Electronic supplementary information

Synthesis, characterization and evaluation of surface properties of cyclohexanoxy carbonyl methyl pyridinium and imidazolium ionic liquids

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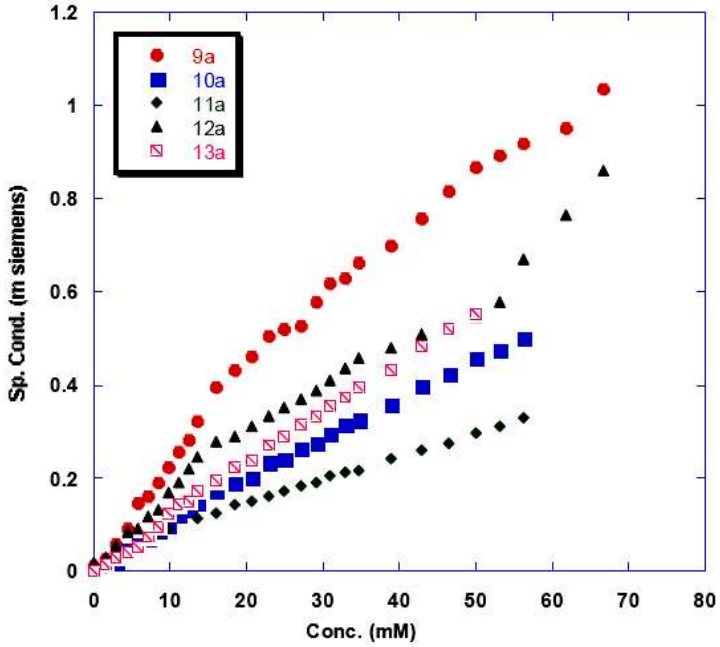


Figure S1. Specific Conductivity vs Concentration plot of ionic liquids 9a-13a

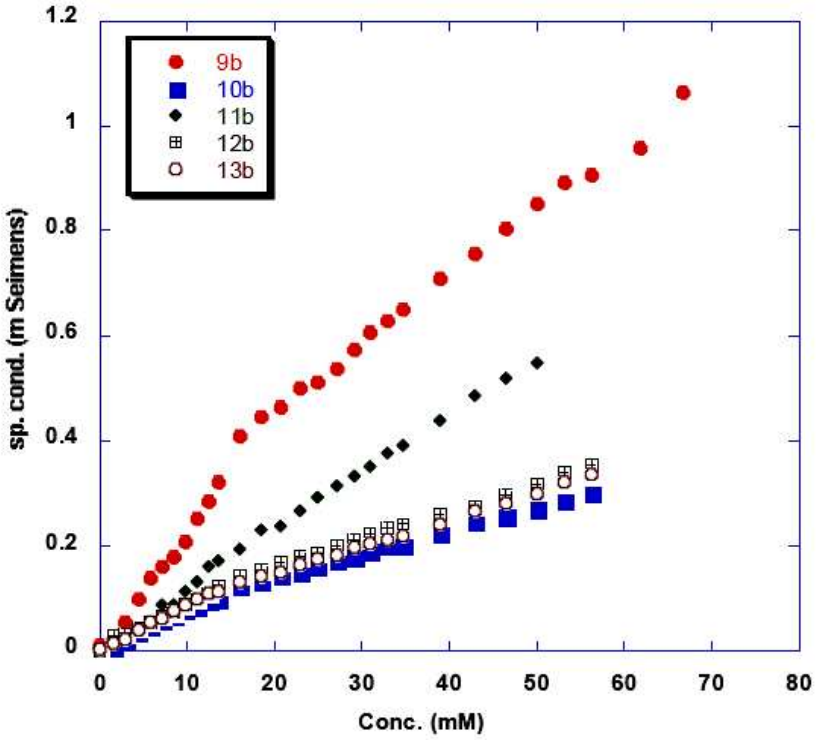
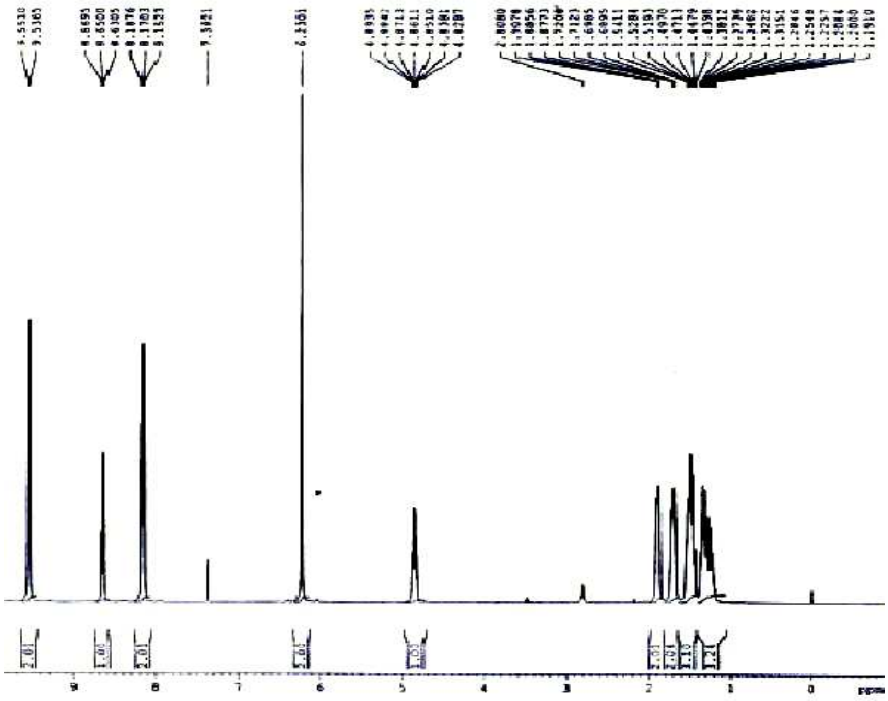
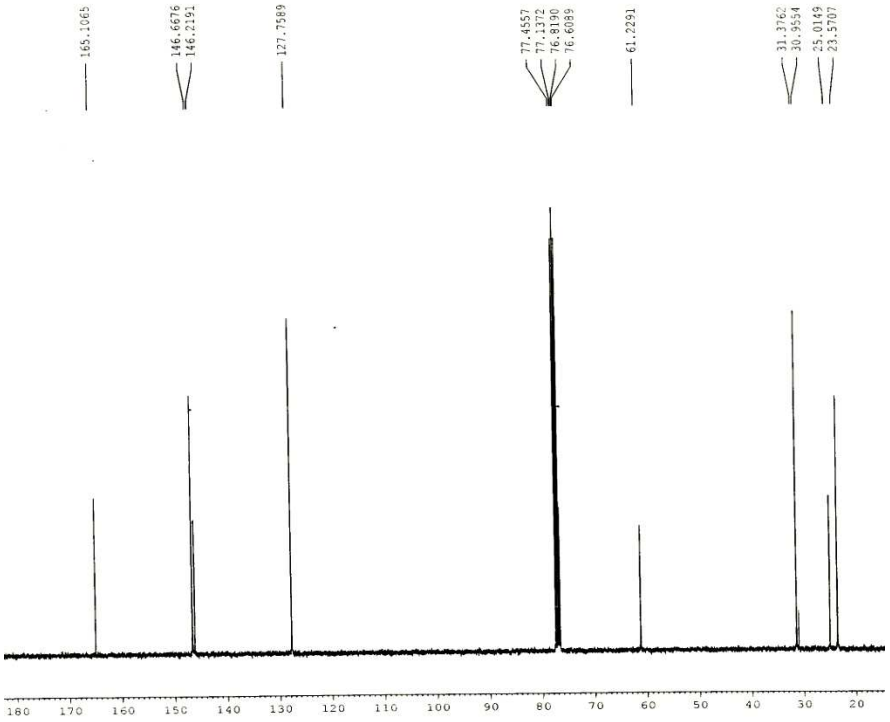


Figure S2. Specific Conductivity vs Concentration plot of ionic liquids 9b-13b



^{1}H spectra of *N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (9a)



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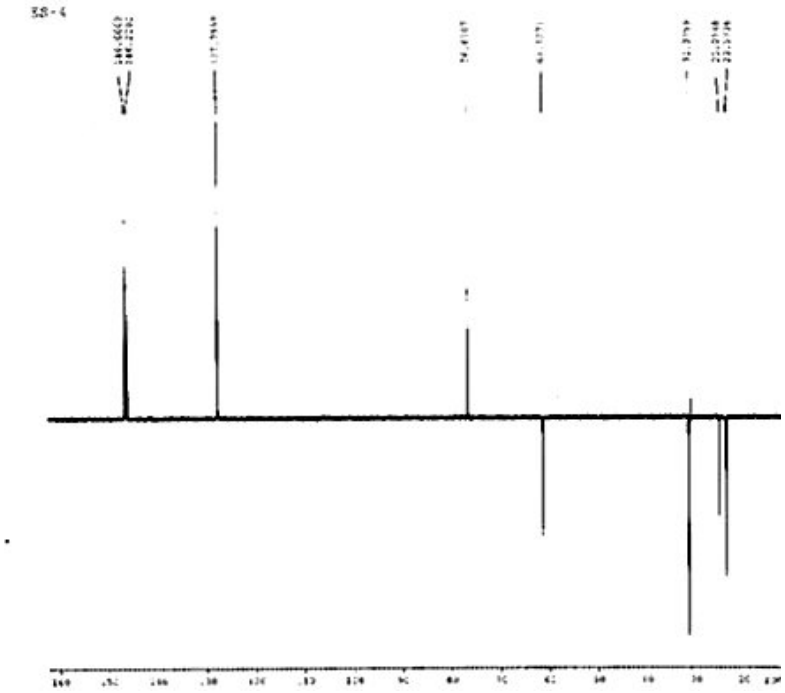
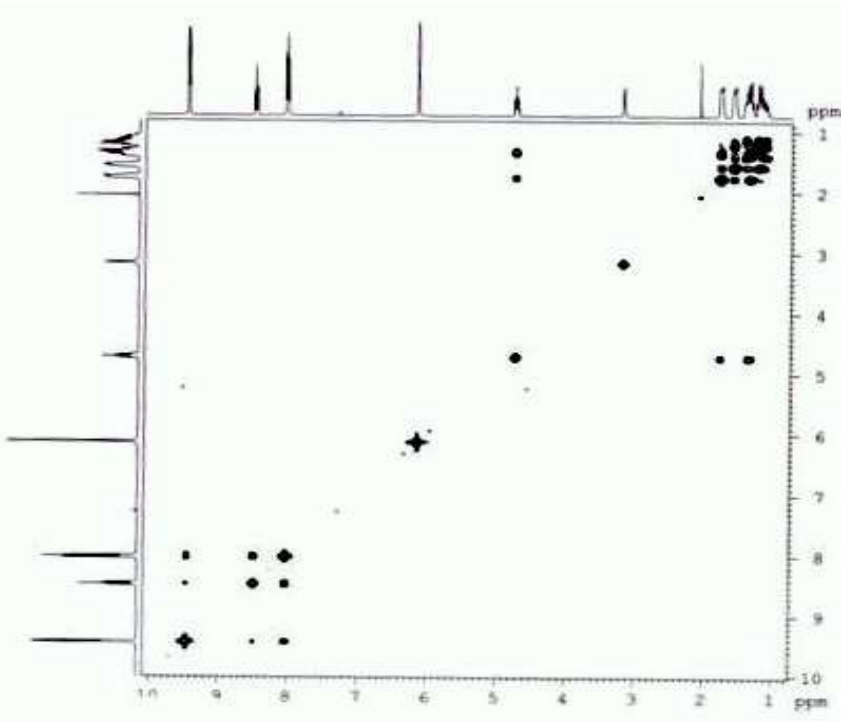
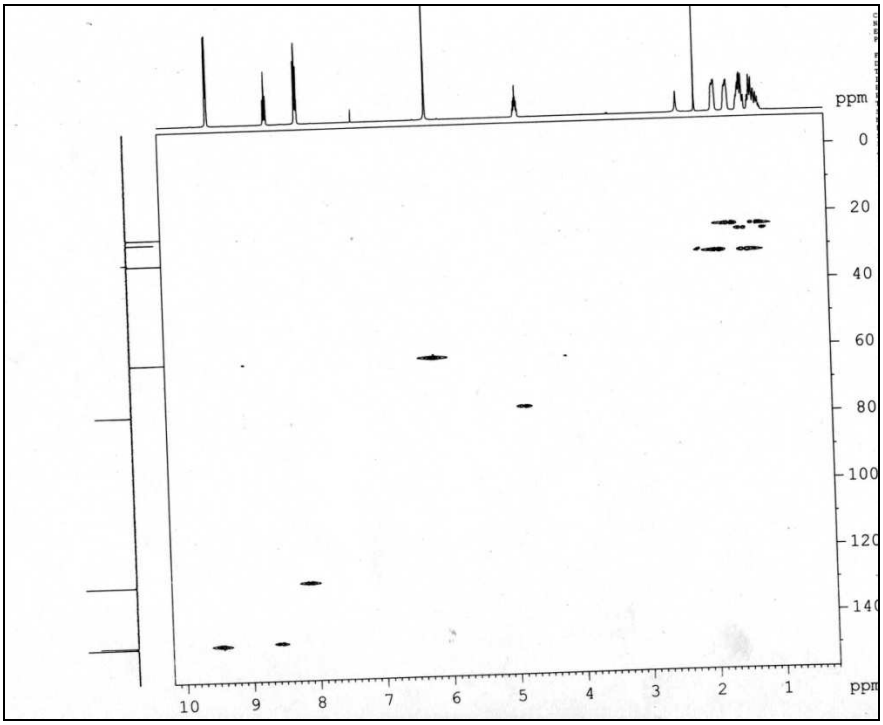


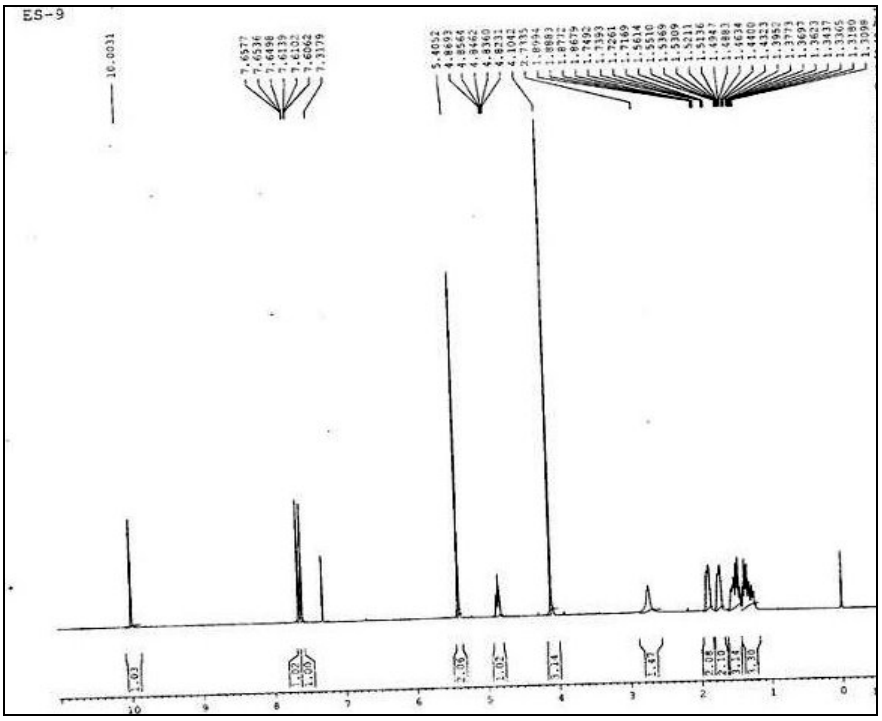
^{13} C DEPT spectra of *N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (9a)



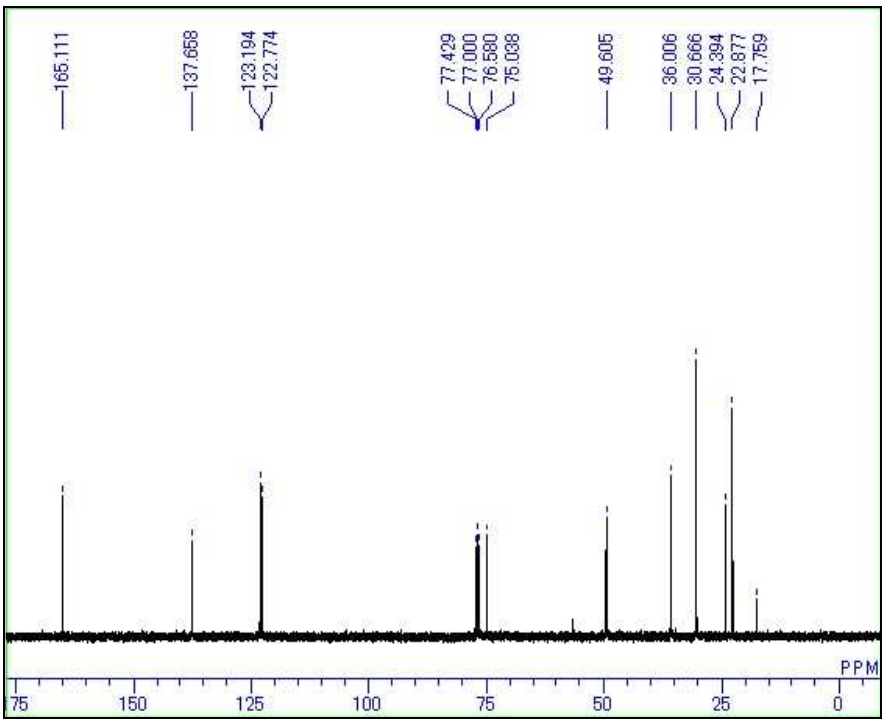
2D- COSY ^{1}H-^{1}H spectra of *N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (9a)



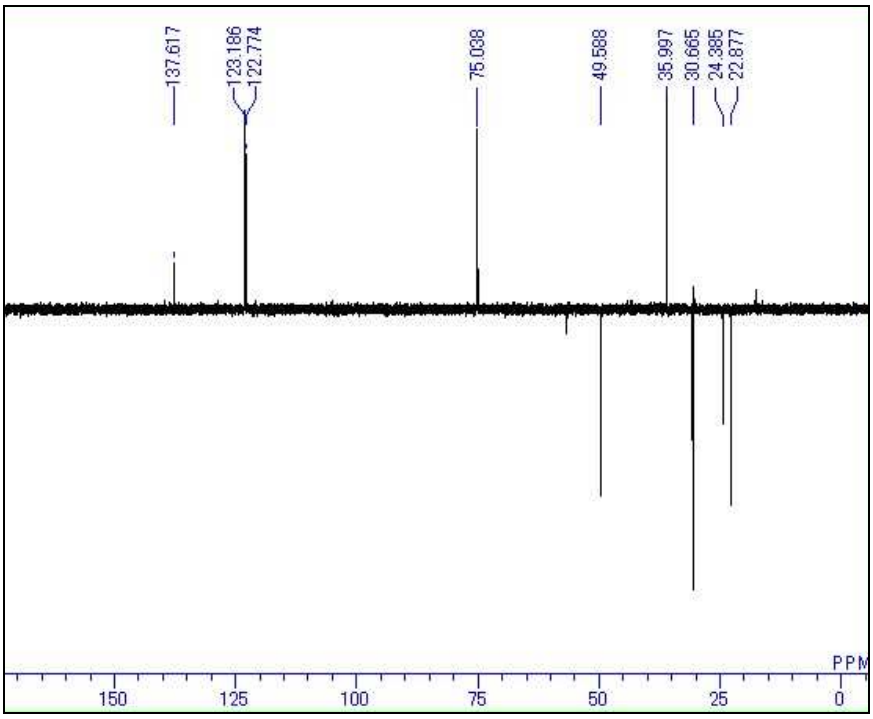
2D- HETCOR ^{1}H-^{13}C spectra of N-(cyclohexanoxycarbonylmethyl) pyridinium bromide (9a)



^{1}H spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)imidazolium bromide (13a)



^{13}C spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)imidazolium bromide (13a)

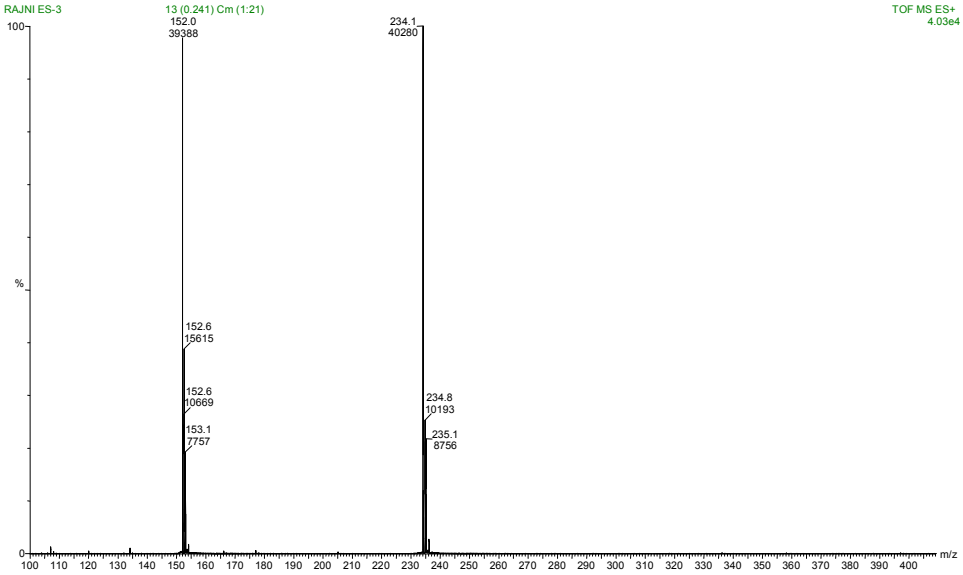


^{13}C DEPT spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)imidazolium bromide (13a)

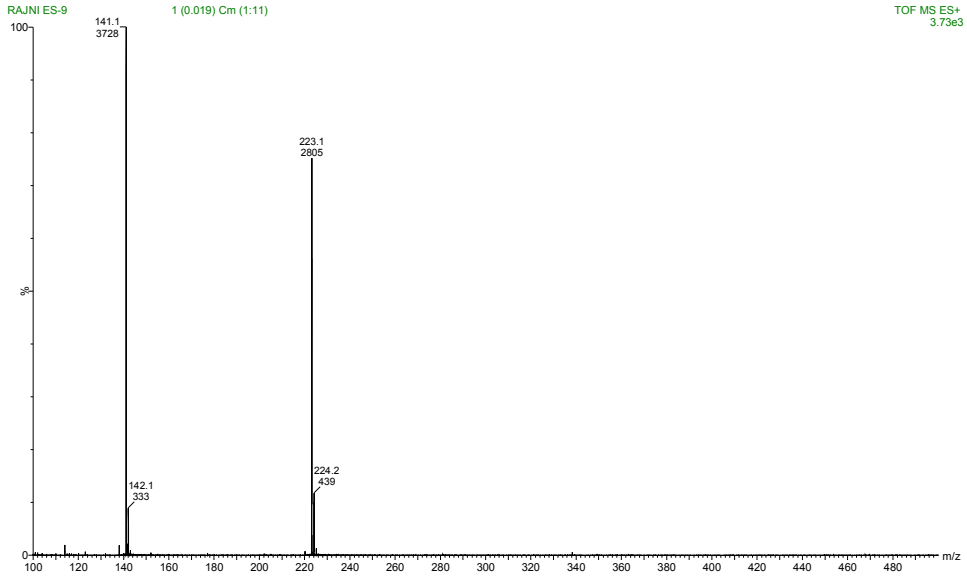
Mass spectra of *N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (9a)

Mass spectra of 2-methyl-*N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (10a)

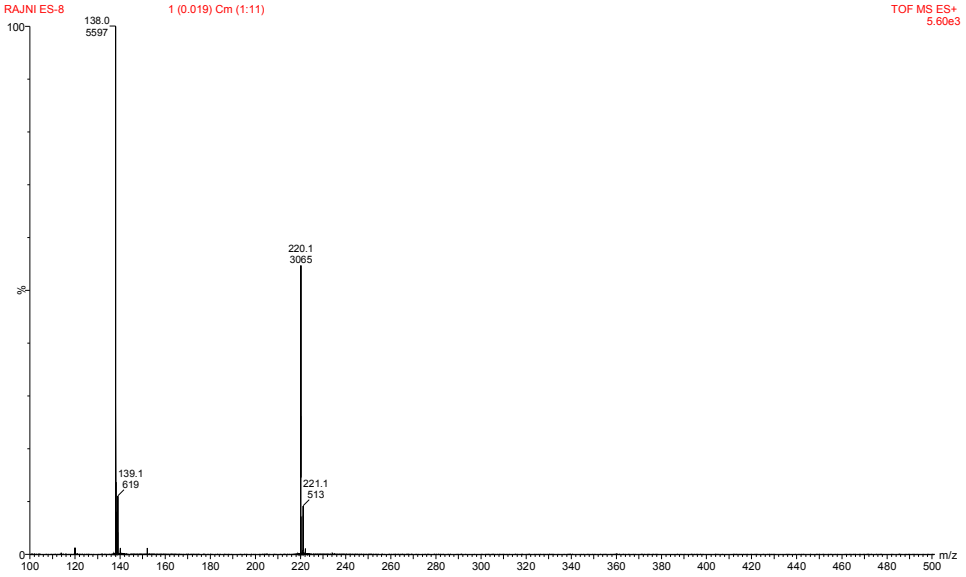
Mass spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (11a)



Mass spectra of 4-methyl-*N*-(cyclohexanoxycarbonylmethyl)pyridinium bromide (12a)



Mass spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)imidazolium bromide (13a)

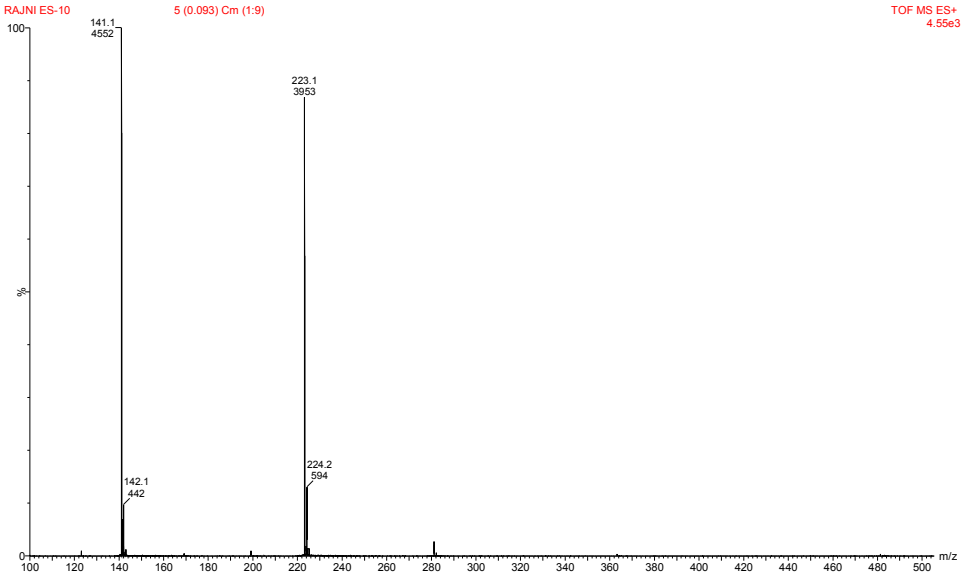


Mass spectra of *N*-(cyclohexanoxycarbonylmethyl)pyridinium chloride (9b)

Mass spectra of 2-methyl -*N*-(cyclohexanoxycarbonylmethyl)pyridinium chloride (10b)

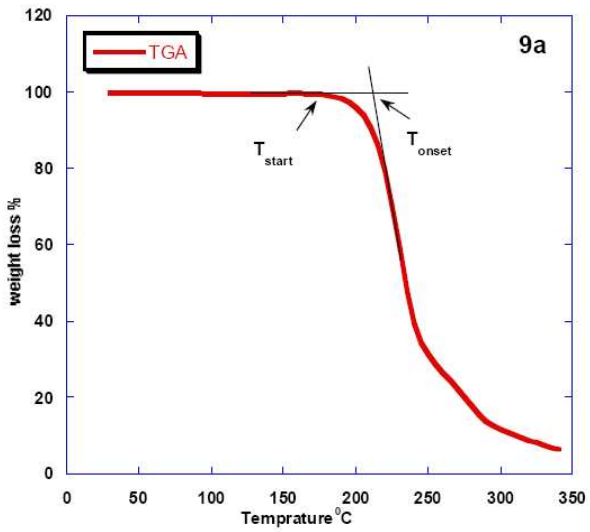
Mass spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)pyridinium chloride (11b)

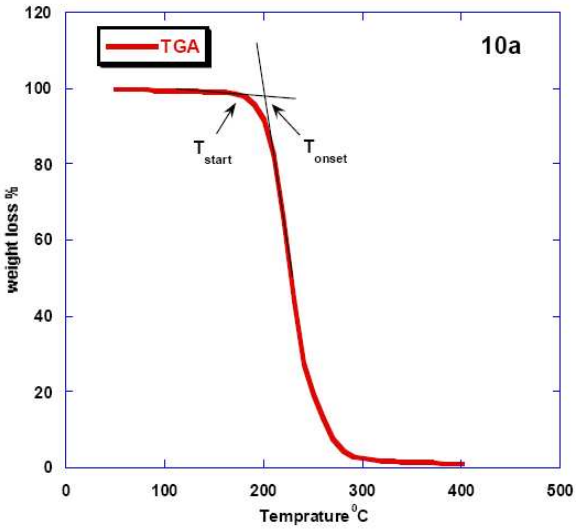
Mass spectra of 4-methyl-*N*-(cyclohexanoxycarbonylmethyl)pyridinium chloride (12b)

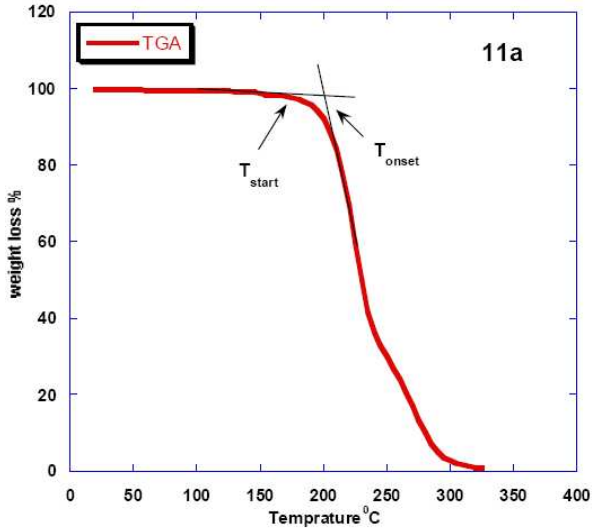


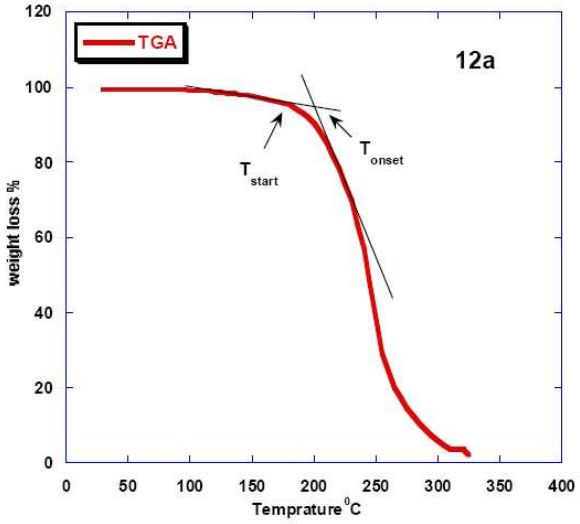
Mass spectra of 3-methyl-*N*-(cyclohexanoxycarbonylmethyl)imidazolium chloride (13b)

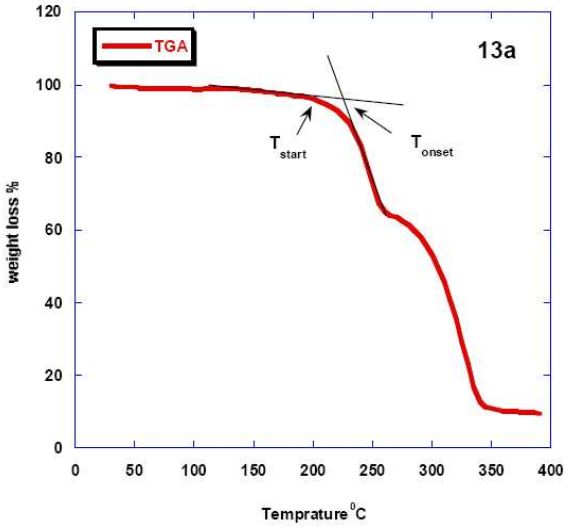
Thermal stability analysis of ionic liquids

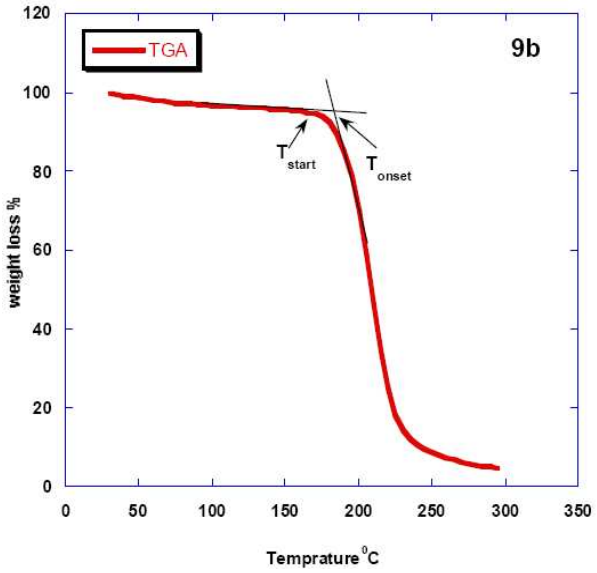








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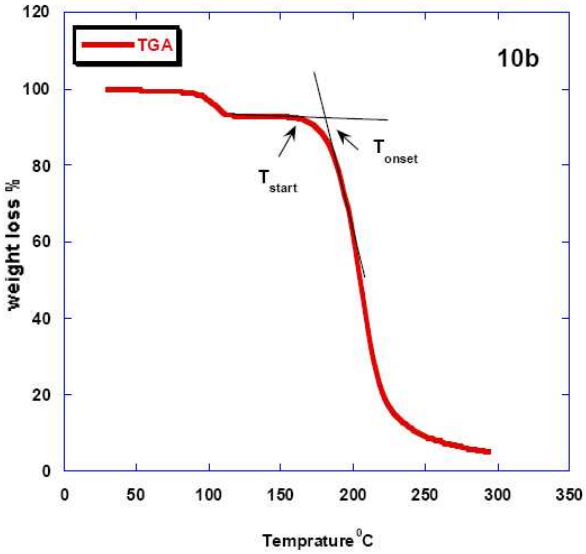
9b
T start
T onset
weight loss %
Temprature °C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10b
T start
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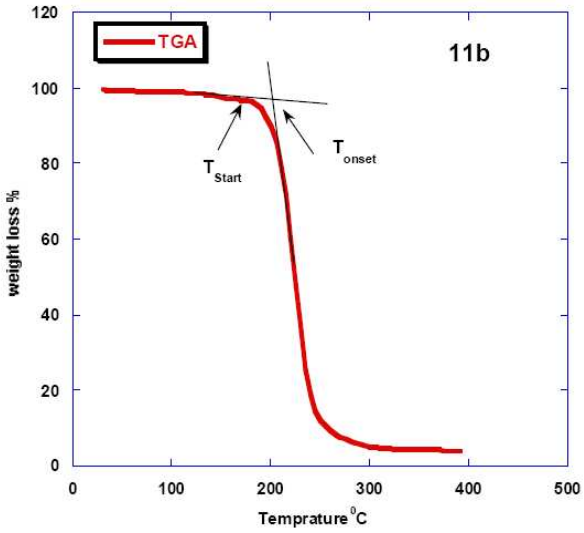
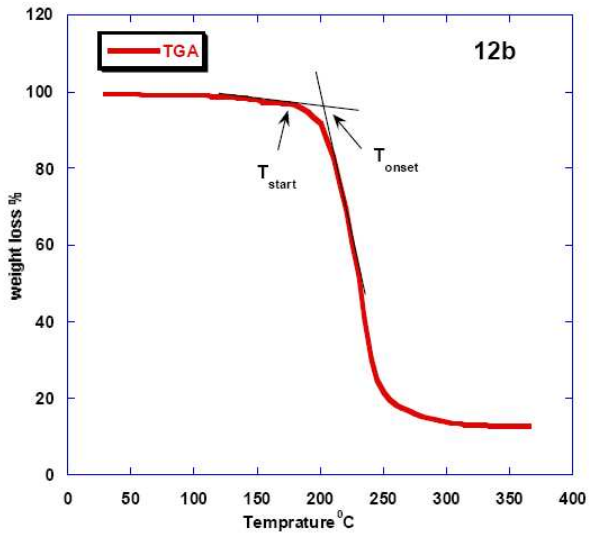
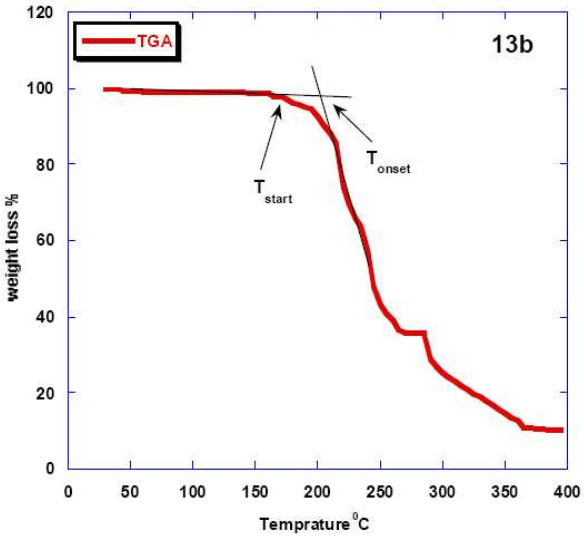
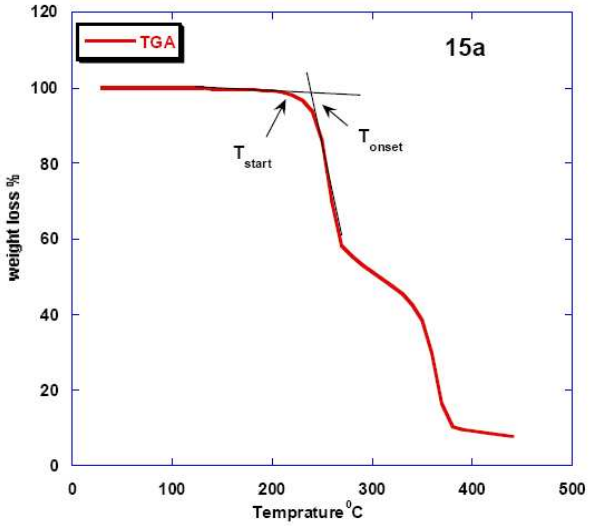
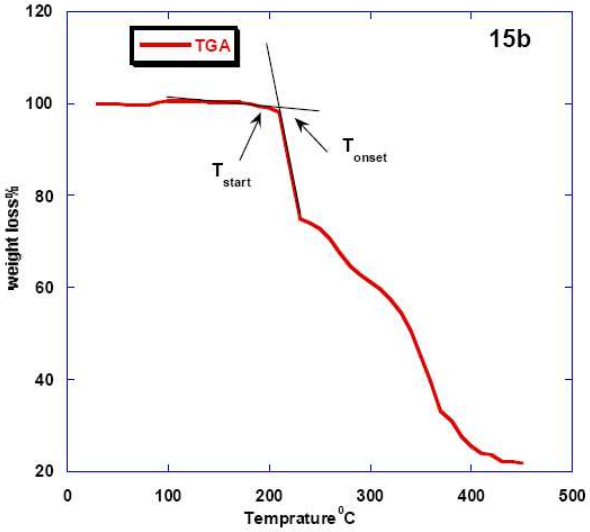
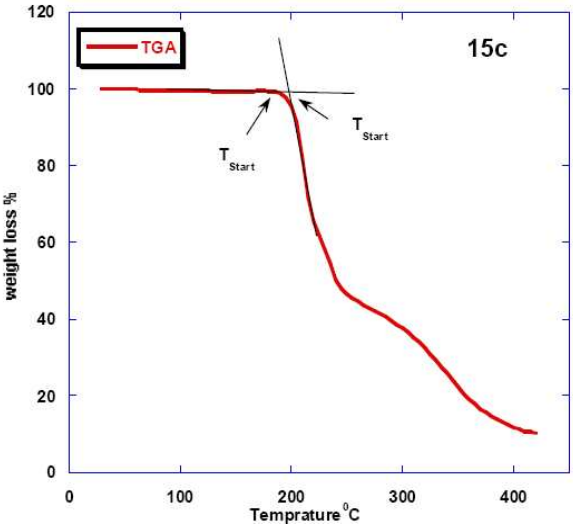

TGA
11b
T Start
T onset
weight loss %
Temprature °C


TGA
12b
T start
T onset
weight loss %
Temprature °C


TGA
13b
T start
T onset
weight loss %
Temprature °C


TGA
15a
T start
T onset
weight loss %
Temprature °C
120
100
80
60
40
20
0
0
100
200
300
400
500


TGA
15b
T start
T onset
weight loss%
Temprature °C
120
100
80
60
40
20
0
100
200
300
400
500


TGA
15c
T Start
T Start
weight loss %
Temprature °C
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100
80
60
40
20
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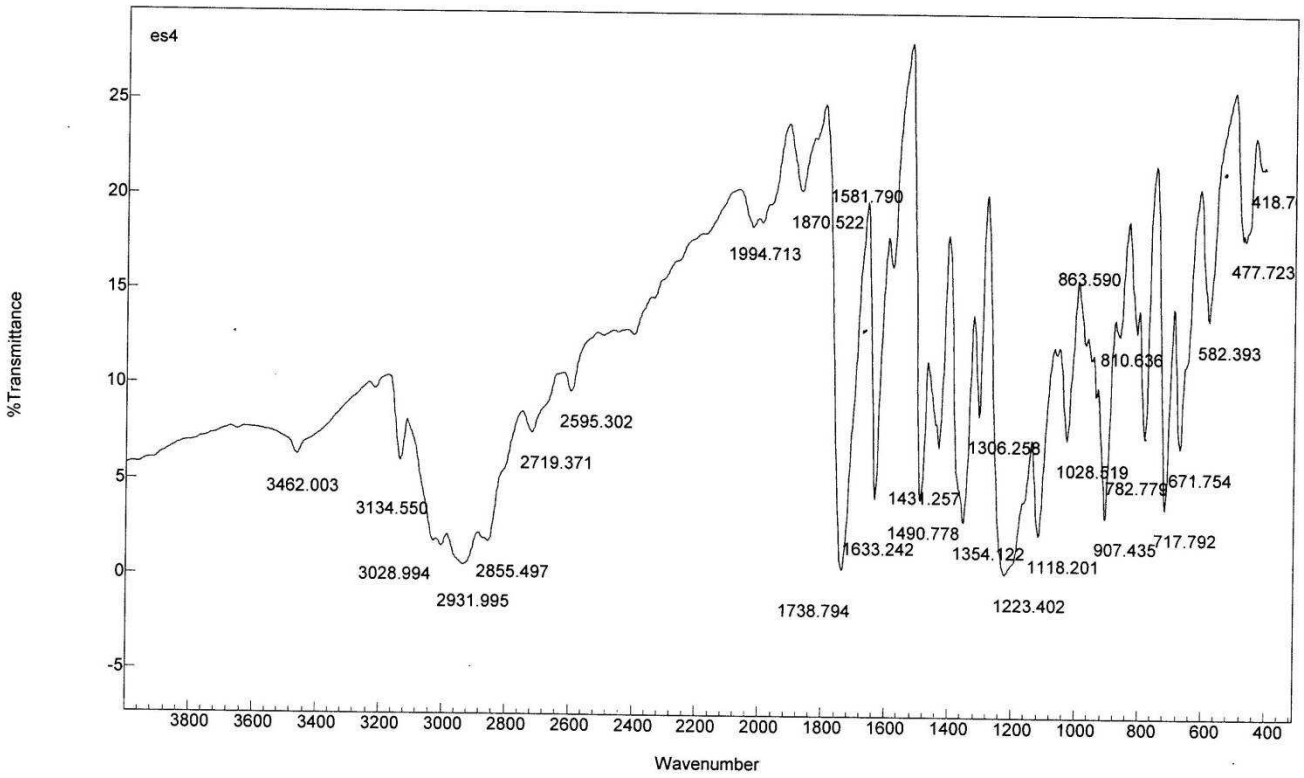
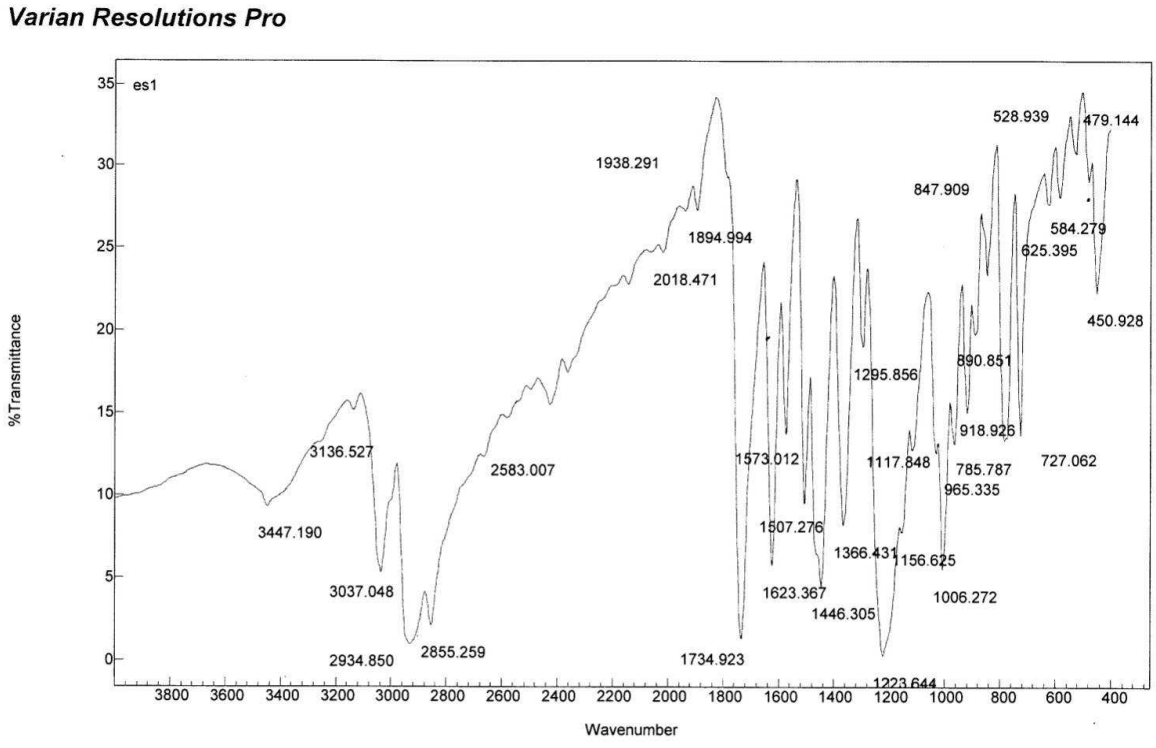
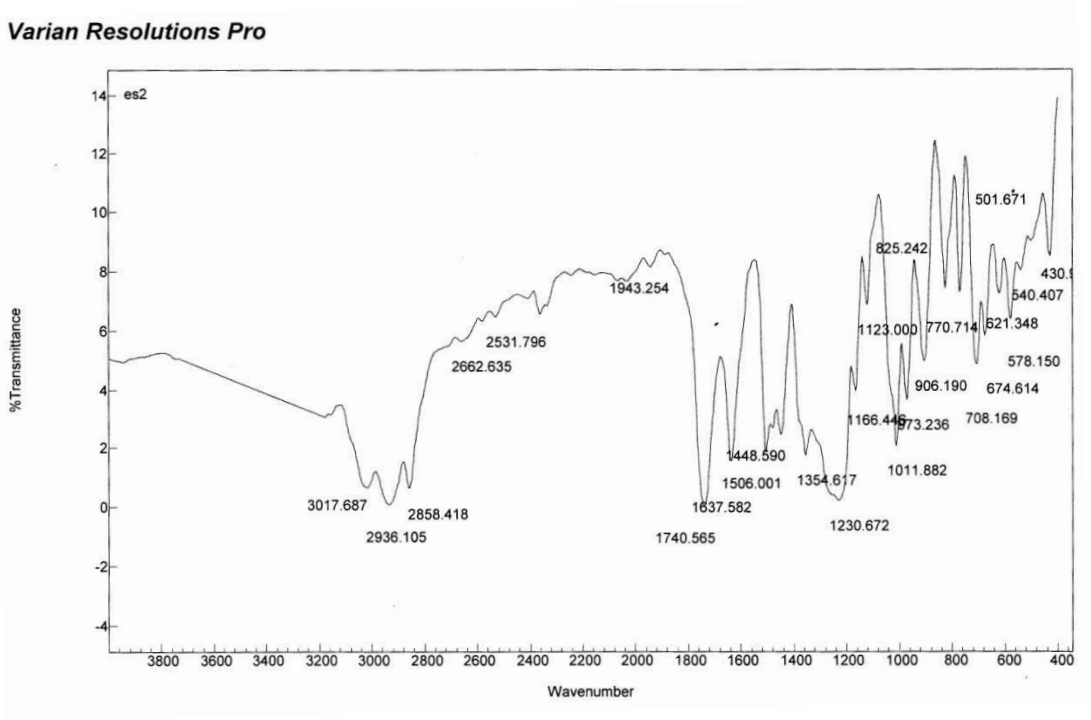
100
200
300
400



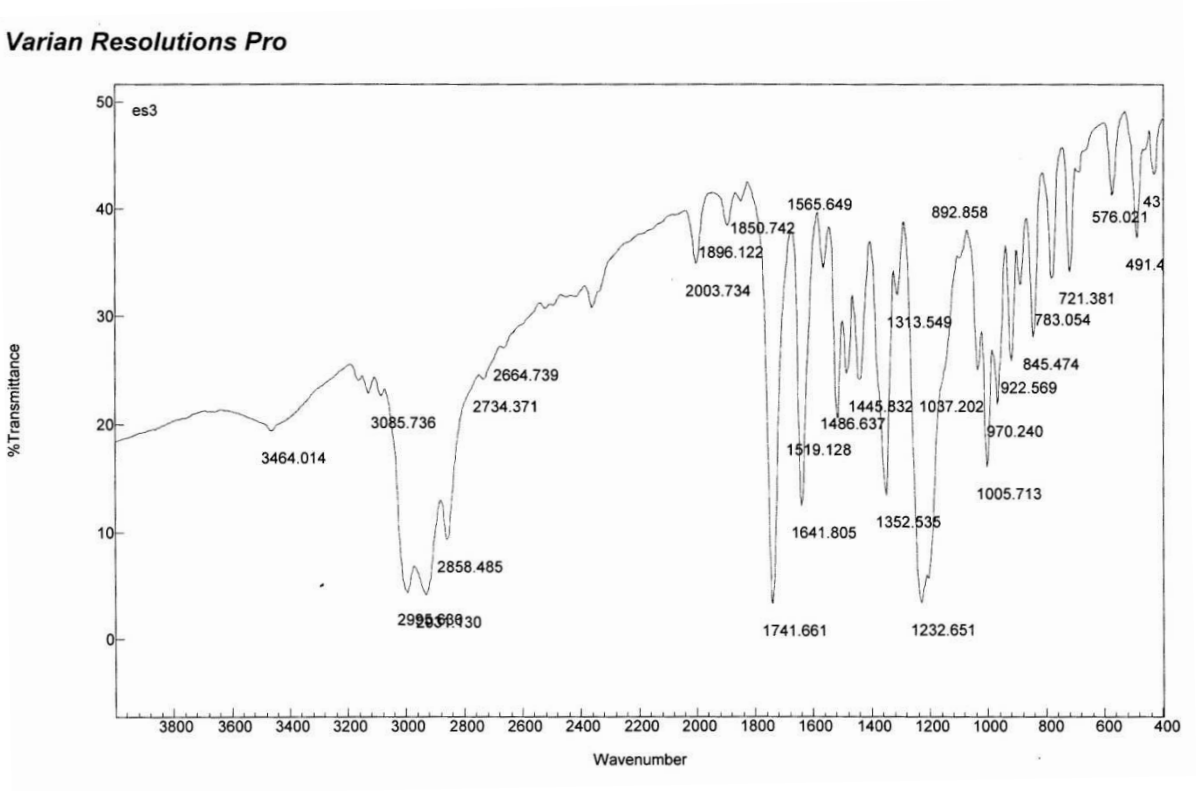
IR spectra of N-(cyclohexanoxycarbonylmethyl)pyridinium bromide (9a)



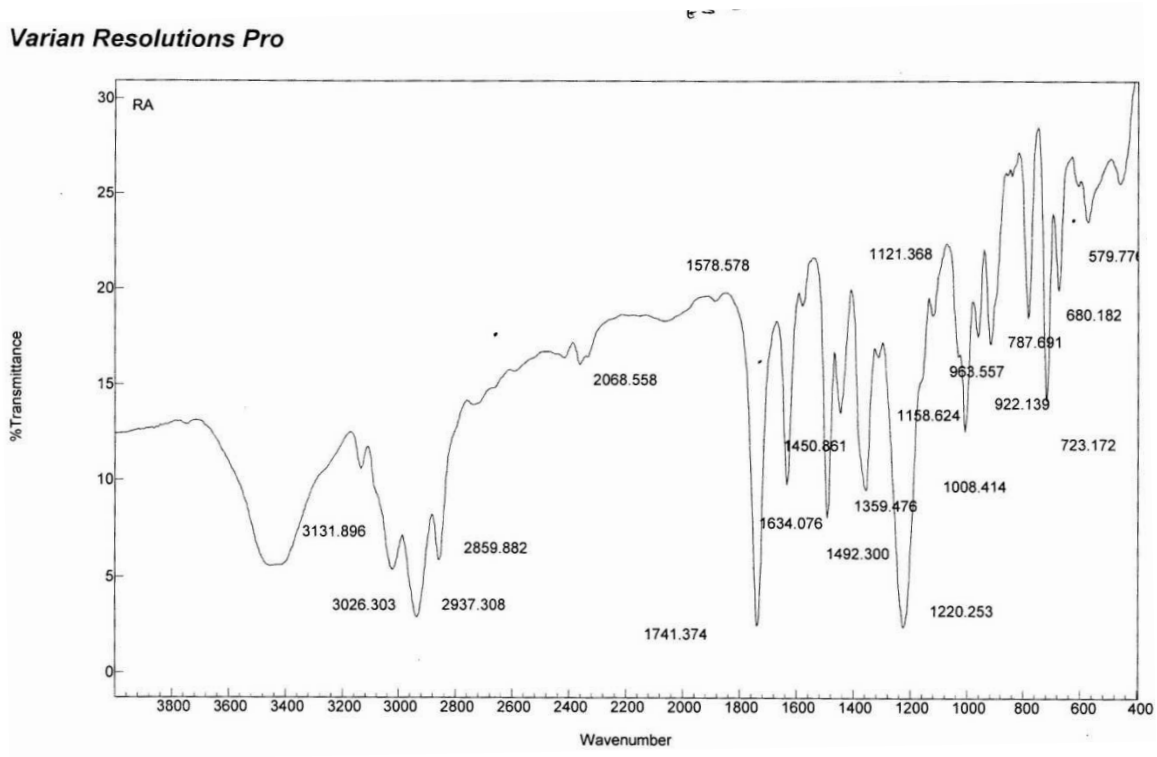
IR spectra of 2-methyl -N-(cyclohexanoxycarbonylmethyl)pyridinium bromide (10a)



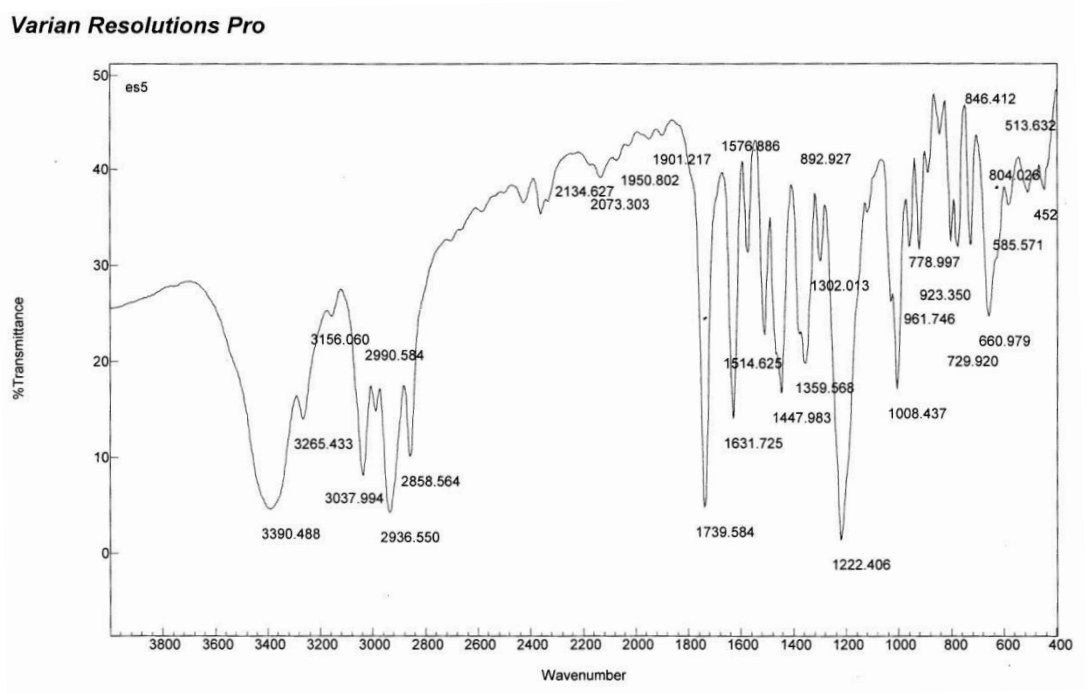
IR spectra of 3-methyl-N-(cyclohexanoxycarbonylmethyl)pyridinium bromide (11a)



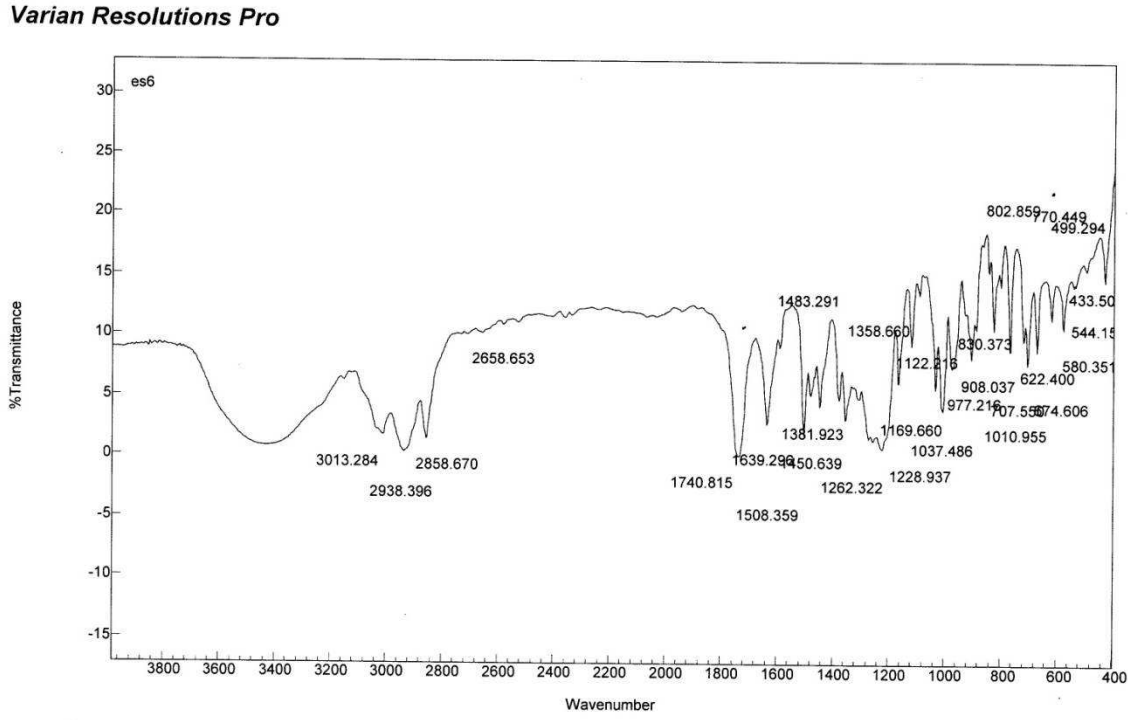
IR spectra of 4-methyl -N-(cyclohexanoxycarbonylmethyl)pyridinium chloride (12a)



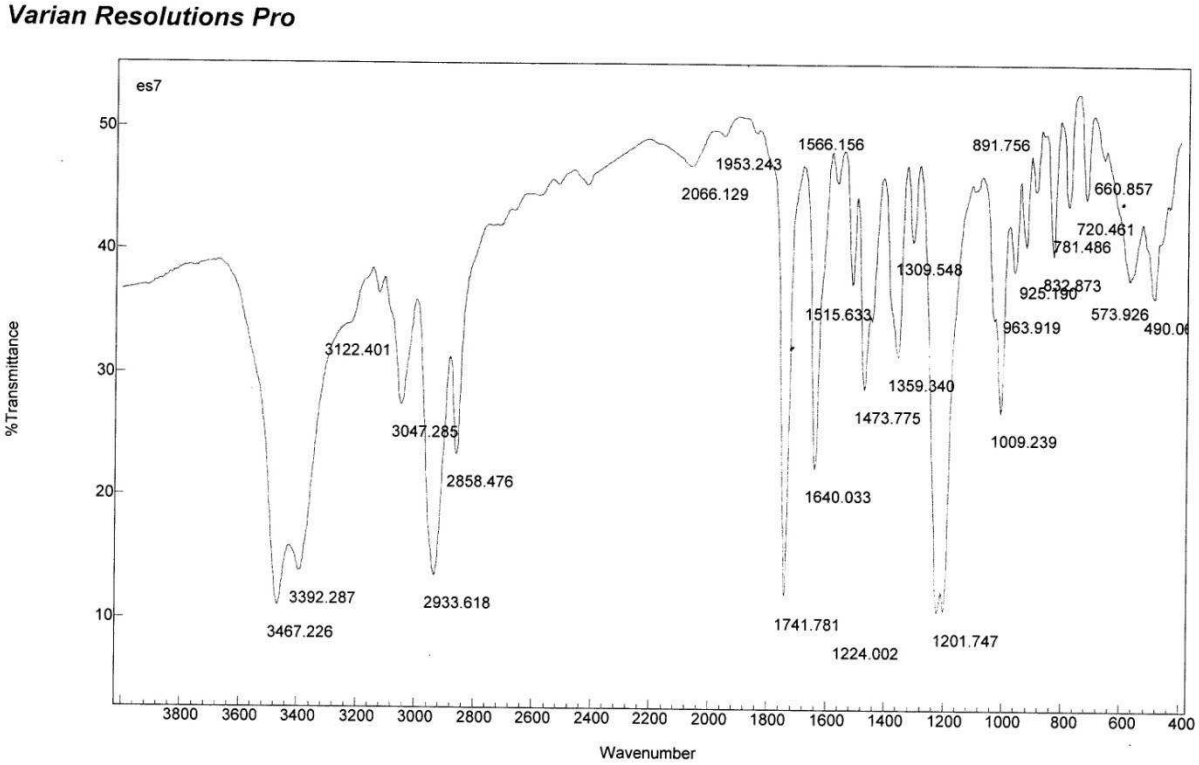
IR spectra of N-(cyclohexanoxycarbonylmethyl)pyridinium bromide (9b)



IR spectra of 2-methyl -N-(cyclohexanoxycarbonylmethyl)pyridinium chloride (10b)



IR spectra of 3-methyl -N-(cyclohexanoxycarbonylmethyl)pyridinium chloride (11b)



IR spectra of 4-methyl -N-(cyclohexanoxycarbonylmethyl)pyridinium chloride (12b)

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **15a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6425(7)	2500	5621(4)	63(1)
C(2)	7417(6)	1032(5)	5440(3)	84(1)
C(3)	8147(7)	1059(7)	4302(4)	98(2)
C(4)	9156(11)	2500	4131(6)	118(3)
C(5)	4298(6)	2500	6946(4)	59(1)
C(6)	4057(6)	2500	8166(4)	64(1)
C(7)	1465(7)	1105(6)	8459(4)	94(2)
C(8)	-194(8)	1033(12)	8633(5)	154(4)
C(9)	-1067(10)	2500	8727(8)	212(11)
N(1)	2271(5)	2500	8386(3)	59(1)
O(1)	5911(4)	2500	6774(3)	74(1)
O(2)	3203(5)	2500	6304(3)	105(2)
F(1)	5988(8)	2500	1150(11)	270(6)
F(2)	4650(9)	1173(5)	2280(4)	192(2)
F(3)	2411(10)	2500	1868(10)	239(4)
F(4)	3774(7)	1169(5)	634(3)	165(2)
P(1)	4210(2)	2500	1477(1)	65(1)

Table 2. Bond lengths [Å] and angles [°] for **15a**.

C(1)-O(1)	1.485(6)
C(1)-C(2)	1.492(5)
C(1)-C(2)#1	1.492(5)
C(1)-H(1)	0.9800
C(2)-C(3)	1.529(6)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.479(7)
C(3)-H(3A)	0.9700

C(3)-H(3B)	0.9700
C(4)-C(3)#1	1.479(7)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-O(2)	1.156(6)
C(5)-O(1)	1.301(6)
C(5)-C(6)	1.517(7)
C(6)-N(1)	1.447(6)
C(6)-H(6A)	1.06(4)
C(7)-C(8)	1.338(8)
C(7)-N(1)	1.349(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.430(10)
C(8)-H(8)	0.9300
C(9)-C(8)#1	1.430(10)
C(9)-H(9)	0.9300
N(1)-C(7)#1	1.349(5)
F(1)-P(1)	1.475(6)
F(2)-P(1)	1.531(3)
F(3)-P(1)	1.517(6)
F(4)-P(1)	1.564(3)
P(1)-F(2)#1	1.531(3)
P(1)-F(4)#1	1.564(3)

O(1)-C(1)-C(2)	107.6(3)
O(1)-C(1)-C(2)#1	107.6(3)
C(2)-C(1)-C(2)#1	113.2(5)
O(1)-C(1)-H(1)	109.5
C(2)-C(1)-H(1)	109.5
C(2)#1-C(1)-H(1)	109.5
C(1)-C(2)-C(3)	109.8(4)
C(1)-C(2)-H(2A)	109.7
C(3)-C(2)-H(2A)	109.7
C(1)-C(2)-H(2B)	109.7
C(3)-C(2)-H(2B)	109.7
H(2A)-C(2)-H(2B)	108.2
C(4)-C(3)-C(2)	111.2(4)

C(4)-C(3)-H(3A)	109.4
C(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3B)	109.4
C(2)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
C(3)-C(4)-C(3)#1	111.6(6)
C(3)-C(4)-H(4A)	109.3
C(3)#1-C(4)-H(4A)	109.3
C(3)-C(4)-H(4B)	109.3
C(3)#1-C(4)-H(4B)	109.3
H(4A)-C(4)-H(4B)	108.0
O(2)-C(5)-O(1)	127.7(5)
O(2)-C(5)-C(6)	124.2(5)
O(1)-C(5)-C(6)	108.1(4)
N(1)-C(6)-C(5)	109.6(4)
N(1)-C(6)-H(6A)	105(2)
C(5)-C(6)-H(6A)	120(2)
C(8)-C(7)-N(1)	121.3(6)
C(8)-C(7)-H(7)	119.4
N(1)-C(7)-H(7)	119.4
C(7)-C(8)-C(9)	116.9(7)
C(7)-C(8)-H(8)	121.6
C(9)-C(8)-H(8)	121.6
C(8)-C(9)-C(8)#1	121.0(7)
C(8)-C(9)-H(9)	119.5
C(8)#1-C(9)-H(9)	119.5
C(7)#1-N(1)-C(7)	122.7(6)
C(7)#1-N(1)-C(6)	118.6(3)
C(7)-N(1)-C(6)	118.6(3)
C(5)-O(1)-C(1)	116.8(4)
F(1)-P(1)-F(3)	177.3(6)
F(1)-P(1)-F(2)#1	88.5(4)
F(3)-P(1)-F(2)#1	89.7(4)
F(1)-P(1)-F(2)	88.5(4)
F(3)-P(1)-F(2)	89.7(4)
F(2)#1-P(1)-F(2)	94.7(4)
F(1)-P(1)-F(4)	90.8(4)

F(3)-P(1)-F(4)	91.0(4)
F(2)#1-P(1)-F(4)	178.7(2)
F(2)-P(1)-F(4)	86.4(3)
F(1)-P(1)-F(4)#1	90.8(4)
F(3)-P(1)-F(4)#1	91.0(4)
F(2)#1-P(1)-F(4)#1	86.4(3)
F(2)-P(1)-F(4)#1	178.7(2)
F(4)-P(1)-F(4)#1	92.4(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **15a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	60(3)	70(3)	58(2)	0	2(2)	0
C(2)	105(3)	74(2)	72(2)	-6(2)	5(2)	13(2)
C(3)	102(3)	121(4)	72(2)	-19(2)	7(2)	29(3)
C(4)	95(5)	190(10)	69(3)	0	23(3)	0
C(5)	60(3)	48(2)	69(3)	0	-2(2)	0
C(6)	55(3)	71(3)	66(3)	0	-1(2)	0
C(7)	96(3)	99(3)	88(3)	-9(2)	6(2)	-35(3)
C(8)	98(4)	257(11)	107(4)	-5(5)	5(4)	-102(6)
C(9)	47(4)	500(30)	90(6)	0	5(4)	0
N(1)	55(2)	68(2)	55(2)	0	5(2)	0
O(1)	53(2)	108(3)	61(2)	0	4(1)	0
O(2)	64(2)	187(5)	65(2)	0	-3(2)	0
F(1)	90(4)	200(8)	525(19)	0	90(6)	0
F(2)	332(7)	109(3)	133(3)	47(2)	-40(4)	30(3)
F(3)	140(5)	195(7)	390(12)	0	127(7)	0
F(4)	273(6)	114(3)	107(2)	-35(2)	-19(3)	-25(3)
P(1)	72(1)	55(1)	68(1)	0	-9(1)	0

Table 4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **15b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3791(3)	1996(2)	9771(2)	63(1)
C(2)	4765(4)	1694(4)	9095(2)	95(1)
C(3)	3694(5)	817(4)	8468(2)	117(2)
C(4)	2820(5)	-185(3)	8835(2)	102(1)
C(5)	1856(5)	123(3)	9520(2)	97(1)
C(6)	2918(4)	1002(3)	10161(2)	84(1)
C(7)	4749(3)	3748(2)	10611(2)	56(1)
C(8)	6141(3)	4497(2)	11150(2)	61(1)
C(9)	8409(3)	3942(2)	10579(2)	57(1)
C(10)	9728(3)	3560(3)	10631(2)	68(1)
C(11)	10199(3)	3281(2)	11363(2)	69(1)
C(12)	9309(4)	3375(2)	12023(2)	67(1)
C(13)	7961(3)	3761(2)	11949(2)	57(1)
C(14)	3524(5)	1717(2)	12850(2)	83(1)
C(15)	8449(3)	1772(2)	4974(2)	54(1)
C(16)	8384(5)	1895(3)	4093(2)	86(1)
C(17)	8604(7)	884(4)	3586(2)	125(2)
C(18)	7421(5)	-157(3)	3768(2)	91(1)
C(19)	7505(6)	-296(3)	4641(2)	94(1)
C(20)	7269(5)	717(2)	5172(2)	86(1)
C(21)	9053(3)	3656(2)	5607(1)	48(1)
C(22)	8374(3)	4511(2)	6061(2)	58(1)
C(23)	5541(3)	3923(2)	5574(2)	54(1)
C(24)	3939(3)	3556(2)	5674(2)	66(1)
C(25)	3442(3)	3336(2)	6427(2)	70(1)
C(26)	4555(4)	3483(2)	7066(2)	69(1)
C(27)	6177(3)	3869(2)	6943(2)	55(1)
C(28)	8830(4)	1721(2)	7853(2)	70(1)
N(1)	7546(2)	4046(2)	11232(1)	48(1)
N(2)	6635(2)	4091(1)	6198(1)	44(1)

O(1)	4951(2)	2763(2)	10385(1)	67(1)
O(2)	3617(2)	4070(2)	10429(1)	73(1)
O(3)	5363(3)	3553(2)	13526(2)	92(1)
O(4)	2509(3)	3194(2)	13667(2)	113(1)
O(5)	3649(4)	3593(2)	12401(2)	108(1)
O(6)	7988(2)	2676(1)	5448(1)	55(1)
O(7)	10425(2)	3892(2)	5422(1)	64(1)
O(8)	8626(3)	3582(2)	8565(1)	89(1)
O(9)	10127(3)	3607(2)	7391(2)	97(1)
O(10)	11206(3)	3177(2)	8622(2)	112(1)
F(1)	2109(3)	1266(2)	12427(2)	136(1)
F(2)	4669(4)	1570(2)	12373(2)	144(1)
F(3)	3530(5)	1158(2)	13457(2)	165(1)
F(4)	7456(3)	1586(2)	7423(2)	115(1)
F(5)	8448(3)	1180(2)	8489(2)	126(1)
F(6)	9739(3)	1237(2)	7418(2)	132(1)
S(1)	9824(1)	3175(1)	8147(1)	55(1)
S(2)	3777(1)	3167(1)	13155(1)	56(1)

Table 5. Bond lengths [Å] and angles [°] for **15b**.

C(1)-O(1)	1.472(3)
C(1)-C(2)	1.494(4)
C(1)-C(6)	1.487(4)
C(1)-H(1)	0.9800
C(2)-C(3)	1.512(5)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.475(6)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.502(5)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.526(4)
C(5)-H(5A)	0.9700

C(5)-H(5B)	0.9700
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-O(2)	1.193(3)
C(7)-O(1)	1.312(3)
C(7)-C(8)	1.504(3)
C(8)-N(1)	1.476(3)
C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700
C(9)-C(10)	1.351(4)
C(9)-N(1)	1.342(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.370(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.362(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.380(4)
C(12)-H(12)	0.9300
C(13)-N(1)	1.334(3)
C(13)-H(13)	0.9300
C(14)-F(3)	1.280(4)
C(14)-F(2)	1.318(4)
C(14)-F(1)	1.336(5)
C(14)-S(2)	1.788(3)
C(15)-O(6)	1.463(2)
C(15)-C(16)	1.477(4)
C(15)-C(20)	1.504(4)
C(15)-H(15)	0.9800
C(16)-C(17)	1.505(5)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.485(6)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.470(5)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700

C(19)-C(20)	1.531(4)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-O(7)	1.194(3)
C(21)-O(6)	1.314(3)
C(21)-C(22)	1.502(3)
C(22)-N(2)	1.478(3)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-N(2)	1.335(3)
C(23)-C(24)	1.351(4)
C(23)-H(23)	0.9300
C(24)-C(25)	1.355(4)
C(24)-H(24)	0.9300
C(25)-C(26)	1.366(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.376(4)
C(26)-H(26)	0.9300
C(27)-N(2)	1.334(3)
C(27)-H(27)	0.9300
C(28)-F(5)	1.309(4)
C(28)-F(6)	1.303(3)
C(28)-F(4)	1.322(4)
C(28)-S(1)	1.799(3)
O(3)-S(2)	1.415(2)
O(4)-S(2)	1.405(2)
O(5)-S(2)	1.415(2)
O(8)-S(1)	1.434(2)
O(9)-S(1)	1.412(2)
O(10)-S(1)	1.405(2)

O(1)-C(1)-C(2)	106.3(2)
O(1)-C(1)-C(6)	108.5(2)
C(2)-C(1)-C(6)	111.8(3)
O(1)-C(1)-H(1)	110.1

C(2)-C(1)-H(1)	110.1
C(6)-C(1)-H(1)	110.1
C(1)-C(2)-C(3)	110.3(3)
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2B)	109.6
C(3)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(2)	112.1(3)
C(4)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3B)	109.2
C(2)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
C(3)-C(4)-C(5)	110.5(4)
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(4)-C(5)-C(6)	111.6(3)
C(4)-C(5)-H(5A)	109.3
C(6)-C(5)-H(5A)	109.3
C(4)-C(5)-H(5B)	109.3
C(6)-C(5)-H(5B)	109.3
H(5A)-C(5)-H(5B)	108.0
C(1)-C(6)-C(5)	110.0(3)
C(1)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6A)	109.7
C(1)-C(6)-H(6B)	109.7
C(5)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
O(2)-C(7)-O(1)	126.6(2)
O(2)-C(7)-C(8)	120.5(3)
O(1)-C(7)-C(8)	112.9(2)
N(1)-C(8)-C(7)	114.3(2)
N(1)-C(8)-H(8A)	108.7

C(7)-C(8)-H(8A)	108.7
N(1)-C(8)-H(8B)	108.7
C(7)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(10)-C(9)-N(1)	121.0(2)
C(10)-C(9)-H(9)	119.5
N(1)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	119.5(3)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(12)-C(11)-C(10)	119.3(3)
C(12)-C(11)-H(11)	120.4
C(10)-C(11)-H(11)	120.4
C(11)-C(12)-C(13)	119.8(3)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
N(1)-C(13)-C(12)	119.7(2)
N(1)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
F(3)-C(14)-F(2)	108.3(3)
F(3)-C(14)-F(1)	106.8(3)
F(2)-C(14)-F(1)	107.3(3)
F(3)-C(14)-S(2)	112.7(3)
F(2)-C(14)-S(2)	111.1(2)
F(1)-C(14)-S(2)	110.3(3)
O(6)-C(15)-C(16)	110.8(2)
O(6)-C(15)-C(20)	105.1(2)
C(16)-C(15)-C(20)	112.3(3)
O(6)-C(15)-H(15)	109.5
C(16)-C(15)-H(15)	109.5
C(20)-C(15)-H(15)	109.5
C(15)-C(16)-C(17)	111.5(3)
C(15)-C(16)-H(16A)	109.3
C(17)-C(16)-H(16A)	109.3
C(15)-C(16)-H(16B)	109.3
C(17)-C(16)-H(16B)	109.3
H(16A)-C(16)-H(16B)	108.0

C(18)-C(17)-C(16)	111.7(3)
C(18)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17A)	109.3
C(18)-C(17)-H(17B)	109.3
C(16)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	107.9
C(19)-C(18)-C(17)	111.5(3)
C(19)-C(18)-H(18A)	109.3
C(17)-C(18)-H(18A)	109.3
C(19)-C(18)-H(18B)	109.3
C(17)-C(18)-H(18B)	109.3
H(18A)-C(18)-H(18B)	108.0
C(18)-C(19)-C(20)	111.6(3)
C(18)-C(19)-H(19A)	109.3
C(20)-C(19)-H(19A)	109.3
C(18)-C(19)-H(19B)	109.3
C(20)-C(19)-H(19B)	109.3
H(19A)-C(19)-H(19B)	108.0
C(15)-C(20)-C(19)	110.4(3)
C(15)-C(20)-H(20A)	109.6
C(19)-C(20)-H(20A)	109.6
C(15)-C(20)-H(20B)	109.6
C(19)-C(20)-H(20B)	109.6
H(20A)-C(20)-H(20B)	108.1
O(7)-C(21)-O(6)	126.2(2)
O(7)-C(21)-C(22)	120.9(2)
O(6)-C(21)-C(22)	112.87(18)
N(2)-C(22)-C(21)	113.52(19)
N(2)-C(22)-H(22A)	108.9
C(21)-C(22)-H(22A)	108.9
N(2)-C(22)-H(22B)	108.9
C(21)-C(22)-H(22B)	108.9
H(22A)-C(22)-H(22B)	107.7
N(2)-C(23)-C(24)	121.7(2)
N(2)-C(23)-H(23)	119.2
C(24)-C(23)-H(23)	119.2
C(23)-C(24)-C(25)	118.7(3)

C(23)-C(24)-H(24)	120.6
C(25)-C(24)-H(24)	120.6
C(24)-C(25)-C(26)	120.0(3)
C(24)-C(25)-H(25)	120.0
C(26)-C(25)-H(25)	120.0
C(25)-C(26)-C(27)	119.8(3)
C(25)-C(26)-H(26)	120.1
C(27)-C(26)-H(26)	120.1
N(2)-C(27)-C(26)	119.1(2)
N(2)-C(27)-H(27)	120.4
C(26)-C(27)-H(27)	120.4
F(5)-C(28)-F(6)	107.9(3)
F(5)-C(28)-F(4)	105.9(3)
F(6)-C(28)-F(4)	108.2(3)
F(5)-C(28)-S(1)	111.6(2)
F(6)-C(28)-S(1)	111.6(2)
F(4)-C(28)-S(1)	111.3(2)
C(13)-N(1)-C(9)	120.7(2)
C(13)-N(1)-C(8)	120.4(2)
C(9)-N(1)-C(8)	118.9(2)
C(23)-N(2)-C(27)	120.7(2)
C(23)-N(2)-C(22)	119.7(2)
C(27)-N(2)-C(22)	119.6(2)
C(7)-O(1)-C(1)	118.83(19)
C(21)-O(6)-C(15)	119.21(17)
O(10)-S(1)-O(9)	115.23(18)
O(10)-S(1)-O(8)	116.25(18)
O(9)-S(1)-O(8)	111.80(16)
O(10)-S(1)-C(28)	104.48(15)
O(9)-S(1)-C(28)	103.21(16)
O(8)-S(1)-C(28)	103.93(14)
O(4)-S(2)-O(5)	114.7(2)
O(4)-S(2)-O(3)	116.34(17)
O(5)-S(2)-O(3)	112.23(18)
O(4)-S(2)-C(14)	104.78(16)
O(5)-S(2)-C(14)	102.69(18)
O(3)-S(2)-C(14)	104.18(17)

Symmetry transformations used to generate equivalent atoms:

Table 6. Anisotropic displacement parameters ($Å^2$x 10^3)for **15b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(1)	65(2)	71(2)	-2(1)	-17(1)	11(1)
C(2)	73(2)	122(3)	65(2)	0(2)	6(2)	-14(2)
C(3)	90(3)	161(4)	69(2)	-21(2)	0(2)	-5(3)
C(4)	98(3)	91(3)	101(3)	-27(2)	-14(2)	15(2)
C(5)	87(2)	89(2)	90(2)	0(2)	0(2)	-16(2)
C(6)	72(2)	95(2)	68(2)	-3(2)	11(2)	-2(2)
C(7)	44(1)	67(2)	56(1)	11(1)	4(1)	11(1)
C(8)	49(1)	60(1)	73(2)	0(1)	1(1)	14(1)
C(9)	50(1)	70(2)	45(1)	7(1)	1(1)	6(1)
C(10)	51(1)	82(2)	67(2)	-3(1)	9(1)	13(1)
C(11)	54(1)	68(2)	85(2)	2(1)	-3(1)	18(1)
C(12)	72(2)	60(2)	63(2)	10(1)	-13(1)	12(1)
C(13)	58(1)	57(1)	47(1)	0(1)	4(1)	2(1)
C(14)	101(2)	51(2)	96(2)	0(2)	27(2)	23(2)
C(15)	50(1)	55(1)	59(1)	-5(1)	6(1)	25(1)
C(16)	120(3)	72(2)	56(2)	6(1)	14(2)	7(2)
C(17)	186(5)	93(3)	75(2)	-20(2)	53(3)	8(3)
C(18)	109(3)	76(2)	78(2)	-27(2)	2(2)	24(2)
C(19)	133(3)	60(2)	93(2)	-6(2)	4(2)	37(2)
C(20)	135(3)	52(2)	69(2)	5(1)	29(2)	23(2)
C(21)	46(1)	52(1)	51(1)	10(1)	7(1)	20(1)
C(22)	47(1)	46(1)	80(2)	5(1)	14(1)	12(1)
C(23)	63(1)	56(1)	51(1)	6(1)	5(1)	29(1)
C(24)	58(1)	66(2)	77(2)	-9(1)	-8(1)	30(1)
C(25)	49(1)	58(2)	104(2)	6(2)	17(1)	16(1)
C(26)	89(2)	55(1)	72(2)	14(1)	36(2)	25(1)
C(27)	70(1)	53(1)	49(1)	2(1)	5(1)	28(1)
C(28)	62(2)	58(2)	84(2)	-6(1)	4(1)	11(1)
N(1)	42(1)	49(1)	47(1)	1(1)	-1(1)	5(1)

N(2)	46(1)	37(1)	53(1)	2(1)	8(1)	18(1)
O(1)	56(1)	60(1)	80(1)	-4(1)	-23(1)	15(1)
O(2)	49(1)	87(1)	86(1)	5(1)	-2(1)	25(1)
O(3)	84(2)	97(2)	83(2)	-15(1)	-11(1)	15(1)
O(4)	107(2)	92(2)	140(2)	-15(2)	59(2)	35(2)
O(5)	132(2)	95(2)	98(2)	46(2)	-16(2)	21(2)
O(6)	52(1)	48(1)	66(1)	1(1)	17(1)	19(1)
O(7)	43(1)	73(1)	80(1)	11(1)	12(1)	20(1)
O(8)	108(2)	81(2)	80(1)	-13(1)	16(1)	36(1)
O(9)	111(2)	101(2)	85(2)	43(1)	28(1)	26(2)
O(10)	86(2)	87(2)	148(2)	5(2)	-62(2)	9(1)
F(1)	126(2)	81(1)	163(2)	-41(2)	5(2)	-16(1)
F(2)	152(2)	109(2)	173(3)	-39(2)	60(2)	54(2)
F(3)	255(4)	82(2)	181(3)	71(2)	40(3)	63(2)
F(4)	78(1)	108(2)	132(2)	-34(1)	-27(1)	2(1)
F(5)	147(2)	77(1)	152(2)	50(2)	24(2)	11(1)
F(6)	114(2)	89(2)	186(3)	-49(2)	26(2)	37(1)
S(1)	58(1)	50(1)	52(1)	3(1)	-3(1)	8(1)
S(2)	65(1)	45(1)	57(1)	1(1)	6(1)	18(1)

Table 7. Torsion angles [°] for **15b**.

O(1)-C(1)-C(2)-C(3)	174.6(3)
C(6)-C(1)-C(2)-C(3)	56.4(5)
C(1)-C(2)-C(3)-C(4)	-56.2(6)
C(2)-C(3)-C(4)-C(5)	55.8(5)
C(3)-C(4)-C(5)-C(6)	-55.4(5)
O(1)-C(1)-C(6)-C(5)	-173.0(3)
C(2)-C(1)-C(6)-C(5)	-56.1(4)
C(4)-C(5)-C(6)-C(1)	55.4(5)
O(2)-C(7)-C(8)-N(1)	-172.1(2)
O(1)-C(7)-C(8)-N(1)	7.6(3)
N(1)-C(9)-C(10)-C(11)	-0.5(4)
C(9)-C(10)-C(11)-C(12)	1.2(4)
C(10)-C(11)-C(12)-C(13)	-0.8(4)

C(11)-C(12)-C(13)-N(1)	-0.4(4)
O(6)-C(15)-C(16)-C(17)	-171.3(3)
C(20)-C(15)-C(16)-C(17)	-54.0(4)
C(15)-C(16)-C(17)-C(18)	54.8(6)
C(16)-C(17)-C(18)-C(19)	-55.9(6)
C(17)-C(18)-C(19)-C(20)	55.7(5)
O(6)-C(15)-C(20)-C(19)	173.9(3)
C(16)-C(15)-C(20)-C(19)	53.4(4)
C(18)-C(19)-C(20)-C(15)	-54.1(5)
O(7)-C(21)-C(22)-N(2)	176.8(2)
O(6)-C(21)-C(22)-N(2)	-2.9(3)
N(2)-C(23)-C(24)-C(25)	-1.2(4)
C(23)-C(24)-C(25)-C(26)	-0.3(4)
C(24)-C(25)-C(26)-C(27)	1.0(4)
C(25)-C(26)-C(27)-N(2)	-0.2(4)
C(12)-C(13)-N(1)-C(9)	1.2(3)
C(12)-C(13)-N(1)-C(8)	-177.8(2)
C(10)-C(9)-N(1)-C(13)	-0.7(4)
C(10)-C(9)-N(1)-C(8)	178.3(2)
C(7)-C(8)-N(1)-C(13)	-113.1(3)
C(7)-C(8)-N(1)-C(9)	67.9(3)
C(24)-C(23)-N(2)-C(27)	1.9(3)
C(24)-C(23)-N(2)-C(22)	-179.0(2)
C(26)-C(27)-N(2)-C(23)	-1.2(3)
C(26)-C(27)-N(2)-C(22)	179.7(2)
C(21)-C(22)-N(2)-C(23)	-72.9(3)
C(21)-C(22)-N(2)-C(27)	106.2(2)
O(2)-C(7)-O(1)-C(1)	7.6(4)
C(8)-C(7)-O(1)-C(1)	-172.0(2)
C(2)-C(1)-O(1)-C(7)	124.2(3)
C(6)-C(1)-O(1)-C(7)	-115.5(3)
O(7)-C(21)-O(6)-C(15)	-2.7(4)
C(22)-C(21)-O(6)-C(15)	177.0(2)
C(16)-C(15)-O(6)-C(21)	-79.4(3)
C(20)-C(15)-O(6)-C(21)	159.1(2)
F(5)-C(28)-S(1)-O(10)	59.4(3)
F(6)-C(28)-S(1)-O(10)	-61.5(3)

F(4)-C(28)-S(1)-O(10)	177.5(3)
F(5)-C(28)-S(1)-O(9)	-179.8(2)
F(6)-C(28)-S(1)-O(9)	59.4(3)
F(4)-C(28)-S(1)-O(9)	-61.6(3)
F(5)-C(28)-S(1)-O(8)	-63.0(3)
F(6)-C(28)-S(1)-O(8)	176.2(3)
F(4)-C(28)-S(1)-O(8)	55.2(3)
F(3)-C(14)-S(2)-O(4)	-57.0(4)
F(2)-C(14)-S(2)-O(4)	-178.8(3)
F(1)-C(14)-S(2)-O(4)	62.4(3)
F(3)-C(14)-S(2)-O(5)	-177.1(3)
F(2)-C(14)-S(2)-O(5)	61.1(3)
F(1)-C(14)-S(2)-O(5)	-57.8(3)
F(3)-C(14)-S(2)-O(3)	65.7(3)
F(2)-C(14)-S(2)-O(3)	-56.1(3)
F(1)-C(14)-S(2)-O(3)	-175.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **15c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(10)	6081(12)	5250(40)	2860(20)	144(9)
C(1)	8939(9)	1703(19)	8530(20)	87(6)
C(2)	9707(11)	1772(19)	9164(14)	82(5)
C(3)	10253(9)	1230(20)	8640(20)	91(6)
C(4)	10034(8)	618(19)	7609(16)	67(4)
C(5)	9270(9)	548(19)	6989(16)	87(5)
C(6)	7937(7)	1100(30)	6768(14)	95(6)
C(7)	7766(8)	2656(17)	6025(15)	77(5)
C(8)	6788(7)	4520(20)	4880(18)	97(6)
C(9)	6395(12)	3700(40)	3820(20)	149(9)
C(11)	5579(12)	6310(40)	3220(30)	180(13)
C(12)	5930(20)	7270(40)	4440(30)	203(13)

C(13)	6279(11)	5680(30)	5399(19)	135(8)
B(1)	11796(10)	1290(20)	6280(20)	77(6)
N(1)	8753(6)	985(17)	7500(13)	69(4)
O(1)	8261(5)	3382(13)	5682(8)	78(3)
O(2)	7046(5)	3000(14)	5682(10)	99(4)
F(1)	12144(9)	20(20)	6740(20)	285(15)
F(2)	12035(10)	1410(30)	5293(16)	222(9)
F(3)	11937(11)	2770(20)	6660(20)	262(11)
F(4)	11055(6)	876(18)	5710(12)	154(5)

Table 9. Bond lengths [Å] and angles [°] for **15c**.

C(10)-C(11)	1.36(3)
C(10)-C(9)	1.62(3)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(1)-N(1)	1.31(2)
C(1)-C(2)	1.40(2)
C(1)-H(1)	0.9300
C(2)-C(3)	1.39(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.29(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.38(2)
C(4)-H(4)	0.9300
C(5)-N(1)	1.314(18)
C(5)-H(5)	0.9300
C(6)-C(7)	1.44(2)
C(6)-N(1)	1.505(17)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-O(1)	1.223(15)
C(7)-O(2)	1.284(15)
C(8)-C(9)	1.42(3)
C(8)-O(2)	1.469(18)
C(8)-C(13)	1.53(3)
C(8)-H(8)	0.9800
C(9)-H(9A)	0.9700

C(9)-H(9B)	0.9700
C(11)-C(12)	1.61(4)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.65(4)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
B(1)-F(3)	1.18(2)
B(1)-F(1)	1.179(19)
B(1)-F(4)	1.366(19)
B(1)-F(2)	1.40(3)
C(11)-C(10)-C(9)	107(2)
C(11)-C(10)-H(10A)	110.3
C(9)-C(10)-H(10A)	110.3
C(11)-C(10)-H(10B)	110.3
C(9)-C(10)-H(10B)	110.3
H(10A)-C(10)-H(10B)	108.5
N(1)-C(1)-C(2)	119.4(16)
N(1)-C(1)-H(1)	120.3
C(2)-C(1)-H(1)	120.3
C(3)-C(2)-C(1)	117.9(17)
C(3)-C(2)-H(2)	121.0
C(1)-C(2)-H(2)	121.0
C(4)-C(3)-C(2)	119.3(14)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	122.1(15)
C(3)-C(4)-H(4)	119.0
C(5)-C(4)-H(4)	119.0
N(1)-C(5)-C(4)	118.5(17)
N(1)-C(5)-H(5)	120.7
C(4)-C(5)-H(5)	120.7
C(7)-C(6)-N(1)	114.8(12)
C(7)-C(6)-H(6A)	108.6
N(1)-C(6)-H(6A)	108.6

C(7)-C(6)-H(6B)	108.6
N(1)-C(6)-H(6B)	108.6
H(6A)-C(6)-H(6B)	107.6
O(1)-C(7)-O(2)	126.2(13)
O(1)-C(7)-C(6)	121.1(12)
O(2)-C(7)-C(6)	112.2(12)
C(9)-C(8)-O(2)	105.8(16)
C(9)-C(8)-C(13)	114.0(15)
O(2)-C(8)-C(13)	105.1(16)
C(9)-C(8)-H(8)	110.6
O(2)-C(8)-H(8)	110.6
C(13)-C(8)-H(8)	110.6
C(8)-C(9)-C(10)	110(2)
C(8)-C(9)-H(9A)	109.6
C(10)-C(9)-H(9A)	109.6
C(8)-C(9)-H(9B)	109.6
C(10)-C(9)-H(9B)	109.6
H(9A)-C(9)-H(9B)	108.1
C(10)-C(11)-C(12)	115.2(18)
C(10)-C(11)-H(11A)	108.5
C(12)-C(11)-H(11A)	108.5
C(10)-C(11)-H(11B)	108.5
C(12)-C(11)-H(11B)	108.5
H(11A)-C(11)-H(11B)	107.5
C(11)-C(12)-C(13)	109(2)
C(11)-C(12)-H(12A)	109.9
C(13)-C(12)-H(12A)	109.9
C(11)-C(12)-H(12B)	109.9
C(13)-C(12)-H(12B)	109.9
H(12A)-C(12)-H(12B)	108.3
C(8)-C(13)-C(12)	105.0(18)
C(8)-C(13)-H(13A)	110.8
C(12)-C(13)-H(13A)	110.8
C(8)-C(13)-H(13B)	110.8
C(12)-C(13)-H(13B)	110.8
H(13A)-C(13)-H(13B)	108.8
F(3)-B(1)-F(1)	121(2)

F(3)-B(1)-F(4)	118.7(17)
F(1)-B(1)-F(4)	112.6(16)
F(3)-B(1)-F(2)	101(2)
F(1)-B(1)-F(2)	102(2)
F(4)-B(1)-F(2)	94.9(18)
C(1)-N(1)-C(5)	122.0(13)
C(1)-N(1)-C(6)	119.1(13)
C(5)-N(1)-C(6)	117.0(15)
C(7)-O(2)-C(8)	118.0(10)

Table 10. Anisotropic displacement parameters ($Å^2$x 10^3)for **15c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(10)	108(15)	180(20)	110(20)	31(17)	-12(13)	23(15)
C(1)	87(12)	54(9)	128(19)	47(11)	42(11)	5(7)
C(2)	121(14)	69(10)	46(12)	2(8)	6(10)	15(9)
C(3)	74(10)	50(9)	130(20)	35(10)	-11(11)	5(7)
C(4)	71(10)	66(9)	68(13)	-3(9)	24(8)	2(7)
C(5)	86(11)	65(9)	121(16)	1(9)	47(11)	14(7)
C(6)	48(8)	153(17)	86(14)	-12(12)	23(7)	-23(8)
C(7)	75(10)	42(7)	120(15)	26(8)	38(9)	1(7)
C(8)	40(7)	94(11)	141(19)	30(12)	-2(9)	-15(7)
C(9)	93(12)	220(30)	140(20)	40(20)	43(14)	-15(15)
C(11)	87(14)	240(30)	170(30)	40(20)	-25(15)	48(16)
C(12)	210(30)	140(20)	290(50)	20(30)	120(30)	60(20)
C(13)	132(15)	170(20)	112(19)	59(16)	41(13)	45(14)
B(1)	78(11)	47(10)	98(19)	11(10)	14(10)	6(8)
N(1)	62(7)	92(9)	53(10)	-6(7)	19(6)	1(6)
O(1)	66(5)	97(7)	70(8)	39(6)	20(5)	7(5)
O(2)	40(5)	96(7)	146(11)	24(7)	4(5)	-13(5)
F(1)	226(15)	112(11)	370(30)	70(14)	-142(18)	-46(10)
F(2)	205(14)	330(20)	153(16)	-51(16)	82(12)	-67(15)
F(3)	270(20)	153(13)	320(30)	-133(15)	24(16)	43(12)
F(4)	92(7)	202(13)	155(12)	12(10)	13(7)	-25(7)

Table 11- H-bonding parameters (Å,°) for 15a-15c compounds.

15a

X-H…Y	X…Y	H…Y	√X-H…Y
C1-H1...O2	2.708(7)	2.29	104
C3-H3B...F2	3.669(8)	2.70	175
C3-H3A...O2[1]	3.282(6)	2.83	109
C6-H6A...F2[1]	3.330(5)	2.68	119
C6-H6A...F4[1]	3.831(5)	2.79	163
C7-H7...F1[1]	3.688(7)	2.79	163
C7-H7...F2[1]	3.766(8)	2.97	144
C7-H7...F1[2]	3.688(7)	2.79	163
C3-H3A...O2[2]	3.282(6)	2.83	109
C4-H4A...F3[3]	3.844(13)	2.97	151
C4-H4A...F3[4]	3.844(13)	2.97	151
C6-H6A...F4[5]	3.250(6)	2.55	123
C8-H8...F3[6]	3.520(10)	2.63	160
C8-H8...F4[6]	3.533(9)	2.76	141
C8-H8...F3[7]	3.520(10)	2.63	160
C9-H9...O1[8]	3.341(9)	2.91	110
C9-H9...O1[9]	3.341(9)	2.91	110

(1) -x+1,-y,-z+1 (2) -x+1,+y-1/2,-z+1 (3) x+1,+y,+z (4) x+1,-y+1/2,+z
(5) x,+y,+z+1 (6) -x,-y,-z+1 (7) -x,+y-1/2,-z+1 (8) x-1,+y,+z
(9) x-1,-y+1/2,+z

15b

X-H…Y	X…Y	H…Y	√X-H…Y
C1-H1...O2	2.758(4)	2.36	103
C2-H2A...F5	3.555(5)	2.90	126
C2-H2B...O8	3.705(4)	2.95	135
C3-H3B...F4	3.654(5)	2.89	137
C8-H8B...O5	3.091(4)	2.36	132
C9-H9...O8	3.324(3)	2.62	133
C10-H10...O10	3.617(4)	2.71	164

C13-H13...O3	3.465(4)	2.55	168
C16-H16A...O7	3.228(3)	2.76	111
C20-H20B...F4	3.747(4)	2.90	146
C22-H22A...O9	3.100(4)	2.44	125
C27-H27...O8	3.465(4)	2.57	161
C27-H27...O9	3.567(4)	2.90	130
C24-H2...O7[1]	3.186(3)	2.60	121
C25-H25...O7[1]	3.307(4)	2.84	112
C25-H25...O9[1]	3.387(4)	2.62	141
C1-H1...O10[1]	3.585(4)	2.63	164
C5-H5B...F5[1]	3.941(5)	2.97	175
C8-H8A...O2[2]	3.290(4)	2.51	137
C22-H22B...O4[2]	3.163(4)	2.59	118
C8-H8A...O10[3]	3.155(3)	2.45	129
C10-H10...O2[4]	3.267(3)	2.75	116
C11-H11...O2[4]	3.317(3)	2.84	113
C11-H11...O5[4]	3.292(4)	2.58	134
C17-H17B...F1[5]	3.567(6)	2.98	120
C16-H16A...O4[5]	3.604(5)	2.80	140
C18-H18B...F6[6]	3.631(5)	2.86	137
C20-H20B...F3[7]	3.374(5)	2.66	131
C22-H22B...O7[8]	3.326(3)	2.45	150
C24-H24...O4[9]	3.439(4)	2.60	150
C23-H23...O3[9]	3.354(3)	2.54	147

(1) x-1,+y,+z (2) -x+1,-y+1,-z+2 (3) -x+2,-y+1,-z+2 (4) x+1,+y,+z

(5) x+1,+y,+z-1 (6) -x+2,-y,-z+1 (7) -x+1,-y,-z+2 (8) -x+2,-y+1,-z+1 (9) x,+y,+z-1

15 c

X-H…Y	X…Y	H…Y	√X-H…Y
C4-H4...F4	3.377(26)	2.57	145
C8-H8...O1	2.718(15)	2.31	104
C3-H3...F4[1]	3.277(24)	2.82	111
C1-H1...O1[1]	3.219(27)	2.52	132
C2-H2...F4[1]	3.140(20)	2.56	121
C3-H3...F2[1]	3.694(24)	2.88	148
C1-H1...F1[2]	3.084(22)	2.44	126
C1-H1...F4[2]	3.180(20)	2.80	106
C3-H3...O1[3]	3.337(18)	2.75	122
C5-H5...F2[4]	3.424(23)	2.65	141
C5-H5...F4[4]	3.344(23)	2.42	171
C6-H6A...F2[4]	3.107(28)	2.25	147
C8-H8...F2[5]	3.729(27)	2.84	151
C10-H10A...F3[5]	3.779(31)	2.88	155
C12-H12B...F2[5]	3.791(38)	2.96	144

(1) x,-y+1/2,+z+1/2 (2) -x+2,+y+1/2,-z+1/2+1 (3) -x+2,+y-1/2,-z+1/2+1

(4) -x+2,-y,-z+1 (5) -x+2,-y+1,-z+1

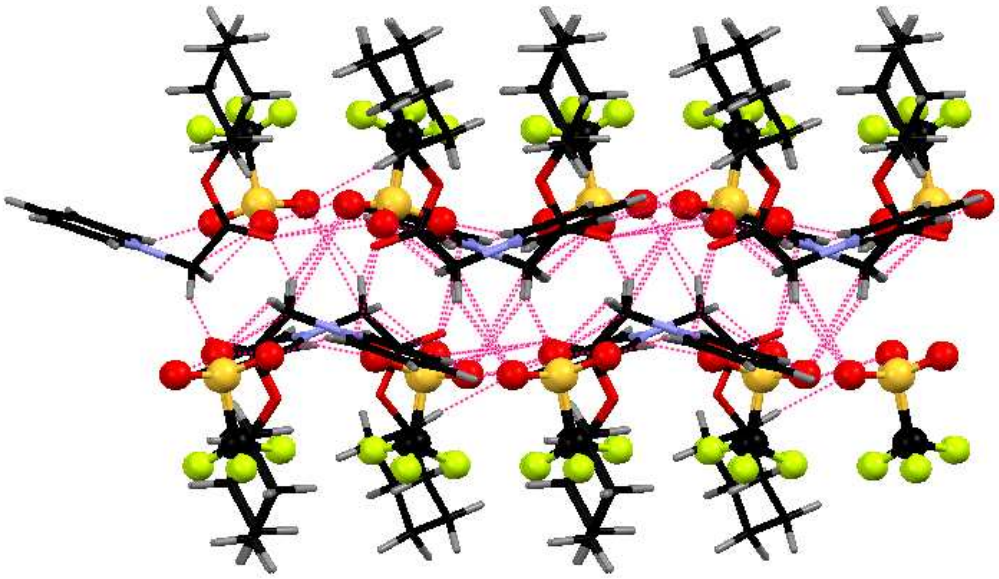


Fig. S3 – Packing of 15b forming 3D network, shown down the c axis

Table 12- crystal data and structure refinement parameters for compounds 15a-15c.

Identification code	**15a**	**15b**	**15c**
Empirical formula	$C_{13}H_{18}F_6NO_2P$	$C_{14}H_{18}F_3NO_5S$	$C_{13}H_{18}BF_4NO_2$
Formula weight	365.25	369.35	307.10
Temperature	295(2) K	295(2) K	296 (2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_{1/m}$	P - 1	$P2_{1/c}$
Unit cell dimensions	a= 7.9197(2)Å α= 90° b = 8.4851(2)Å β= 91.5930(10)° c = 12.286(3)Å γ = 90°	a = 8.6090(6) Å α= 95.806(3)° b = 12.5350(9) Å β= 91.687(3)° c = 16.4900(13) Å γ = 105.799(2)°	a = 18.259(13)Å α= 90° b= 7.324(6)Å β= 106.74(3)° c= 12.251(9) Å γ= 90°
Volume	825.33(3) $Å^3$	1700.5(2) $Å^3$	1569(2)$Å^3$
Z	2	4	4
Density(Mg/m^3)	1.470	1.443	1.300
Absorption coeff.	0.234 mm^{-1}	0.245 mm^{-1}	0.117 mm^{-1}
F(000)	376	768	640
Crystal size (mm^3)	0.16x0.13x0.09	0.20x0.18x0.16	0.20 x 0.18 x 0.10
Theta range for data collection	1.66 to 27.84°	1.24 to 31.94°	1.16 to 25.10°

Index ranges	-10<=h<=10 -11<=k<=11 -16<=l<=16	-12<=h<=12, -17<=k<=18, -24<=l<=24	-21<=h<=19, -7<=k<=7, -12<=l<=11
Reflections collected	7782	41666	5238
Independent reflections	2096[R(int)= 0.0210]	11308[R(int)= 0.0302]	1839 [R(int)= 0.1060]
Completeness to absorption correction	theta=27.84°, 99.8%	theta=31.94°, 96.1%	theta=25.1°,65.9 %
Max. and minimum transmission	Semi empirical 0.981 & 0.959	Semi empirical 0.7463 & 0.6676	Semi empirical 0.9884 & 0.9770
Data / restraints / parameters	2096 / 0 / 124	11308 / 0 / 433	1839 / 6 / 190
Goodness-of-fit on F^2	1.366	1.366	1.637
Final R indices[I>2sigma(I)]	R1=0.0954 WR2=0.3237	R1=0.0709,WR2=0.2140	R1=0.2242,WR2=4724
Final R indices	R1=0.1221,WR2=0.3548	R1=0.1213 WR2=0.2595	R1=0.3605,WR2=0.5412
Largest diff. peak and hole	0.784 & - 0.617 e.Å^{-3}	0.569 & -0.333 e.Å^{-3}	0.689& -0.548 e.Å^{-3}
CCDC Number	892805	892803	892802

Table 13-Torsion angles (°) around the –CH_2COO groups in 15a-15c.

15a	**15b (molecule 1)**	**15b (molecule 2)**	**15c**
C1-O1-C5-O2 0.0	C1-O1-C7-O2 7.62	C15-O6-C21-O7 -2.67	C8-O2-C7-O1 -7.05
C1-O1-C5-C6 180.0	C1-O1-C7-C8 172.0	C15-O6-C21-C22 177.0	C8-O2-C7-C6 178.2
O1-C5-C6-N1 180.0	O1-C7-C8-N1 7.60	O6-C21-C22-N2 -2.89	O2-C7-C6-N1 158.1
O2-C5-C6-N1 0.0	O2-C7-C8-N1 172.1	O7-C21-C22-N2 176.8	O1-C7-C6-N1 30.3