Electronic Supplementary Information for

Supramolecular complexes formed by dimethoxypillar[5]arene and imidazolium salts: a joint experimental and computational investigation

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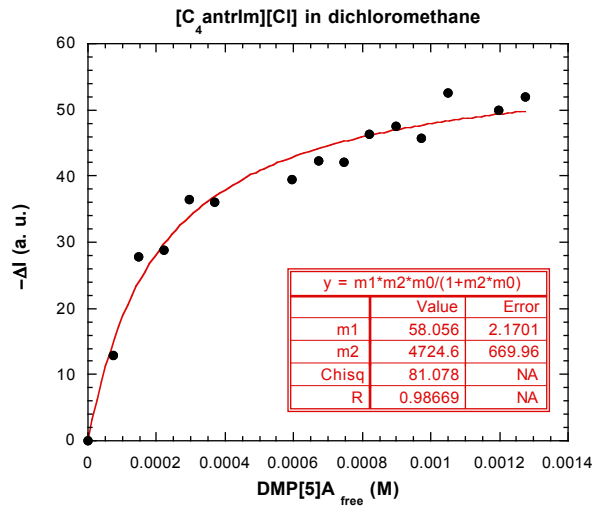
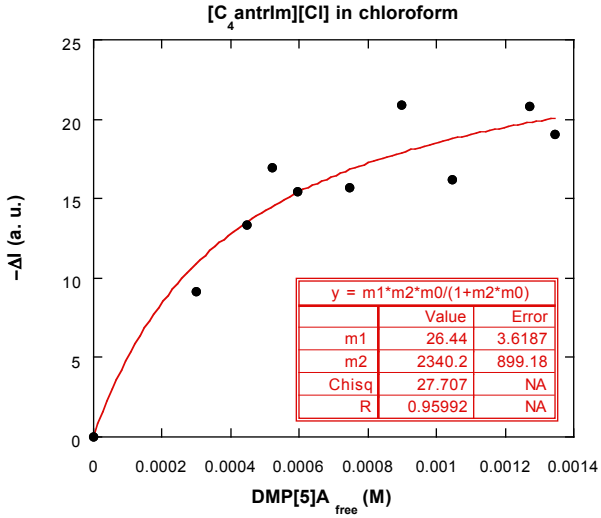
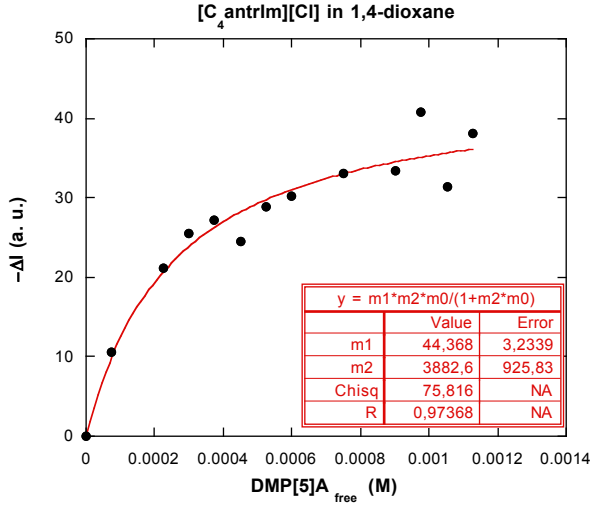
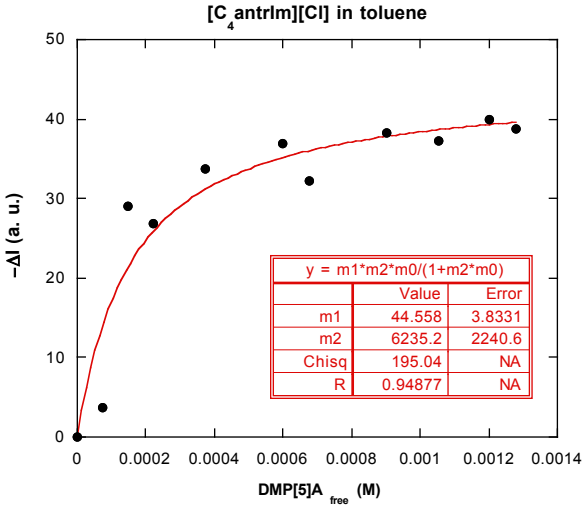
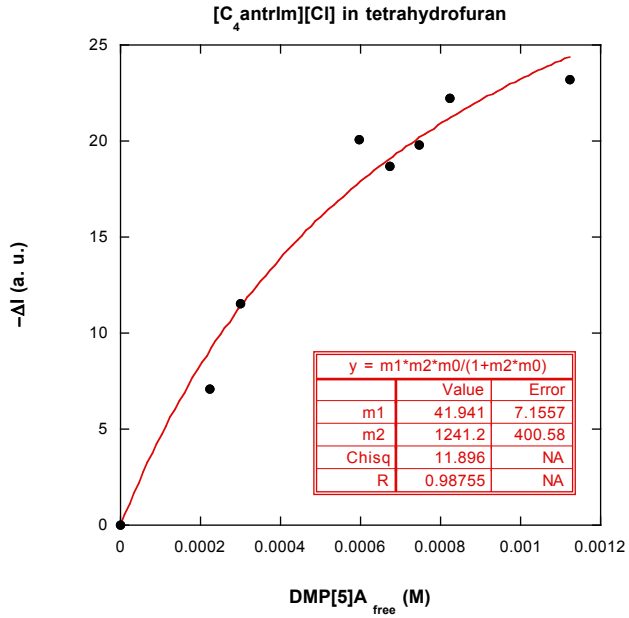
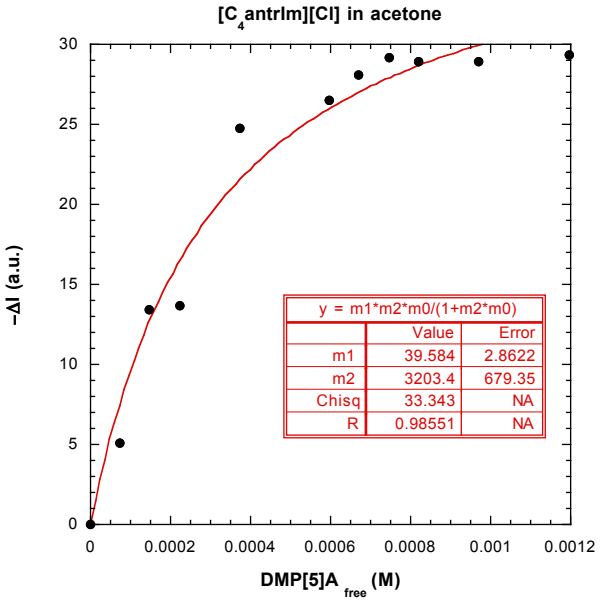

[C4antrIm][Cl] in dichloromethane
−ΔI (a. u.)
DMP[5]A free (M)
y = m1*m2*m0/(1+m2*m0)
Value Error
m1 58.056 2.1701
m2 4724.6 669.96
Chisq 81.078 NA
R 0.98669 NA


[C4antrIm][Cl] in chloroform
−ΔI (a. u.)
DMP[5]A free (M)
y = m1*m2*m0/(1+m2*m0)
Value Error
m1 26.44 3.6187
m2 2340.2 899.18
Chisq 27.707 NA
R 0.95992 NA


[C4antrIm][Cl] in 1,4-dioxane
−ΔI (a. u.)
DMP[5]A free (M)
y = m1*m2*m0/(1+m2*m0)
Value Error
m1 44,368 3,2339
m2 3882,6 925,83
Chisq 75,816 NA
R 0,97368 NA


[C4antrIm][Cl] in toluene
−ΔI (a. u.)
DMP[5]A free (M)
y = m1*m2*m0/(1+m2*m0)
Value Error
m1 44.558 3.8331
m2 6235.2 2240.6
Chisq 195.04 NA
R 0.94877 NA


[C4antrIm][Cl] in tetrahydrofuran
−ΔI (a. u.)
DMP[5]A free (M)
y = m1*m2*m0/(1+m2*m0)
Value Error
m1 41.941 7.1557
m2 1241.2 400.58
Chisq 11.896 NA
R 0.98755 NA


[C4antrIm][Cl] in acetone
−ΔI (a.u.)
DMP[5]A free (M)
y = m1*m2*m0/(1+m2*m0)
Value Error
m1 39.584 2.8622
m2 3203.4 679.35
Chisq 33.343 NA
R 0.98551 NA

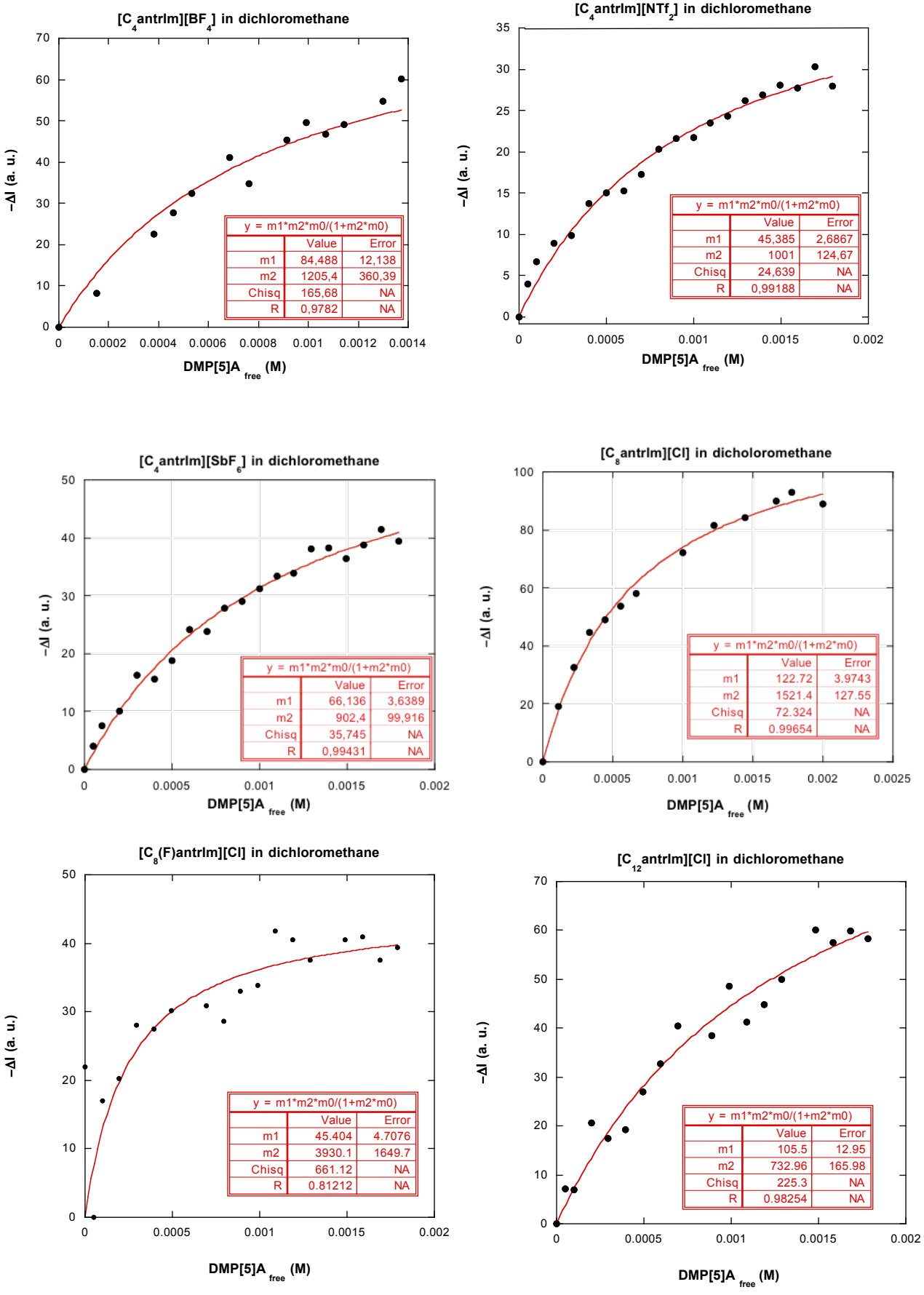


Figure S1.Hyperbolic fits of inclusion complexes obtained by differences of fluorescence intensity values as function of concentration of free host.

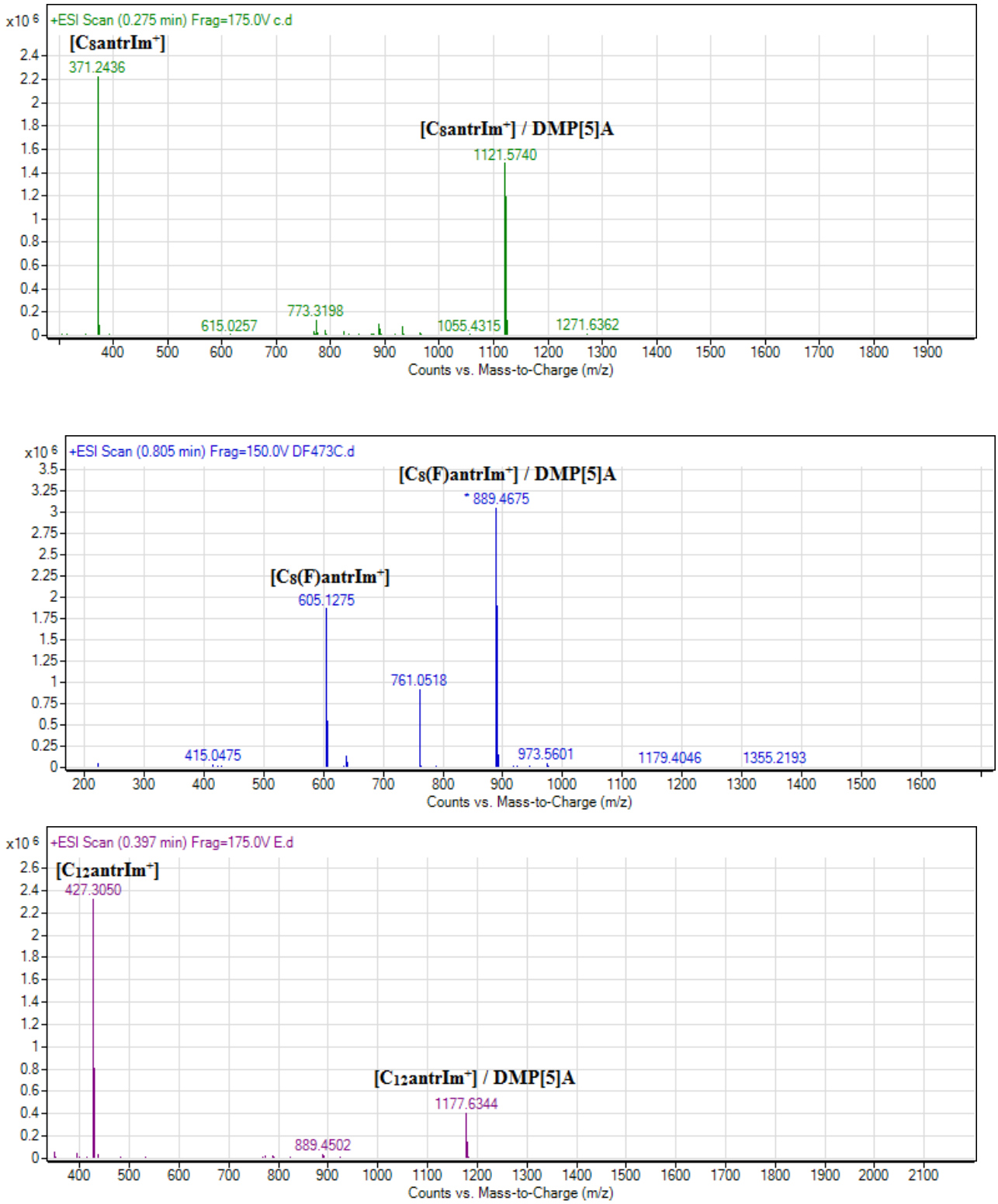


Figure S2. High resolution ESI mass spectra of equimolar mixtures of guests and the host.

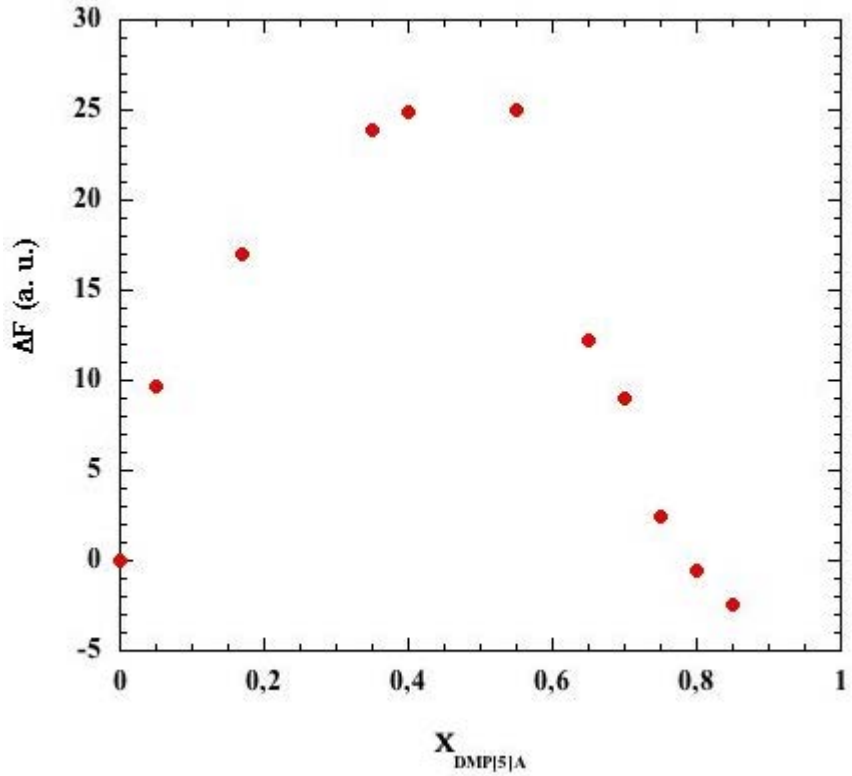
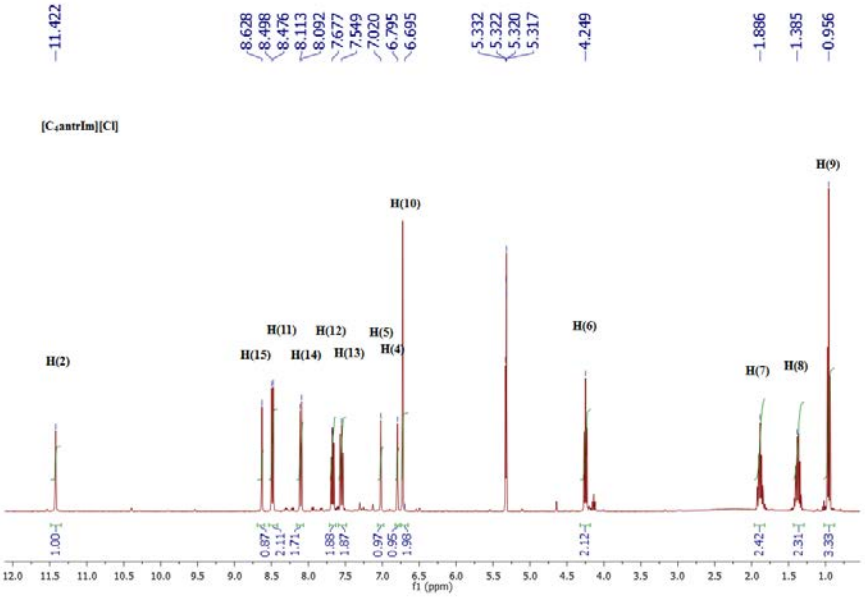
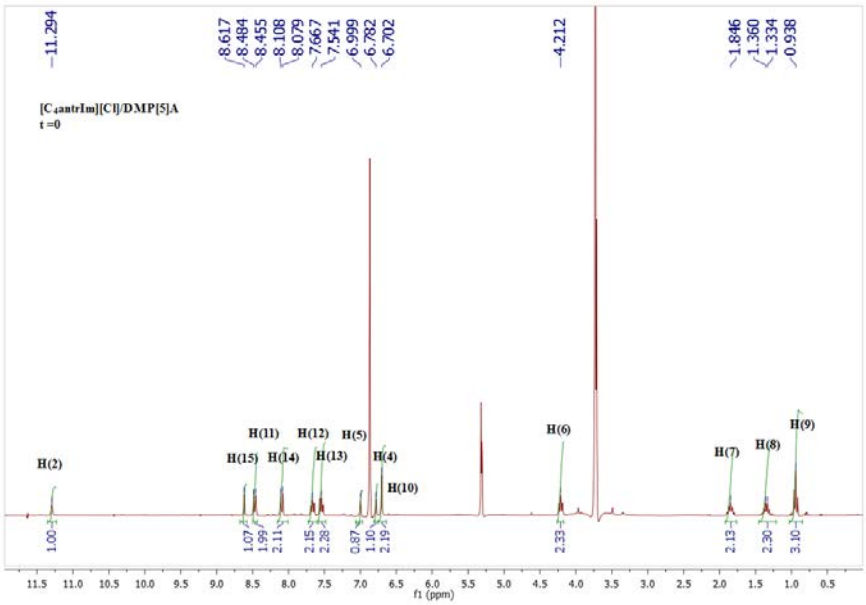
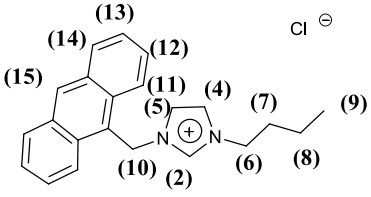


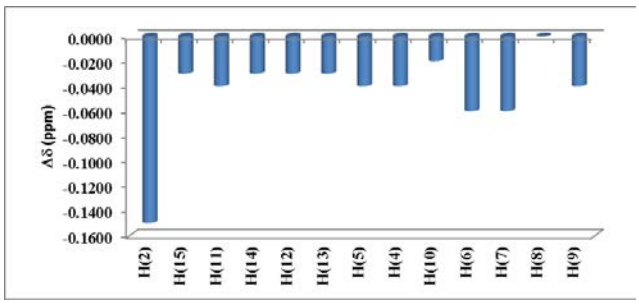
Figure S3. Job's plot for **[C_{12}antrIm][Cl]/DMP[5]A** complex.

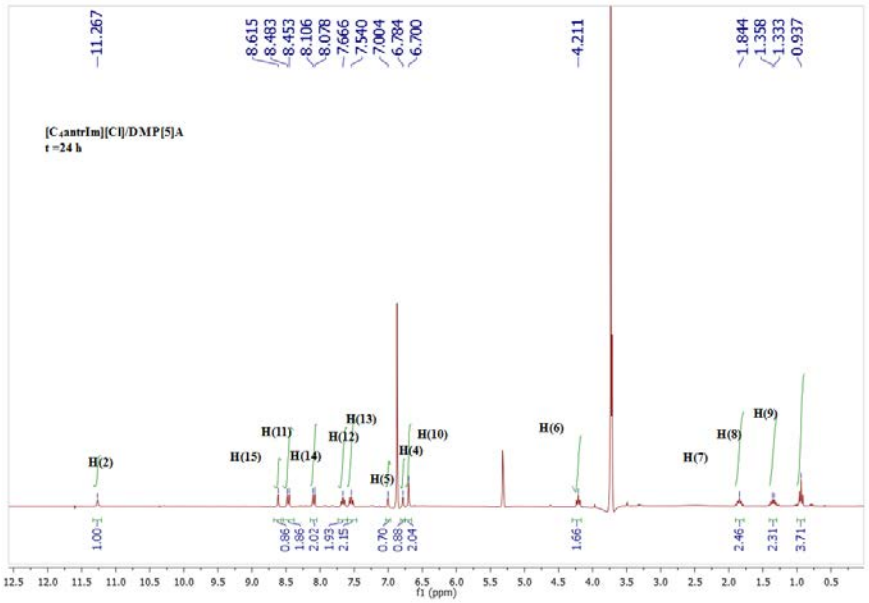
a)


11.422
8.628
8.498
8.476
8.113
8.092
7.677
7.549
7.020
6.795
6.695
5.332
5.322
5.320
5.317
4.249
1.886
1.385
0.956
[C4antrIm][Cl]
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)
f1 (ppm)

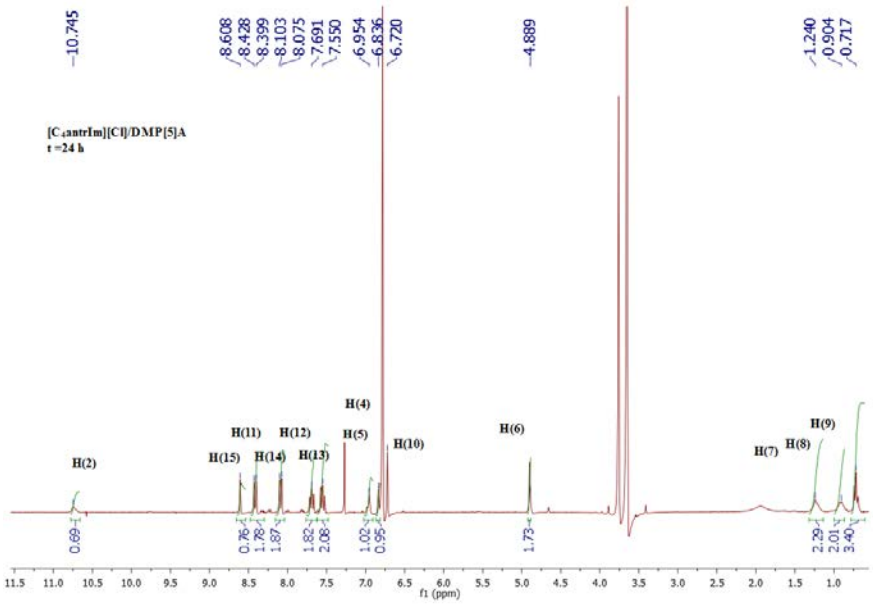

11.294
8.617
8.484
8.455
8.108
8.079
7.667
7.541
6.999
6.782
6.702
4.212
1.846
1.360
1.334
0.938
[C4antrIm][Cl]/DMP[5]A
t =0
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)
f1 (ppm)

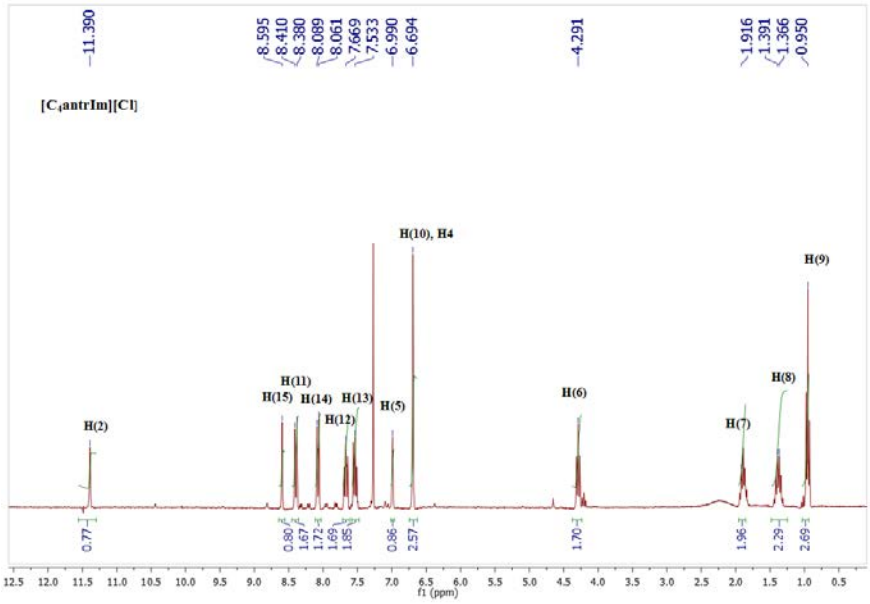

(13)
(14)
(12)
(15)
(11)
(4)
(5)
(7)
(9)
Cl
(10)
(2)
(6)
(8)

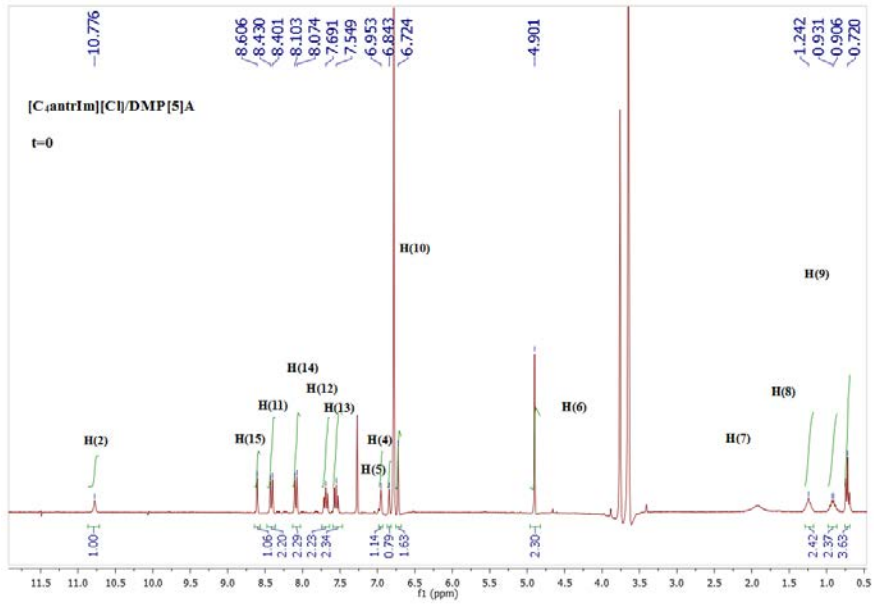

0.0000
-0.0200
-0.0400
-0.0600
-0.0800
-0.1000
-0.1200
-0.1400
-0.1600
Δδ (ppm)
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)

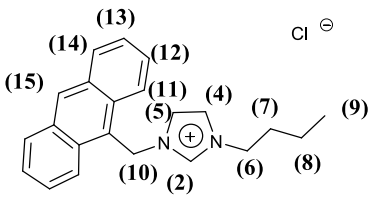

11.267
8.615
8.483
8.453
8.106
8.078
7.666
7.540
7.004
6.784
6.700
4.211
1.844
1.358
1.333
0.937
[C4antrIm][Cl]/DMP[5]A
t =24 h
H(2)
H(15)
H(11)
H(14)
H(13)
H(12)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)
f1 (ppm)

b)


10.745
8.608
8.428
8.399
8.103
8.075
7.691
7.550
6.954
6.836
6.720
4.889
1.240
0.904
0.717
[C4antrIm][Cl]/DMP[5]A
t =24 h
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(4)
H(5)
H(10)
H(6)
H(7)
H(8)
H(9)
f1 (ppm)

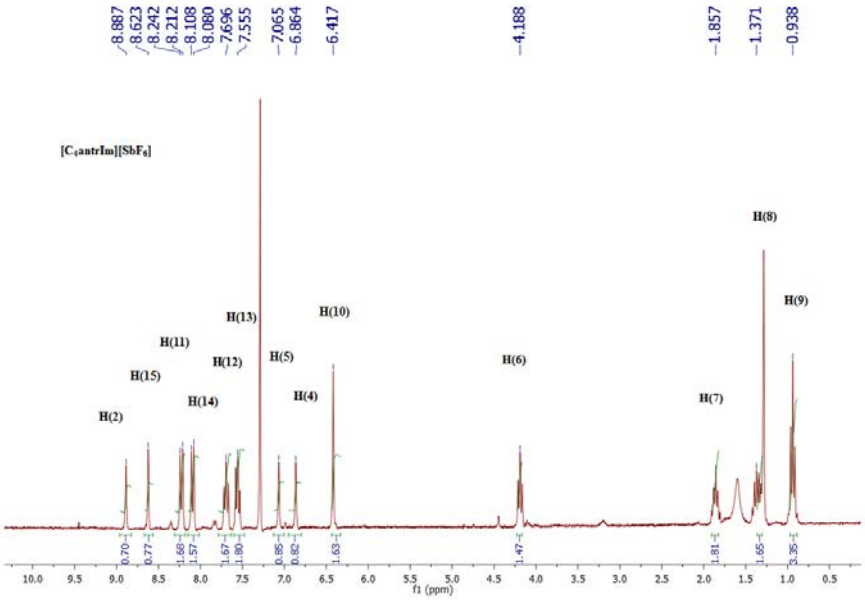

11.390
8.595
8.410
8.380
8.089
8.061
7.669
7.533
6.990
6.694
4.291
1.916
1.391
1.366
0.950
[C4antrIm][Cl]
H(10), H4
H(9)
H(11)
H(15)
H(14)
H(13)
H(12)
H(5)
H(6)
H(8)
H(7)
H(2)
f1 (ppm)

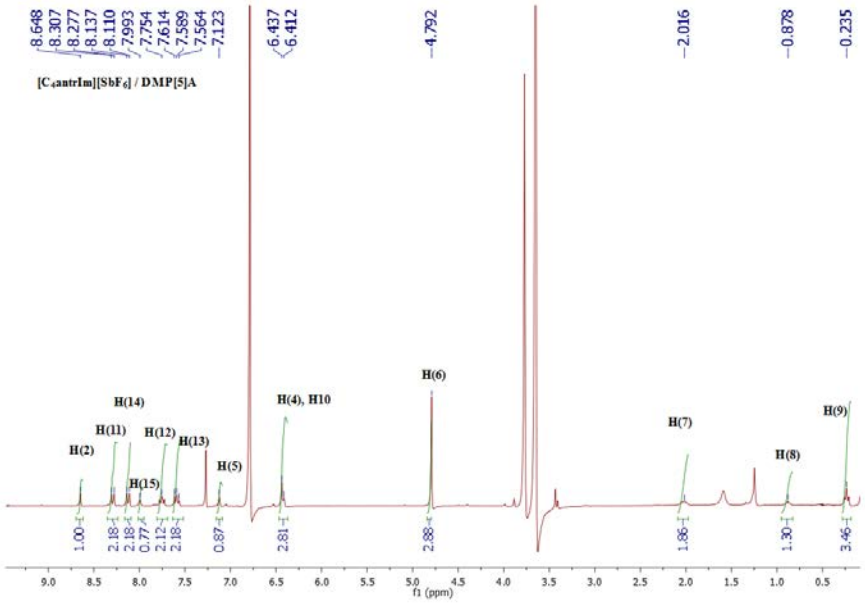

10.776
8.606
8.430
8.401
8.103
8.074
7.691
7.549
6.953
6.843
6.724
4.901
1.242
0.931
0.906
0.720
[C4antrIm][Cl]/DMP[5]A
t=0
H(10)
H(9)
H(14)
H(12)
H(11)
H(13)
H(6)
H(8)
H(2)
H(15)
H(4)
H(5)
H(7)
f1 (ppm)

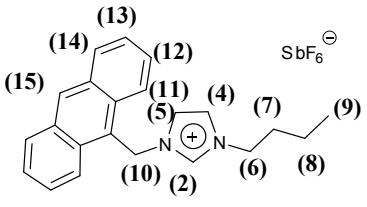

(13)
(14)
(12)
(15)
(11)
(4)
(5)
(7)
(9)
N
N
(10)
(2)
(6)
(8)
Cl

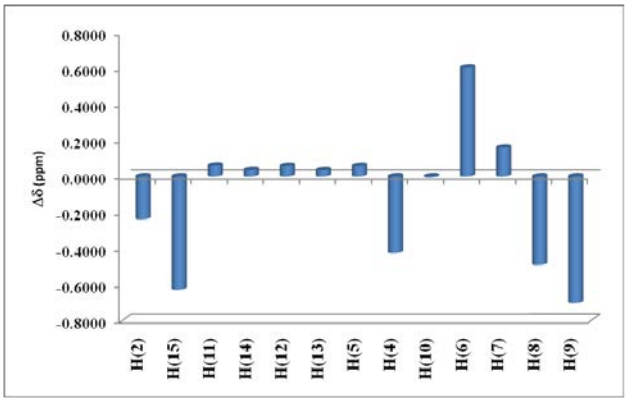

0.800
0.600
0.400
0.200
0.000
-0.200
-0.400
-0.600
-0.800
Δδ (ppm)
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)

c)

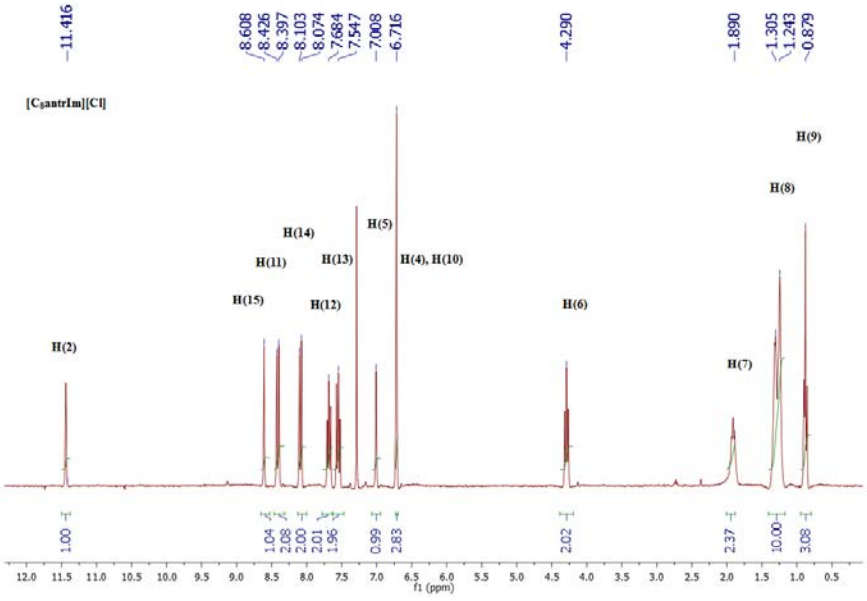

8.887
8.623
8.242
8.212
8.108
8.080
7.696
7.555
7.065
6.864
6.417
4.188
1.857
1.371
0.938
[C4antrIm][SbF6]
H(8)
H(9)
H(13)
H(10)
H(11)
H(12)
H(5)
H(6)
H(15)
H(14)
H(4)
H(7)
H(2)
f1 (ppm)

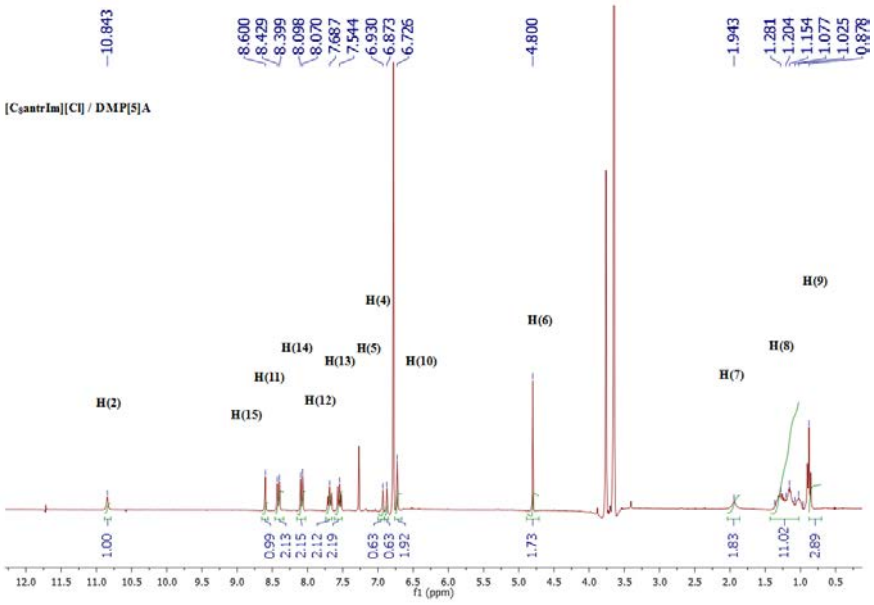

8.648
8.307
8.277
8.137
8.110
7.993
7.754
7.614
7.589
7.564
7.123
6.437
6.412
4.792
2.016
0.878
0.235
[C4antrIm][SbF6] / DMP[5]A
H(6)
H(14)
H(4), H10
H(7)
H(9)
H(11)
H(12)
H(13)
H(2)
H(8)
H(5)
H(15)
f1 (ppm)

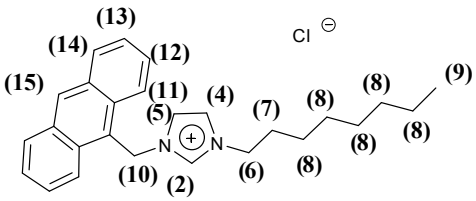

(13)
(14)
(12)
SbF6
(15)
(11)
(4)
(5)
(7)
(9)
N
N
(10)
(2)
(6)
(8)

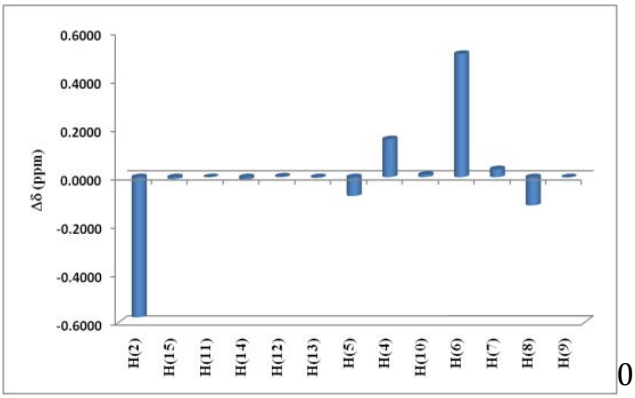

0.8000
0.6000
0.4000
0.2000
0.0000
-0.2000
-0.4000
-0.6000
-0.8000
Δδ (ppm)
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)

d)


[C8antrIm][Cl]
11.416
8.608
8.426
8.397
8.103
8.074
7.684
7.547
7.008
6.716
4.290
1.890
1.305
1.243
0.879
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4), H(10)
H(6)
H(7)
H(8)
H(9)
f1 (ppm)

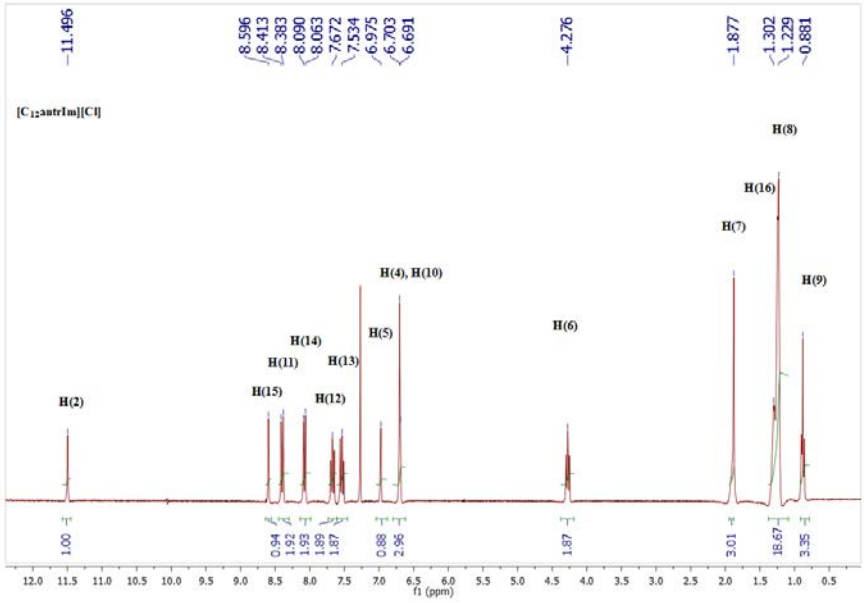

[C8antrIm][Cl] / DMP[5]A
10.843
8.600
8.429
8.399
8.098
8.070
7.687
7.544
6.930
6.873
6.726
4.800
1.943
1.281
1.204
1.154
1.077
1.025
0.878
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)
f1 (ppm)

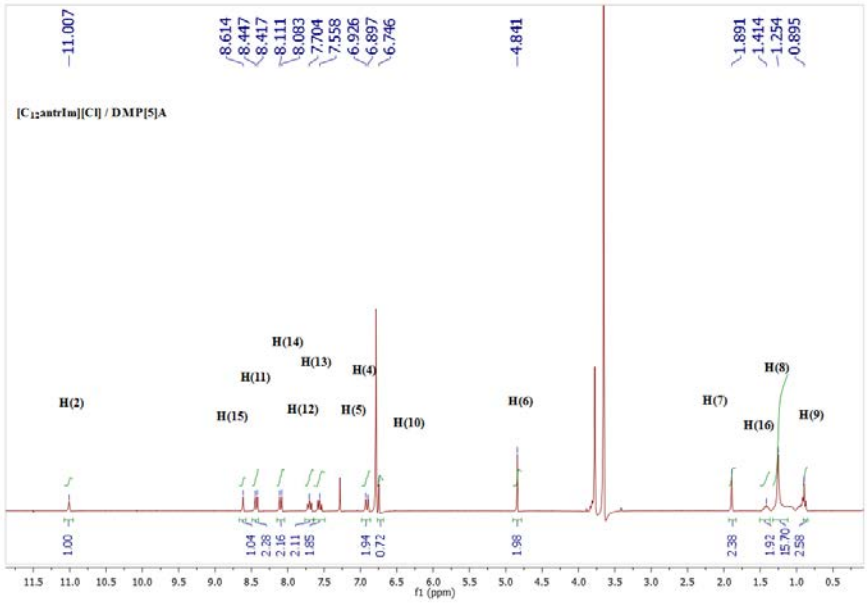

(13)
(14)
(12)
(15)
(11)
(4)
(5)
(7)
(8)
(8)
(9)
(8)
(8)
(6)
(8)
(10)
(2)
Cl ⊖

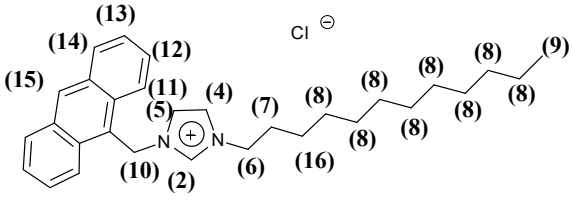

0.6000
0.4000
0.2000
0.0000
-0.2000
-0.4000
-0.6000
Δδ (ppm)
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(8)
H(9)

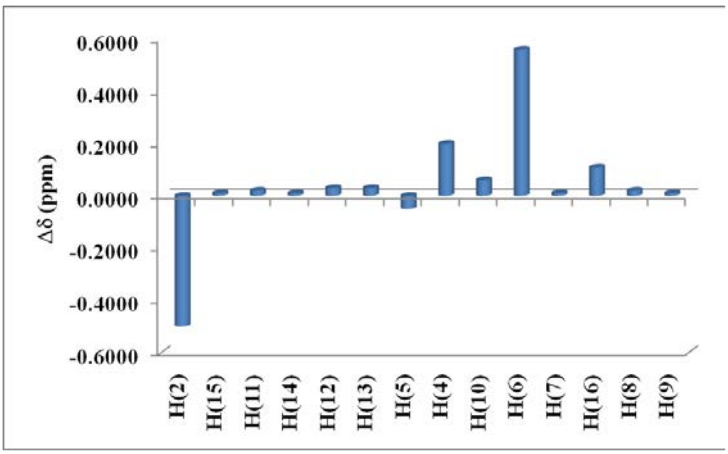
0

e)

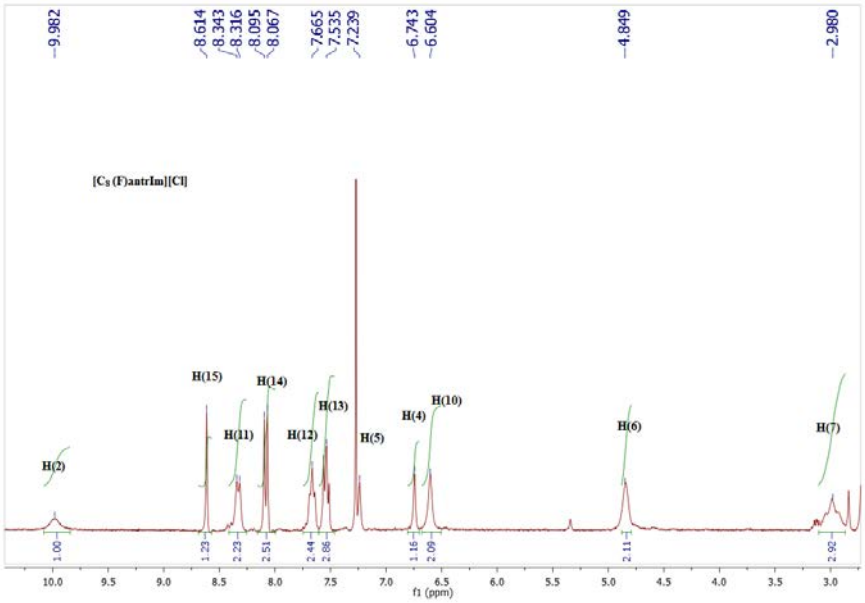

11.496
8.596
8.413
8.383
8.090
8.063
7.672
7.534
6.975
6.703
6.691
4.276
1.877
1.302
1.229
0.881
[C12antrIm][Cl]
H(2)
H(15)
H(11)
H(14)
H(13)
H(12)
H(4), H(10)
H(5)
H(6)
H(7)
H(8)
H(16)
H(9)
1.00
0.94
1.92
1.93
1.89
1.87
0.88
2.96
1.87
3.01
18.67
3.35
f1 (ppm)


11.007
8.614
8.447
8.417
8.111
8.083
7.704
7.558
6.926
6.897
6.746
4.841
1.891
1.414
1.254
0.895
[C12antrIm][Cl] / DMP[5]A
H(2)
H(15)
H(11)
H(14)
H(13)
H(12)
H(4)
H(5)
H(10)
H(6)
H(7)
H(16)
H(8)
H(9)
1.00
1.04
2.28
2.16
2.11
1.85
1.94
0.72
1.98
2.38
1.92
15.70
2.58
f1 (ppm)


(13)
(14)
(12)
(15)
(11)
(4)
(5)
(7)
(8)
(8)
(8)
(8)
(9)
(8)
(8)
(8)
(8)
(16)
(6)
(10)
(2)
N
N
Cl


0.6000
0.4000
0.2000
0.0000
-0.2000
-0.4000
-0.6000
Δδ (ppm)
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)
H(16)
H(8)
H(9)

f)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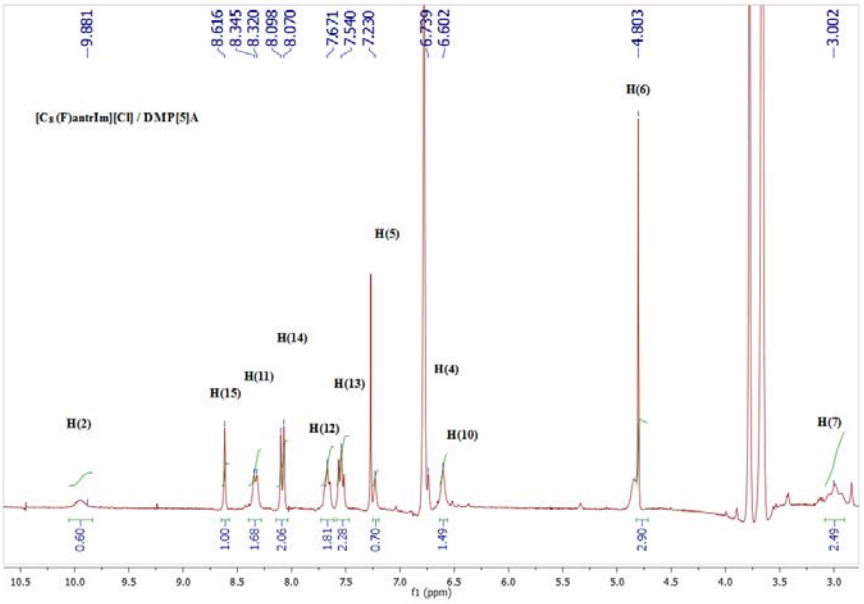
8.095
8.067
7.665
7.535
7.239
6.743
6.604
4.849
2.980
[C8 (F)antrIm][Cl]
H(15)
H(14)
H(13)
H(11)
H(12)
H(5)
H(4)
H(10)
H(6)
H(7)
H(2)
f1 (ppm)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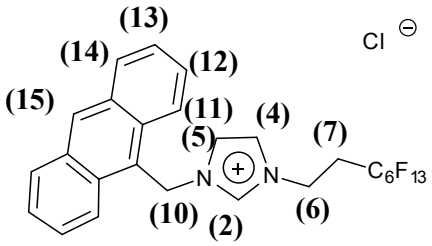
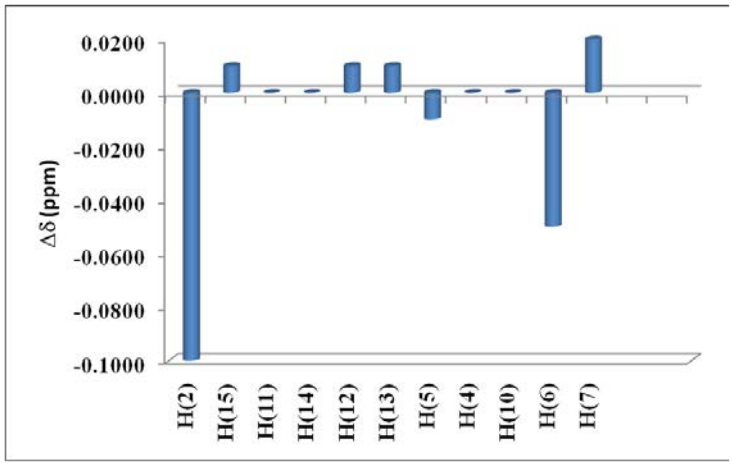
8.320
8.098
8.070
7.671
7.540
7.230
6.739
6.602
4.803
3.002
[C8 (F)antrIm][Cl] / DMP[5]A
H(6)
H(5)
H(14)
H(11)
H(15)
H(13)
H(4)
H(2)
H(12)
H(10)
H(7)
f1 (ppm)


(13)
(14)
(12)
(15)
(11)
(4)
(5)
(7)
Cl
N
N
C6F13
(10)
(2)
(6)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0.0000
-0.0200
-0.0400
-0.0600
-0.0800
-0.1000
Δδ (ppm)
H(2)
H(15)
H(11)
H(14)
H(12)
H(13)
H(5)
H(4)
H(10)
H(6)
H(7)

g)

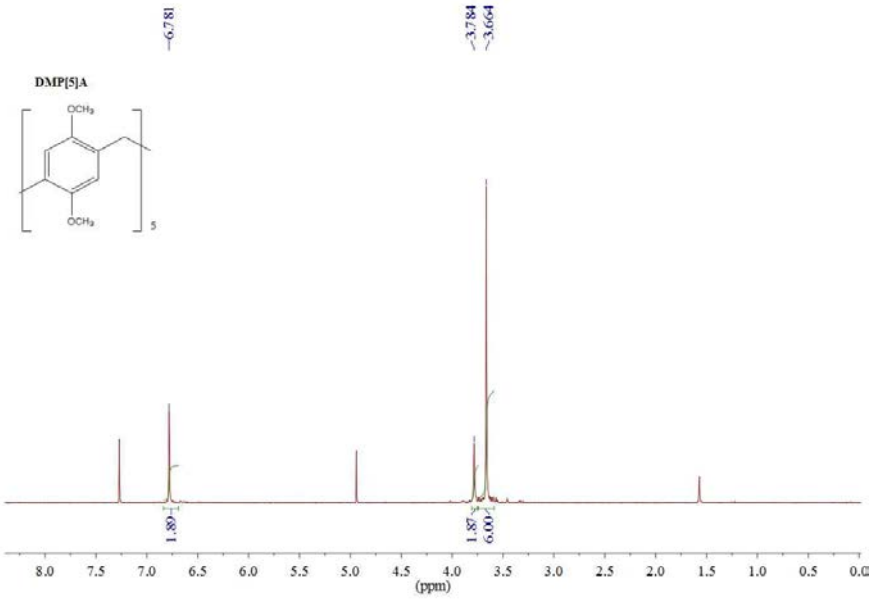


Figure S4. ^{1}H NMR spectra of the organic salts and equimolar mixtures of organic salts and DMP[5]A in $CDCl_3$, plots of chemical shift differences and legend of the protons:**a)** CD_2Cl_2; **b)-g)** $CDCl_3$.

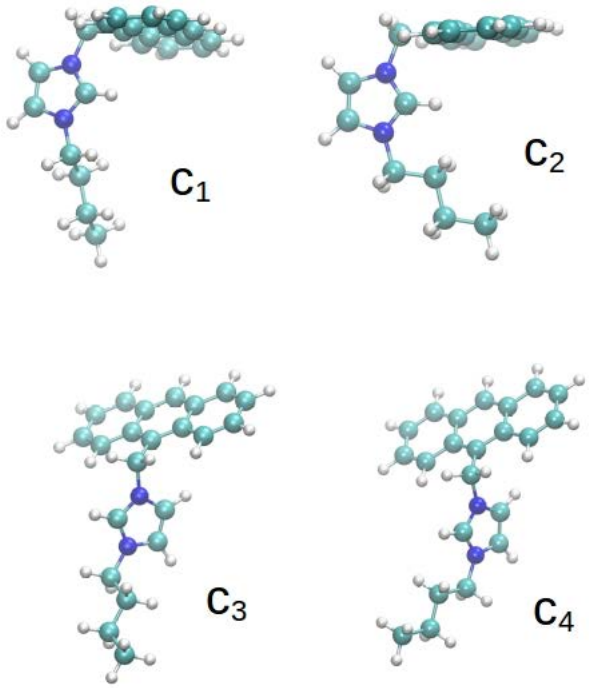


Figure S5. Four different conformations of the **[C_4antrIm$^+$]**cation in the isolated state.

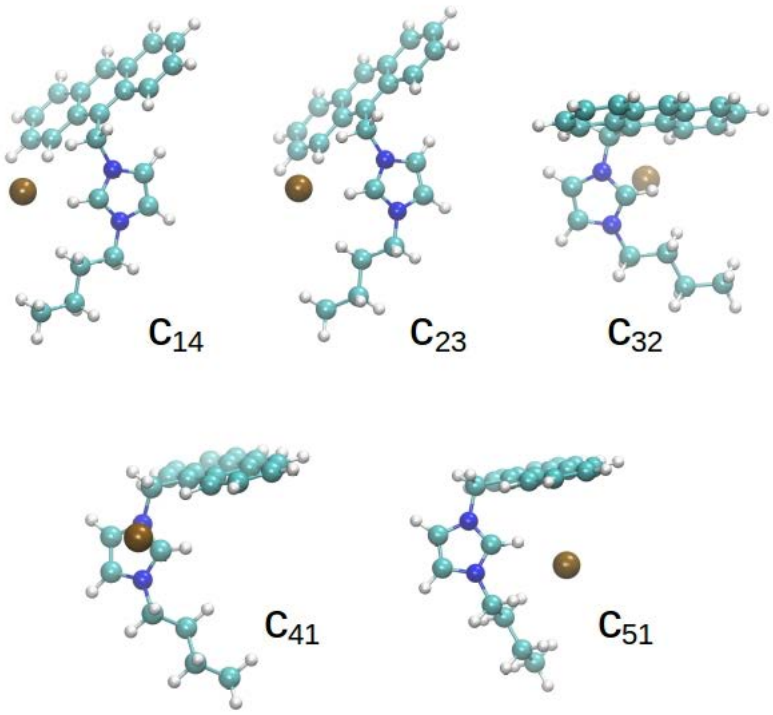


Figure S6. Conformations of the **[C_4antrIm][Cl]** ionic pair in the isolated state.

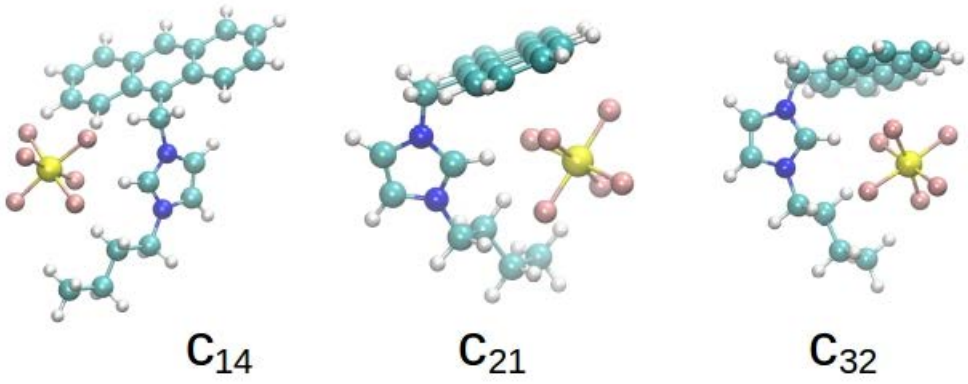
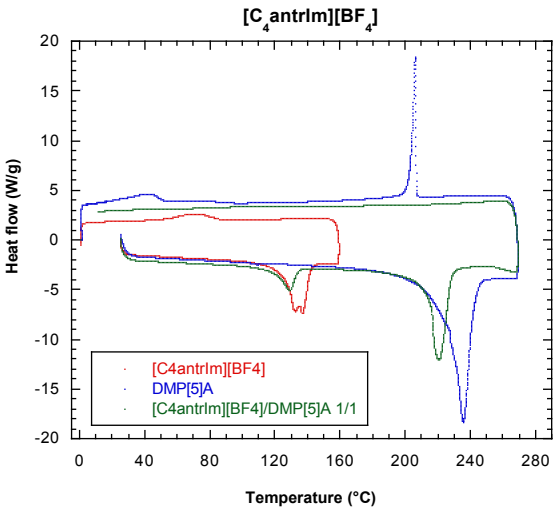
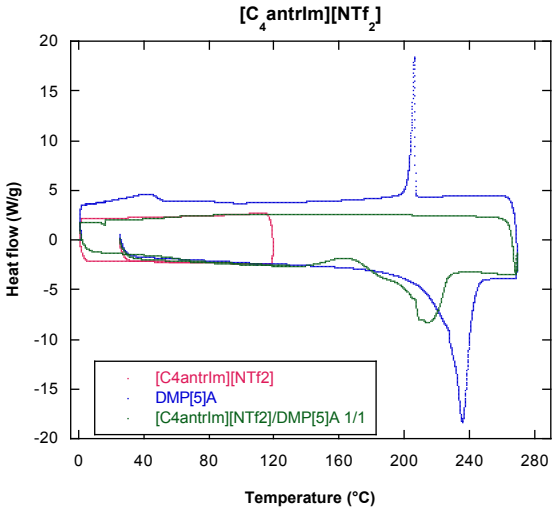
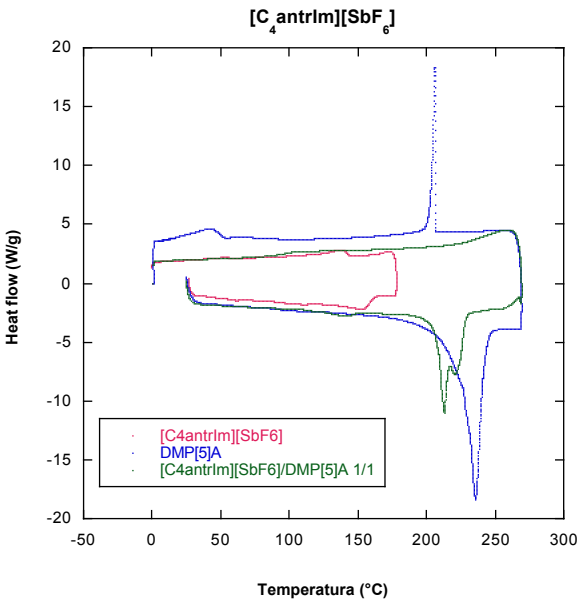
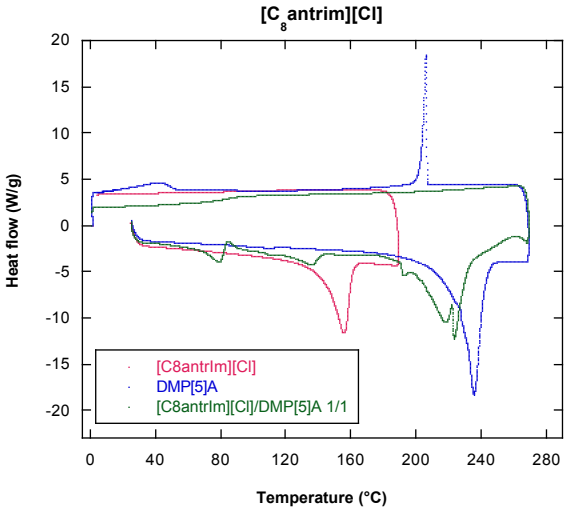


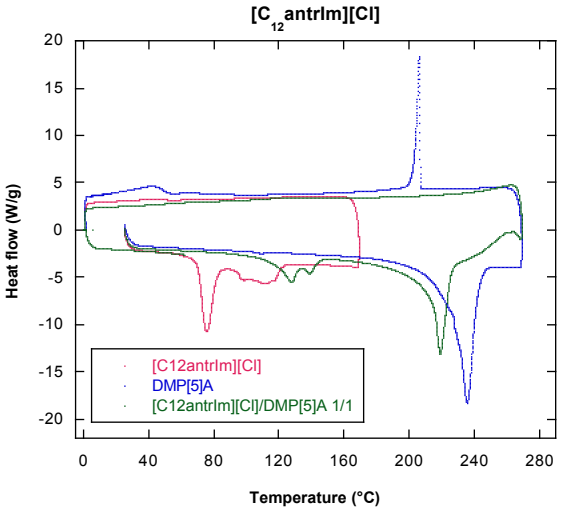
Figure S7. Possible conformations of the **[C_4antrIm][SbF_6]** species in the isolated state.


[C4antrIm][BF4]
DMP[5]A
[C4antrIm][BF4]/DMP[5]A 1/1
Heat flow (W/g)
Temperature (°C)


[C4antrIm][NTf2]
DMP[5]A
[C4antrIm][NTf2]/DMP[5]A 1/1
Heat flow (W/g)
Temperature (°C)


[C4antrIm][SbF6]
DMP[5]A
[C4antrIm][SbF6]/DMP[5]A 1/1
Heat flow (W/g)
Temperatura (°C)


[C8antrIm][Cl]
DMP[5]A
[C8antrIm][Cl]/DMP[5]A 1/1
Heat flow (W/g)
Temperature (°C)


[C12antrIm][Cl]
DMP[5]A
[C12antrIm][Cl]/DMP[5]A 1/1
Heat flow (W/g)
Temperature (°C)

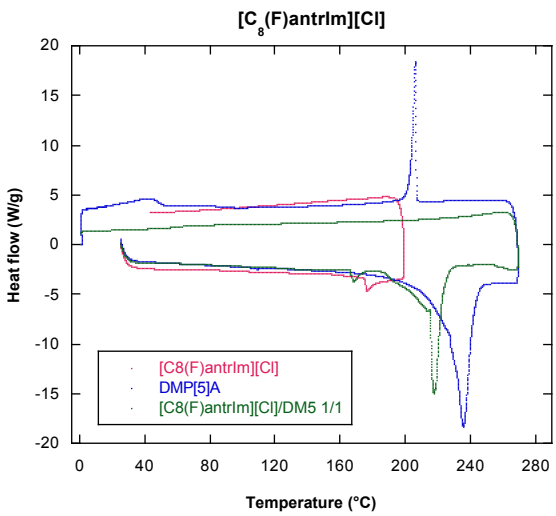
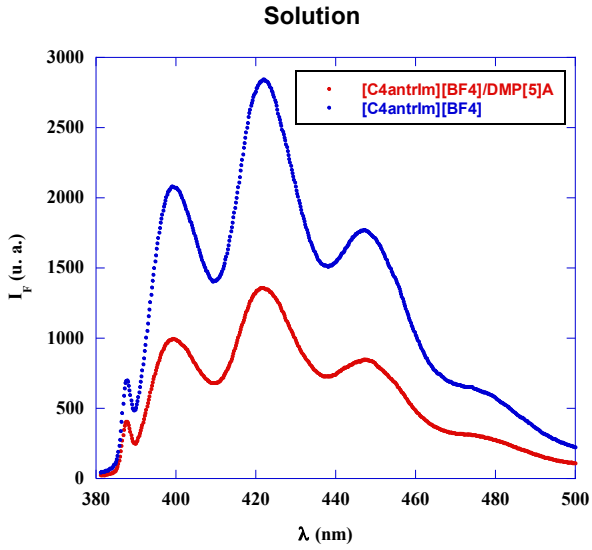
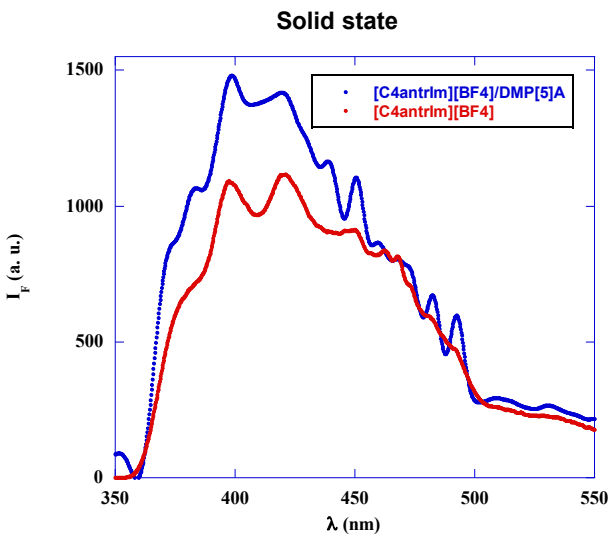
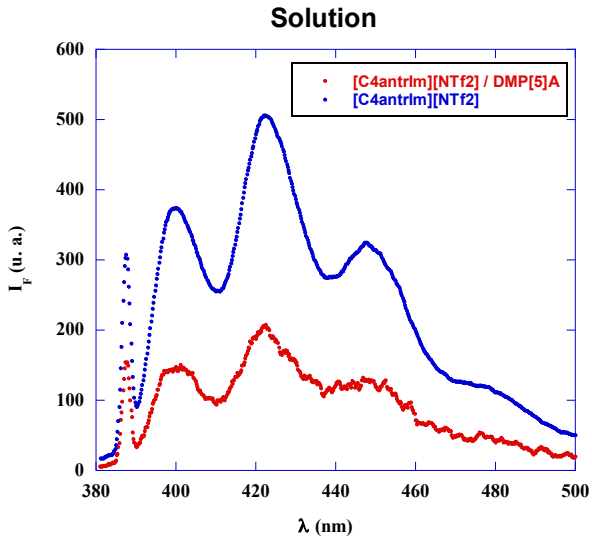
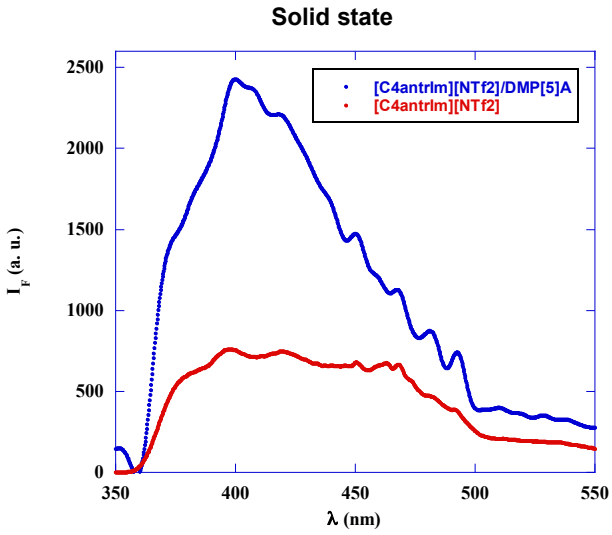

[C8(F)antrIm][Cl]
DMP[5]A
[C8(F)antrIm][Cl]/DM5 1/1
Heat flow (W/g)
Temperature (°C)

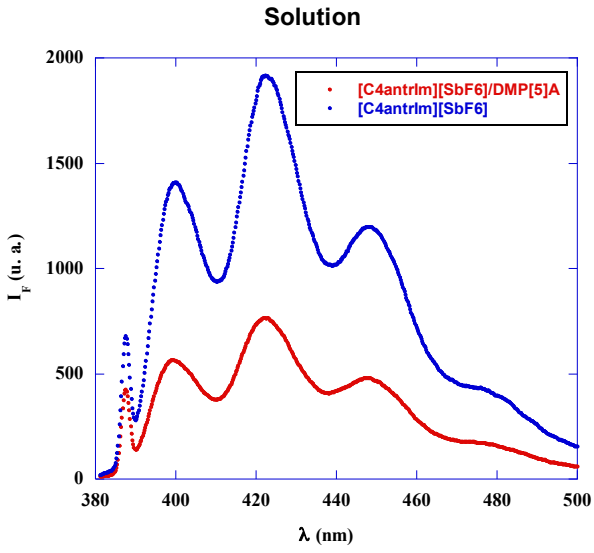
Figure S8. OverlappedDSC traces of salt, **DMP[5]A** and complexes obtained from CH_2Cl_2.

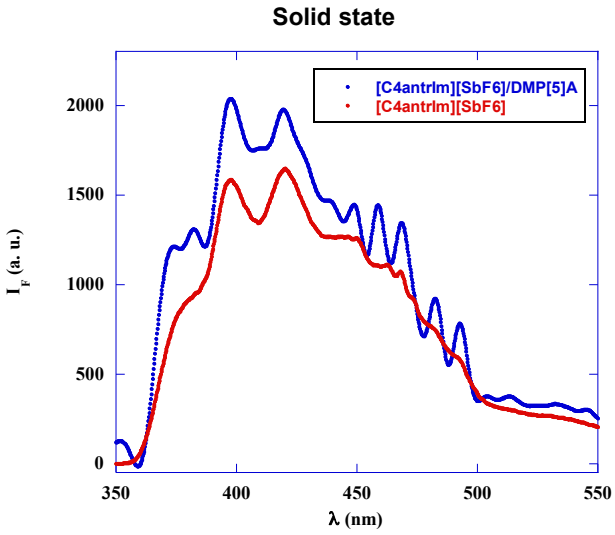












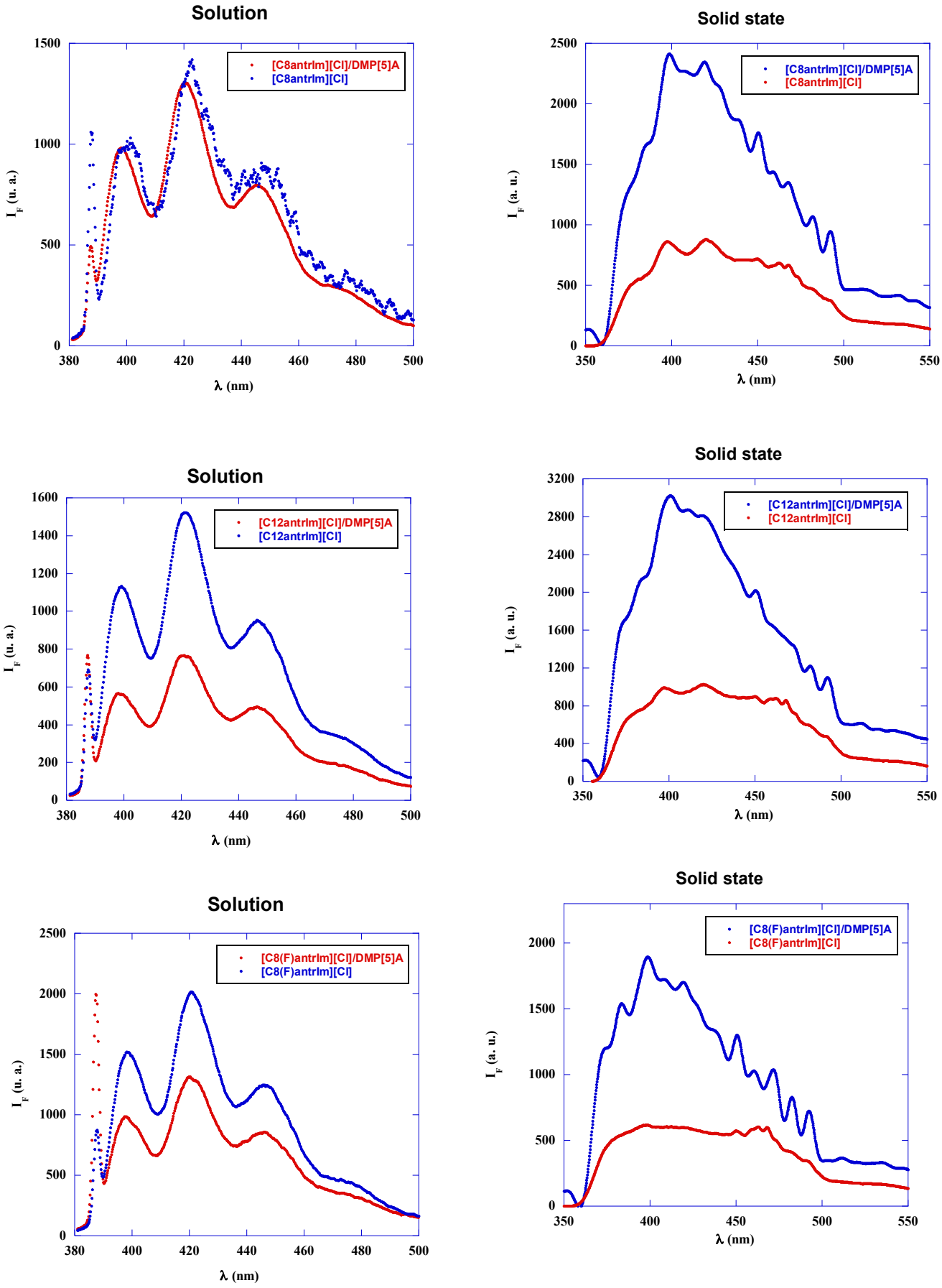


Figure S9. Solution (left) and solid-state (right) fluorescence spectra of guest salts and host-guest complexes.

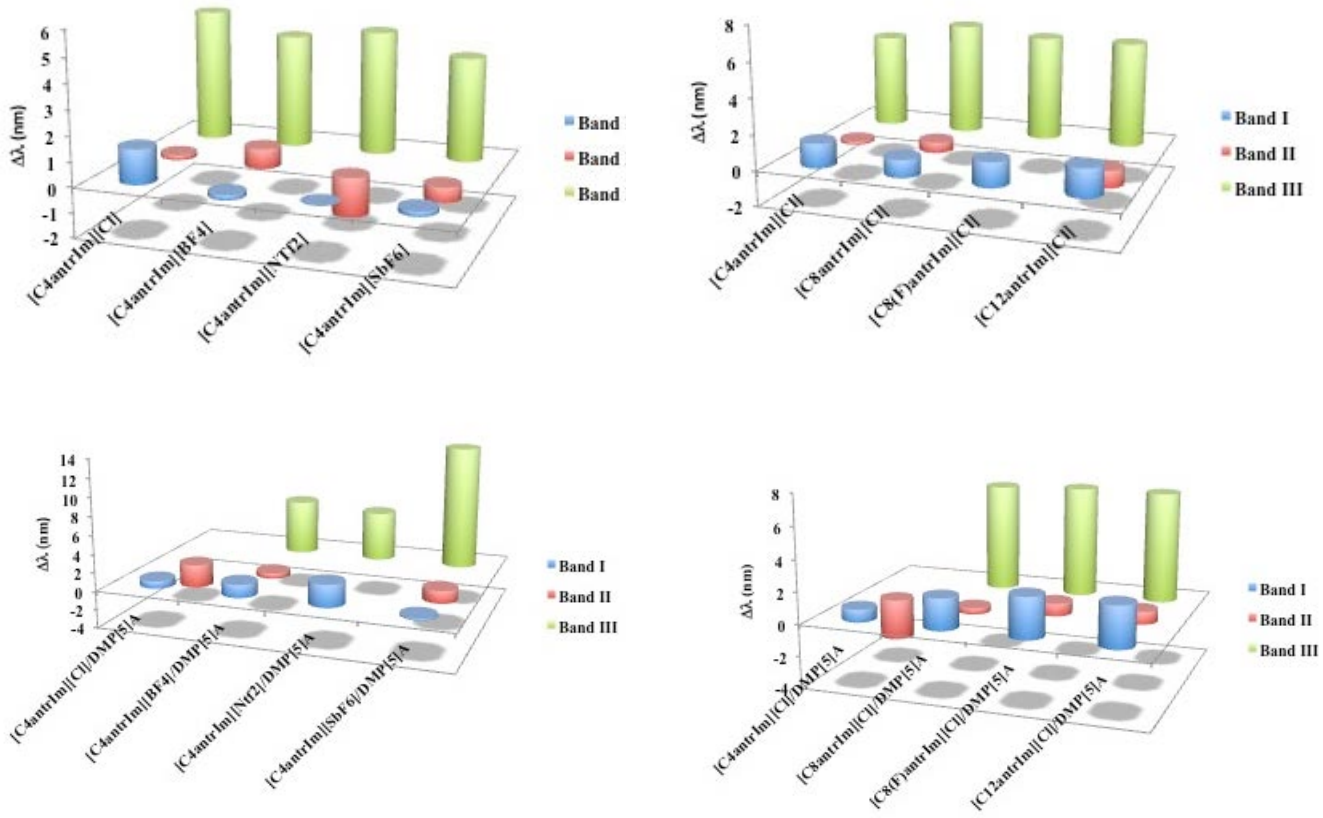


Figure S10. Changes in λ values ($\Delta\lambda = \lambda_{solid\ state} - \lambda_{solution}$) corresponding to main emission bands of **[$C_n$antrIm][X]** and **[$C_n$antrIm][X]/DMP[5]A** mixtures, as a function of the anion and alkyl chain, on going from solution to solid state.

Table S1. Calculated chemical shift differences, Δδ, for H nuclei of the **[C_8antrIm][Cl]** and **[C_8(F)antrIm][Cl]** guest molecules incapsulated in **DMP[5]A**.

H2	H4	H5	H6	H7	H8	H9	H10	H11	H12	H13	H14	H15
[C_8antrIm][Cl]/DMP[5]A - *IN*												
-6.15	-0.07	-0.85	-3.15	-4.04	-0.47[a]	+0.03	-0.27	+0.08	-0.06	+0.02	+0.05	+0.08
[C_8antrIm][Cl]/DMP[5]A - *OUT*												
-0.11	-0.04	+0.01	+0.02	-0.25	-2.37[a]	-0.53	+0.01	-0.04	+0.05	+0.03	+0.04	+0.05

[a]Value averaged over ten H nuclei

Table S2.Melting temperature ($T_{heating}$), enthalpy variation of melting process ($\Delta H_{heating}$), crystallization temperature ($T_{cooling}$), enthalpy variation of crystallization process($\Delta H_{cooling}$) of organic salts and relative complexes with **DMP[5]A**.

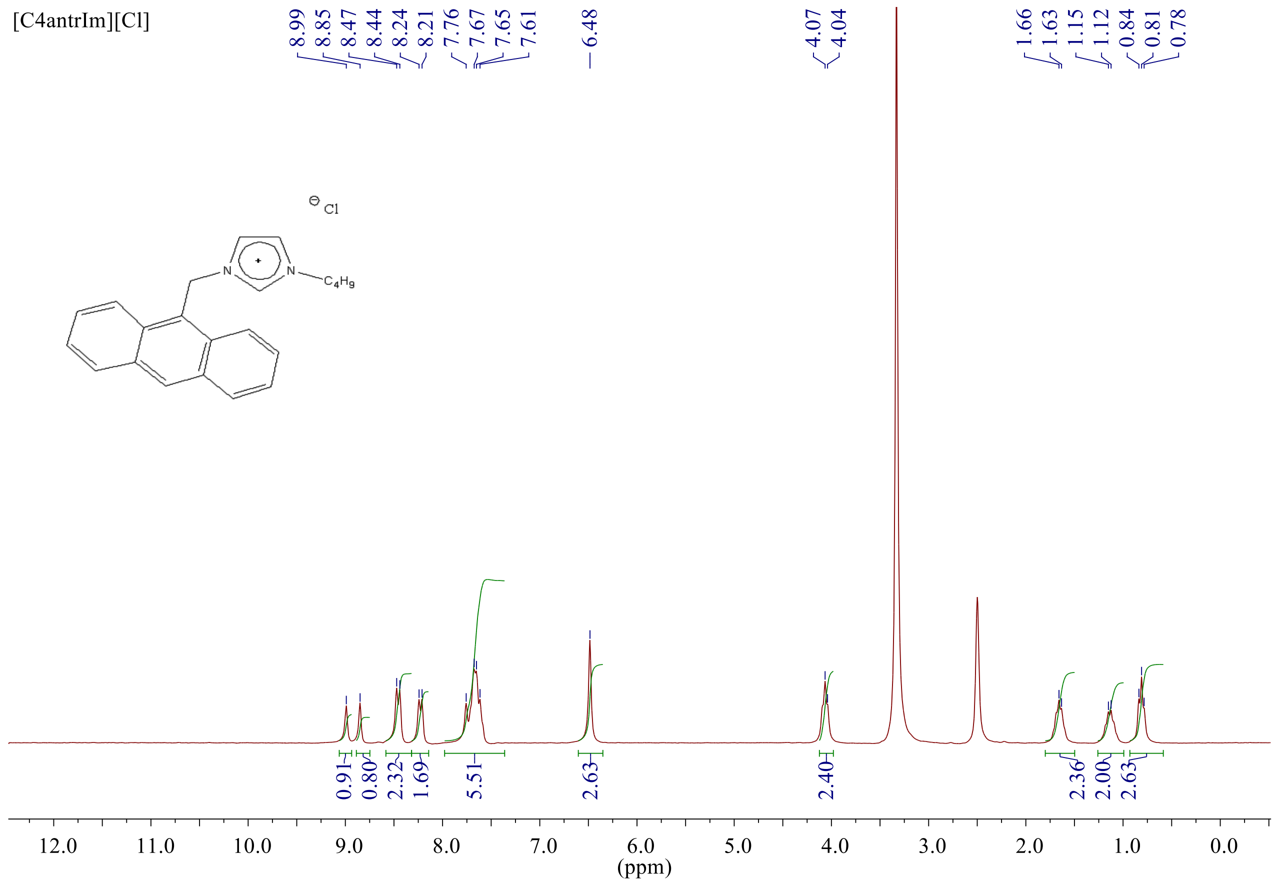
	$T_{heating}$(°C)	$\Delta H_{heating}$(J/g)	$T_{cooling}$(°C)	$\Delta H_{cooling}$(J/g)
[C_4antrIm][NTf_2]	-[a]	-	-	-
[C_4antrIm][NTf_2] / DMP[5]A (1:1)[b]	213.5	-	-	-
[C_4antrIm][SbF_6]	58.8	-	54.5	
	145.5	7.7	127.6	6.3
[C_4antrIm][SbF_6] / DMP[5]A (1:1)[b]	138.8	6.2	-	-
	213.2 (220.8)[c]	-	-	-
[C_4antrIm][BF_4]	136.8	-	68.4	-
[C_4antrIm][BF_4] / DMP[5]A (1:1)[b]	129.1	20.3	-	-
	220.9	76.1	-	-
[C_8antrIm][Cl]	155.7	77.2	-	-
[C_8antrIm][Cl] / DMP[5]A (1:1)[b]	79.3	-	-	-
	136.3	-	-	-
	218.4 (223.7)[c]	-	-	-
[C_{12}antrIm][Cl]	75.5	39.6	-	-
	112.9	-	-	-
[C_{12}antrIm][Cl] / DMP[5]A (1:1)[b]	127.8 (138.9)[c]	-	-	-
	219.3	-	-	-
[C_8(F)antrIm][Cl]	176.7	5.9	-	-
[C_8(F)antrIm][Cl] /DMP[5]A (1:1)[b]	168.5	3.6	-	-
	217.7	-	-	-

[a]nosignal,[b] from CH_2Cl_2 solution, [c]temperature in brackets indicates shoulder peak.

Table S3. Changes in λ values ($\Delta\lambda = \lambda_{solid\ state} - \lambda_{solution}$) corresponding to main emission bands of **[$C_n$antrIm][X]** and **[$C_n$antrIm][X]/DMP[5]A** mixtures, as a function of the anion and alkyl chain, on going from solution to solid state.

	Solution (λ, nm)	**Solid State (λ, nm)**	
	[C_4antrIm][Cl]	[C_4antrIm][Cl]	Dl (nm)
Band I	397.2	398.6	1.4
Band II	420	420.2	0.2
Band III	444.8	450.2	5.4
	[C_4antrIm][Cl]/DMP[5]A	**[C_4antrIm][Cl]/DMP[5]A**	
Band I	397.2	398	0.8
Band II	420.4	417.8	-2.6
Band III	444.8		
	[C_4antrIm][BF_4]	**[C_4antrIm][BF_4]**	
Band I	397.6	397.4	-0.2
Band II	420.4	421.2	0.8
Band III	445	449.6	4.6
	[C_4antrIm][BF_4]/DMP[5]A	**[C_4antrIm][BF_4]/DMP[5]A**	
Band I	397.2	398.6	1.4
Band II	420.2	419.6	-0.6
Band III	444.6	450.6	6
	[C_4antrIm][NTf_2]	[C_4antrIm][NTf_2]	
Band I	397.8	397.8	0
Band II	421	419.4	-1.6
Band III	445.4	450.4	5
	[C_4antrIm][NTf_2]/DMP[5]A	**[C_4antrIm][NTf_2]/DMP[5]A**	
Band I	397.6	400	2.4
Band II	420.6		
Band III	444.6	450	5.4
	[C_4antrIm][SbF_6]	**[C_4antrIm][SbF_6]**	
Band I	397.6	397.8	0.2
Band II	420.8	420.2	-0.6
Band III	445.6	449.8	4.2
	[C_4antrIm][SbF_6]/DMP[5]A	**[C_4antrIm][SbF_6]/DMP[5]A**	
Band I	397.6	397.4	-0.2
Band II	420.8	419.4	-1.4
Band III	445.2	458.6	13.4
	[C_8antrIm][Cl]	**[C_8antrIm][Cl]**	
Band I	396.6	397.6	1
Band II	419.4	420	0.6

Band III		443.8	450.2	6.4
	[C_8antrIm][Cl]/DMP[5]A		**[C_8antrIm][Cl]/DMP[5]A**	
Band I		396.6	398.6	2
Band II		419.4	419	-0.4
Band III		443.6	450.4	6.8
	[C_{12}antrIm][Cl]		**[C_{12}antrIm][Cl]**	
Band I		397	398.6	1.6
Band II		420	419	-1
Band III		444.4	450.4	6
	[C_{12}antrIm][Cl]/DMP[5]A		**[C_{12}antrIm][Cl]/DMP[5]A**	
Band I		397	400.8	3.8
Band II		420	422	2
Band III		444.4	450.4	6
	[C_8(F)antrIm][Cl]		**[C_8(F)antrIm][Cl]**	
Band I		396.8	398.2	1.4
Band II		419.6		
Band III		444	450	6
	[C_8(F)antrIm][Cl]/DMP[5]A		**[C_8(F)antrIm][Cl]/DMP[5]A**	
Band I		396.2	398.8	2.6
Band II		419	419.8	0.8
Band III		443.6	450.6	7


[C4antrIm][Cl]
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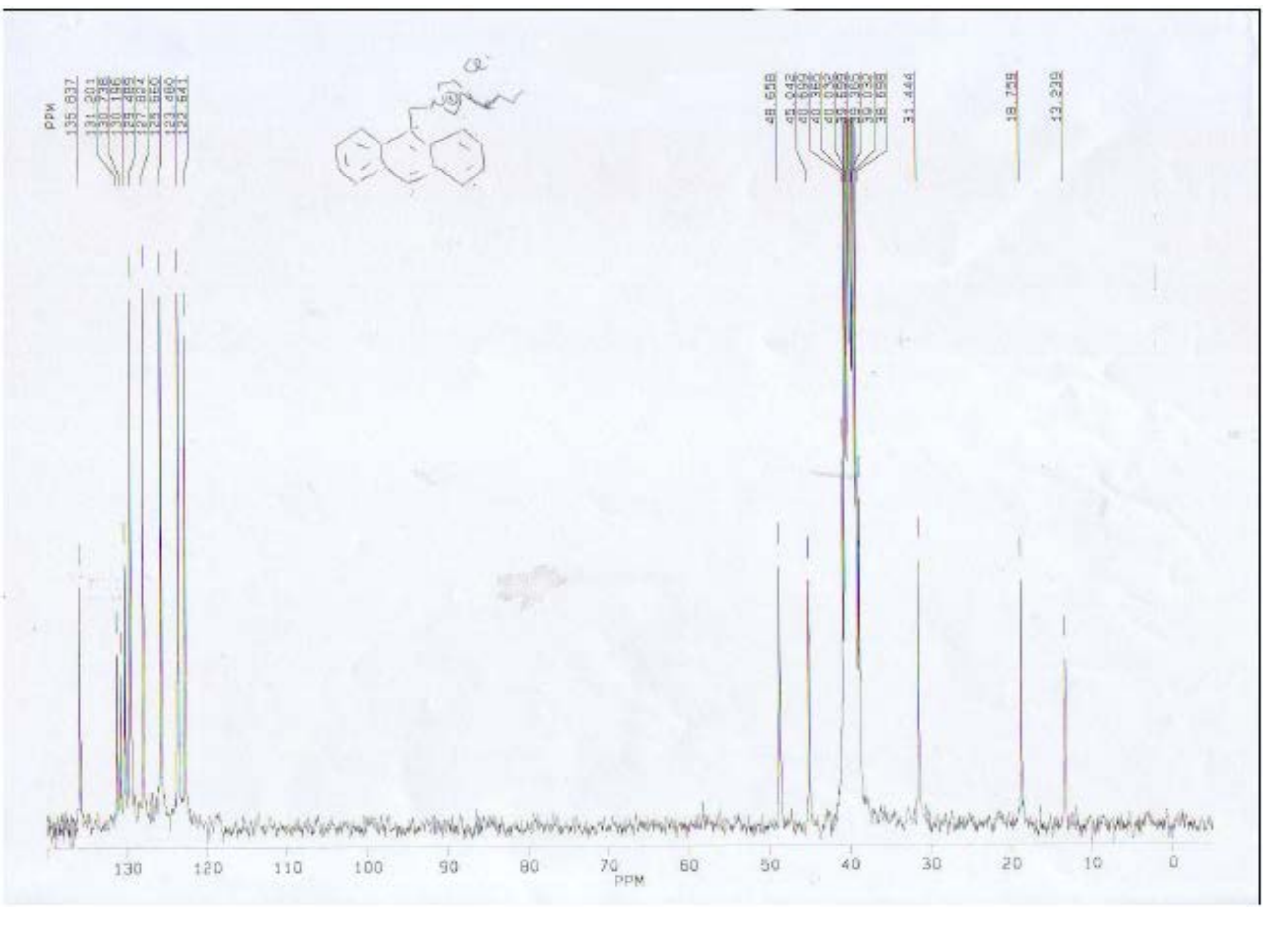
6.48
4.07 4.04
1.66 1.63 1.15 1.12 0.84 0.81 0.78
0.91 0.80 2.32 1.69 5.51 2.63 2.40 2.36 2.00 2.63
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
(ppm)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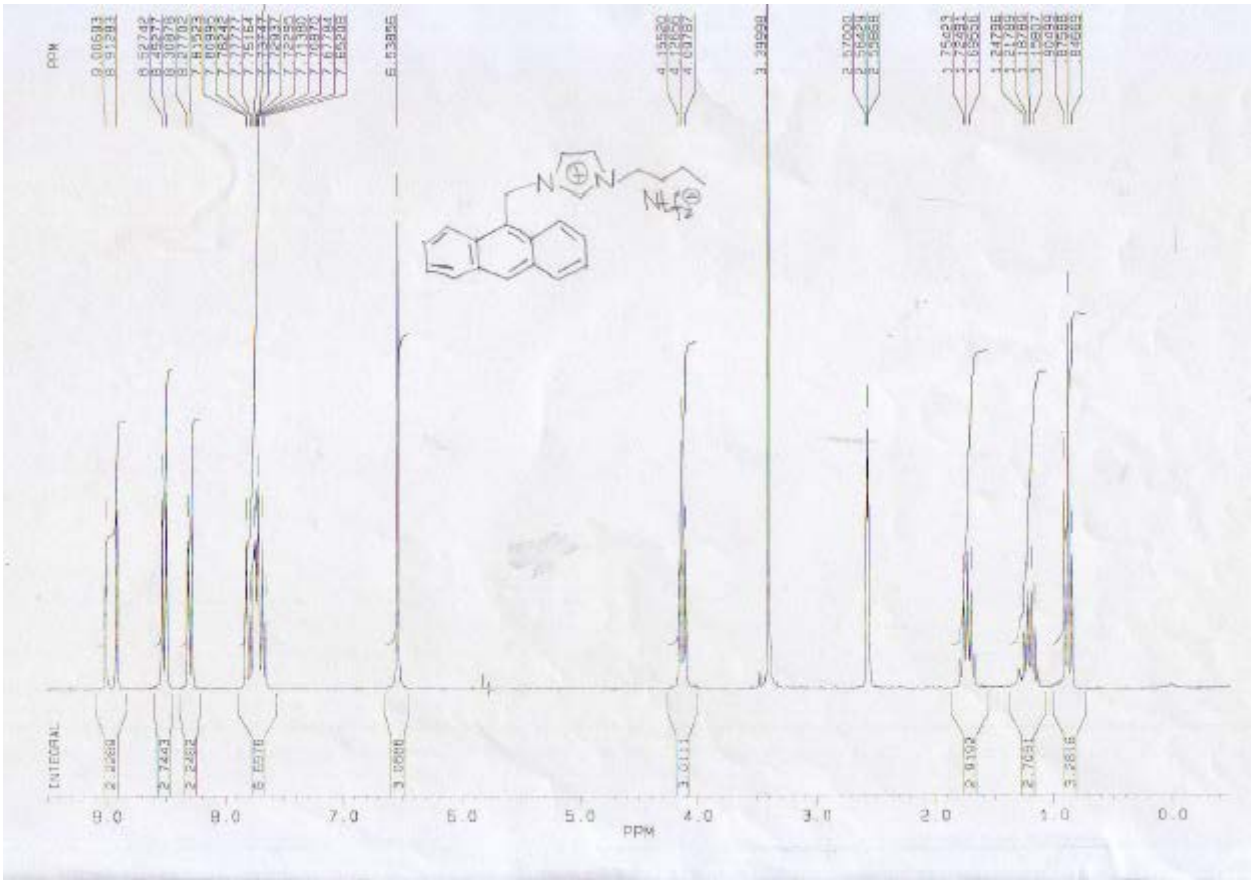
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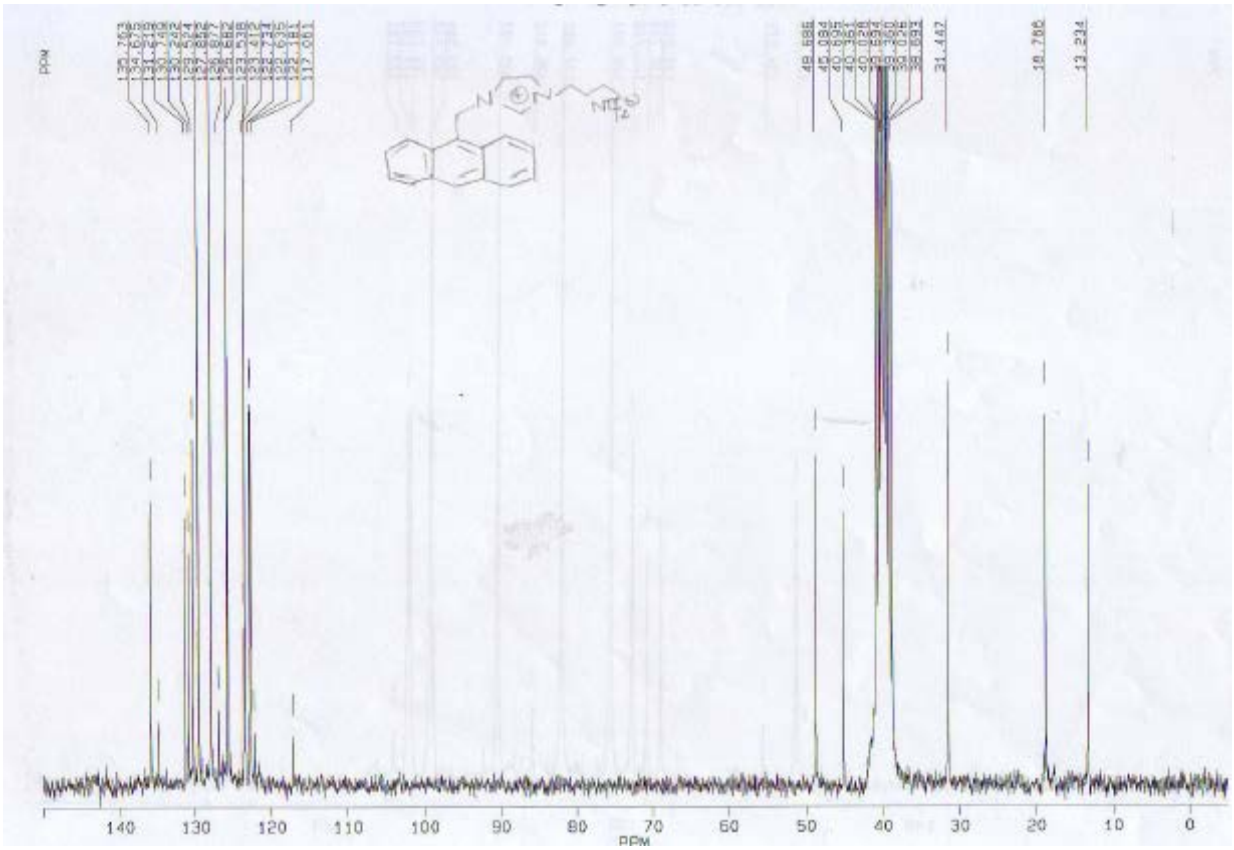
INTEGRAL
PPM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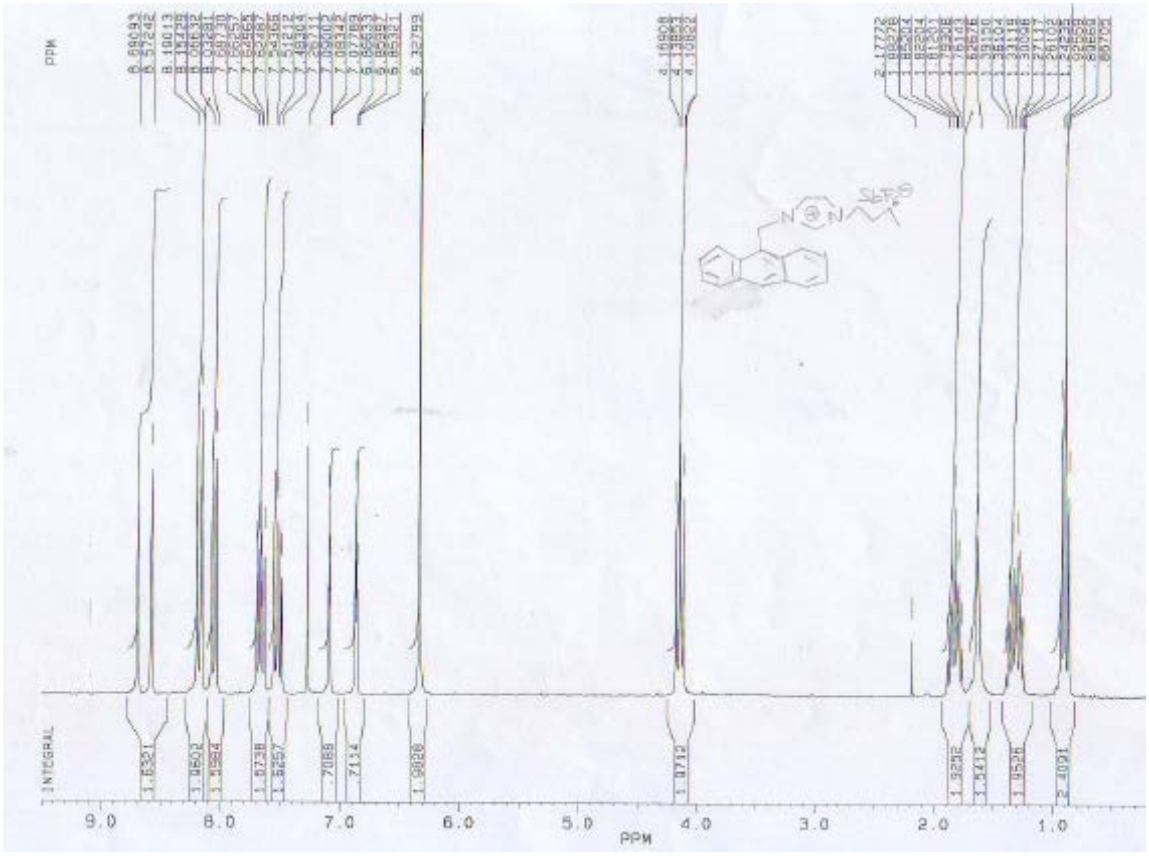
PPM


PPM
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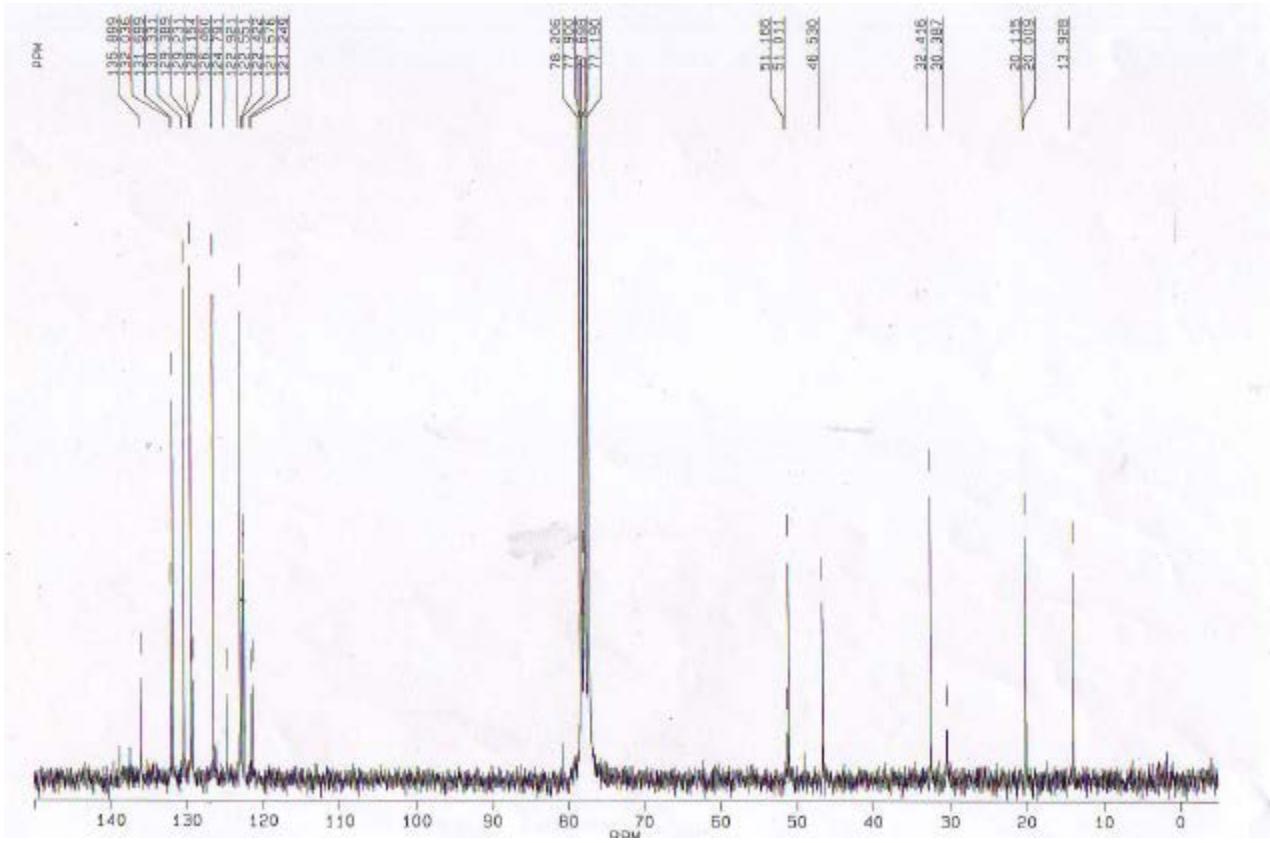
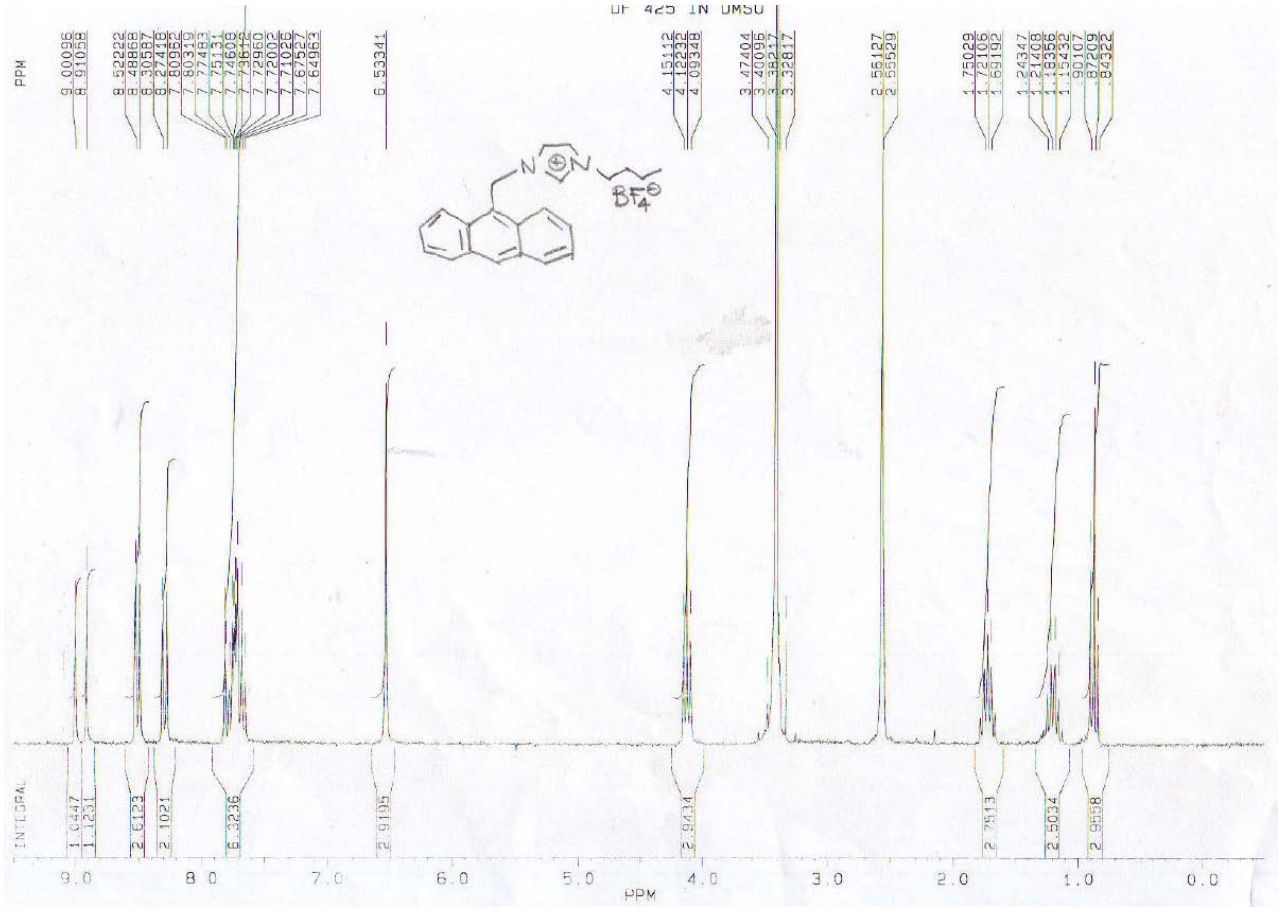
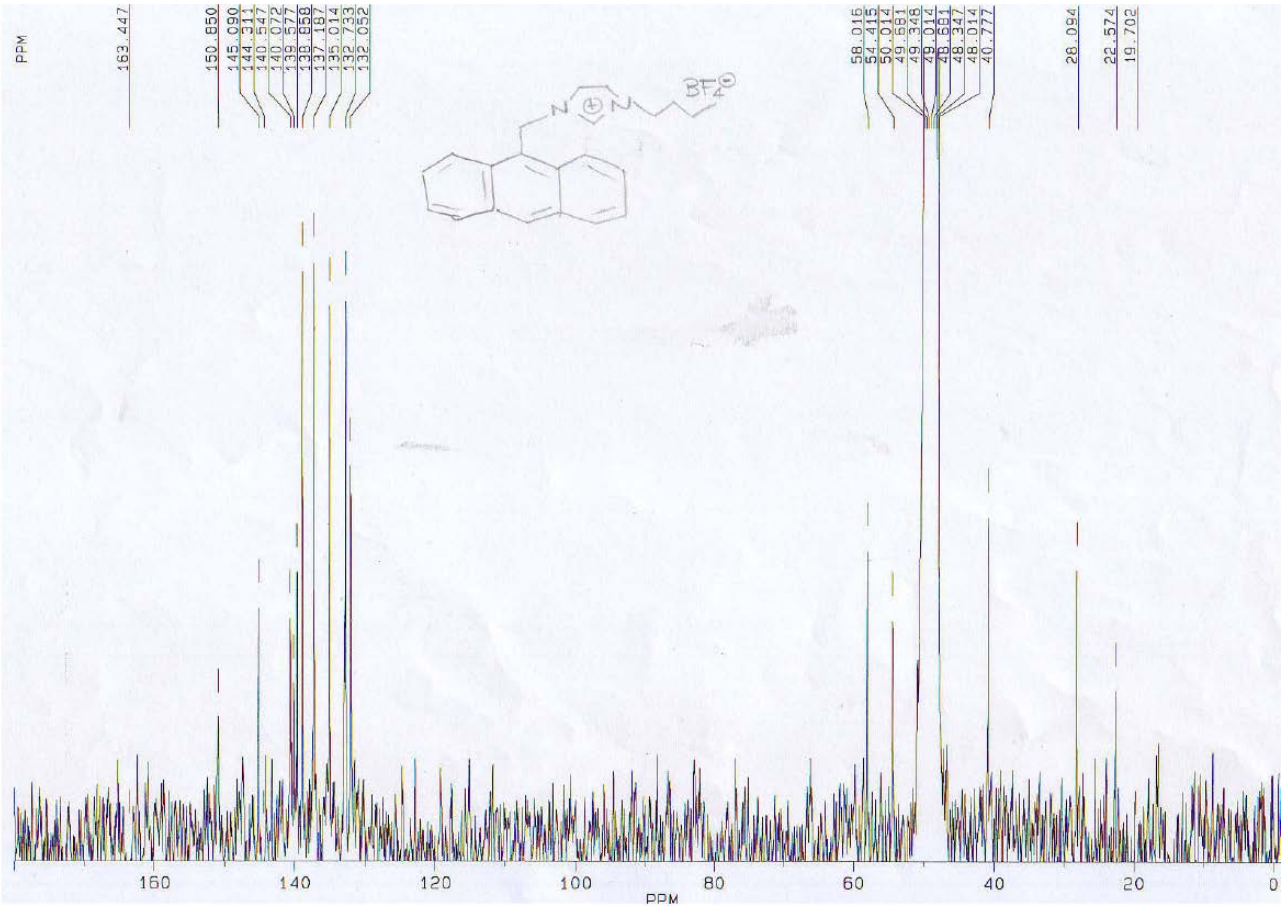
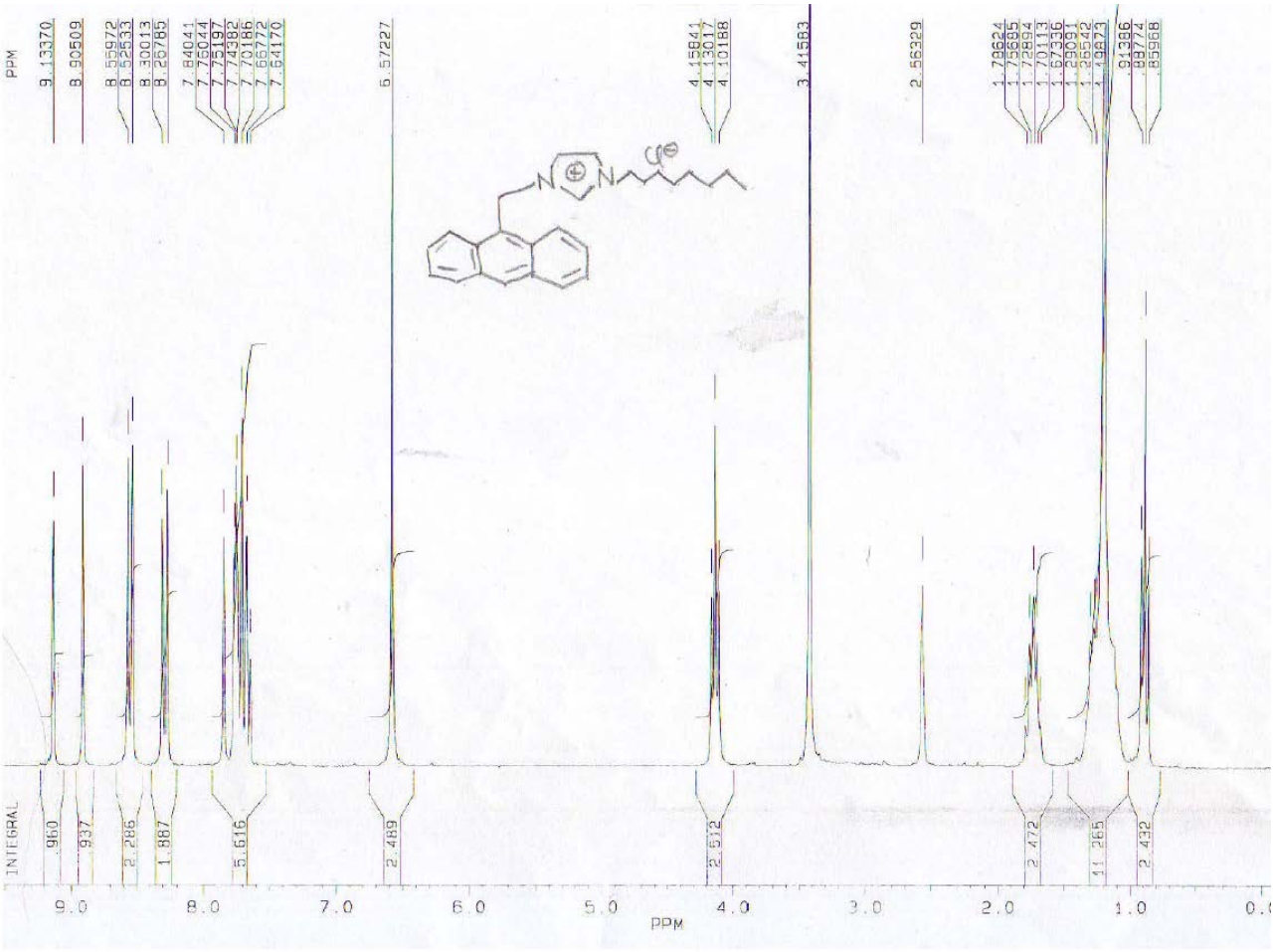
7.0
6.0
5.0
4.0
3.0
2.0
1.0
PPM


PPM
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM


PPM
INTEGRAL
PPM


PPM
PPM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7.74382
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7.69772
7.64170
5.57227
4.15841
4.13017
4.10188
3.41583
2.56329
1.79624
1.75865
1.72894
1.71113
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1.65091
1.62542
1.61873
1.61366
1.58772
1.55968
INTEGRAL
.960
.937
2.285
1.887
5.616
2.489
2.512
2.472
11.265
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8.0
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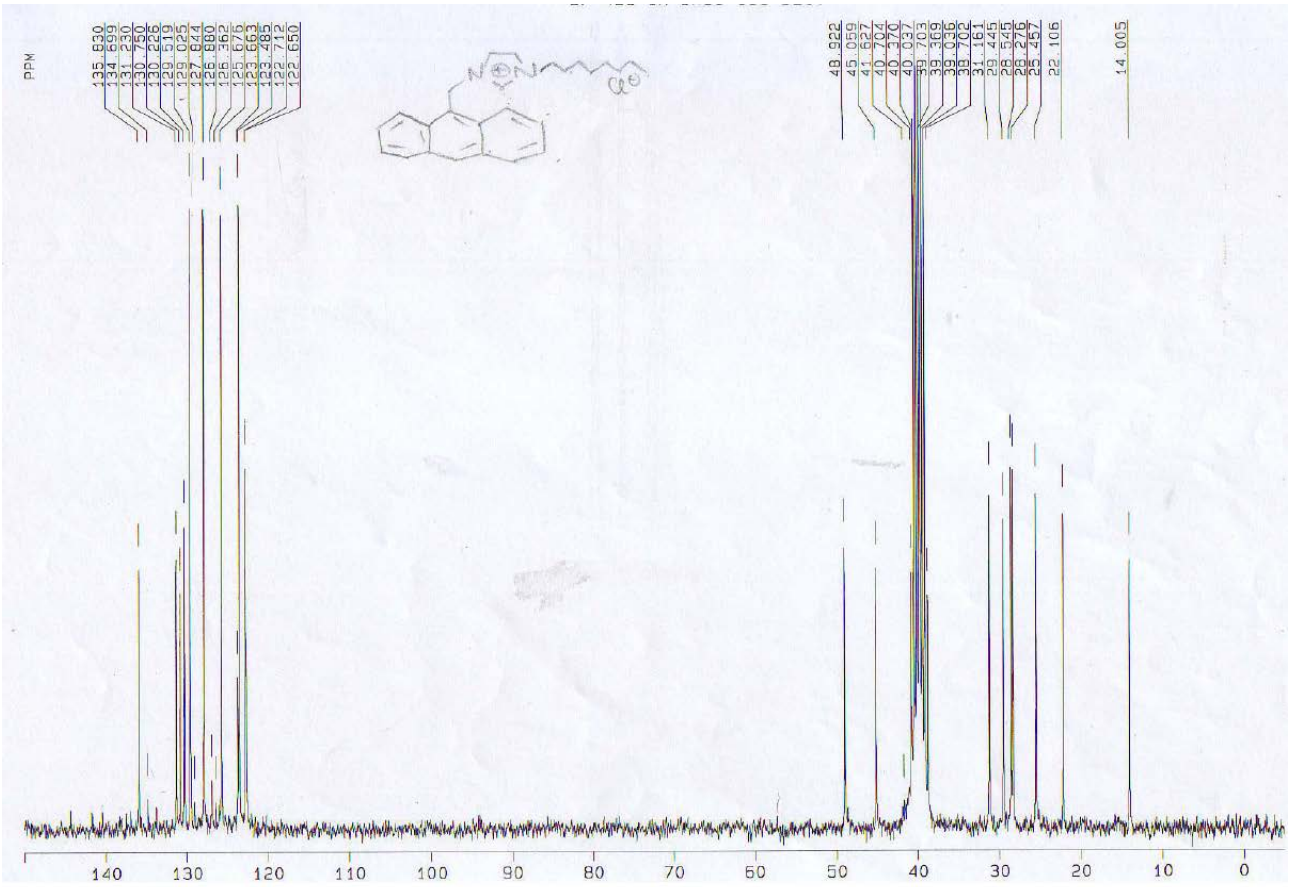
4.0
3.0
2.0
1.0
PPM


PPM
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131.230
130.750
130.226
129.519
129.025
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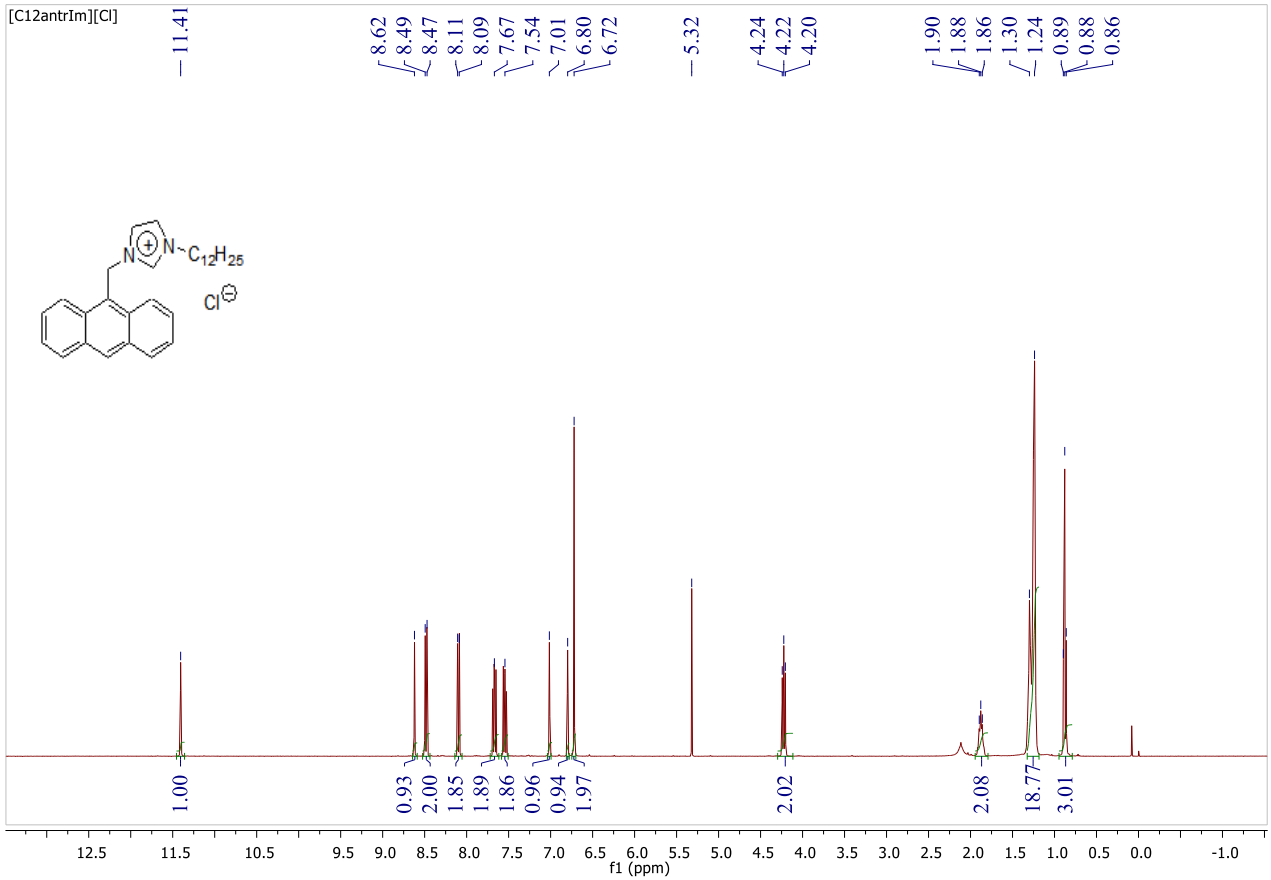
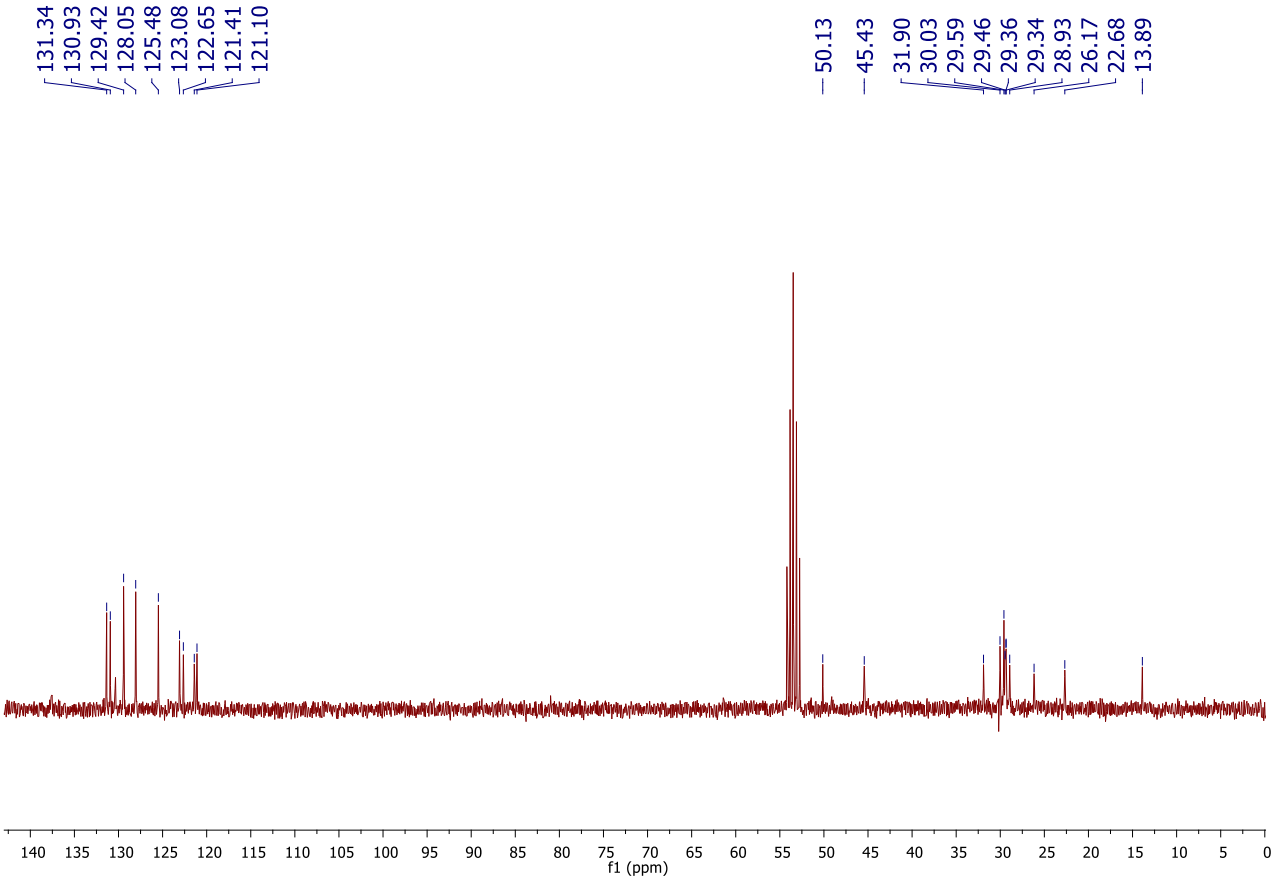
126.880
126.362
125.676
123.663
123.485
122.712
122.650
48.922
45.059
41.527
40.274
40.137
39.963
39.789
39.616
39.442
39.269
39.095
38.702
31.161
29.445
28.245
26.276
25.457
22.106
14.005
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


[C12antrIm][Cl]
11.41
8.62
8.49
8.47
8.11
8.09
7.67
7.54
7.01
6.80
6.72
5.32
4.24
4.22
4.20
1.90
1.88
1.86
1.30
1.24
0.89
0.88
0.86
$C_{12}H_{25}$
Cl
1.00
0.93
2.00
1.85
1.89
1.86
0.96
0.94
1.97
2.02
2.08
18.77
3.01
f1 (ppm)


131.34
130.93
129.42
128.05
125.48
123.08
122.65
121.41
121.10
50.13
45.43
31.90
30.03
29.59
29.46
29.36
29.34
28.93
26.17
22.68
13.89
f1 (ppm)

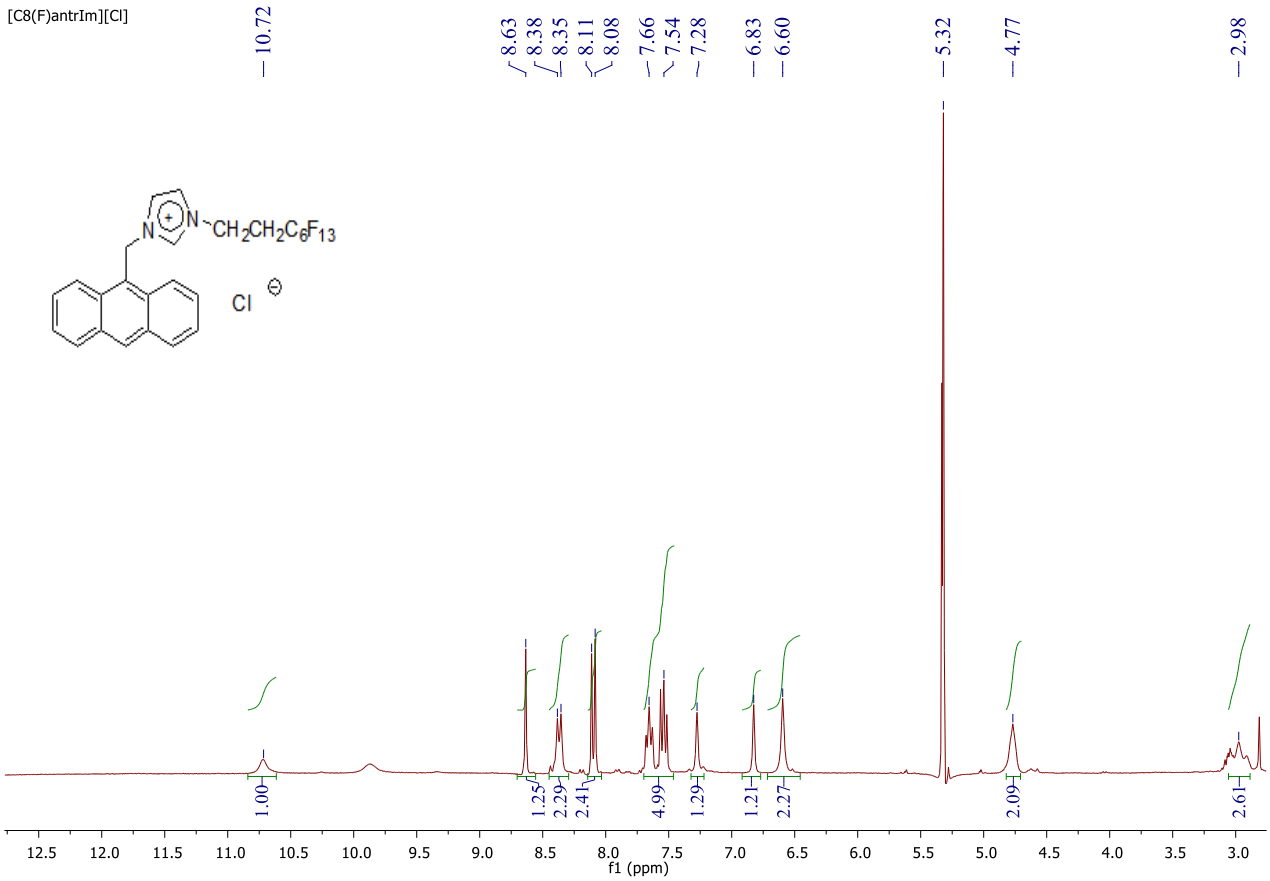


Figure S11. ^{1}H NMR and ^{13}C NMR spectra of all new synthesize compounds at 0.026M.

Table S4. Atom coordinates and absolute energies.

$[C_4antrIm]^+$ (conformation c_1) in chloroform-PCM

Total M06-2X energy: -961.239552 u.a.

imaginary frequencies: 0

C	-1.248486	5.414974	3.554264
N	-1.454541	4.095493	3.891008
C	-1.048806	3.326703	2.880242
N	-0.582629	4.112381	1.908071
C	-0.696465	5.426019	2.308341
C	-2.089552	3.616811	5.126775
C	-3.601730	3.792143	5.091931
C	-4.248737	3.294358	6.381661
C	-5.764097	3.460578	6.360812
C	-0.007675	3.662024	0.620230
C	-0.183323	2.182940	0.406340
C	0.830784	1.289802	0.815241
C	0.674454	-0.116194	0.554298
C	-0.483128	-0.574012	-0.078526
C	-1.511956	0.297105	-0.444458
C	-1.370845	1.704955	-0.189936
C	2.018262	1.708803	1.505229
C	2.972018	0.805319	1.882618
C	2.821502	-0.585219	1.598867
C	1.703736	-1.028726	0.954757
C	-2.468235	2.558557	-0.547186
C	-3.597959	2.051005	-1.125929
C	-3.722128	0.655515	-1.396570
C	-2.707279	-0.193225	-1.062848
H	3.862195	1.150032	2.409579
H	3.599506	-1.284965	1.903688
H	1.566226	-2.088820	0.735378
H	2.166220	2.759653	1.752900
H	-0.592448	-1.642117	-0.280124
H	-2.785863	-1.264419	-1.255478
H	-4.630051	0.275871	-1.864978
H	-4.418277	2.721002	-1.384906
H	-2.418445	3.628532	-0.346078
H	-1.089660	2.241617	2.850266
H	-0.372040	6.246238	1.677855
H	-1.504536	6.226602	4.226760
H	-0.501822	4.243355	-0.165038
H	1.048373	3.949836	0.619469
H	-1.638142	4.175478	5.957253
H	-1.813041	2.561129	5.239655
H	-4.007304	3.240374	4.228446
H	-3.842997	4.856931	4.939318
H	-3.823101	3.843715	7.237259
H	-3.989914	2.233357	6.531214
H	-6.041156	4.518365	6.238431

H	-6.215738	3.098023	7.293809
H	-6.209137	2.897371	5.526972

$[C_4antrIm]^+$ (conformation c_2) in chloroform-PCM

Total M06-2X energy: -961.238575 u.a.

imaginary frequencies: 0

C	2.879117	0.467125	1.491884
C	2.715642	-0.895695	1.101625
C	1.606716	-1.272402	0.401848
C	0.599519	-0.316748	0.049272
C	1.945435	1.410599	1.164996
C	0.767725	1.062133	0.421518
C	-0.548525	-0.706223	-0.644287
C	-1.557646	0.205284	-0.962285
C	-0.225871	1.999525	0.063556
C	-1.406498	1.586889	-0.592023
C	-2.744368	-0.218902	-1.643490
C	-3.743312	0.665932	-1.926879
C	-3.611317	2.033056	-1.539216
C	-2.488786	2.478881	-0.899279
H	3.762730	0.758089	2.060652
H	3.476837	-1.628283	1.369472
H	1.460197	-2.310980	0.100848
H	2.103238	2.437645	1.493627
H	-0.666418	-1.752969	-0.933540
H	-2.829607	-1.269878	-1.924977
H	-4.644993	0.336522	-2.442989
H	-4.420177	2.731051	-1.757134
H	-2.433551	3.527852	-0.609030
N	-1.446519	3.605694	3.711338
C	-1.114256	2.937866	2.606251
N	-0.545976	3.787791	1.748555
C	-0.512763	5.039704	2.322536
C	-1.079382	4.924711	3.555906
H	-1.273886	1.881004	2.421846
H	-0.092519	5.896277	1.807391
H	-1.253660	5.661945	4.331794
C	-0.030674	3.453088	0.401368
H	-0.547256	4.105200	-0.309989
H	1.028071	3.731527	0.385804
C	-2.090771	3.049985	4.914937
C	-2.437589	1.578603	4.776440
H	-2.993488	3.648723	5.095655
H	-1.397360	3.210678	5.751378
C	-3.120540	1.060640	6.041480
H	-1.521506	0.993830	4.591038
H	-3.107003	1.432243	3.912717
C	-3.477957	-0.416997	5.931218
H	-4.030087	1.653341	6.230072
H	-2.454960	1.222198	6.904636

H	-4.162565	-0.593867	5.088286
H	-3.968736	-0.773868	6.846400
H	-2.577695	-1.028256	5.768785

$[C_4antrIm]^+$ (conformation c_3) in chloroform-PCM

Total M06-2X energy: -961.238330 u.a.

imaginary frequencies: 0

C	-1.026324	4.074525	4.102973
N	-1.389807	5.255677	3.494885
C	-0.987819	5.221427	2.224807
N	-0.384501	4.053665	1.997489
C	-0.397852	3.315841	3.160610
C	-2.068559	6.382151	4.151634
C	-1.136717	7.132546	5.093690
C	-1.855888	8.288384	5.784589
C	-0.934420	9.048508	6.731980
C	0.216643	3.633980	0.712261
C	0.001862	2.165114	0.453442
C	1.034423	1.238816	0.714252
C	0.818679	-0.152379	0.411480
C	-0.408580	-0.562528	-0.111545
C	-1.449157	0.342455	-0.334611
C	-1.248315	1.734670	-0.042082
C	2.300885	1.599588	1.289820
C	3.267441	0.661364	1.520794
C	3.054359	-0.711572	1.194872
C	1.862869	-1.102114	0.658543
C	-2.350395	2.625896	-0.266002
C	-3.543653	2.167247	-0.751046
C	-3.731324	0.785560	-1.052223
C	-2.711330	-0.097764	-0.848127
H	4.216704	0.965262	1.962908
H	3.843458	-1.439586	1.382262
H	1.675852	-2.148181	0.410457
H	2.505607	2.632840	1.567545
H	-0.562634	-1.619189	-0.342005
H	-2.836336	-1.159029	-1.069319
H	-4.690257	0.443895	-1.441580
H	-4.365883	2.865572	-0.909947
H	-2.252432	3.687412	-0.039396
H	-1.132055	6.012226	1.494162
H	0.024891	2.318025	3.211009
H	-1.255583	3.869289	5.142931
H	-0.248425	4.248810	-0.065774
H	1.277715	3.896695	0.738724
H	-2.932560	5.968218	4.687989
H	-2.446205	7.035652	3.354995
H	-0.273436	7.510883	4.522800
H	-0.743168	6.433497	5.849775
H	-2.723263	7.896209	6.340411
H	-2.257390	8.975140	5.021549

H	-0.542989	8.383458	7.516254
H	-1.465153	9.875079	7.222885
H	-0.075494	9.471158	6.189610

$[C_4antrIm]^+$ (conformation c_4) in chloroform-PCM

Total M06-2X energy: -961.237313 u.a.

imaginary frequencies: 0

C	3.446879	0.697808	0.604572
C	3.209203	-0.702168	0.462088
C	1.934851	-1.158143	0.295106
C	0.826360	-0.250992	0.254664
C	2.418048	1.596218	0.560746
C	1.060037	1.165142	0.372189
C	-0.478240	-0.725880	0.110717
C	-1.575387	0.138966	0.094070
C	-0.040158	2.047494	0.315577
C	-1.358615	1.554673	0.204763
C	-2.910234	-0.364491	-0.029367
C	-3.980913	0.481762	-0.030069
C	-3.773834	1.887796	0.093235
C	-2.513593	2.406247	0.205123
H	4.466499	1.054818	0.752275
H	4.047500	-1.397966	0.493642
H	1.729975	-2.225110	0.193370
H	2.648388	2.653428	0.687062
H	-0.645959	-1.801523	0.019373
H	-3.048645	-1.443144	-0.120009
H	-4.994652	0.092185	-0.121903
H	-4.634982	2.556709	0.098674
H	-2.399964	3.485457	0.308237
N	-0.694478	5.418428	3.326728
C	-0.602969	5.275090	2.004582
N	-0.106632	4.065128	1.738212
C	0.128327	3.411451	2.926995
C	-0.240551	4.263527	3.924621
H	-0.882744	6.013571	1.260971
H	0.522930	2.401569	2.958541
H	-0.227172	4.147985	5.002524
C	0.174844	3.536679	0.384576
H	-0.491742	4.066963	-0.304657
H	1.198837	3.816454	0.122893
C	-1.199039	6.594994	4.057125
C	-1.712673	7.690781	3.140647
H	-0.372113	6.962658	4.679587
H	-1.996779	6.235414	4.720768
C	-2.226795	8.878752	3.952801
H	-2.527752	7.299672	2.508946
H	-0.904261	8.030787	2.472351
C	-2.751420	9.995589	3.058198
H	-1.413369	9.259925	4.590823

H	-3.024026	8.534924	4.631032
H	-1.960150	10.369120	2.391189
H	-3.117376	10.841061	3.655623
H	-3.581974	9.639181	2.430801

[C_4antrIm][Cl] (conformation c_{14}) in chloroform-PCM

Total M06-2X energy: -1421.609538 u.a.

imaginary frequencies: 0

C	0.306255	4.397705	3.930180
N	-0.423293	5.424747	3.366509
C	-0.456557	5.256661	2.042926
N	0.231627	4.152461	1.746412
C	0.716848	3.593444	2.910198
C	-1.087044	6.507074	4.108003
C	-1.764870	7.505364	3.185078
C	-2.461678	8.607254	3.979082
C	-3.135367	9.623177	3.063229
C	0.408829	3.637450	0.373881
C	0.054771	2.172087	0.297651
C	1.061116	1.188785	0.412544
C	0.695088	-0.202670	0.355531
C	-0.646411	-0.557088	0.203690
C	-1.651124	0.408456	0.107817
C	-1.300783	1.802359	0.153113
C	2.453268	1.495594	0.602128
C	3.391251	0.507758	0.713183
C	3.020418	-0.868653	0.640773
C	1.710636	-1.207621	0.467290
C	-2.361492	2.765088	0.048530
C	-3.660944	2.361064	-0.085236
C	-4.004554	0.976458	-0.125031
C	-3.025375	0.030204	-0.034299
H	4.438993	0.773815	0.856718
H	3.786157	-1.639778	0.726611
H	1.405724	-2.254319	0.413170
H	2.781860	2.532357	0.665882
H	-0.916876	-1.615011	0.164560
H	-3.267123	-1.033660	-0.068753
H	-5.048721	0.681675	-0.234015
H	-4.445768	3.113516	-0.171326
H	-2.152681	3.837221	0.050291
H	-0.975661	5.870479	1.283009
H	1.297502	2.677154	2.914297
H	0.463703	4.326818	5.000420
H	-0.232848	4.260768	-0.262591
H	1.444014	3.826875	0.075092
H	-0.319560	6.997375	4.722804
H	-1.818242	6.038707	4.781657
H	-2.497052	6.988314	2.544008
H	-1.018467	7.950520	2.506771

H	-1.726486	9.114488	4.625530
H	-3.209641	8.154211	4.650439
H	-2.397321	10.108236	2.407286
H	-3.644030	10.406000	3.642293
H	-3.880541	9.134309	2.418496
Cl	-1.978181	6.376979	-0.542601

[C_4antrIm][Cl] (conformation c_{23}) in chloroform-PCM

Total M06-2X energy: -1421.609389 u.a.

imaginary frequencies: 0

C	1.150197	4.665426	3.816053
N	0.239789	5.637155	3.457748
C	-0.183316	5.396706	2.214616
N	0.430875	4.299560	1.770744
C	1.269788	3.818892	2.754102
C	-0.232793	6.752939	4.289945
C	-1.753677	6.825910	4.321153
C	-2.236836	7.994245	5.175764
C	-3.758751	8.078577	5.215791
C	0.195067	3.708389	0.438323
C	-0.066506	2.225944	0.545295
C	0.985915	1.302249	0.368024
C	0.712612	-0.106483	0.486221
C	-0.580862	-0.534744	0.790013
C	-1.623421	0.373104	0.989866
C	-1.368432	1.782820	0.866545
C	2.342652	1.688980	0.089256
C	3.329820	0.757081	-0.069300
C	3.045953	-0.637980	0.033030
C	1.774403	-1.051458	0.303057
C	-2.464649	2.685450	1.081120
C	-3.708556	2.211583	1.393940
C	-3.957026	0.811646	1.516719
C	-2.942596	-0.079226	1.317142
H	4.349194	1.082752	-0.278917
H	3.847893	-1.363820	-0.102535
H	1.537992	-2.113514	0.390246
H	2.605892	2.743127	0.007239
H	-0.780377	-1.605206	0.880690
H	-3.113850	-1.153876	1.401865
H	-4.959090	0.460563	1.765015
H	-4.524921	2.919192	1.543717
H	-2.335432	3.765243	0.980020
H	-0.942882	5.952078	1.632433
H	1.860630	2.918891	2.622043
H	1.627981	4.655743	4.788998
H	-0.657306	4.256805	0.016276
H	1.065359	3.928715	-0.186608
H	0.199914	7.681406	3.892381
H	0.178036	6.588324	5.294135

H	-2.148353	5.876221	4.718014
H	-2.142267	6.932043	3.294133
H	-1.822225	8.933146	4.773189
H	-1.839475	7.889354	6.199179
H	-4.168894	8.203856	4.202758
H	-4.095109	8.926975	5.827326
H	-4.191076	7.160267	5.640859
Cl	-2.589526	6.277655	0.299469

[C_4antrIm][Cl] (conformation c_{32}) in chloroform-PCM

Total M06-2X energy: -1421.605518 u.a.

imaginary frequencies: 0

C	-0.081279	4.117696	4.141636
N	-1.068324	3.154580	4.092669
C	-1.180037	2.728504	2.838416
N	-0.268553	3.346814	2.089254
C	0.415464	4.243765	2.881339
C	-1.988281	2.841554	5.192960
C	-3.049966	1.831238	4.796481
C	-3.997175	1.549073	5.960283
C	-5.073462	0.536512	5.585567
C	-0.258540	3.290334	0.619456
C	-0.194452	1.874555	0.098066
C	1.056437	1.223053	0.026265
C	1.135083	-0.101138	-0.526752
C	-0.030563	-0.729684	-0.972176
C	-1.277393	-0.111269	-0.869467
C	-1.372349	1.214244	-0.313404
C	2.275699	1.820532	0.491912
C	3.469405	1.160414	0.401228
C	3.541721	-0.147850	-0.163625
C	2.405646	-0.756831	-0.612103
C	-2.682628	1.793458	-0.184070
C	-3.793202	1.109461	-0.593939
C	-3.690416	-0.191337	-1.173604
C	-2.467633	-0.781932	-1.302931
H	4.379329	1.637275	0.767004
H	4.504614	-0.654632	-0.230318
H	2.440324	-1.759129	-1.042884
H	2.259089	2.812308	0.942135
H	0.034243	-1.733010	-1.400022
H	-2.368519	-1.780645	-1.732068
H	-4.591900	-0.709930	-1.501253
H	-4.775513	1.566677	-0.468993
H	-2.818842	2.771611	0.285149
H	-1.899138	2.007622	2.468908
H	1.191587	4.887987	2.484069
H	0.179729	4.621381	5.065021
H	-1.160930	3.820698	0.291685
H	0.609109	3.871924	0.290810

H	-2.462410	3.791092	5.478234
H	-1.386012	2.479860	6.038008
H	-2.571465	0.890002	4.476957
H	-3.617431	2.236008	3.941862
H	-4.467981	2.493247	6.278562
H	-3.418611	1.179037	6.822912
H	-5.674389	0.901410	4.739407
H	-5.752473	0.346317	6.427951
H	-4.623417	-0.423001	5.288829
Cl	-3.303578	4.583223	2.046594

[C_4antrIm][Cl] (conformation c_{41}) in chloroform-PCM

Total M06-2X energy: -1421.604956 u.a.

imaginary frequencies: 0

C	-0.608282	5.357376	3.563728
N	0.081616	4.253097	4.016883
C	0.407626	3.498804	2.970156
N	-0.091649	4.052598	1.867669
C	-0.713459	5.234275	2.211784
C	0.605406	4.042012	5.369367
C	0.122788	2.738019	5.987615
C	0.676237	2.555713	7.398259
C	0.215948	1.248053	8.032491
C	0.261212	3.614509	0.508739
C	-0.003779	2.144273	0.289658
C	1.051694	1.210186	0.368528
C	0.783810	-0.176807	0.085024
C	-0.513296	-0.578751	-0.236582
C	-1.572374	0.331841	-0.272440
C	-1.319261	1.719799	0.000675
C	2.393553	1.569503	0.742103
C	3.379087	0.624053	0.803451
C	3.115284	-0.743561	0.489517
C	1.853148	-1.129261	0.144903
C	-2.439742	2.616447	-0.027995
C	-3.699268	2.168991	-0.315091
C	-3.940244	0.791708	-0.599496
C	-2.904555	-0.096886	-0.577098
H	4.383768	0.922183	1.105496
H	3.922811	-1.474691	0.537418
H	1.627121	-2.171860	-0.085838
H	2.639497	2.594867	1.029923
H	-0.707168	-1.631627	-0.455128
H	-3.069595	-1.155013	-0.788178
H	-4.951879	0.457176	-0.829990
H	-4.532812	2.872017	-0.325404
H	-2.298254	3.672827	0.197370
H	1.004853	2.594376	3.000408
H	-1.175900	5.877302	1.471681
H	-0.966590	6.125627	4.238950

H	-0.329362	4.228836	-0.179236
H	1.316753	3.877074	0.371417
H	0.279797	4.902798	5.966759
H	1.701849	4.075723	5.281927
H	0.439453	1.889826	5.358252
H	-0.979170	2.731010	6.008660
H	0.360622	3.406947	8.023869
H	1.777362	2.587472	7.361291
H	-0.881899	1.208622	8.098732
H	0.620990	1.132783	9.047079
H	0.547295	0.385151	7.435350
Cl	3.068876	4.610152	2.601786

[C_4antrIm][Cl] (conformation c_{51}) in chloroform-PCM

Total M06-2X energy: -1421.604695 u.a.

imaginary frequencies: 0

C	0.649477	5.194662	3.741170
N	1.122757	3.914164	3.918778
C	0.926887	3.213170	2.801063
N	0.346229	4.018557	1.905418
C	0.164883	5.264931	2.468885
C	1.689509	3.338715	5.147110
C	0.633939	2.602587	5.959162
C	1.269963	1.875974	7.139328
C	0.238335	1.134368	7.981648
C	0.011835	3.647737	0.516373
C	0.004722	2.153849	0.328207
C	1.213825	1.488750	0.037152
C	1.207466	0.064482	-0.149211
C	0.006941	-0.637034	-0.036175
C	-1.188881	0.006779	0.289059
C	-1.195265	1.429917	0.493769
C	2.477464	2.164237	-0.044874
C	3.630605	1.476326	-0.296796
C	3.614396	0.063666	-0.496891
C	2.435178	-0.617678	-0.426995
C	-2.437661	2.038274	0.877805
C	-3.576452	1.295633	1.019169
C	-3.568411	-0.112326	0.787740
C	-2.405769	-0.733986	0.436546
H	4.579486	2.011897	-0.339834
H	4.547889	-0.463395	-0.693982
H	2.403776	-1.699867	-0.562637
H	2.535070	3.240328	0.120288
H	0.006759	-1.719842	-0.179944
H	-2.374853	-1.812072	0.269377
H	-4.489407	-0.683963	0.903172
H	-4.504502	1.783599	1.319047
H	-2.481967	3.107025	1.084959
H	1.213111	2.150819	2.699621

H	-0.287046	6.083555	1.920247
H	0.698859	5.940623	4.526372
H	-0.963217	4.090869	0.292723
H	0.743181	4.129435	-0.142371
H	2.143572	4.166401	5.707743
H	2.464478	2.629189	4.829668
H	0.157705	1.861030	5.298015
H	-0.140282	3.308816	6.304559
H	1.821755	2.596073	7.767323
H	2.007922	1.162854	6.737654
H	-0.507998	1.829525	8.396369
H	0.712085	0.606128	8.820672
H	-0.296049	0.390279	7.372127
Cl	2.069657	0.290677	3.549085

[C_4antrIm][Cl] (conformation c_{14}) + $CHCl_3$ in chloroform-PCM

Total M06-2X energy: -2840.866434 u.a.

imaginary frequencies: 0

C	-5.820054	-0.631904	-0.706595
C	-4.589256	-0.082217	-0.220821
C	-3.599532	-0.953589	0.355746
C	-3.907177	-2.357139	0.406126
C	-5.091972	-2.843994	-0.071379
C	-6.069062	-1.971468	-0.637284
C	-2.386340	-0.404907	0.827200
C	-2.144421	0.983663	0.744099
C	-3.141765	1.840776	0.161727
C	-4.335106	1.288273	-0.306823
C	-2.896701	3.250331	0.073274
C	-1.737540	3.790492	0.548883
C	-0.753144	2.945482	1.144489
C	-0.940742	1.594653	1.230972
C	-1.323559	-1.311169	1.400957
N	-0.395036	-1.783617	0.353916
C	0.934568	-1.789164	0.476673
N	1.456363	-2.296910	-0.641207
C	0.432673	-2.610537	-1.508075
C	-0.734531	-2.287240	-0.884008
C	2.887376	-2.364058	-0.971734
C	3.773946	-2.140371	0.240015
C	5.249537	-2.159386	-0.149606
C	6.147893	-1.859881	1.045056
Cl	2.142569	0.433681	2.523378
H	0.167923	3.379988	1.536682
H	-1.559363	4.864131	0.481241
H	-3.664997	3.879318	-0.379994
H	-0.144271	0.999412	1.679559
H	-5.089156	1.942935	-0.750251
H	-6.553968	0.052048	-1.136681
H	-7.007863	-2.381064	-1.010308

H	-5.295716	-3.913871	-0.016976
H	-3.189337	-3.060448	0.827852
H	1.479417	-1.359958	1.327991
H	-1.763640	-2.369757	-1.215551
H	0.621647	-3.027646	-2.490739
H	-1.758131	-2.190896	1.886728
H	-0.700846	-0.803583	2.145842
H	3.074188	-1.592112	-1.733683
H	3.066273	-3.349605	-1.423438
H	3.573602	-2.920285	0.993879
H	3.535850	-1.169794	0.705398
H	5.422240	-1.410713	-0.941198
H	5.507566	-3.139256	-0.584640
H	5.908860	-0.873176	1.469510
H	7.208805	-1.863967	0.759769
H	6.005692	-2.607669	1.839720
Cl	3.763514	1.174276	-1.013588
C	2.113455	1.729847	-0.637433
Cl	1.961018	3.466499	-0.965978
Cl	0.919553	0.808560	-1.588543
H	1.941529	1.529423	0.431998

[C_4antrIm][SbF_6] (conformation c_{14}) in chloroform-PCM

Total M06-2X energy: -1565.829661 u.a.

imaginary frequencies: 0

C	3.244811	-2.857356	1.994448
C	3.543140	-1.775668	1.104147
C	2.473270	-1.117911	0.403168
C	1.138796	-1.593780	0.629007
C	0.893584	-2.629834	1.486346
C	1.958642	-3.271945	2.185406
C	2.772541	-0.045523	-0.466691
C	4.104560	0.385871	-0.647944
C	5.164797	-0.290627	0.052634
C	4.858827	-1.350237	0.908046
C	6.520170	0.138933	-0.126162
C	6.823932	1.189417	-0.941379
C	5.778513	1.875438	-1.629401
C	4.474286	1.490853	-1.490917
C	1.643910	0.660549	-1.178333
N	1.047286	1.706063	-0.318074
C	-0.259209	1.893736	-0.119069
N	-0.418180	2.919921	0.719481
C	0.825761	3.403802	1.063208
C	1.747537	2.640485	0.414991
C	-1.689939	3.437457	1.258219
C	-2.887405	2.700545	0.694919
C	-4.204482	3.172288	1.301424
C	-5.373985	2.371523	0.736396
F	-1.061755	-0.799289	-1.591363

H	6.025274	2.717635	-2.276668
H	7.857493	1.511045	-1.070045
H	7.303788	-0.396958	0.412510
H	3.710169	2.046462	-2.033654
H	5.668029	-1.855597	1.440620
H	4.074261	-3.340352	2.514132
H	1.739175	-4.096648	2.864036
H	-0.134431	-2.968765	1.615913
H	0.293471	-1.150496	0.111209
H	-1.048884	1.283674	-0.544813
H	2.831519	2.673124	0.420645
H	0.944122	4.239958	1.742891
H	0.830260	-0.021054	-1.442427
H	1.978911	1.142393	-2.101598
H	-1.724984	4.509622	1.021222
H	-1.637467	3.325829	2.350064
H	-2.775876	1.625561	0.886555
H	-2.920478	2.822248	-0.399353
H	-4.347841	4.247681	1.104970
H	-4.163905	3.053561	2.396723
H	-5.459560	2.521598	-0.350071
H	-6.324714	2.667769	1.200272
H	-5.223516	1.294664	0.904887
Sb	-2.621982	-1.190211	-0.567398
F	-1.862851	-2.811941	0.005140
F	-4.153364	-1.422893	0.490613
F	-1.763496	-0.335968	0.899555
F	-3.414346	-2.031321	-2.040366
F	-3.243059	0.501172	-1.145289

[C_4antrIm][SbF_6] (conformation c_{31}) in chloroform-PCM

Total M06-2X energy: -1565.826191 u.a.

imaginary frequencies: 0

C	-1.262102	-1.217433	3.002789
C	-1.889742	-0.565754	1.893394
C	-1.632348	0.824115	1.649811
C	-0.770777	1.513010	2.568087
C	-0.202641	0.860920	3.625385
C	-0.441329	-0.528135	3.845729
C	-2.208902	1.449728	0.524354
C	-3.056247	0.732695	-0.347582
C	-3.347897	-0.645639	-0.055775
C	-2.750831	-1.261638	1.044761
C	-4.217247	-1.384939	-0.919251
C	-4.766874	-0.808060	-2.026839
C	-4.466216	0.551436	-2.335155
C	-3.645571	1.292008	-1.530625
C	-1.896118	2.901259	0.282657
N	-0.494114	3.120400	-0.137816
C	0.367284	2.201931	-0.585364

N	1.524239	2.812774	-0.857490
C	1.400283	4.152061	-0.568583
C	0.130186	4.348570	-0.118129
C	2.756976	2.154617	-1.323561
C	3.458063	1.400483	-0.202305
C	4.654120	0.615523	-0.732380
C	5.271180	-0.265186	0.349025
H	-4.894772	1.005500	-3.229396
H	-5.424558	-1.379103	-2.682362
H	-4.420920	-2.428179	-0.671494
H	-3.436384	2.321754	-1.815756
H	-2.941250	-2.320304	1.232612
H	-1.450754	-2.282111	3.145421
H	0.036685	-1.030320	4.687040
H	0.449591	1.406467	4.308512
H	-0.549445	2.571123	2.424615
H	0.168283	1.136141	-0.676647
H	-0.382830	5.246151	0.208035
H	2.221461	4.845312	-0.710907
H	-2.028282	3.487478	1.201073
H	-2.535884	3.347683	-0.482581
H	3.387600	2.949895	-1.741523
H	2.474933	1.463445	-2.124695
H	2.742408	0.697527	0.243923
H	3.773710	2.107898	0.582726
H	5.407478	1.309046	-1.142596
H	4.308088	-0.017812	-1.564898
H	5.587167	0.334568	1.216598
H	6.151420	-0.803702	-0.029111
H	4.536519	-1.009074	0.690933
F	-0.699749	-0.831112	-1.066460
Sb	0.859279	-1.684383	-0.415717
F	1.803405	-0.523311	-1.586265
F	2.499210	-2.358565	0.215034
F	0.946137	-0.337393	0.915276
F	-0.121947	-2.809239	0.725735
F	0.782513	-2.975660	-1.774817

[C_4antrIm][SbF_6] (conformation c_{32}) in chloroform-PCM

Total M06-2X energy: -1565.825690 u.a.

imaginary frequencies: 0

C	-1.838713	1.186714	3.329344
C	-2.113081	0.850600	1.967091
C	-1.906585	1.828517	0.938891
C	-1.414056	3.114812	1.337732
C	-1.161171	3.401387	2.651867
C	-1.375640	2.426214	3.668402
C	-2.171500	1.489173	-0.407625
C	-2.639974	0.204563	-0.749705
C	-2.824666	-0.769823	0.294836

C	-2.557297	-0.427114	1.618122
C	-3.279814	-2.088019	-0.034327
C	-3.561453	-2.430461	-1.322132
C	-3.390889	-1.468432	-2.362459
C	-2.944542	-0.207327	-2.092275
C	-1.883164	2.518310	-1.470704
N	-0.425393	2.705892	-1.643775
C	0.503234	1.763476	-1.465816
N	1.704000	2.312944	-1.655332
C	1.539234	3.644096	-1.963620
C	0.198803	3.892206	-1.961308
C	2.988056	1.620567	-1.449450
C	3.224030	1.304015	0.022104
C	4.497107	0.484934	0.209014
C	4.741548	0.144558	1.675227
H	-3.614698	-1.749453	-3.392326
H	-3.908569	-3.434555	-1.566679
H	-3.386142	-2.808881	0.777479
H	-2.819596	0.484864	-2.923277
H	-2.681165	-1.181534	2.397495
H	-2.003113	0.422639	4.091203
H	-1.164486	2.673964	4.708793
H	-0.788984	4.389142	2.926334
H	-1.229971	3.888865	0.592444
H	0.316701	0.736250	-1.168002
H	-0.360442	4.801226	-2.151612
H	2.383574	4.296912	-2.153320
H	-2.281049	3.502882	-1.197188
H	-2.306128	2.255478	-2.443162
H	3.762868	2.283566	-1.854885
H	2.962162	0.696247	-2.036910
H	2.372060	0.722144	0.400498
H	3.276737	2.243025	0.597988
H	5.359342	1.034194	-0.206021
H	4.394177	-0.444882	-0.373251
H	4.826030	1.058028	2.284098
H	5.669052	-0.431879	1.799640
H	3.908563	-0.458371	2.064001
F	-0.508262	-1.733664	-1.288736
Sb	0.779287	-1.879044	0.080025
F	1.966575	-1.036093	-1.144489
F	2.149758	-1.876585	1.372984
F	0.283363	-0.148425	0.684830
F	-0.447232	-2.657589	1.271997
F	1.316061	-3.567453	-0.536600

[C_8antrIm][Cl] in chloroform-PCM

Total M06-2X energy: -1579.268189 u.a.

imaginary frequencies: 0

C	-6.738729	-0.666034	-0.148395

C	-5.486612	0.028884	-0.090376
C	-4.352828	-0.598983	0.537075
C	-4.540347	-1.925844	1.059175
C	-5.748573	-2.559151	0.975768
C	-6.871593	-1.921472	0.367964
C	-3.125113	0.095155	0.596367
C	-2.994633	1.378805	0.021981
C	-4.132592	1.986846	-0.612639
C	-5.349487	1.301848	-0.646212
C	-4.001530	3.285814	-1.201970
C	-2.809932	3.950284	-1.169717
C	-1.679238	3.352797	-0.536162
C	-1.761602	2.115300	0.039716
C	-1.917418	-0.546147	1.235072
N	-1.066459	-1.194452	0.217130
C	0.252913	-1.015942	0.124482
N	0.699059	-1.739446	-0.904514
C	-0.366383	-2.397175	-1.485036
C	-1.479999	-2.051958	-0.780635
C	2.091915	-1.796924	-1.371639
C	3.040161	-1.036896	-0.459867
C	4.474439	-1.115041	-0.975425
C	5.457546	-0.377229	-0.071851
C	6.893661	-0.436218	-0.582349
C	7.882663	0.296352	0.318661
C	9.319921	0.237574	-0.190570
C	10.298062	0.974172	0.718421
Cl	1.177118	1.306335	2.128650
H	-0.733479	3.894742	-0.501485
H	-2.716839	4.939027	-1.620006
H	-4.879256	3.728614	-1.676341
H	-0.873231	1.713956	0.532517
H	-6.212902	1.770378	-1.124650
H	-7.584061	-0.163395	-0.621854
H	-7.827294	-2.443394	0.317549
H	-5.858069	-3.565778	1.380511
H	-3.709394	-2.452630	1.527362
H	0.821660	-0.343029	0.792438
H	-2.519866	-2.333430	-0.907909
H	-0.240404	-3.044807	-2.345205
H	-2.196285	-1.304637	1.972487
H	-1.271377	0.181112	1.744134
H	2.112393	-1.382286	-2.389224
H	2.369684	-2.858489	-1.428690
H	2.987431	-1.453722	0.559219
H	2.728681	0.017341	-0.383518
H	4.522168	-0.690795	-1.993124
H	4.778749	-2.172443	-1.062947
H	5.142666	0.675819	0.025682
H	5.410261	-0.805829	0.944041
H	7.203049	-1.491967	-0.681606

H	6.937778	-0.005853	-1.598581
H	7.573180	1.351820	0.417993
H	7.837778	-0.132839	1.335340
H	9.625316	-0.818120	-0.289147
H	9.360686	0.665657	-1.206647
H	11.327064	0.921300	0.335369
H	10.024818	2.036847	0.808265
H	10.291846	0.543528	1.731630

DMP[5]A in chloroform-PCM

Total M06-2X energy: -2496.306068 u.a.

imaginary frequencies: n.a.

C	-4.063246	0.666069	1.206677
C	-4.309196	-0.000288	0.005016
C	-4.078483	0.672168	-1.202823
C	-3.629510	1.994952	-1.190502
C	-3.382733	2.661490	0.010947
C	-3.593399	1.981097	1.218550
C	-4.765729	-1.443150	0.002184
C	-3.585020	-2.390085	-0.000287
C	-3.010642	-2.809665	-1.201669
C	-1.889739	-3.643287	-1.212595
C	-1.334036	-4.085694	-0.003945
C	-1.907615	-3.664538	1.197181
C	-3.017327	-2.816170	1.208371
C	-0.100247	-4.962841	-0.006581
C	1.166477	-4.133276	-0.006455
C	1.756746	-3.732544	-1.206563
C	2.898479	-2.927761	-1.215698
C	3.484648	-2.529186	-0.006358
C	2.894348	-2.929293	1.193744
C	1.740080	-3.716349	1.203023
C	4.703968	-1.632407	-0.007380
C	4.309619	-0.171072	-0.006554
C	4.092352	0.509477	-1.205925
C	3.674096	1.842321	-1.213288
C	3.486530	2.525543	-0.003719
C	3.704411	1.844662	1.195470
C	4.103076	0.505572	1.203292
C	3.000379	3.959470	-0.003056
C	1.487828	4.029813	0.000697
C	0.782486	4.026158	1.212073
C	-0.613832	4.069122	1.207952
C	-1.331052	4.090010	0.010385
C	-0.626603	4.074749	-1.201335
C	0.770420	4.054769	-1.196789
C	-2.845032	4.076806	0.015394
H	-1.182734	4.058361	2.136354
O	1.539611	3.984703	2.352630
H	1.338577	4.033922	-2.125560

O	-1.383719	4.079425	-2.342660
H	3.381505	4.471925	-0.895155
H	3.388776	4.470335	0.886984
O	3.427621	2.555806	-2.355839
H	4.231746	-0.044534	-2.133241
O	4.309961	-0.220248	2.346206
H	3.528742	2.387478	2.122896
H	5.307684	-1.842918	-0.898937
H	5.308238	-1.845781	0.882960
O	3.509668	-2.486615	-2.359150
H	1.279184	-4.047251	-2.133264
O	1.107036	-4.126835	2.346200
H	3.352859	-2.586753	2.120371
H	-0.111714	-5.600126	-0.899430
H	-0.113615	-5.605720	0.882466
O	-1.273408	-4.077451	-2.356119
H	-3.454158	-2.444922	-2.127022
O	-3.611131	-2.354388	2.353069
H	-1.443184	-4.001033	2.122781
H	-5.378928	-1.628361	-0.888445
H	-5.377731	-1.628471	0.893599
H	-3.206799	4.598967	0.910068
H	-3.215528	4.604946	-0.871875
O	-4.316671	-0.040314	-2.347995
H	-3.436724	2.535241	-2.116232
O	-3.317313	2.679408	2.363609
H	-4.227016	0.115456	2.131903
C	-3.492206	2.000781	3.589787
H	-3.208143	2.709057	4.376096
H	-4.541538	1.696756	3.734926
H	-2.847277	1.108945	3.648692
C	-3.033426	-2.745691	3.580981
H	-3.631196	-2.271325	4.367114
H	-3.064949	-3.839787	3.709111
H	-1.988110	-2.404839	3.657947
C	1.654388	-3.698651	3.575742
H	1.009654	-4.111776	4.359433
H	2.680671	-4.076290	3.712253
H	1.662554	-2.598887	3.648614
C	4.086045	0.438231	3.575307
H	4.287682	-0.299200	4.360136
H	4.764751	1.297643	3.699724
H	3.044157	0.787968	3.658473
C	0.849494	3.963279	3.584754
H	1.616765	3.920371	4.365720
H	0.241721	4.872545	3.720491
H	0.196147	3.078952	3.662560
C	-4.060689	0.610419	-3.575025
H	-4.289109	-0.116877	-4.361957
H	-4.703124	1.496904	-3.701277
H	-3.004803	0.916916	-3.653113

C	-1.799061	-3.620296	-3.584789
H	-1.170262	-4.055663	-4.369247
H	-2.839955	-3.953837	-3.725599
H	-1.761770	-2.520826	-3.651705
C	2.921607	-2.858956	-3.588051
H	3.538062	-2.406718	-4.372840
H	2.915452	-3.953698	-3.715085
H	1.889317	-2.481368	-3.668676
C	3.592304	1.879717	-3.584760
H	3.341272	2.602440	-4.369074
H	4.632177	1.541346	-3.721084
H	2.918600	1.010328	-3.656890
C	-0.692466	4.037853	-3.573562
H	-1.458988	4.034314	-4.356371
H	-0.045510	4.921002	-3.700939
H	-0.077651	3.126939	-3.657173

[C_4antrIm][Cl]/DMP[5]A in vacuo

Total M06-2X energy: -3917.941212 u.a.

imaginary frequencies: n.a.

C	1.324572	-1.853637	-0.040579
N	0.520577	-0.734095	0.000623
C	1.280422	0.322244	0.259993
N	2.557518	-0.066613	0.332831
C	2.602773	-1.438092	0.174908
C	-0.945645	-0.736687	-0.032687
C	-1.522961	0.579183	-0.531464
C	-2.955147	0.370809	-1.017243
C	-3.594847	1.678415	-1.468001
C	3.605248	0.827808	0.859772
C	4.984006	0.221099	0.824378
C	5.303577	-0.767810	1.783807
C	6.601441	-1.383808	1.763825
C	7.536211	-0.980811	0.808013
C	7.247341	0.019778	-0.120591
C	5.949862	0.644859	-0.115053
C	4.366641	-1.193366	2.788168
C	4.710015	-2.162477	3.689219
C	5.996671	-2.779288	3.659891
C	6.914134	-2.398401	2.724880
C	5.723890	1.689690	-1.077176
C	6.687812	2.058359	-1.972068
C	7.962714	1.417445	-1.982864
C	8.229141	0.432094	-1.079516
H	3.985512	-2.462380	4.447414
H	6.243023	-3.550381	4.390749
H	7.905518	-2.854064	2.691665
H	3.368458	-0.746445	2.851456
H	8.521763	-1.452816	0.792615
H	9.201666	-0.063462	-1.063067

H	8.717504	1.725563	-2.706633
H	6.483031	2.858684	-2.684186
H	4.769076	2.214074	-1.099616
H	0.932728	1.339322	0.396183
H	3.532683	-1.991324	0.220151
H	0.917056	-2.843287	-0.217904
H	3.534805	1.756585	0.286635
H	3.292822	1.047686	1.892114
H	-1.295046	-0.953603	0.989623
H	-1.235193	-1.567492	-0.694327
H	-0.914359	0.952587	-1.373042
H	-1.496925	1.338478	0.271303
H	-3.557778	-0.100811	-0.218825
H	-2.924158	-0.339094	-1.861141
H	-3.746646	2.354464	-0.611974
H	-4.569621	1.509880	-1.954132
H	-2.935781	2.201064	-2.181381
Cl	1.101919	0.419655	3.100611
C	-2.496350	0.288029	4.054140
C	-3.544133	-0.304521	3.350259
C	-4.299858	0.482468	2.468306
C	-4.001014	1.833884	2.302791
C	-2.964114	2.428285	3.025958
C	-2.212594	1.650854	3.915731
C	-3.897207	-1.763982	3.543187
C	-3.433000	-2.633384	2.397683
C	-4.298734	-2.988535	1.366617
C	-3.857615	-3.755150	0.286925
C	-2.530871	-4.197295	0.233886
C	-1.663131	-3.855163	1.277174
C	-2.100443	-3.072047	2.350725
C	-2.034265	-4.962343	-0.975041
C	-1.485964	-4.005518	-2.014490
C	-2.350343	-3.156254	-2.714818
C	-1.860061	-2.192392	-3.593866
C	-0.479787	-2.075971	-3.816277
C	0.379772	-2.934421	-3.135116
C	-0.110562	-3.885775	-2.236062
C	0.055662	-1.017031	-4.752764
C	0.234794	0.315901	-4.061480
C	-0.705609	1.337594	-4.204148
C	-0.527501	2.573400	-3.581555
C	0.587073	2.801430	-2.757013
C	1.531079	1.780997	-2.627897
C	1.368093	0.551303	-3.274331
C	0.732622	4.104205	-1.995768
C	-0.103819	4.108051	-0.730593
C	0.439337	3.754846	0.511471
C	-0.374161	3.689628	1.647752
C	-1.729282	4.010584	1.580797
C	-2.270085	4.382806	0.342720

C	-1.462783	4.431639	-0.791335
C	-2.611457	3.880540	2.801929
H	0.026425	3.342805	2.602984
O	1.787420	3.468979	0.559287
H	-1.875083	4.702940	-1.759814
O	-3.615938	4.653054	0.319246
H	0.410477	4.933421	-2.640186
H	1.787213	4.253605	-1.733237
O	-1.403595	3.617486	-3.726729
H	-1.580999	1.137872	-4.820580
O	2.273529	-0.473371	-3.197794
H	2.403913	1.962661	-1.997527
H	-0.638108	-0.893223	-5.593872
H	1.026994	-1.347823	-5.143402
O	-2.655548	-1.308305	-4.274113
H	-3.417187	-3.258074	-2.522789
O	0.710036	-4.696645	-1.485994
H	1.449163	-2.814267	-3.298991
H	-2.865599	-5.533263	-1.408103
H	-1.248171	-5.663947	-0.674974
O	-4.666322	-4.112085	-0.767128
H	-5.322376	-2.624004	1.421493
O	-1.319369	-2.672977	3.388765
H	-0.632274	-4.210233	1.228853
H	-4.988439	-1.856537	3.634660
H	-3.437590	-2.117893	4.474465
H	-2.079024	4.261982	3.680700
H	-3.524638	4.469319	2.656188
O	-5.328224	-0.157073	1.816468
H	-4.572724	2.466068	1.622122
O	-1.247668	2.306210	4.617041
H	-1.890506	-0.339410	4.705998
C	-0.653901	1.616379	5.701150
H	-0.000305	2.344287	6.196109
H	-1.427637	1.275714	6.410865
H	-0.048931	0.773175	5.340685
C	0.065677	-2.945189	3.319429
H	0.515485	-2.458207	4.190712
H	0.256808	-4.032242	3.341147
H	0.514637	-2.493161	2.421465
C	2.060683	-4.785227	-1.887324
H	2.517079	-5.560036	-1.261167
H	2.140845	-5.070278	-2.948917
H	2.592653	-3.830409	-1.733573
C	3.609474	-0.124950	-2.898633
H	4.216935	-1.018919	-3.087190
H	3.958941	0.701189	-3.540017
H	3.728683	0.162602	-1.845707
C	2.406274	3.679427	1.827531
H	3.489096	3.659111	1.647771
H	2.122897	4.666375	2.226043

H	2.128072	2.887608	2.541671
C	-6.204091	0.650782	1.066905
H	-6.990636	-0.013198	0.687689
H	-6.660099	1.436570	1.692333
H	-5.688487	1.126554	0.216254
C	-6.002737	-3.671480	-0.723286
H	-6.480570	-4.046014	-1.636101
H	-6.532571	-4.073953	0.155837
H	-6.062673	-2.569517	-0.700510
C	-4.050059	-1.501236	-4.182822
H	-4.507796	-0.746411	-4.832483
H	-4.336911	-2.508243	-4.527853
H	-4.410360	-1.359397	-3.149893
C	-2.421843	3.477796	-4.692638
H	-2.947914	4.439018	-4.723896
H	-2.000680	3.256502	-5.686997
H	-3.134461	2.682436	-4.416746
C	-4.139249	5.193204	-0.872028
H	-5.194416	5.412534	-0.672621
H	-3.616387	6.122662	-1.152546
H	-4.067482	4.475589	-1.707357

[C_4antrIm][Cl]/DMP[5]A in chloroform-PCM

Total M06-2X energy: -3917.951934 u.a.

imaginary frequencies: n.a.

C	2.960500	2.072415	-0.275678
N	2.044892	1.046829	-0.383605
C	2.568121	0.073109	-1.130972
N	3.798806	0.447200	-1.500745
C	4.067310	1.690510	-0.973002
C	0.746772	1.043984	0.307206
C	-0.325004	0.172753	-0.315121
C	-1.640285	0.498343	0.395767
C	-2.763955	-0.423166	-0.035989
C	4.766804	-0.389170	-2.238268
C	5.873634	-0.819679	-1.301933
C	7.080732	-0.089807	-1.231915
C	8.069671	-0.457031	-0.251147
C	7.815759	-1.514361	0.623788
C	6.627438	-2.245092	0.559496
C	5.640447	-1.907105	-0.430288
C	7.390075	1.023009	-2.089191
C	8.571242	1.701756	-1.979012
C	9.545083	1.328329	-1.004912
C	9.296944	0.278700	-0.170270
C	4.445477	-2.704716	-0.482911
C	4.249973	-3.731064	0.400424
C	5.220258	-4.043183	1.399511
C	6.377971	-3.324237	1.468077
H	8.776180	2.537254	-2.649152

H	10.481304	1.882521	-0.936216
H	10.028680	-0.024775	0.580629
H	6.684130	1.338731	-2.856142
H	8.563520	-1.775094	1.376579
H	7.140532	-3.557535	2.213349
H	5.036754	-4.864065	2.093368
H	3.339538	-4.328450	0.334797
H	3.693363	-2.533717	-1.256593
H	2.081960	-0.845186	-1.480847
H	5.016093	2.191315	-1.132649
H	2.733760	2.983403	0.273536
H	4.192765	-1.224693	-2.658198
H	5.133647	0.203775	-3.079935
H	0.408189	2.086190	0.311635
H	0.933042	0.753924	1.350378
H	-0.088872	-0.900515	-0.199852
H	-0.421183	0.379190	-1.396432
H	-1.893282	1.552651	0.177720
H	-1.485674	0.425173	1.488735
H	-2.882207	-0.399677	-1.127743
H	-3.726952	-0.134101	0.414898
H	-2.547089	-1.458487	0.261132
Cl	2.062849	-2.287889	-3.301005
C	-2.918953	-0.050224	-3.880501
C	-3.724682	0.984475	-3.399432
C	-4.871892	0.661132	-2.661798
C	-5.196469	-0.677452	-2.420962
C	-4.380011	-1.710252	-2.884803
C	-3.234235	-1.388076	-3.628012
C	-3.376409	2.432162	-3.674604
C	-2.570270	3.094743	-2.576431
C	-3.189725	3.876469	-1.601304
C	-2.446153	4.537271	-0.618397
C	-1.048716	4.420148	-0.588747
C	-0.428431	3.645462	-1.575435
C	-1.172082	2.973299	-2.550938
C	-0.236036	5.065620	0.519701
C	-0.098771	4.130671	1.713023
C	-1.237032	3.506099	2.228715
C	-1.151503	2.529293	3.215465
C	0.100755	2.115641	3.696897
C	1.234427	2.783370	3.233131
C	1.143474	3.796684	2.268145
C	0.188295	0.963983	4.677498
C	-0.306780	-0.351931	4.105826
C	-1.567988	-0.847658	4.443376
C	-2.040299	-2.052651	3.921829
C	-1.241956	-2.801861	3.044824
C	0.020166	-2.309535	2.703866
C	0.492526	-1.101242	3.231776
C	-1.751892	-4.117644	2.491783

C	-2.523104	-3.937074	1.201156
C	-1.869984	-4.063611	-0.033454
C	-2.577309	-3.856200	-1.221597
C	-3.923516	-3.484607	-1.206882
C	-4.568949	-3.337614	0.028958
C	-3.874893	-3.585531	1.215935
C	-4.647909	-3.149846	-2.496783
H	-2.083548	-3.936134	-2.188424
O	-0.542526	-4.384294	0.013030
H	-4.354660	-3.468100	2.186363
O	-5.876330	-2.926742	-0.014128
H	-2.406211	-4.583860	3.239424
H	-0.899676	-4.783134	2.310035
O	-3.265070	-2.583406	4.227138
H	-2.181250	-0.252908	5.117739
O	1.730953	-0.579591	2.955454
H	0.626041	-2.902565	2.018701
H	-0.416428	1.200194	5.565330
H	1.233235	0.853352	4.996688
O	-2.240021	1.907170	3.747998
H	-2.202946	3.789963	1.819061
O	2.244105	4.453606	1.767465
H	2.206040	2.470798	3.616073
H	-0.727211	5.997600	0.833018
H	0.762545	5.322873	0.146543
O	-3.008692	5.316384	0.357695
H	-4.275321	3.957085	-1.634007
O	-0.623482	2.189312	-3.526186
H	0.660802	3.575351	-1.567405
H	-4.305299	3.000397	-3.812964
H	-2.799256	2.480909	-4.607348
H	-4.295912	-3.815757	-3.294227
H	-5.725675	-3.299730	-2.361798
O	-5.612610	1.720620	-2.206845
H	-6.063819	-0.949314	-1.820179
O	-2.479280	-2.439052	-4.060250
H	-2.024499	0.218738	-4.440120
C	-1.244284	-2.135445	-4.685184
H	-0.755241	-3.095374	-4.883393
H	-1.401791	-1.598915	-5.635566
H	-0.591602	-1.545201	-4.023962
C	0.784669	2.176246	-3.642648
H	1.018739	1.514287	-4.482978
H	1.176877	3.187527	-3.838313
H	1.258043	1.774316	-2.732536
C	3.451891	4.336453	2.499030
H	4.150355	5.052805	2.052885
H	3.293884	4.583033	3.560368
H	3.875449	3.320976	2.422606
C	2.567195	-1.338899	2.104140
H	3.488911	-0.758557	1.966492

H	2.813740	-2.316378	2.549823
H	2.092753	-1.511681	1.122486
C	0.118143	-4.566654	-1.227856
H	1.149405	-4.848741	-0.988099
H	-0.352757	-5.375661	-1.810294
H	0.138666	-3.642427	-1.825505
C	-6.754752	1.419534	-1.434238
H	-7.203515	2.380803	-1.159847
H	-7.485427	0.827380	-2.008732
H	-6.485788	0.865655	-0.519302
C	-4.417897	5.425213	0.370016
H	-4.666583	6.070049	1.219652
H	-4.793466	5.882724	-0.559019
H	-4.892531	4.438947	0.504356
C	-3.496440	2.184776	3.162504
H	-4.221538	1.543557	3.675981
H	-3.780941	3.240627	3.301771
H	-3.492955	1.947937	2.085666
C	-4.059871	-1.884334	5.160943
H	-4.973751	-2.474768	5.289001
H	-3.547502	-1.787824	6.131739
H	-4.322974	-0.879503	4.792506
C	-6.519694	-2.707998	1.222277
H	-7.531097	-2.358981	0.985902
H	-6.584233	-3.635559	1.814262
H	-5.994706	-1.940979	1.816322

[C_4antrIm][Cl]/DMP[5]A + 2$CHCl_3$ in chloroform-PCM

Total M06-2X energy: -6756.44679104 u.a.

imaginary frequencies: n.a.

C	-2.849620	-0.811404	-3.365453
C	-1.685589	-1.562513	-3.475659
C	-0.486756	-0.895850	-3.798550
C	-0.484707	0.478302	-4.031600
C	-1.664566	1.228369	-3.932627
C	-2.840946	0.569500	-3.580732
C	-1.677776	-3.039317	-3.151210
C	-1.414668	-3.230660	-1.674289
C	-2.470772	-3.410896	-0.771816
C	-2.204781	-3.500711	0.599331
C	-0.900568	-3.417064	1.089462
C	0.153231	-3.255012	0.178940
C	-0.108371	-3.158709	-1.185458
C	-0.597953	-3.495034	2.568248
C	-0.313134	-2.140698	3.179135
C	-1.382653	-1.289914	3.524072
C	-1.144108	-0.064930	4.144801
C	0.163438	0.361414	4.417471
C	1.221009	-0.460812	4.032458
C	0.981869	-1.700877	3.432680

C	0.410689	1.718233	5.043508
C	0.324721	2.791838	3.983225
C	-0.908190	3.376353	3.663309
C	-0.992852	4.290138	2.613397
C	0.128245	4.620042	1.848129
C	1.358239	4.025114	2.158965
C	1.450340	3.138957	3.236289
C	-0.000740	5.574792	0.681215
C	-0.423348	4.852728	-0.579538
C	0.530202	4.392409	-1.488817
C	0.152210	3.695108	-2.640445
C	-1.206084	3.465808	-2.903041
C	-2.158723	3.911494	-1.985891
C	-1.779460	4.597417	-0.829897
O	-2.667659	5.069837	0.098607
C	-4.035264	4.784847	-0.109891
C	-1.634555	2.724554	-4.150673
O	1.037182	3.215653	-3.562024
C	2.413430	3.286620	-3.237740
O	-1.977971	2.998588	4.428444
C	-3.241630	3.520869	4.070280
O	2.419798	4.344895	1.352295
C	3.714036	4.063836	1.849492
O	-2.628086	-1.758558	3.230832
C	-3.728521	-0.973992	3.649733
O	2.529165	-0.041521	4.236173
C	3.093962	-0.549965	5.441766
O	-3.728967	-3.484072	-1.305941
C	-4.730374	-4.091113	-0.511467
O	1.415460	-3.202477	0.712495
C	2.488115	-3.183158	-0.206396
O	0.634481	-1.667360	-3.859968
C	1.874381	-0.995486	-4.019195
O	-4.009150	1.297163	-3.396793
C	-4.926121	1.176465	-4.481223
C	4.239264	-0.152278	-0.604522
N	3.588003	0.113655	0.531135
C	4.187874	-0.568550	1.566624
C	5.238056	-1.255367	1.032237
N	5.244994	-0.985189	-0.319449
C	2.380081	0.938154	0.669481
C	1.133103	0.239518	0.153225
C	-0.100056	1.095702	0.420209
C	-1.364312	0.428521	-0.098267
C	6.177106	-1.554135	-1.315968
C	7.596888	-1.522604	-0.807626
C	8.354530	-0.341244	-0.963206
C	9.702034	-0.295624	-0.463322
C	10.242364	-1.421490	0.162543
C	9.498760	-2.590990	0.330710
C	8.143720	-2.647114	-0.152346

C	10.470097	0.904016	-0.614631
C	9.937443	2.001897	-1.225452
C	8.602218	1.959141	-1.728150
C	7.835022	0.834058	-1.605038
C	7.409315	-3.860688	0.084758
C	7.979579	-4.923209	0.727976
C	9.330546	-4.865522	1.185198
C	10.062834	-3.731170	0.990842
Cl	4.811162	0.652620	-3.744949
H	8.188553	2.836025	-2.227558
H	10.527758	2.911778	-1.338086
H	11.491259	0.915310	-0.229280
H	6.828076	0.838743	-2.027435
H	11.268596	-1.384230	0.535783
H	11.095367	-3.664861	1.338612
H	9.767074	-5.727384	1.690155
H	7.395893	-5.829264	0.893672
H	6.372923	-3.945732	-0.241653
H	4.051284	0.247927	-1.611656
H	5.979081	-1.898910	1.493863
H	3.805049	-0.487895	2.581792
H	5.844008	-2.574659	-1.532229
H	6.035955	-0.968055	-2.233637
H	2.549674	1.896062	0.155312
H	2.276260	1.140607	1.744472
H	1.034362	-0.737223	0.657870
H	1.228118	0.046910	-0.931890
H	0.027473	2.084409	-0.054710
H	-0.181500	1.277252	1.507707
H	-1.299082	0.249196	-1.184891
H	-2.247170	1.057717	0.088631
H	-1.528341	-0.547023	0.391605
H	0.433743	1.004545	-4.285168
H	-3.777646	-1.312977	-3.077327
H	-2.647530	-3.478173	-3.411918
H	-0.893265	-3.539295	-3.732755
H	-3.016137	-3.625273	1.316618
H	0.692985	-3.015271	-1.907574
H	-1.456708	-3.944683	3.084064
H	0.277930	-4.139237	2.723003
H	-1.962739	0.596357	4.422406
H	1.825949	-2.335441	3.154264
H	-0.339489	1.903141	5.822251
H	1.406205	1.740964	5.503072
H	-1.939011	4.756880	2.347792
H	2.399063	2.668057	3.498294
H	-0.747719	6.340361	0.928212
H	0.963180	6.068036	0.507672
H	-0.935135	2.952960	-4.964983
H	-2.633551	3.071676	-4.442928
H	-3.206482	3.700289	-2.199559

H	1.579885	4.583711	-1.267174
H	2.955591	2.728842	-4.008156
H	2.762473	4.331692	-3.203783
H	2.612171	2.808817	-2.263446
H	4.419617	4.528327	1.152086
H	3.851599	4.489062	2.856388
H	3.912076	2.979754	1.888573
H	4.122863	-0.174374	5.498223
H	2.522499	-0.197613	6.315716
H	3.099207	-1.651389	5.437046
H	3.406968	-3.209863	0.391292
H	2.458029	-4.058436	-0.875524
H	2.471372	-2.266785	-0.822350
H	2.657347	-1.755863	-3.929456
H	1.952309	-0.511602	-5.005072
H	2.020386	-0.228731	-3.242272
H	-4.572572	5.228002	0.736169
H	-4.401477	5.233246	-1.047474
H	-4.221431	3.698191	-0.132886
H	-3.964608	3.074571	4.761900
H	-3.266910	4.617487	4.174375
H	-3.505027	3.250463	3.034319
H	-4.627978	-1.522663	3.348125
H	-3.727504	-0.840127	4.743518
H	-3.723502	0.014127	3.161740
H	-5.601652	-4.226415	-1.163173
H	-4.391141	-5.069961	-0.134695
H	-5.022984	-3.453148	0.337062
H	-5.824210	1.742664	-4.204579
H	-4.490192	1.596218	-5.402276
H	-5.192752	0.121768	-4.654317
C	-5.479896	-0.020247	-0.969879
H	-4.848684	0.551338	-1.659526
Cl	-6.329635	-1.260228	-1.926395
Cl	-4.457617	-0.759414	0.265263
Cl	-6.655312	1.107227	-0.246812
Cl	-7.577231	-2.055215	1.472480
C	-8.891818	-1.840527	0.298872
Cl	-9.059072	-3.277993	-0.727896
H	-8.630621	-0.993330	-0.339447
Cl	-10.418806	-1.466296	1.120134

[C_4antrIm][SbF_6]/DMP[5]A in chloroform-PCM

Total M06-2X energy: -4062.213021 u.a.

imaginary frequencies: n.a.

C	-8.018998	3.593964	-2.808726
C	-7.857529	2.775427	-1.644536
C	-6.849311	1.750912	-1.630793
C	-6.027868	1.614288	-2.800263
C	-6.210437	2.415760	-3.892280

C	-7.223734	3.420432	-3.904036
C	-6.715420	0.922989	-0.495052
C	-7.536935	1.117562	0.636426
C	-8.534551	2.155455	0.612739
C	-8.674259	2.951031	-0.525037
C	-9.378057	2.354835	1.754125
C	-9.246803	1.579198	2.867642
C	-8.256975	0.551226	2.902024
C	-7.436572	0.326348	1.832054
C	-5.714404	-0.202742	-0.518761
N	-4.354250	0.210599	-0.123448
C	-3.246383	-0.185400	-0.747156
N	-2.188888	0.155754	-0.012274
C	-2.634239	0.788325	1.127487
C	-3.997183	0.826033	1.056947
C	-0.820375	-0.336421	-0.247153
C	0.269633	0.598427	0.245096
C	1.637266	-0.009370	-0.063793
C	2.778438	0.866168	0.437775
H	-8.157068	-0.065650	3.795101
H	-9.892488	1.736575	3.731890
H	-10.129002	3.145446	1.707010
H	-6.694840	-0.468875	1.902659
H	-9.441936	3.728247	-0.541122
H	-8.798684	4.357611	-2.797110
H	-7.356144	4.042847	-4.789083
H	-5.575759	2.285416	-4.769360
H	-5.239018	0.863942	-2.829979
H	-3.213123	-0.768075	-1.661453
H	-4.735498	1.243935	1.733037
H	-1.942286	1.158147	1.880528
H	-5.624362	-0.647283	-1.513709
H	-5.995227	-1.025359	0.145700
H	-0.736645	-0.514695	-1.326564
H	-0.752933	-1.315338	0.254878
H	0.185968	0.748884	1.334743
H	0.174917	1.592888	-0.224573
H	1.732899	-0.165515	-1.153638
H	1.697103	-1.007872	0.404392
H	2.760932	1.855266	-0.049340
H	3.750544	0.396140	0.229152
H	2.693961	1.023845	1.526042
F	-4.730894	-2.926907	-1.115307
Sb	-3.217549	-3.700117	-0.258034
F	-2.137712	-2.629776	-1.421302
F	-1.638804	-4.312537	0.597163
F	-3.285953	-2.251474	0.980502
F	-4.310980	-4.728552	0.879767
F	-3.141572	-5.098406	-1.517107
C	0.792949	3.970361	1.808936
C	2.042833	4.475598	1.467100

C	3.155564	4.099581	2.239848
C	2.993739	3.252399	3.333145
C	1.733429	2.745796	3.675184
C	0.632059	3.105732	2.895511
C	2.225739	5.357186	0.252920
C	2.618436	4.535777	-0.954908
C	3.961479	4.349485	-1.287051
C	4.330559	3.564014	-2.381408
C	3.345154	2.973672	-3.184644
C	2.002490	3.146738	-2.843543
C	1.635329	3.906680	-1.731191
C	3.738102	2.135332	-4.380680
C	3.914746	0.681217	-4.004962
C	5.151584	0.201415	-3.570230
C	5.312316	-1.132210	-3.186556
C	4.229026	-2.018255	-3.263383
C	2.991842	-1.537569	-3.696463
C	2.824141	-0.197265	-4.048567
C	4.375989	-3.451072	-2.799718
C	3.992347	-3.558143	-1.340194
C	4.942933	-3.359072	-0.337829
C	4.575053	-3.369081	1.008756
C	3.239025	-3.593745	1.371343
C	2.287458	-3.793496	0.369065
C	2.655705	-3.770967	-0.979601
C	2.843247	-3.589551	2.830921
C	2.532849	-2.198208	3.338216
C	1.227304	-1.694538	3.257312
C	0.933598	-0.429799	3.773017
C	1.928508	0.367490	4.339191
C	3.242708	-0.119343	4.383382
C	3.531236	-1.395721	3.895037
C	1.602717	1.764690	4.818283
H	-0.080120	-0.028813	3.735199
O	0.296386	-2.500865	2.664322
H	4.541605	-1.799931	3.930542
O	4.182104	0.714797	4.930231
H	3.663465	-4.009263	3.427376
H	1.955604	-4.220752	2.961049
O	5.457310	-3.175723	2.039323
H	5.970745	-3.168508	-0.644163
O	1.774486	-3.946426	-2.009999
H	1.249179	-3.947384	0.667967
H	5.414921	-3.776015	-2.931558
H	3.724881	-4.097459	-3.400649
O	6.491043	-1.654813	-2.725598
H	5.978350	0.908571	-3.520528
O	1.626068	0.339555	-4.444411
H	2.160011	-2.239599	-3.723251
H	4.679659	2.516766	-4.794756
H	2.958851	2.218966	-5.148663

O	5.628691	3.332661	-2.748020
H	4.710068	4.823432	-0.654424
O	0.336325	4.089601	-1.331329
H	1.256289	2.656930	-3.467553
H	3.009370	6.098929	0.453441
H	1.286157	5.885134	0.045938
H	0.576822	1.788007	5.205235
H	2.292055	2.048433	5.623201
O	4.358332	4.615320	1.849268
H	3.843518	2.940280	3.938169
O	-0.598698	2.567869	3.222093
H	-0.059979	4.245956	1.188721
C	-1.705080	3.448738	3.079290
H	-2.545083	2.983928	3.611129
H	-1.482242	4.429528	3.526489
H	-1.985172	3.589423	2.021676
C	-0.674312	3.587264	-2.180011
H	-1.629301	3.869232	-1.721669
H	-0.604904	4.027222	-3.187970
H	-0.621300	2.488224	-2.264978
C	0.527757	-0.542679	-4.534429
H	-0.327029	0.061719	-4.858450
H	0.711466	-1.340839	-5.271767
H	0.302193	-1.007944	-3.559894
C	0.400197	-3.850613	-1.691894
H	-0.144610	-3.835095	-2.642125
H	0.053090	-4.701681	-1.088729
H	0.191862	-2.924124	-1.138910
C	-1.062190	-2.222749	2.943578
H	-1.637685	-3.033855	2.492377
H	-1.237036	-2.170163	4.030655
H	-1.388293	-1.275465	2.481916
C	5.500972	4.199550	2.569142
H	6.358902	4.684674	2.090616
H	5.447053	4.512682	3.624283
H	5.623471	3.105060	2.523623
C	6.637667	3.873670	-1.920772
H	7.592483	3.549132	-2.349176
H	6.600587	4.975109	-1.907609
H	6.551101	3.498076	-0.887914
C	7.590136	-0.774316	-2.627144
H	8.423813	-1.366662	-2.234079
H	7.866990	-0.364743	-3.612239
H	7.375216	0.059695	-1.938899
C	6.804231	-2.932587	1.694052
H	7.344680	-2.799445	2.638001
H	7.237908	-3.783092	1.143289
H	6.903437	-2.020803	1.082191
C	5.512015	0.241179	4.978764
H	6.107072	1.042389	5.430879
H	5.592810	-0.666655	5.598096

H	5.896232	0.022620	3.968719

[C_8antrIm][Cl]/DMP[5]A in chloroform-PCM (C_8^{IN})

Total M06-2X energy: -4075.144352 u.a.

imaginary frequencies: n.a.

C	1.619315	-3.778342	1.758570
C	0.241089	-3.710833	1.532759
C	-0.529426	-2.894709	2.371649
C	0.081704	-2.134978	3.375106
C	1.457447	-2.200126	3.591473
C	2.227357	-3.034701	2.769089
C	-0.379664	-4.475190	0.379036
C	-0.257360	-3.708330	-0.923123
C	0.939362	-3.735758	-1.659139
C	1.080211	-2.951681	-2.806288
C	0.028288	-2.160356	-3.272795
C	-1.180258	-2.160606	-2.564050
C	-1.310641	-2.924343	-1.399061
C	0.166877	-1.335261	-4.533501
C	0.457484	0.118844	-4.237606
C	1.778953	0.556612	-4.057834
C	2.038815	1.893339	-3.757695
C	1.001491	2.820760	-3.612102
C	-0.314298	2.385770	-3.804431
C	-0.574770	1.048245	-4.118307
C	1.305003	4.237675	-3.168414
C	1.715264	4.253447	-1.710407
C	3.061261	4.092001	-1.356962
C	3.429146	4.033925	-0.011179
C	2.475229	4.121120	1.000733
C	1.125303	4.282805	0.652481
C	0.757380	4.354827	-0.695587
C	2.869933	4.020112	2.456369
C	2.656598	2.633825	3.025141
C	1.589600	2.356711	3.880022
C	1.425159	1.087137	4.444900
C	2.321844	0.061982	4.117296
C	3.384559	0.332335	3.250865
C	3.562571	1.607353	2.715137
O	4.605799	1.949509	1.892229
C	5.650242	1.008627	1.763431
C	2.112699	-1.338504	4.647201
O	0.443919	0.771294	5.335530
C	-0.306205	1.844946	5.873237
O	3.959574	3.997904	-2.389688
C	5.308456	3.755587	-2.048526
O	0.254349	4.349360	1.696939
C	-1.125793	4.418874	1.395155
O	2.757868	-0.391893	-4.183576
C	4.091179	0.078206	-4.244218

O	-1.309336	3.314314	-3.611282
C	-2.596066	2.987609	-4.104576
O	1.926381	-4.558079	-1.186488
C	3.067879	-4.735037	-2.001723
O	-2.186469	-1.395180	-3.087281
C	-3.509208	-1.733938	-2.718982
O	-1.890753	-2.868247	2.160420
C	-2.678446	-2.552616	3.307614
O	3.576886	-3.052359	3.005955
C	4.324062	-4.058621	2.353359
C	-1.643923	-0.183347	0.403857
N	-0.964415	0.701600	-0.316044
C	-1.862929	1.506738	-0.983727
C	-3.111439	1.067843	-0.661838
N	-2.951066	-0.004785	0.190837
C	0.492423	0.883006	-0.315506
C	1.254515	-0.396026	0.001778
C	2.693233	-0.265876	-0.491007
C	3.566469	-1.477805	-0.178687
C	-3.973568	-0.687664	1.007381
C	-5.383125	-0.468121	0.522500
C	-5.990554	0.784899	0.767673
C	-7.328286	1.030198	0.303976
C	-8.017971	0.017257	-0.365980
C	-7.444787	-1.237690	-0.579809
C	-6.104117	-1.498444	-0.121815
C	-7.933191	2.307584	0.538998
C	-7.256527	3.288476	1.203982
C	-5.931229	3.045375	1.676451
C	-5.314341	1.842875	1.468582
C	-5.583800	-2.821302	-0.341202
C	-6.319054	-3.781618	-0.977007
C	-7.637889	-3.505451	-1.447892
C	-8.180436	-2.270362	-1.248793
Cl	-1.962641	1.212766	2.973824
H	-5.401627	3.831057	2.216792
H	-7.723694	4.257592	1.381945
H	-8.949171	2.472548	0.175690
H	-4.298177	1.696486	1.847382
H	-9.033618	0.206785	-0.721686
H	-9.191412	-2.041050	-1.590336
H	-8.205388	-4.285661	-1.955410
H	-5.894424	-4.775519	-1.122500
H	-4.586612	-3.084595	0.010479
H	-1.218350	-0.925312	1.069750
H	-4.088093	1.414546	-0.976874
H	-1.537389	2.317310	-1.627529
H	-3.693230	-1.743618	1.018973
H	-3.834371	-0.292737	2.024484
H	0.727213	1.673341	0.415267
H	0.751060	1.247840	-1.321835

H	0.777185	-1.246225	-0.513799
H	1.232440	-0.600304	1.087724
H	3.156618	0.644786	-0.064046
H	2.667610	-0.125141	-1.587403
H	3.782119	-1.516648	0.904833
C	4.863027	-1.447027	-0.986234
H	3.007281	-2.403802	-0.404584
H	-0.506136	-1.445998	3.985325
H	2.207862	-4.418434	1.106008
H	0.129593	-5.442705	0.275734
H	-1.439841	-4.658012	0.592561
H	2.011425	-2.943258	-3.371882
H	-2.244921	-2.917692	-0.834472
H	0.979711	-1.749348	-5.142969
H	-0.769008	-1.400422	-5.103906
H	3.055970	2.247775	-3.601126
H	-1.595321	0.692431	-4.248220
H	2.121214	4.644225	-3.779238
H	0.417090	4.863403	-3.311438
H	4.467753	3.896670	0.283204
H	-0.287028	4.483488	-0.984349
H	3.932501	4.284244	2.550094
H	2.279923	4.736377	3.042353
H	1.473319	-1.297957	5.536149
H	3.077880	-1.778585	4.925507
H	4.071929	-0.482858	3.020942
H	0.879530	3.154342	4.093662
H	-0.962750	1.403467	6.631957
H	0.360870	2.583656	6.349543
H	-0.919446	2.317794	5.094594
H	-1.650047	4.412490	2.356086
H	-1.364712	5.339705	0.837249
H	-1.451073	3.534918	0.824051
H	-3.207007	3.889159	-3.988180
H	-2.549352	2.702798	-5.167423
H	-3.051428	2.162352	-3.531912
H	-4.173374	-1.144404	-3.362486
H	-3.701305	-2.808706	-2.871150
H	-3.715816	-1.477336	-1.671291
H	-3.713435	-2.812203	3.052048
H	-2.352443	-3.156165	4.168876
H	-2.611809	-1.480873	3.552431
H	6.415920	1.479368	1.135390
H	6.082759	0.756330	2.745675
H	5.302571	0.082729	1.277814
H	5.854097	3.673037	-2.995125
H	5.729703	4.584052	-1.456672
H	5.412922	2.816993	-1.478258
H	4.717289	-0.796937	-4.451817
H	4.212027	0.820276	-5.049854
H	4.402806	0.527289	-3.286799

H	3.699153	-5.469559	-1.488646
H	2.789860	-5.117263	-2.997040
H	3.627768	-3.792321	-2.119342
H	5.353502	-3.963192	2.716788
H	3.935388	-5.060781	2.597447
H	4.311144	-3.922144	1.260432
C	5.908934	-2.471807	-0.563315
H	4.614579	-1.595069	-2.052914
H	5.307909	-0.436052	-0.923674
C	7.185905	-2.402490	-1.396047
H	6.157752	-2.323138	0.503558
H	5.484051	-3.489264	-0.638539
C	8.227216	-3.431261	-0.969319
H	6.930432	-2.548702	-2.459770
H	7.610624	-1.387016	-1.319115
H	9.138966	-3.363469	-1.579342
H	8.513697	-3.285145	0.083594
H	7.831233	-4.453962	-1.066764

[C_8antrIm][Cl]/DMP[5]A in chloroform-PCM (C_8^{OUT})

Total M06-2X energy: -4075.138810 u.a.

imaginary frequencies: n.a.

C	11.546851	-1.542675	0.200124
C	10.432846	-0.664918	-0.005518
C	9.175382	-1.203379	-0.455087
C	9.103584	-2.625399	-0.657534
C	10.187050	-3.430466	-0.443165
C	11.433410	-2.885384	-0.011201
C	8.084778	-0.330421	-0.659286
C	8.211925	1.053466	-0.406592
C	9.471055	1.573687	0.053548
C	10.549170	0.704764	0.236662
C	9.601817	2.975314	0.318543
C	8.546008	3.821404	0.140850
C	7.296672	3.311114	-0.323125
C	7.129701	1.980144	-0.588591
C	6.749509	-0.873055	-1.106790
N	5.865120	-1.115733	0.052039
C	4.604835	-0.686029	0.131972
N	4.103257	-1.079583	1.305304
C	5.073957	-1.776949	1.993780
C	6.185464	-1.799372	1.205712
C	2.761573	-0.746130	1.806787
C	1.711316	-0.740237	0.707006
C	0.325753	-0.393501	1.249205
C	-0.723600	-0.351777	0.142566
C	-2.101707	0.063742	0.640601
C	-3.173994	-0.114201	-0.424964
C	-4.555444	0.333375	0.042153
C	-5.653728	-0.166328	-0.891017

Cl	3.959690	1.236257	-2.367194
C	-3.962807	0.169610	3.938902
C	-2.962835	-0.766422	4.241212
C	-1.645912	-0.326335	4.364416
C	-1.314349	1.020221	4.186580
C	-2.317868	1.958797	3.923333
C	-3.637928	1.517756	3.799691
C	-3.304403	-2.234903	4.348276
C	-3.333922	-2.882432	2.981326
C	-4.524725	-2.965991	2.257258
C	-4.555819	-3.535142	0.982694
C	-3.384962	-4.063157	0.421261
C	-2.191311	-3.966641	1.139043
C	-2.155471	-3.370956	2.401791
C	-3.417606	-4.698949	-0.950974
C	-3.276347	-3.659096	-2.038418
C	-4.400358	-3.086028	-2.633376
C	-4.274893	-2.066198	-3.580877
C	-3.003537	-1.641009	-3.984435
C	-1.877423	-2.221520	-3.395462
C	-2.004829	-3.204967	-2.416120
O	-0.937189	-3.774447	-1.771428
C	0.350171	-3.375219	-2.195532
C	-2.843341	-0.517442	-4.985116
C	-2.594306	0.789552	-4.266370
C	-1.287744	1.166441	-3.925847
C	-1.067489	2.349159	-3.217432
C	-2.131593	3.158632	-2.820151
C	-3.440878	2.765553	-3.130375
C	-3.661332	1.595087	-3.861463
O	-5.343426	-1.426367	-4.153505
C	-6.627293	-1.948434	-3.882100
O	-5.691173	-3.632923	0.223308
C	-6.893513	-3.172505	0.805290
O	-1.009553	-3.235703	3.145024
C	0.157330	-3.842218	2.633598
O	-5.232176	-0.322865	3.797311
C	-6.258002	0.611654	3.529969
C	-1.983623	3.418069	3.702463
C	-1.946327	3.730044	2.223335
C	-3.108357	4.135158	1.554473
C	-3.074594	4.370170	0.178078
C	-1.901679	4.188829	-0.553290
C	-0.745150	3.750217	0.108873
C	-0.772366	3.540304	1.489841
O	-0.027050	1.494945	4.242434
C	0.949779	0.619078	4.760041
O	-4.235762	4.284211	2.321004
C	-5.421790	4.661691	1.654461
C	-1.877609	4.431103	-2.044717
O	0.358197	3.563736	-0.673209

C	1.524165	3.065669	-0.048632
O	-0.282016	0.332787	-4.328480
C	1.017724	0.611821	-3.834663
O	-4.439298	3.592750	-2.687328
C	-5.765356	3.229795	-3.007215
H	6.461043	3.994558	-0.478966
H	8.652186	4.887425	0.343879
H	10.567773	3.347101	0.665096
H	6.161023	1.646618	-0.966151
H	11.505042	1.105253	0.582808
H	12.489702	-1.106193	0.534541
H	12.285575	-3.546027	0.149021
H	10.100029	-4.505105	-0.606603
H	8.172145	-3.086402	-0.984341
H	4.118085	-0.083216	-0.654273
H	7.165957	-2.233981	1.368254
H	4.893645	-2.191618	2.978908
H	6.849703	-1.815133	-1.653803
H	6.204334	-0.176699	-1.756926
H	2.819526	0.236146	2.298455
H	2.524037	-1.497811	2.571580
H	1.690878	-1.731042	0.222284
H	1.990632	-0.010986	-0.073416
H	0.354566	0.581768	1.771048
H	0.014599	-1.132692	2.010532
H	-0.396649	0.343092	-0.655295
H	-0.796487	-1.354894	-0.321303
H	-0.901275	-1.856855	-3.709598
H	-5.379397	-3.430615	-2.303499
H	-4.369091	-5.230210	-1.081857
H	-2.597207	-5.424025	-1.028404
H	-5.423633	-2.557461	2.714923
H	-1.289741	-4.360091	0.672471
H	-4.288758	-2.349223	4.820252
H	-2.554442	-2.735849	4.973490
H	-4.398111	2.261943	3.568433
H	-0.880375	-1.073895	4.568116
H	-2.744524	4.041897	4.188242
H	-1.008445	3.642105	4.150048
H	-3.964275	4.686259	-0.364602
H	0.114880	3.205161	2.028091
H	-2.646343	5.171515	-2.299102
H	-0.896640	4.831851	-2.330274
H	-1.994749	-0.737423	-5.645155
H	-3.751046	-0.436211	-5.594200
H	-4.669756	1.267094	-4.115509
H	-0.060709	2.664788	-2.949253
H	1.663989	-0.204575	-4.174815
H	1.410283	1.564336	-4.222390
H	1.031063	0.651708	-2.733865
H	2.255592	2.879391	-0.844328

H	1.927372	3.790342	0.678629
H	1.312147	2.117817	0.474352
H	1.885804	1.187999	4.801739
H	0.681116	0.274539	5.772142
H	1.085177	-0.261948	4.110790
H	0.941964	-3.678612	3.381947
H	0.015575	-4.925049	2.485130
H	0.460336	-3.386507	1.674531
H	1.064130	-3.934450	-1.579521
H	0.515166	-3.617350	-3.258064
H	0.504393	-2.293230	-2.047103
H	-6.408546	4.007917	-2.580940
H	-5.918871	3.188006	-4.097928
H	-6.030825	2.254213	-2.568534
H	-6.203273	4.707851	2.421175
H	-5.319143	5.650626	1.179159
H	-5.703081	3.921848	0.886527
H	-7.186161	0.034229	3.452526
H	-6.350923	1.347570	4.345212
H	-6.075621	1.143716	2.581631
H	-7.678355	-3.336027	0.057978
H	-7.134963	-3.735535	1.721506
H	-6.835749	-2.097642	1.044674
H	-7.331531	-1.355933	-4.476638
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H	-6.883087	-1.854265	-2.814281
H	-2.366046	-0.543812	1.525369
H	-2.073652	1.114926	0.981898
H	-2.893522	0.442283	-1.339683
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H	-4.731521	-0.057683	1.062373
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H	-6.648549	0.220756	-0.616956
H	-5.442328	0.120067	-1.935502
H	-5.687539	-1.268120	-0.865117