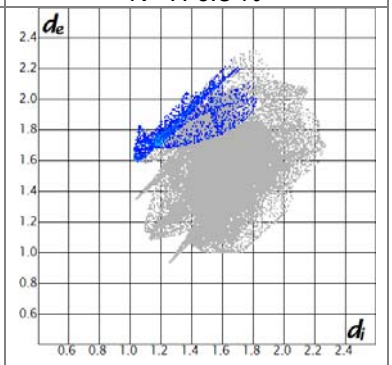
N···H 6.5 %



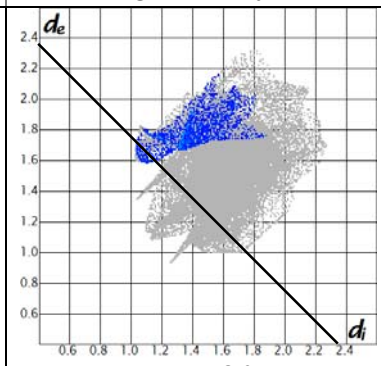
O···C 1.6 %



O···N 1.2 %

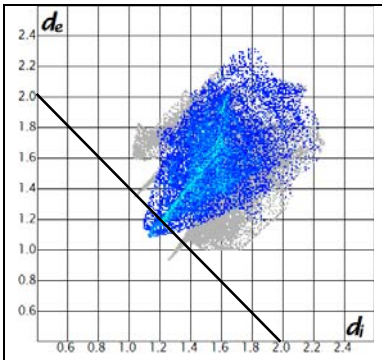


H···C 4.2 %

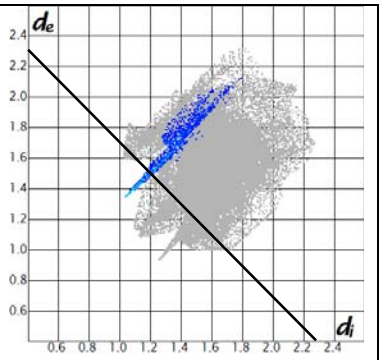


H···N 4.3 %

Anion-anion close contacts



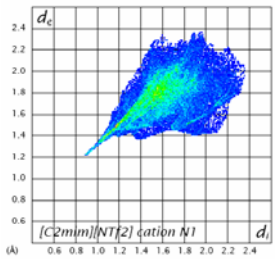
H···H 37.7 %



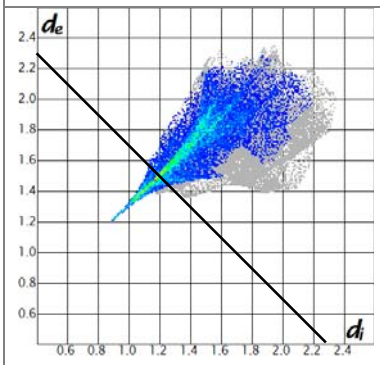
H···O 3.2 %

[C2mim][NTf2]

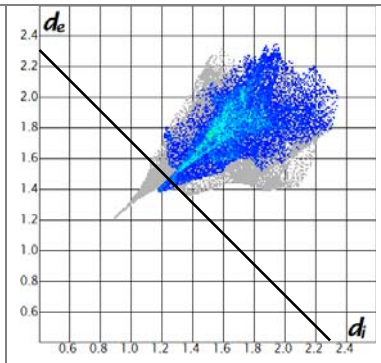
Cation: Full Plot



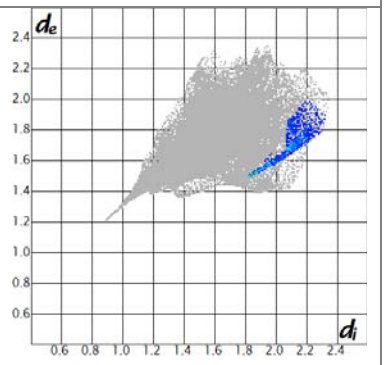
Cation-anion close contacts



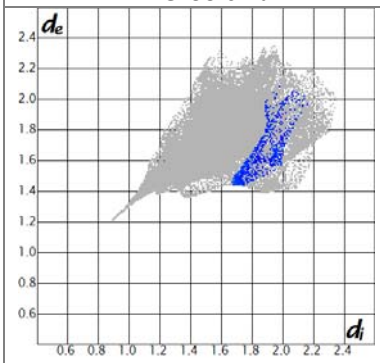
H···O 33.0 %



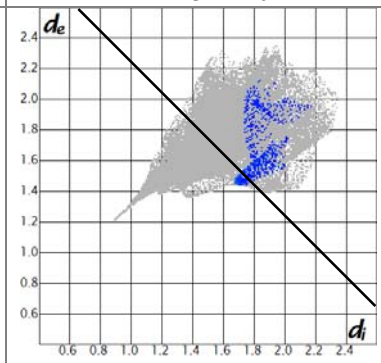
H···F 32.2 %



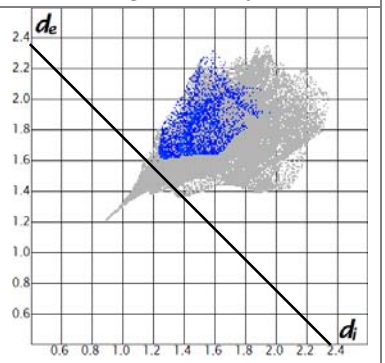
C···F 2.7 %



C···O 1.7 %

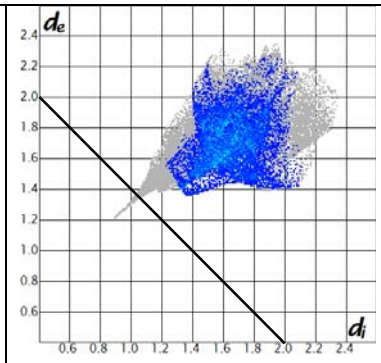


N···O 1.9 %



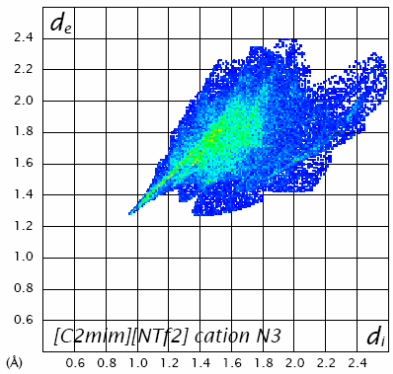
H···N 3.9 %

Cation-cation close contacts

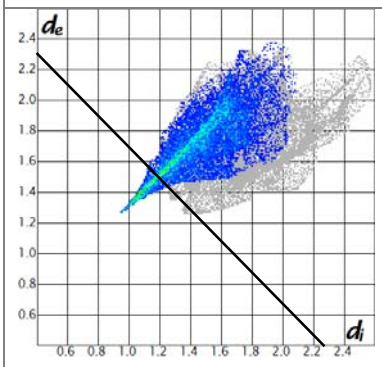


H···H 21.4 %

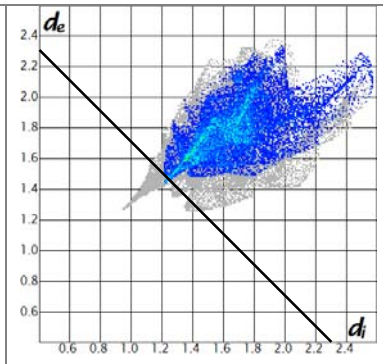
Cation: Full Plot



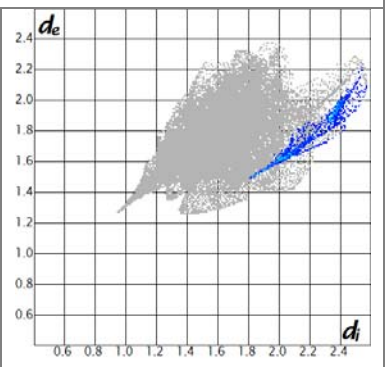
Cation-anion close contacts



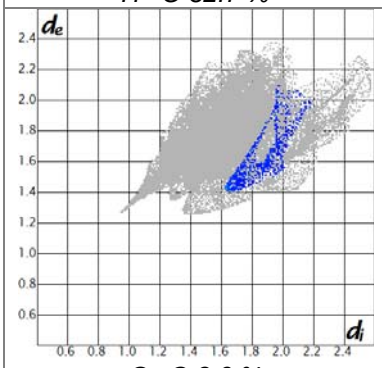
H···O 32.7 %



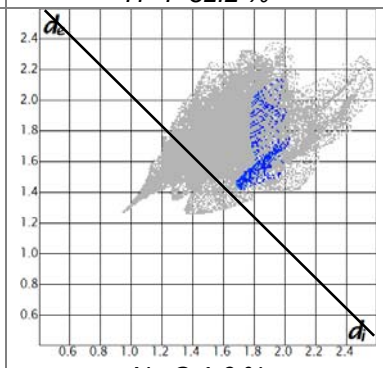
H···F 31.2 %



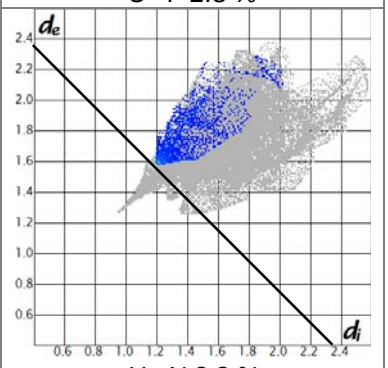
C···F 2.8 %



C···O 2.0 %

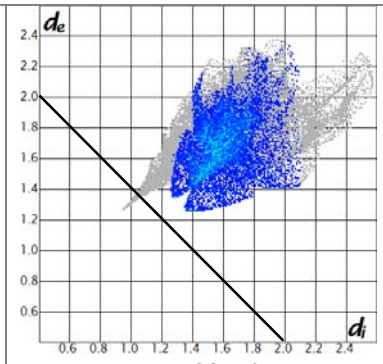


N···O 1.6 %



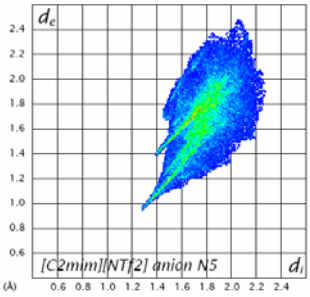
H···N 3.8 %

Cation-Cation close contacts

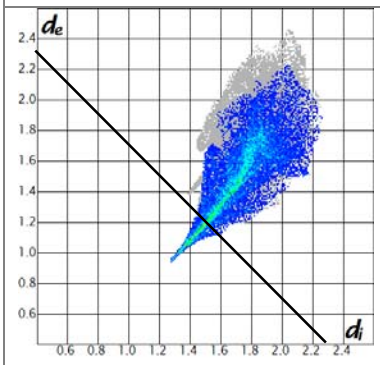


H···H 22.5 %

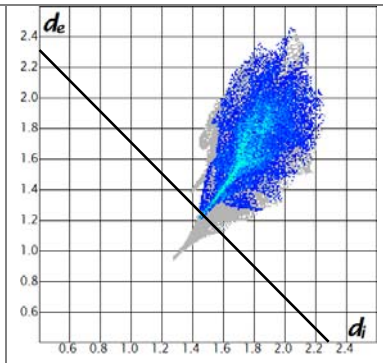
Anion: Full Plot



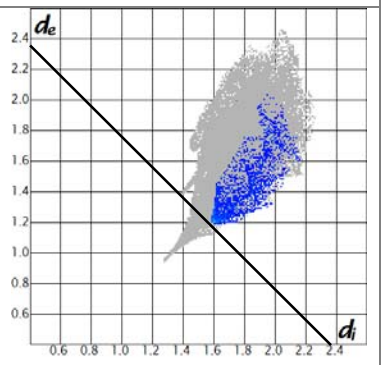
Cation-anion close contacts



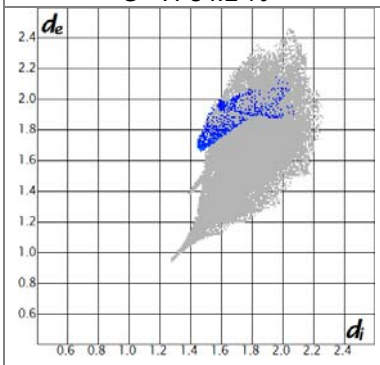
O···H 34.1 %



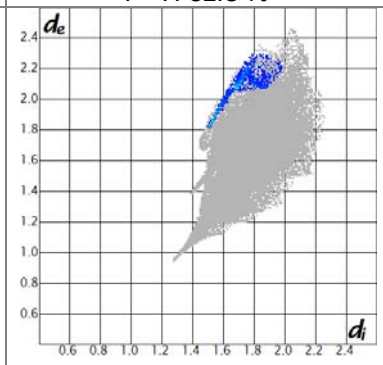
F···H 31.8 %



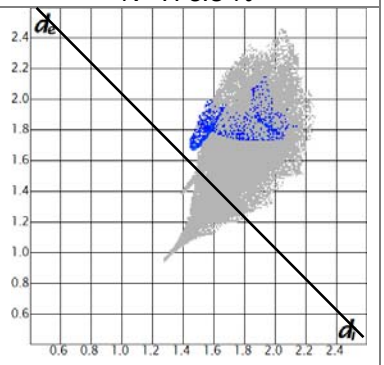
N···H 3.8 %



O···C 1.5 %

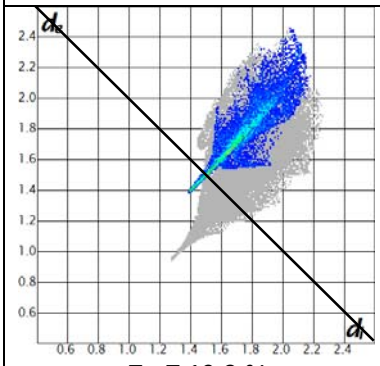


F···C 2.4 %

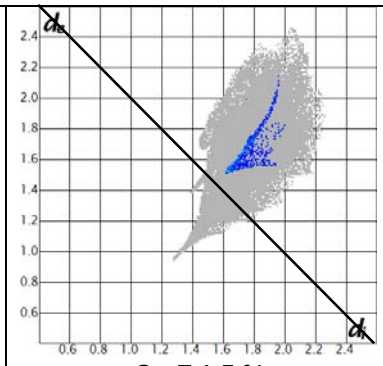


O···N 1.7 %

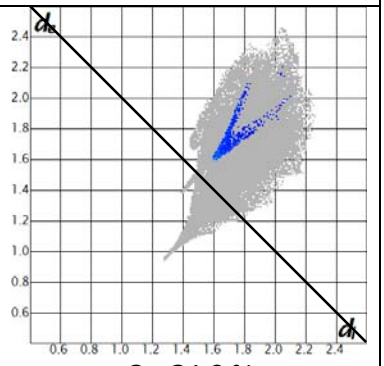
Anion-anion close contacts



F···F 19.2 %

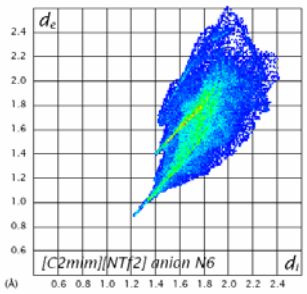


O···F 1.5 %

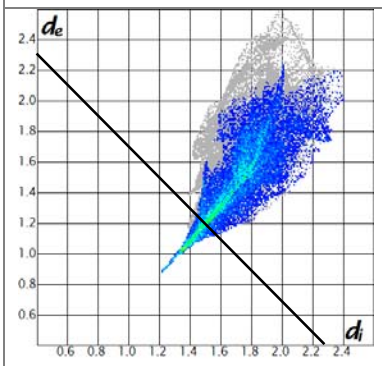


O···O1.3 %

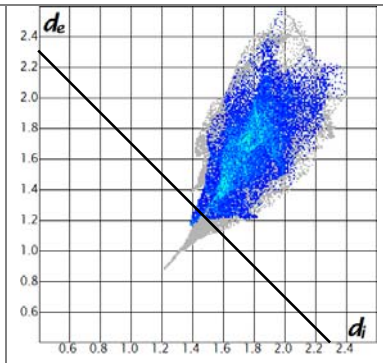
Anion: Full Plot



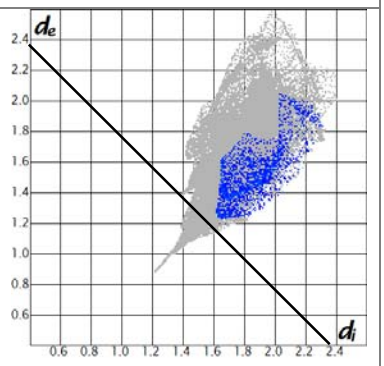
Cation-anion close contacts



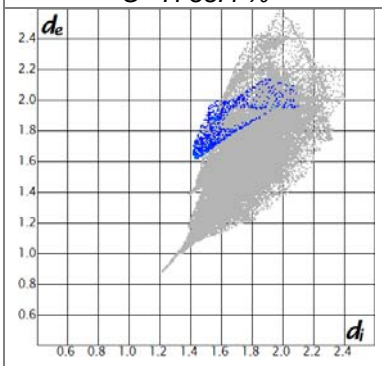
O···H 35.4 %



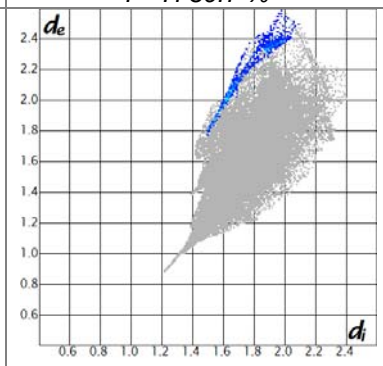
F···H 30.7 %



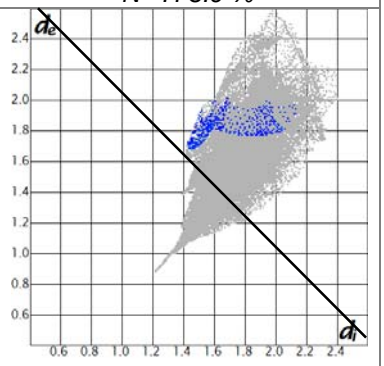
N···H 3.9 %



O···C 1.6 %

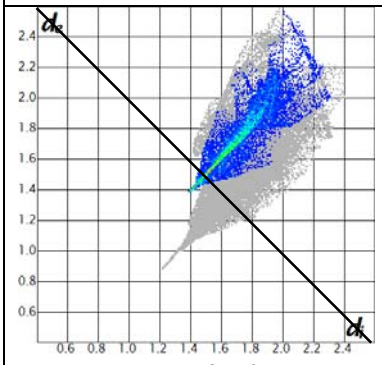


F···C 2.3 %

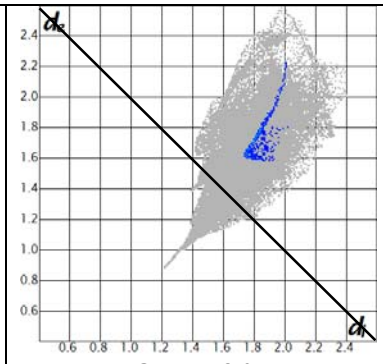


O···N 1.3 %

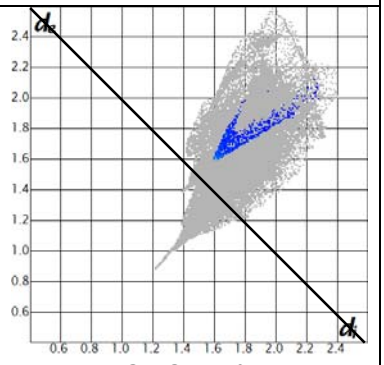
Anion-anion close contacts



F···F 19.7 %



O···F 1.0 %



O···O 1.4 %