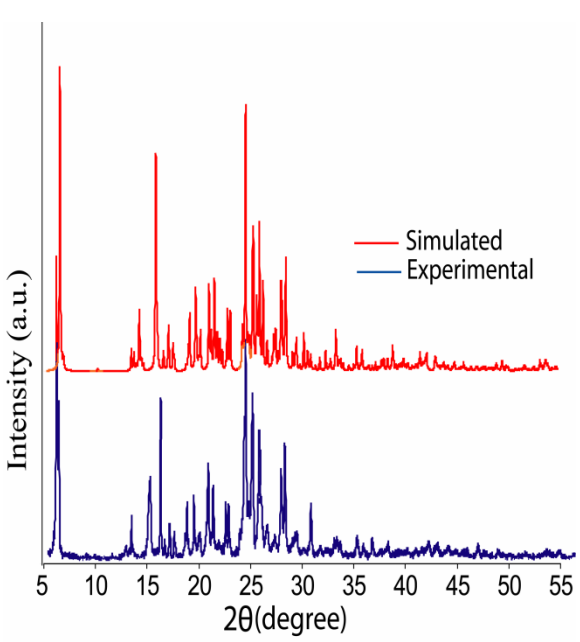
Electronic Supplementary Material (ESI) for New Journal of Chemistry

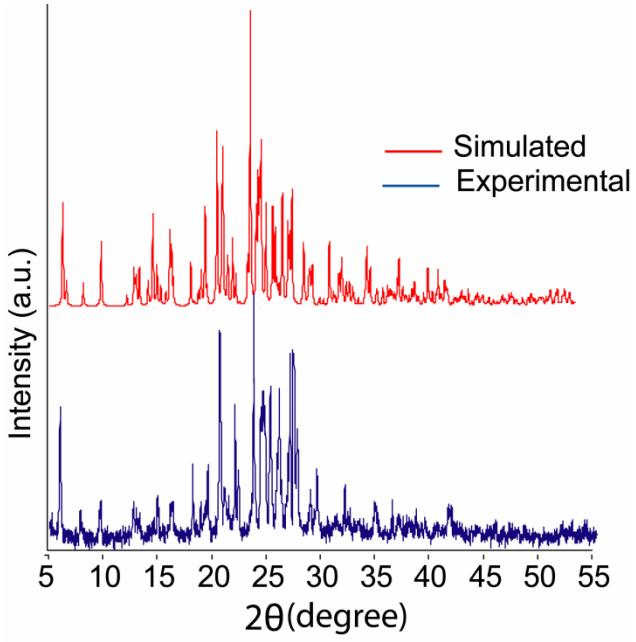
Supporting information

Materials and methods

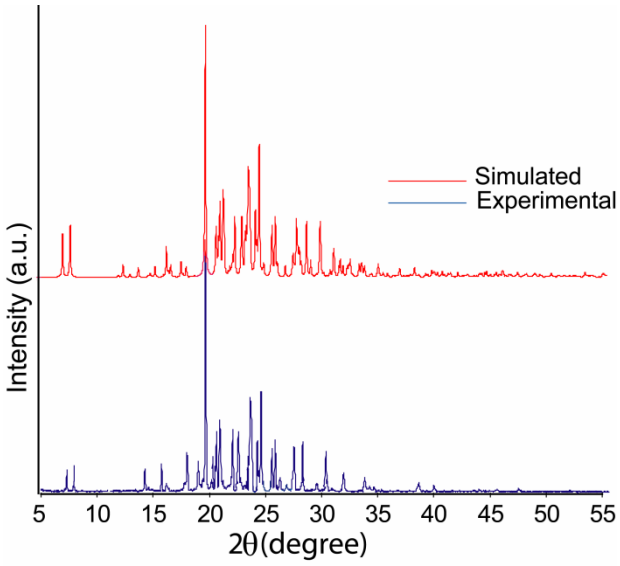
The 1,4,5,8-naphthalenetetracarboxylic dianhydride and 3-(1H-imidazol-1-yl)propan-1-amine are purchased from Sigma-Aldrich (USA). The ^{1}HNMR spectra wre recorded on a Varian FT 400 MHz instrument. The chemical shifts are in parts per million (ppm) on the scale using tetramethylsilane as a reference. The IR spectra were recorded on a Perkin Elmer Spectrum One FT-IR spectrometer with KBr disks in the range 4000-450 cm^{-1}. Fluorescence spectra are recorded with Perkin Elmer spectrometer LS 55. Powder X-ray Diffraction (PXRD) are recorded with Bruker D2 phaser with CuKα source (λ = 154 Å) on a glass surface of air dried sample and thermo-gravimetric analysis are recorded with TA instrument with model SDTQ600 using aluminium pan with a temperature of 5°/minute.



(a)



(b)



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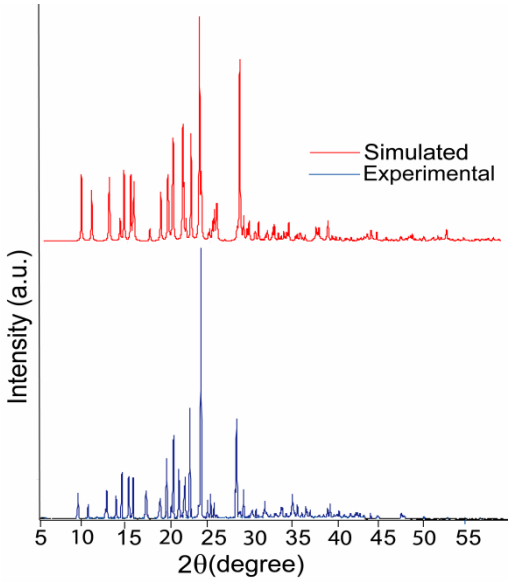
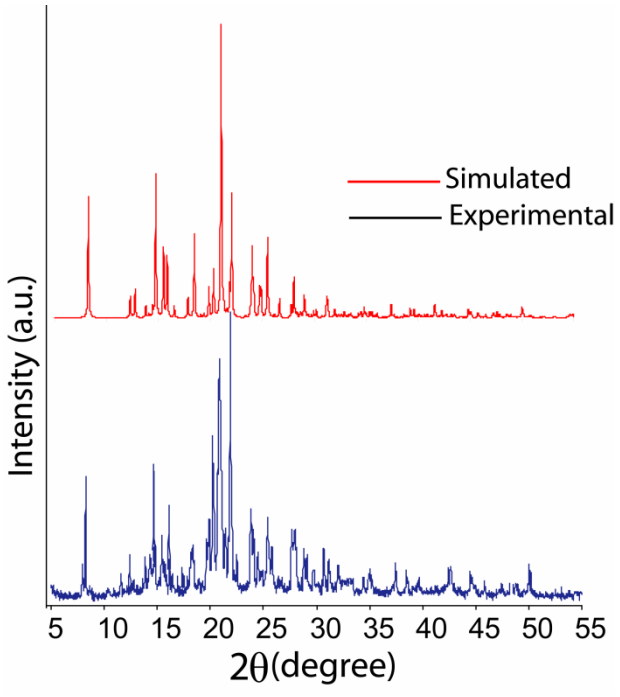
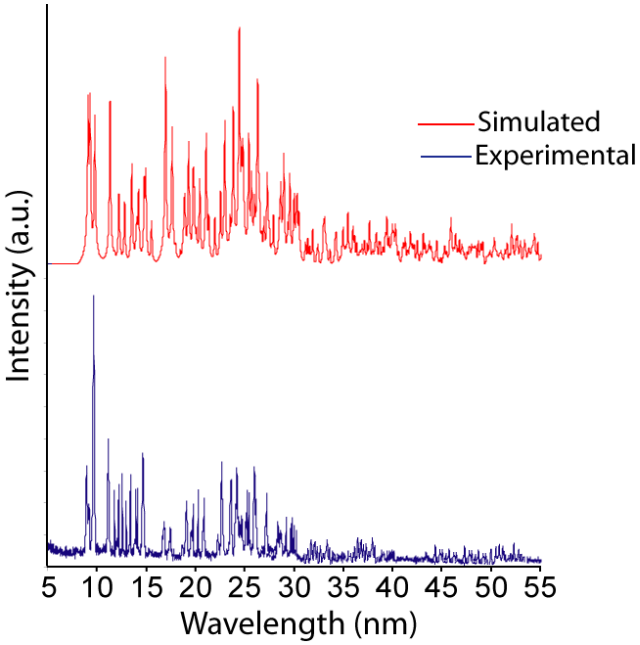


(d)



(e)



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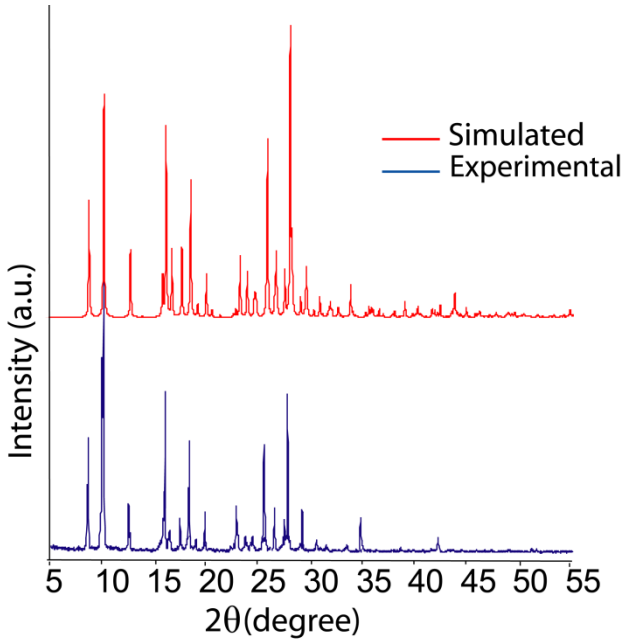
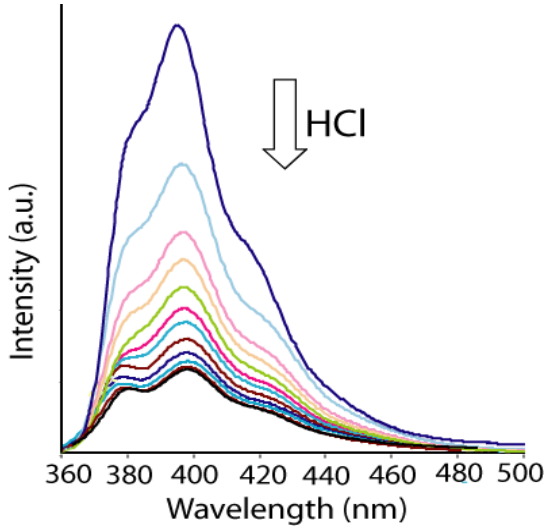
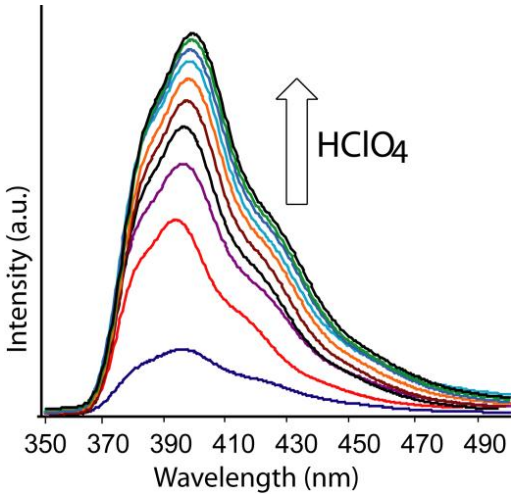


(g)

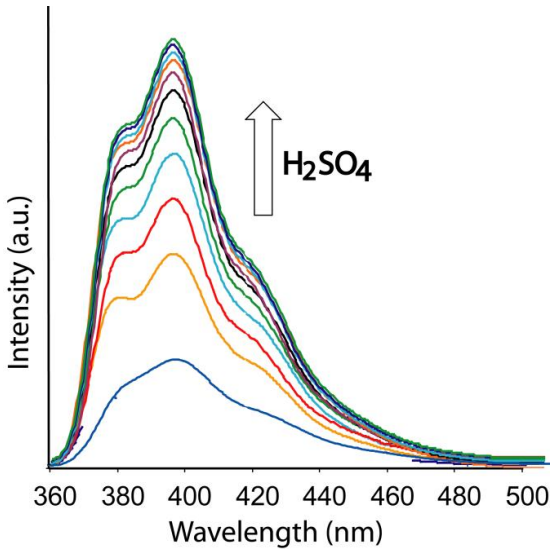
Fig. S1: PXRD pattern of simulated (red) with experimental (blue) of (a) Chloride, (b) bromide, (c) perchlorate, (d) bisulphate, (e) methyl sulphate and (f) Hydrogen phosphate salt (g) nitrate salt.



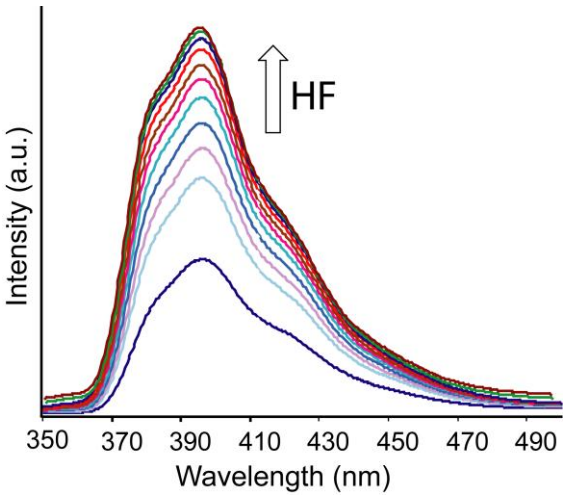
(a)



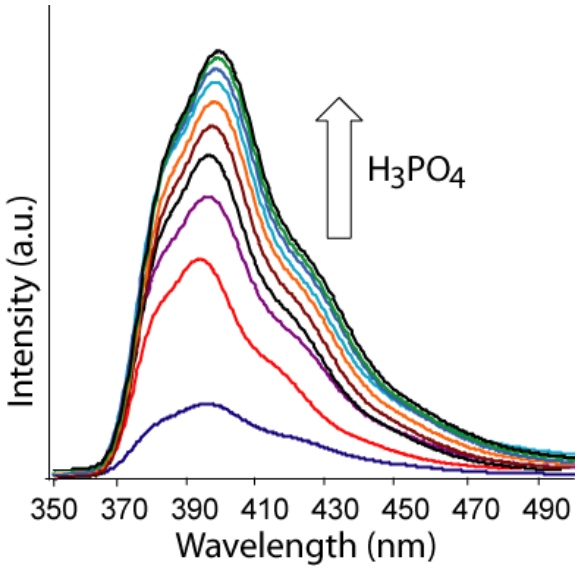
(b)



(c)



(d)



(e)

Fig. 2S: Changes in fluorescence emission intensity (λex = 340nm) of **L** (2ml of 10^{-5}M solution in methanol) with (a) HCl , (b) $HClO_4$, (c) H_2SO_4, (d) HF and (e) H_3PO_4(10 µl in each aliquot from each of the acid solution of concentration 10^{-2} M each)

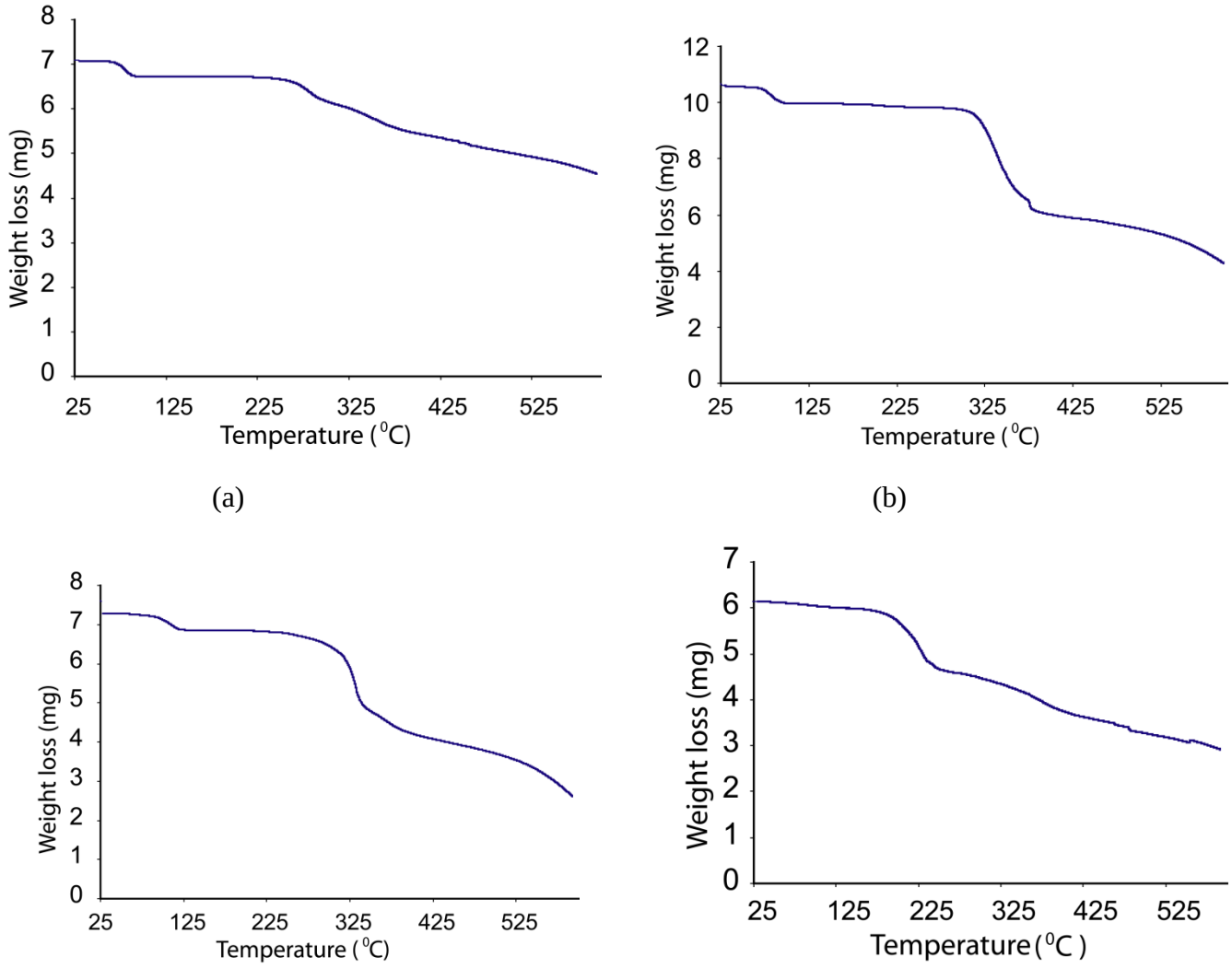
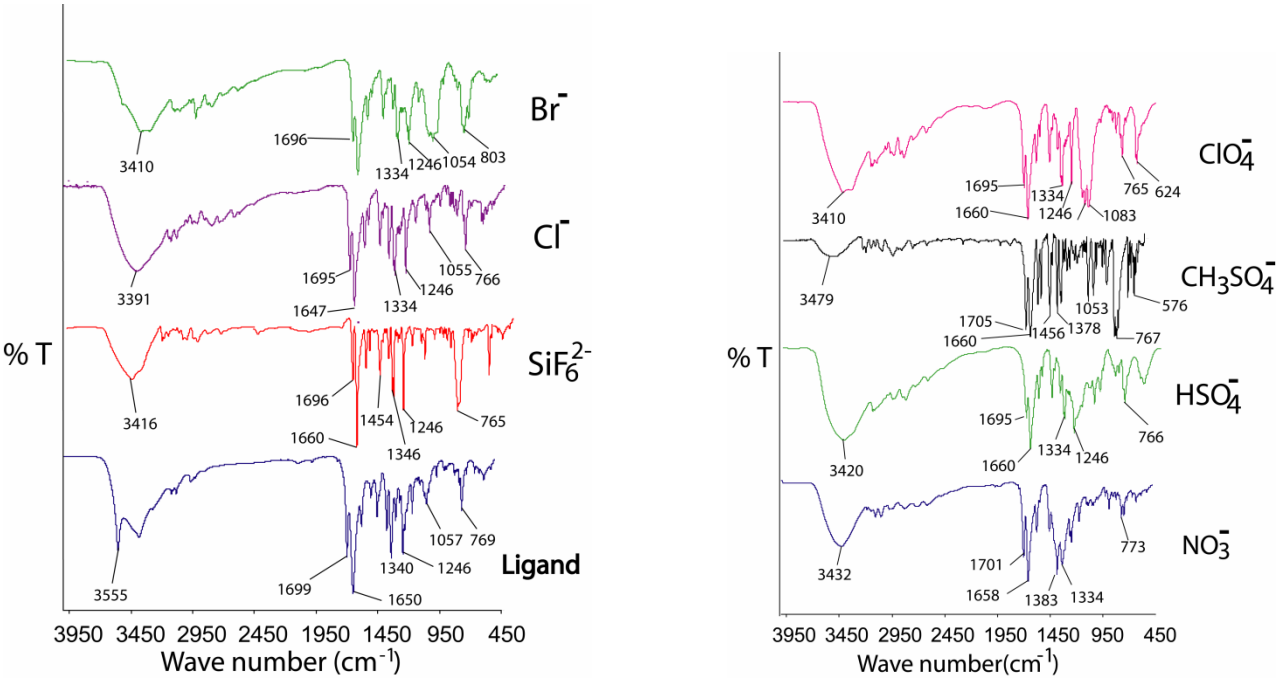


Fig. 3S: Thermo gravimetric analysis diagram of the salt (a) chloride, (b) bromide, (c) bisulphate and (d) hexa-fluorosilicate. The thermogravimetry of the hydrated salt **1** shows loss of water molecules below 74-94°C (wt. loss exptal 5.24%, theoretical 6.09%) and **2** shows it at 70-102°C (wt. loss exptal 5.16%, theoretical 5.29%). Whereas in the case complex **4**, the water of crystallization is lost at around 94-130°C (wt. loss exptal 4.86%, theoretical 5.03%), in this case water molecules are attached to dimeric assemblies of the anions. In the case of **8** no water molecules are lost at low temperature; the weight loss occurs around 192°C probably due to loss of hydrofluoric acid.



(a) (b)

Fig. 4S: IR spectra of the **L** and its different salts (The salts of **L** are denoted by the anions in figures).

Table S1: Crystallographic parameters of salt **8**

Compound No.	Salt **8**
Formulae	$C_{104}H_{102}F_{24}N_{24}O_{19}Si_4$
Mol. wt.	2560.60
Crystal system	Monoclinic
Space group	$P2_1/c$
Temperature /K	298(2)
Wavelength /Å	0.71073
a /Å	19.277(6)
b /Å	9.226(3)
c /Å	34.761(10)
α/°	90.00
β/°	116.698(19)
γ/°	90.00
V/ Å^3	5523(3)
Z	2
Density/Mgm^{-3}	1.536
Abs. Coeff. /mm^{-1}	0.175
F(000)	2624
Total no. of reflections	9817
Reflections, $I > 2\sigma(I)$	3639
Max. 2θ/°	50.50
Ranges (h, k, l)	$-23 \le h \le 23$ $-11 \le k \le 10$ $-41 \le l \le 41$
Complete to 2θ (%)	98.6
Data/ Restraints/Parameters	9817 / 0 / 793
Goof (F^2)	1.116
R indices [$I > 2\sigma(I)$]	0.0817
R indices (all data)	0.1156
$wR_2[I > 2\sigma(I)]$	0.1765
wR_2(all data)	0.2460

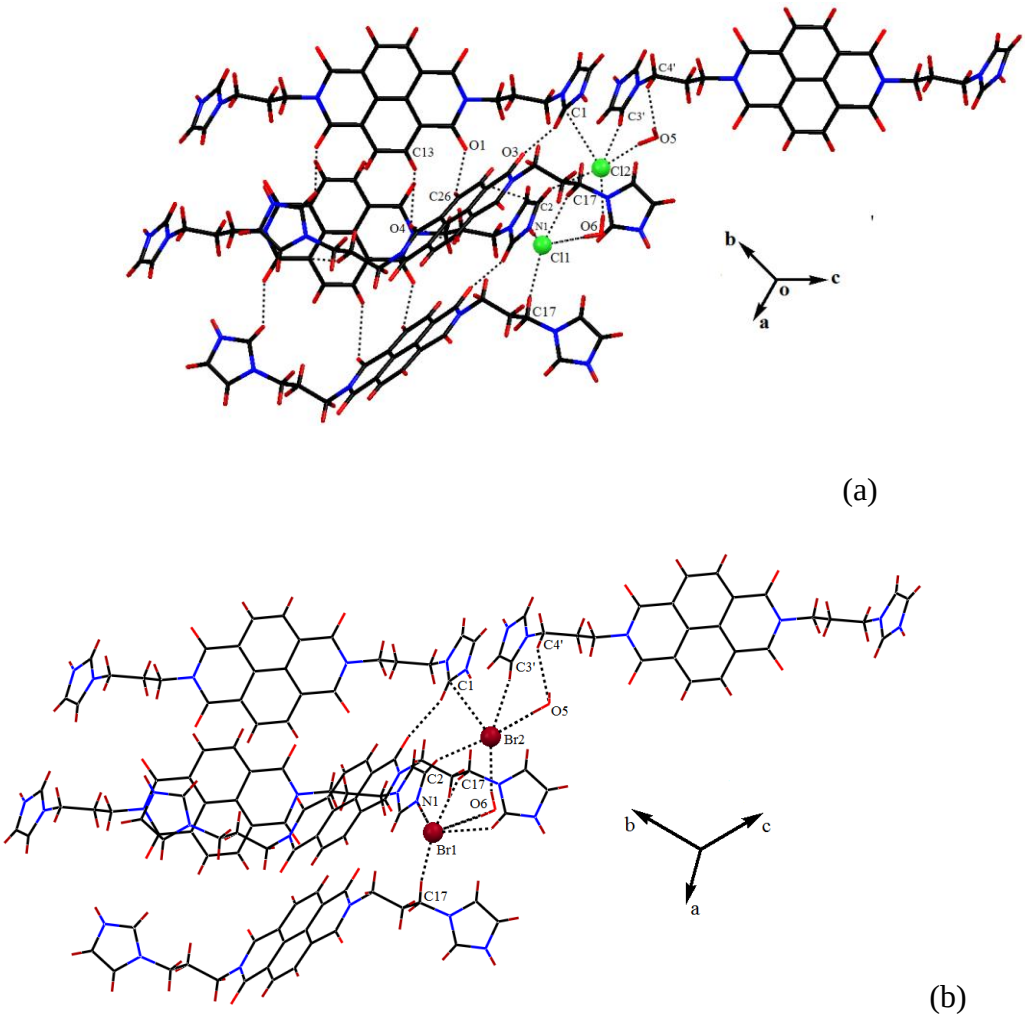
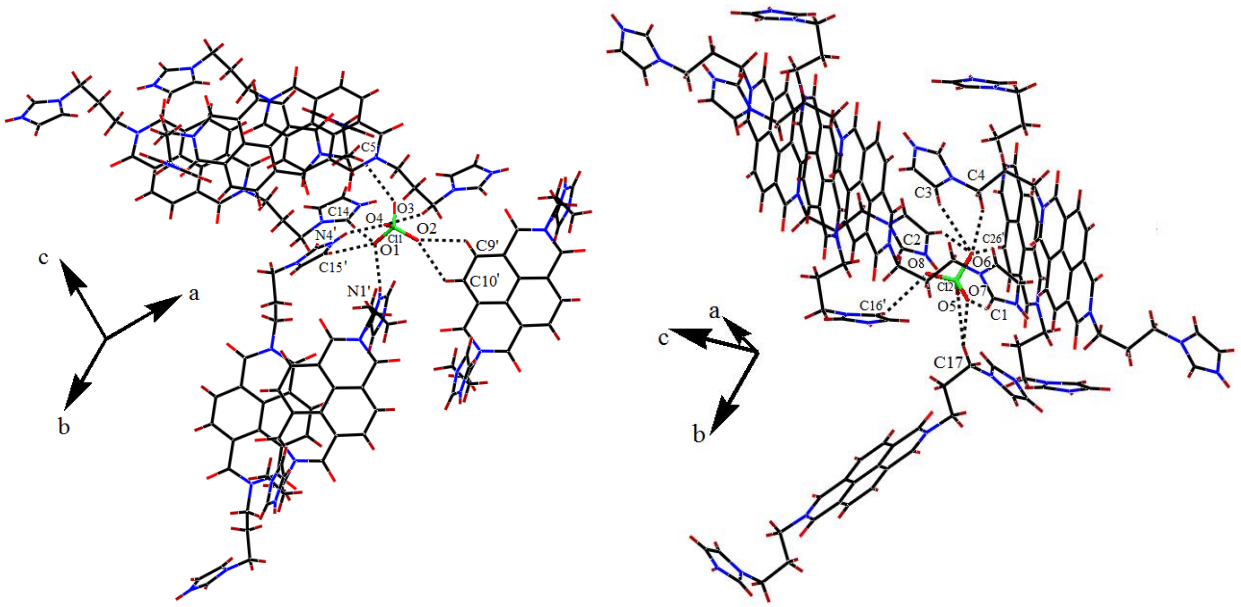


Fig. 4S (a) Coordination environment of chloride ions in salt **1;** and (b) Coordination environment of bromide ions in the salt **2**. [Equivalent atoms are generated by (-x, -y, -z)]



(a) (b)

Fig. 5S (a) Coordination mode of perchlorate anion in the salt **3 (**a) and (b) are two different perchlorate environments [Equivalent atoms are generated by (-x,-y,-z), (1/2-x, 1/2-y, 1/2-z) and (1/2+x, 1/2-y, 1/2+z)]

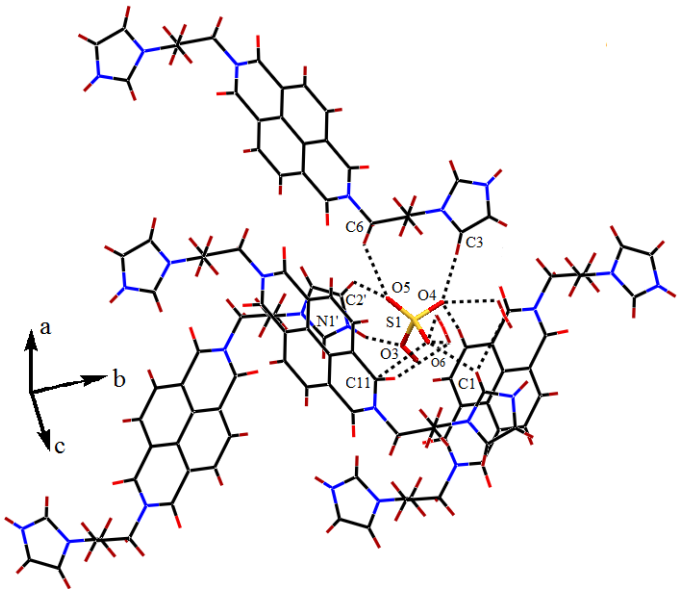


Fig. 6S: Hydrogen bond environment of bisulphate anion in salt **4** [Equivalent atoms are generated by (-x,-y,-z), (1/2-x, 1/2-y, 1/2-z) and (1/2+x, 1/2-y, 1/2+z)]

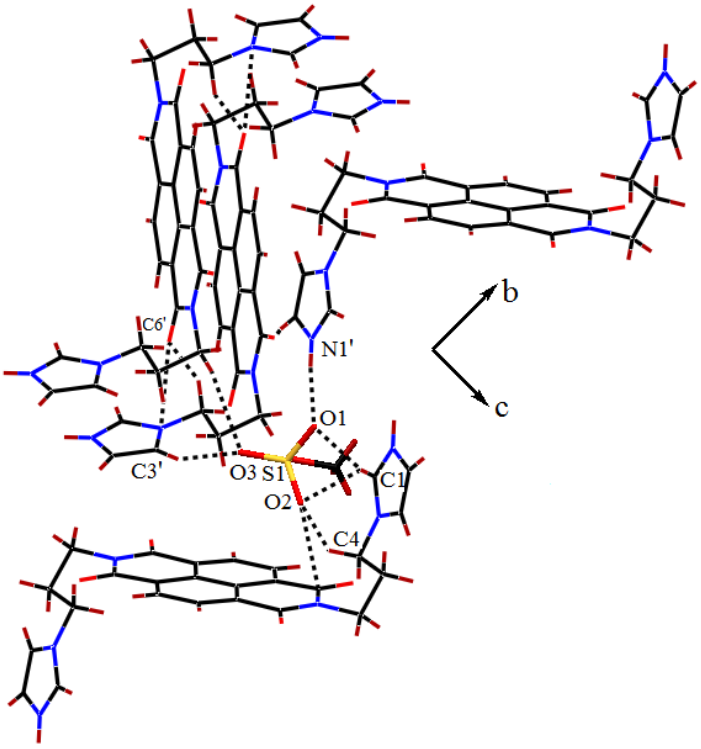


Fig. 7S: The hydrogen bond environment of methylsulphate in salt **5** (portions associated with anion are shown) [Equivalent atoms are generated by (-x,-y,-z), (-x, 1/2+y, 1/2-z) and (x, 1/2-y, 1/2+z)]

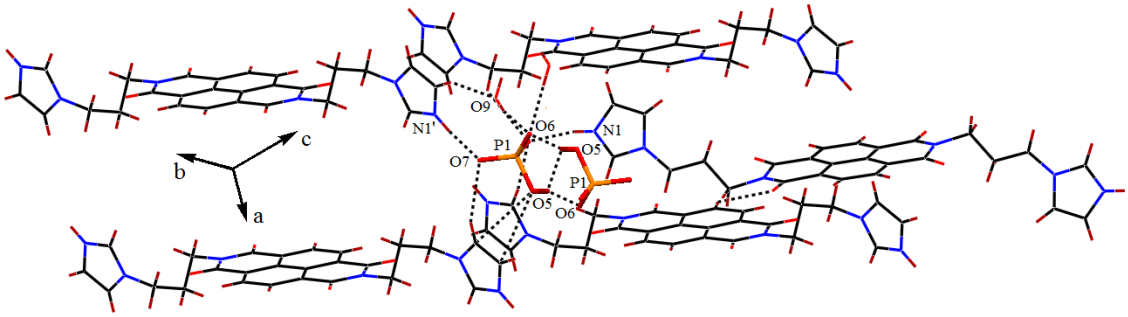


Fig. 8S: Hydrogen bond environment of the hydrogenphosphate anion in the salt **6**. (portions associated with anion are shown) [Equivalent atoms are generated by (-x,-y,-z)]

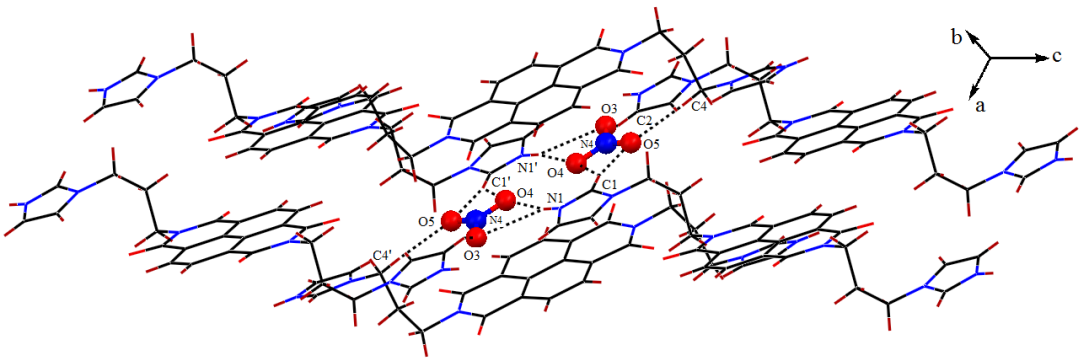
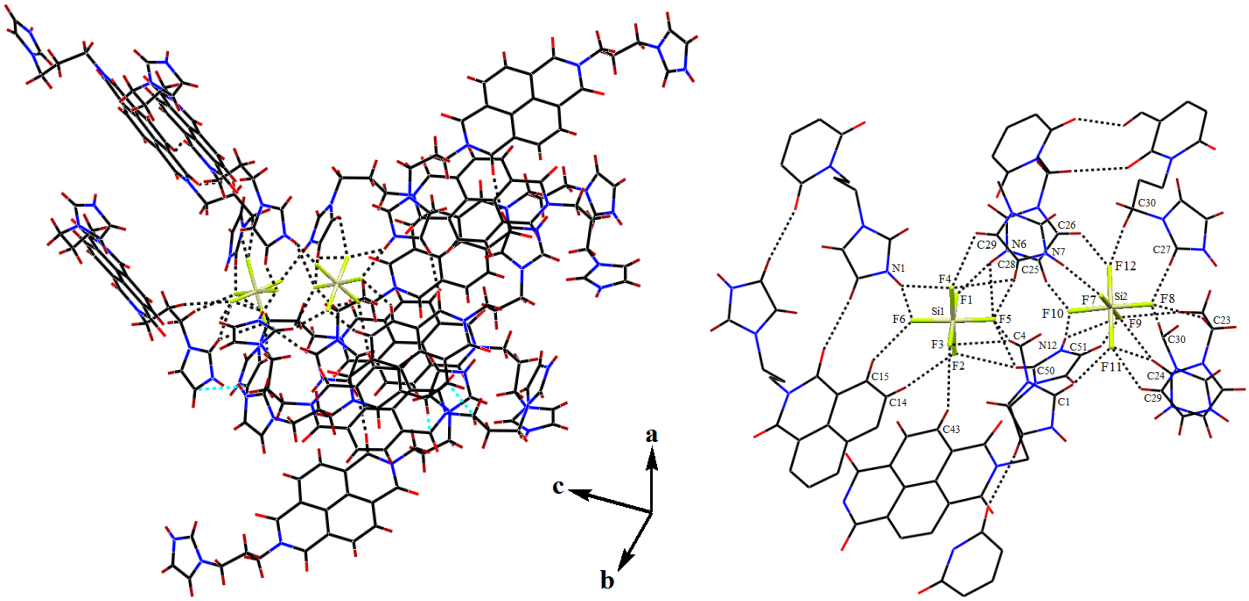


Fig. 9S: Nitrate anions forming layers with $H_2\mathbf{L}^{2+}$. Equivalent atoms are generated by [(-x,-y,-z), (1/2-x, 1/2+y, 1/2-z) and (1/2 + x, 1/2-y, 1/2+z)]



(a) (b)

Fig. 10S: (a)The coordination environments around the two symmetry independent SiF_6^{2-} anions in the salt **8** (b) Only the interested portions in **8** associated with anion is shown. [Equivalent atoms are generated by (-x,-y,-z), (-x, 1/2+y, 1/2-z) and (x, 1/2-y, 1/2+z)]

The hydrogen bond tables of the salts (generated from ins. files):

For salt 1:

1	1 N(1)	--H(1A)	..Cl(1)	[2666.03]	0.86	2.26	3.112(3)	175
2	2 N(4)	--H(4)	..O(5)	[2656.05]	0.86	1.87	2.706(6)	165
3	5 O(5)	--H(5M)	..O(6)	[2665.06]	0.84(6)	1.95(6)	2.757(7)	160(6)
4	5 O(5)	--H(5N)	..Cl(2)	[2665.04]	0.84(4)	2.29(4)	3.087(4)	159(4)
5	6 O(6)	--H(6M)	..Cl(2)	[1655.04]	0.84(4)	2.29(5)	3.123(5)	171(5)
6	6 O(6)	--H(6N)	..Cl(1)	[2666.03]	0.84(3)	2.36(4)	3.195(6)	178(11)
7	1 C(1)	--H(1)	..O(3)	[2566.02]	0.93	2.27	3.122(5)	151
8	1 C(2)	--H(2)	..Cl(2)	[1655.04]	0.93	2.70	3.567(5)	155
9	1 C(3)	--H(3)	..Cl(2)	[2665.04]	0.93	2.78	3.689(4)	167
10	Intra 1 C(6)	--H(6A)	..O(1)	[ ]	0.97	2.34	2.709(5)	102
11	2 C(14)	--H(14)	..O(2)	[2656.01]	0.93	2.49	3.147(5)	127
12	2 C(17)	--H(17A)	..Cl(1)	[ ]	0.97	2.67	3.541(4)	149
13	Intra 2 C(19)	--H(19B)	..O(3)	[ ]	0.97	2.36	2.738(5)	102
14	2 C(26)	--H(26)	..O(1)	[1655.01]	0.93	2.44	3.102(5)	128

Translation of ARU-Code to CIF and Equivalent Position Code

[2566.] =	-x,1-y,1-z
[2666.] =	1-x,1-y,1-z
[1655.] =	1+x,y,z
[2656.] =	1-x,-y,1-z
[2665.] =	1-x,1-y,-z

For salt 2:

1	1 N(1)	--H(1A)	..Br(1)	[2656.03]	0.86	2.41	3.268(4)	176
2	2 N(4)	--H(4)	..O(5)	[ ]	0.86	1.87	2.709(7)	163
3	5 O(5)	--H(5M)	..Br(2)	[2665.04]	0.84(4)	2.43(4)	3.243(5)	163(4)
4	5 O(5)	--H(5N)	..O(6)	[2565.06]	0.85(6)	1.93(7)	2.749(8)	162(8)
5	6 O(6)	--H(6M)	..Br(2)	[ ]	0.83(6)	2.44(5)	3.252(7)	165(6)
6	6 O(6)	--H(6N)	..Br(1)	[1455.03]	0.83(3)	2.54(3)	3.364(6)	175(7)
7	1 C(1)	--H(1)	..O(3)	[2656.02]	0.93	2.30	3.158(7)	154
8	1 C(2)	--H(2)	..Br(2)	[2556.04]	0.93	2.84	3.719(6)	157
9	1 C(3)	--H(3)	..Br(2)	[1456.04]	0.93	2.91	3.820(6)	166
10	Intra 1 C(6)	--H(6B)	..O(1)	[ ]	0.97	2.35	2.718(6)	101
11	2 C(14)	--H(14)	..O(2)	[2566.01]	0.93	2.51	3.159(7)	127
12	2 C(17)	--H(17B)	..Br(1)	[1455.03]	0.97	2.82	3.665(4)	146
13	Intra 2 C(19)	--H(19A)	..O(3)	[ ]	0.97	2.35	2.735(6)	103
14	2 C(25)	--H(25)	..O(1)	[1455.01]	0.93	2.44	3.116(6)	130

Translation of ARU-Code to CIF and Equivalent Position Code

[2656.] =	1-x,-y,1-z
[2556.] =	-x,-y,1-z
[2566.] =	-x,1-y,1-z
[1456.] =	-1+x,y,1+z
[1455.] =	-1+x,y,z
[2665.] =	1-x,1-y,-z
[2565.] =	-x,1-y,-z

For salt 3:

1	1 N(1)	--H(1A)	..O(1)	[ ]	0.86	2.33	3.134(8)	155
2	2 N(4)	--H(4)	..O(4)	[4454.03]	0.86	2.30	3.005(10)	139
3	2 N(4)	--H(4)	..O(12)	[4554.02]	0.86	2.47	3.031(9)	123'
4	1 C(1)	--H(1)	..O(7)	[1655.04]	0.93	2.42	3.166(10)	137
5	1 C(4)	--H(4B)	..O(6)	[3656.04]	0.97	2.48	3.400(7)	158
6	Intra 1 C(6)	--H(6A)	..O(9)	[ ]	0.97	2.31	2.731(6)	105
7	1 C(9)	--H(9)	..O(2)	[1556.03]	0.93	2.52	3.148(10)	126
8	2 C(14)	--H(14)	..O(1)	[ ]	0.93	2.35	3.280(10)	175
9	2 C(15)	--H(15)	..O(1)	[4454.03]	0.93	2.47	3.271(9)	144
10	2 C(17)	--H(17A)	..O(4)	[1455.03]	0.97	2.49	3.429(9)	162
11	2 C(17)	--H(17B)	..O(5)	[ ]	0.97	2.48	3.430(7)	166

12	Intra	2 C(19)	--H(19A)	..O(12)	[ ]	0.97	2.37	2.703(7)	100
13		2 C(26)	--H(26)	..O(6)	[2555.04]	0.93	2.54	3.453(8)	169

Translation of ARU-Code to CIF and Equivalent Position Code

[1655.] =	1+x,y,z
[3656.] =	1-x,-y,1-z
[1556.] =	x,y,1+z
[4454.] =	-1/2+x,1/2-y,-1/2+z
[4554.] =	1/2+x,1/2-y,-1/2+z
[1455.] =	-1+x,y,z
[2555.] =	1/2-x,1/2+y,1/2-z

For salt 4:

1	1 N(1)	--H(1A)	..O(3)	[2655.02]	0.86	2.05	2.824(9)	149
2	2 O(7)	--H(7A)	..O(6)	[4555.02]	0.85(7)	2.32(7)	2.753(8)	112(6)
3	2 O(7)	--H(7B)	..O(6)	[4555.02]	0.84(16)	2.25(15)	2.753(8)	118(10)
4	1 C(1)	--H(1)	..O(6)	[ ]	0.93	2.49	3.296(8)	146
5	1 C(1)	--H(1)	..O(7)	[2655.03]	0.93	2.51	3.132(9)	124'
6	1 C(2)	--H(2)	..O(5)	[2655.02]	0.93	2.48	3.145(8)	129
7	1 C(3)	--H(3)	..O(4)	[1455.02]	0.93	2.32	3.100(9)	141
8	Intra 1 C(6)	--H(6A)	..O(1)	[ ]	0.97	2.35	2.737(7)	103
9	1 C(6)	--H(6A)	..O(5)	[1455.02]	0.97	2.51	3.291(7)	137'
10	1 C(12)	--H(12)	..O(4)	[2645.02]	0.93	2.53	3.377(7)	151
11	1 C(13)	--H(13)	..O(3)	[4554.02]	0.93	2.49	3.246(9)	138

Translation of ARU-Code to CIF and Equivalent Position Code

[2655.] =	1-x,1/2+y,1/2-z
[1455.] =	-1+x,y,z
[2645.] =	1-x,-1/2+y,1/2-z
[4554.] =	x,1/2-y,-1/2+z
[4555.] =	x,1/2-y,1/2+z

For salt 5:

1	1 N(1)	--H(1C)	..O(1)	[2645.02]	0.86	1.85	2.707(4)	174
2	1 C(1)	--H(1)	..O(1)	[4554.02]	0.93	2.40	3.265(5)	154
3	1 C(1)	--H(1)	..O(2)	[4554.02]	0.93	2.59	3.336(5)	138'
4	1 C(2)	--H(2)	..O(5)	[2645.01]	0.93	2.31	3.142(5)	149
5	1 C(3)	--H(3)	..O(3)	[ ]	0.93	2.33	3.203(5)	156
6	1 C(4)	--H(4B)	..O(6)	[1455.01]	0.97	2.59	2.991(5)	105
7	Intra 1 C(6)	--H(6A)	..O(5)	[ ]	0.97	2.38	2.741(5)	101

Translation of ARU-Code to CIF and Equivalent Position Code

[4554.] =	x,1/2-y,-1/2+z
[2645.] =	1-x,-1/2+y,1/2-z
[1455.] =	-1+x,y,z

For salt 6:

1	1 N(1)	--H(1A)	..O(8)	[2756.03]	0.86	1.89	2.696(4)	155
2	2 N(4)	--H(4C)	..O(7)	[ ]	0.89(3)	1.70(3)	2.582(4)	175(4)
3	3 O(5)	--H(5)	..O(6)	[2756.03]	0.82	1.74	2.526(4)	159
4	4 O(9)	--H(9A)	..O(6)	[2666.03]	0.87	2.12	2.992(4)	173
5	4 O(9)	--H(9B)	..O(6)	[1565.03]	0.97	1.82	2.774(4)	164
6	1 C(3)	--H(3)	..O(4)	[1655.02]	0.93	2.52	3.401(4)	159
7	2 C(14)	--H(14)	..O(8)	[2766.03]	0.93	2.32	3.237(5)	167
8	2 C(15)	--H(15)	..O(9)	[1545.04]	0.93	2.52	3.375(5)	153
9	2 C(16)	--H(16)	..O(7)	[1455.03]	0.93	2.52	3.346(5)	149
10	Intra 2 C(19)	--H(19A)	..N(5)	[ ]	0.97	2.60	2.939(4)	101
11	Intra 2 C(19)	--H(19B)	..O(3)	[ ]	0.97	2.37	2.707(4)	100

Translation of ARU-Code to CIF and Equivalent Position Code

[2756.] =	2-x,-y,1-z

[1655.] = 1+x,y,z
[1545.] = x,-1+y,z
[2766.] = 2-x,1-y,1-z
[1455.] = -1+x,y,z
[2666.] = 1-x,1-y,1-z
[1565.] = x,1+y,z

For Salt 7:

1	1 N(1)	--H(1A)	..O(4)	[4454.02]	0.86	1.86	2.712(16)	168
2	1 C(1)	--H(1)	..O(4)	[2545.02]	0.93	2.31	3.049(19)	136
3	1 C(1)	--H(1)	..O(5)	[2545.02]	0.93	2.26	3.17(2)	167'
4	1 C(2)	--H(2)	..O(3)	[2555.02]	0.93	2.46	3.02(2)	118
5	1 C(4)	--H(4B)	..O(5)	[1455.02]	0.97	2.38	3.16(2)	137
6 Intra	1 C(5)	--H(5B)	..O(1)	[ ]	0.97	2.59	3.113(19)	114
7 Intra	1 C(6)	--H(6B)	..O(2)	[ ]	0.97	2.38	2.758(19)	103

Translation of ARU-Code to CIF and Equivalent Position Code
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[4454.] = -1/2+x,1/2-y,-1/2+z
[2545.] = 1/2-x,-1/2+y,1/2-z
[2555.] = 1/2-x,1/2+y,1/2-z
[1455.] = -1+x,y,z

For salt 8 :

1	1 N(1)	--H(1)	..O(2)	[3665.01]	0.86	2.59	3.337(17)	146
2	1 N(6)	--H(6)	..F(10)	[1575.04]	0.86	2.48	3.098(16)	130
3	2 N(7)	--H(7)	..F(7)	[4544.04]	0.86	1.96	2.811(10)	171
4	2 N(12)	--H(12)	..F(9)	[2655.04]	0.86	2.50	2.958(12)	114
5	1 C(2)	--H(2)	..F(4)	[3655.03]	0.93	1.99	2.780(15)	141
6	1 C(2)	--H(2)	..F(6)	[3655.03]	0.93	2.13	2.913(16)	142'
7	1 C(3)	--H(3)	..F(11)	[4554.04]	0.93	2.26	3.173(14)	168
8	1 C(4)	--H(4B)	..F(5)	[3665.03]	0.97	2.38	3.333(13)	170
9 Intra	1 C(6)	--H(6A)	..O(1)	[ ]	0.97	2.33	2.702(13)	102
10	1 C(14)	--H(14)	..F(2)	[1565.03]	0.93	2.46	3.299(12)	150
11	1 C(15)	--H(15)	..F(6)	[1565.03]	0.93	2.30	3.102(12)	144
12 Intra	1 C(21)	--H(21B)	..O(4)	[ ]	0.97	2.36	2.720(12)	101
13 Intra	1 C(21)	--H(21B)	..N(5)	[ ]	0.97	2.60	2.957(14)	102'
14	1 C(23)	--H(23A)	..O(5)	[3575.02]	0.97	2.32	3.248(12)	161
15	1 C(23)	--H(23B)	..F(8)	[1565.04]	0.97	2.32	3.138(11)	142
16	1 C(24)	--H(24)	..F(12)	[1575.04]	0.93	2.46	3.029(18)	120
17	1 C(25)	--H(25)	..F(1)	[2665.03]	0.93	1.82	2.741(12)	168
18	1 C(26)	--H(26)	..F(9)	[1565.04]	0.93	2.21	3.112(11)	164
19	1 C(26)	--H(26)	..F(11)	[1565.04]	0.93	2.50	3.189(12)	131'
20	2 C(27)	--H(27)	..F(8)	[3555.04]	0.93	2.09	3.023(14)	177
21	2 C(28)	--H(28)	..F(5)	[3655.03]	0.93	2.40	3.311(14)	166
22	2 C(29)	--H(29)	..F(11)	[4554.04]	0.93	2.44	3.170(12)	136
23	2 C(30)	--H(30A)	..F(12)	[3555.04]	0.97	2.25	3.211(12)	172
24	2 C(30)	--H(30B)	..F(8)	[4554.04]	0.97	2.33	3.276(11)	165
25 Intra	2 C(32)	--H(32B)	..O(6)	[ ]	0.97	2.36	2.702(13)	100
26	2 C(35)	--H(35)	..O(3)	[3575.01]	0.93	2.44	3.163(12)	135
27 Intra	2 C(47)	--H(47B)	..O(8)	[ ]	0.97	2.36	2.732(12)	102
28	2 C(49)	--H(49A)	..F(1)	[2655.03]	0.97	2.51	3.237(11)	132
29	2 C(50)	--H(50)	..F(2)	[2655.03]	0.93	2.35	3.270(13)	171
30	2 C(51)	--H(51)	..F(9)	[2655.04]	0.93	2.35	2.883(12)	116
31	2 C(51)	--H(51)	..F(10)	[2655.04]	0.93	1.77	2.702(13)	175'
32	2 C(52)	--H(52)	..F(5)	[ ]	0.93	2.41	3.011(12)	122

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[3665.] = 1-x,1-y,-z
[3575.] = -x,2-y,-z
[1575.] = x,2+y,z
[2665.] = 1-x,3/2+y,1/2-z
[3655.] = 1-x,-y,-z

[4554.] = x,1/2-y,-1/2+z
[1565.] = x,1+y,z
[4544.] = x,-1/2-y,-1/2+z
[2655.] = 1-x,1/2+y,1/2-z
[3555.] = -x,-y,-z

Table S2: Hydrogen bond parameters in the salts **1-8**

Salt	D-H...A	d_{D-H} (Å)	$d_{H\cdots A}$(Å)	$d_{D\cdots A}$(Å)	$d_{D-H\cdots A}$ (°)
Chloride salt (salt 1)	N1-H1A...Cl1 [1-x,1-y,1-z]	0.86	2.26	3.112(3)	175
	N4-H4...O5 [1-x,-y,1-z]	0.86	1.87	2.706(6)	165
	O5-H5M...O6 [1-x,1-y,-z]	0.84(6)	1.95(6)	2.757(7)	160(6)
	O5-H5N...Cl2 [1-x,1-y,-z]	0.84(4)	2.29(4)	3.087(4)	159(4)
	O6-H6M...Cl2 [1+x,y,z]	0.84(4)	2.29(5)	3.123(5)	171(5)
	O6-H6N...Cl1 [1-x,1-y,1-z]	0.84(3)	2.36(4)	3.195(6)	178(11)
	C1-H1...O3 [-x,1-y,1-z]	0.93	2.27	3.122(5)	151
	C2-H2...Cl2 [1+ x, y, z]	0.93	2.70	3.567(5)	155
	C3-H3...Cl2 [1-x,1-y,-z]	0.93	2.78	3.69(4)	167
	C14-H14...O2 [1-x,-y,1-z]	0.93	2.49	3.147(5)	127
	C17-H17A...Cl1	0.97	2.67	3.541(4)	149
Bromide salt (salt 2)	N1-H1A...Br1 [1-x,-y,1-z]	0.86	2.41	3.268(4)	176
	N4-H4...O5	0.86	1.87	2.709(7)	163
	O5-H5M...Br2 [1-x,1-y,-z]	0.84(4)	2.43(4)	3.243(5)	163(4)
	O5-H5N...O6 [-x,1-y,-z]	0.85(6)	1.93(7)	2.749(8)	162(8)
	O6-H6M...Br2	0.83(6)	2.44(5)	3.252(7)	165(6)
	O6-H6N...Br1 [-1+x,y,z]	0.83(3)	2.54(3)	3.364(6)	175(7)
	C1-H1...O3 [1-x,-y,1-z]	0.93	2.30	3.158(7)	154
	C1-H1...Br2 [-x,-y,1-z]	0.93	2.84	3.719(6)	157
	C3-H3...Br2 [-1+x,y,1+z]	0.93	2.91	3.820(6)	166
	C6-H6B...O1	0.97	2.35	2.718(6)	101
	C14-H14...O2 [-x,1-y,1-z]	0.93	2.51	3.159(7)	127
	C17-H17B...Br1 [-1+x,y,z]	0.97	2.82	3.665(4)	146
	C19-H19A...O3	0.97	2.35	2.735(6)	103
Perchlorate salt (salt 3)	N(1)-H(1A)...O1	0.86	2.33	3.134(8)	155
	N4-H4...O4 [-1/2+x,1/2-y,-1/2+z]	0.86	2.30	3.005(10)	139
	N4-H4...O12 [1/2+x,1/2-y,-1/2+z]	0.86	2.47	3.031(9)	123
	C1-H1...O7 [1+x,y,z]	0.93	2.42	3.166(10)	137
	C4-H4B...O6 [1-x,-y,1-z]	0.97	2.48	3.400(7)	158
	C6-H6A...O9	0.97	2.31	2.731(6)	105
	C9-H9...O2 [x,y,1+z]	0.93	2.52	3.148(10)	126
	C14-H14...O1	0.93	2.35	3.280(10)	175
	C15-H15...O1 [-1/2+x,1/2-y,-1/2+z]	0.93	2.47	3.271(9)	144
	C17-H17A...O4 [-1+x,y,z]	0.97	2.49	3.429(9)	162
	C17-H17B...O5	0.97	2.48	3.430(7)	166
	C26-H26...O6 [1/2-x,1/2+y,1/2-z]	0.93	2.54	3.453(8)	169
Bisulphate salt (salt 4)	N1-H1A...O3 [1-x,1/2+y,1/2-z]	0.86	2.05	2.824(9)	149
	O7-H7A...O6 [x,1/2-y,1/2+z]	0.85(7)	2.32(7)	2.753(8)	112(6)
	O7-H7B...O6 [x,1/2-y,1/2+z]	0.84(16)	2.25(15)	2.753(8)	118(10)
	C1-H1...O6	0.93	2.49	3.296(8)	146
	C1-H1...O7 [1-x,1/2+y,1/2-z]	0.93	2.51	3.132(9)	124
	C2-H2...O5 [1-x,1/2+y,1/2-z]	0.93	2.48	3.145(8)	129
	C3-H3...O4 [-1+x,y,z]	0.93	2.32	3.100(9)	141
	C5-H5...O3	0.82	2.67	3.447	137
	C6-H6A...O1	0.97	2.35	2.737(7)	103
	C6-H6A...O5 [-1+x,y,z]	0.97	2.51	3.291(7)	137
	C12-H12...O4 [1-x,-1/2+y,1/2-z]	0.93	2.53	3.377(7)	151
	C13-H13...O3 [x,1/2-y,-1/2+z]	0.93	2.49	3.246(9)	138
Methyl sulphate (salt 5)	N1-H1C...O1 [1-x,-1/2+y,1/2-z]	0.86	1.85	2.707(4)	174
	C1-H1...O1 [x,1/2-y,-1/2+z]	0.93	2.40	3.265(5)	154
	C1-H1...O2 [x,1/2-y,-1/2+z]	0.93	2.59	3.336(5)	138
	C2-H2...O5 [1-x,-1/2+y,1/2-z]	0.93	2.31	3.142(5)	149
	C3-H3...O3	0.93	2.33	3.203(5)	156
	C4-H4B...O6 [-1+x,y,z]	0.97	2.59	2.991(5)	105

	C6-H6A...O5 [intra]	0.97	2.38	2.741(5)	101
Hydrogen phosphate salt (salt 6)	N(1)-H(1A)...O(8) [2-x,-y,1-z] N(4)-H(4C)...O(7) O(5)-H(5)...O(6) [2-x,-y,1-z] O(9)-H(9A)...O(6) [1-x,1-y,1-z] O(9)-H(9B)...O(6) [x,1+y,z] C(14)-H(14)...O(8) [2-x,1-y,1-z] C(15)-H(15)...O(9) [x,-1+y,z] C(16)-H(16)...O(7) [-1+x,y,z] C(19)-H(19A)...N(5) [intra] C(19)-H(19B)...O(3) [intra]	0.86 0.89(3) 0.82 0.87 0.97 0.93 0.93 0.93 0.97 0.97	1.89 1.70(3) 1.74 2.12 1.82 2.32 2.52 2.52 2.60 2.37	2.696(4) 2.582(4) 2.526(4) 2.992(4) 2.774(4) 3.237(5) 3.375(5) 3.346(5) 2.939(4) 2.707(4)	155 175(4) 159 173 164 167 153 149 101 100
Nitrate salt (salt 7)	N1-H1A...O4 [-1/2+x,1/2-y,-1/2+z] C1-H1...O4 [1/2-x,-1/2+y,1/2-z] C1-H1...O5 [1/2-x,-1/2+y,1/2-z] C2-H2...O3 [1/2-x,1/2+y,1/2-z] C4-H4B...O5 [-1+x,y,z] C5-H5B...O1 C6-H6B...O2	0.86 0.93 0.93 0.93 0.97 0.97 0.97	1.86 2.31 2.26 2.46 2.38 2.59 2.38	2.712(16) 3.049(19) 3.17(2) 3.02(2) 3.16(2) 3.113(19) 2.758(19)	168 136 167 118 137 114 103
Hexa-fluorosilicate salt (salt 8)	N1-H1...O2 [1-x, 1-y, -z] N6-H6...F10 [x, 2+y, z] N7-H7...F7 [x, -1/2-y, -1/2+z] N12-H12...F9 [1-x,1/2+y,1/2-z] C(2) -H(2) ...F(4) [1-x,1-y, -z] C(2) -H(2) ... F(6) [1-x, 1-y, -z] C(3) -H(3) ...F(11) [x, 1/2-y, -1/2+z] C(4) -H(4B) ...F(5) [1-x,1-y,-z] C(6) -H(6A) ...O(1) [intra] C(14)-H(14) ...F(2) [x, 1+y, z] C(15) -H(15) ...F(6) [x, 1+y, z] C(21) -H(21B) ...O(4) [intra] C(21) -H(21B) ...N(5) [intra] C(23) -H(23A) ...O(5) [-x, 2-y, -z] C(23) -H(23B) ... F(8) [x, 1+y, z] C(24) -H(24) ...F(12) [x, 2+y, z] C(25) -H(25) ... F(1) [1-x, 1/2+y, 1/2-z] C(26) -H(26) ...F(9) [x, 1+y, z] C(26) -H(26) ...F(11) [x, 1+y, z] C(27) -H(27) ...F(8) [-x, -y, -z] C(28) -H(28) ...F(5) [1-x, 1-y, -z] C(29) -H(29) ...F(11) [x, 1/2-y, -1/2+z] C(30) -H(30A) ...F(12) [-x, -y, -z] C(30) -H(30B) ...F(8) [x,1/2-y, -1/2+z] C(32) -H(32B) ...O(6) [Intra] C(35) -H(35) ...O(3) [-x, 2-y, -z] C(47) -H(47B) ...O(8) [Intra] C(49) -H(49A) ...F(1) [1-x,1/2+y, 1/2-z] C(50) -H(50) ...F(2) [1-x,1/2+y,1/2-z] C(51) -H(51) ...F(9) [1-x,1/2+y,1/2-z] C(51) -H(51) ... F(10) [1-x,1/2+y,1/2-z] C(52) -H(52) ... F(5)	0.86 0.86 0.86 0.86 0.93 0.93 0.93 0.97 0.97 0.93 0.93 0.97 0.97 0.97 0.97 0.93 0.93 0.93 0.97 0.97 0.97 0.93 0.93 0.97 0.97 0.93 0.93 0.93 0.93 0.93	2.59 2.48 1.96 2.50 1.99 2.13 2.26 2.38 2.33 2.46 2.30 2.36 2.60 2.32 2.32 2.46 1.82 2.21 2.50 2.09 2.40 2.44 2.25 2.33 2.36 2.44 2.36 2.51 2.35 2.35 1.77 2.41	3.337(17) 3.098(16) 2.811(10) 2.958(12) 2.780(15) 2.913(16) 3.173(14) 3.333(13) 2.702(13) 3.299(12) 3.102(12) 2.720(12) 2.957(14) 3.248(12) 3.138(11) 3.029(18) 2.741(12) 3.112(11) 3.189(12) 3.023(14) 3.311(14) 3.170(12) 3.211(12) 3.276(11) 2.702(13) 3.163(12) 2.732(12) 3.237(11) 3.270(13) 2.883(12) 2.702(13) 3.011(12)	146 130 171 114 141 142 168 170 102 150 144 101 102 161 142 120 168 164 131 177 166 136 172 165 100 135 102 132 171 116 175 122