Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Stereoelectronic Effects: A Simple yet Powerful Tool to Manipulate Anion Affinity

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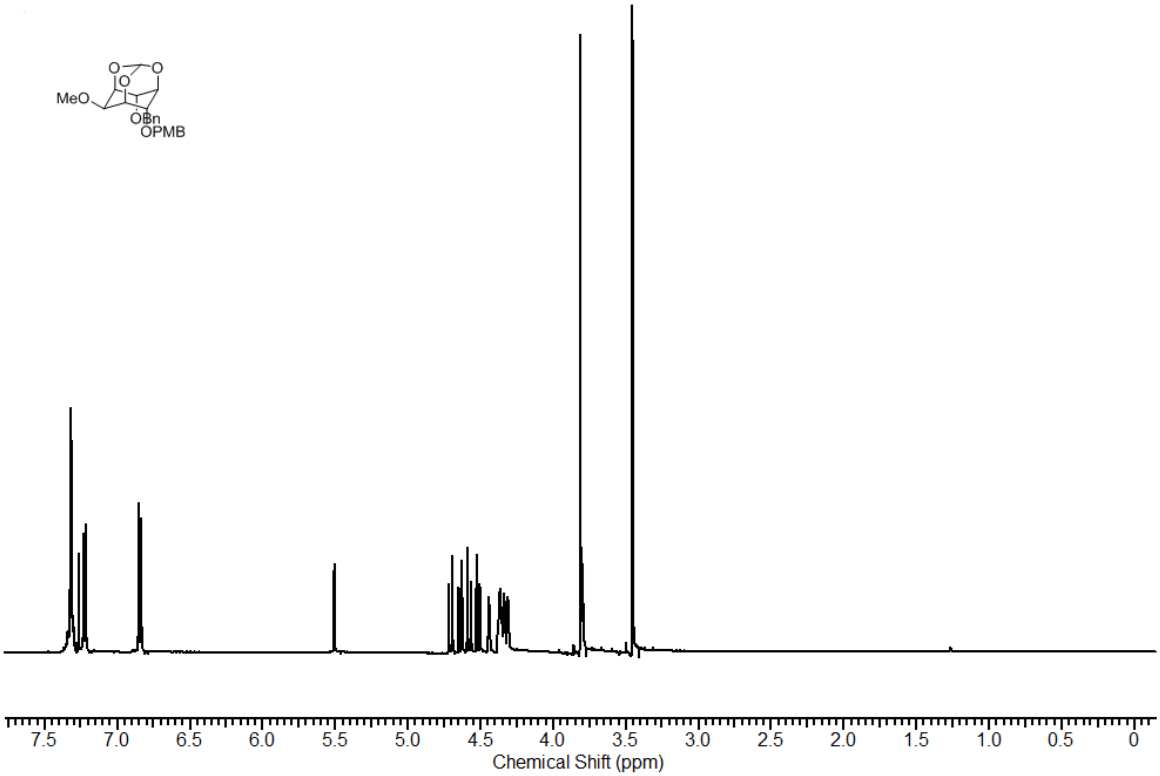
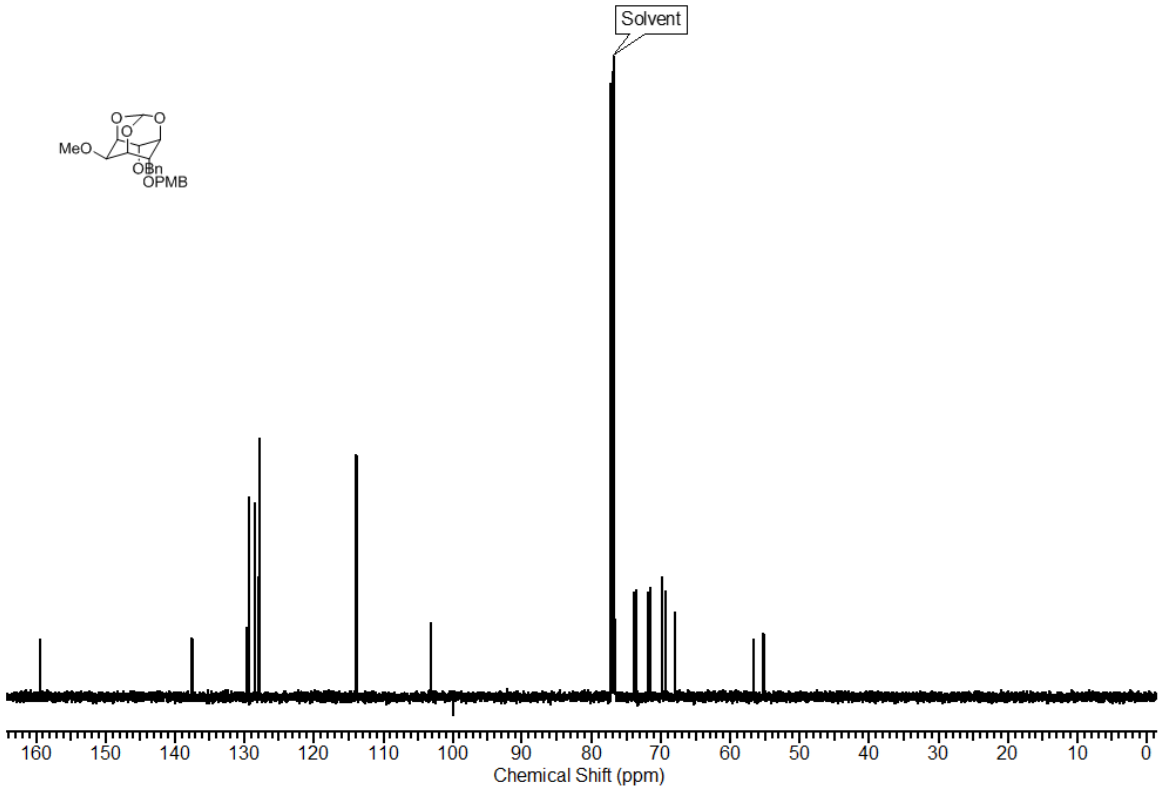
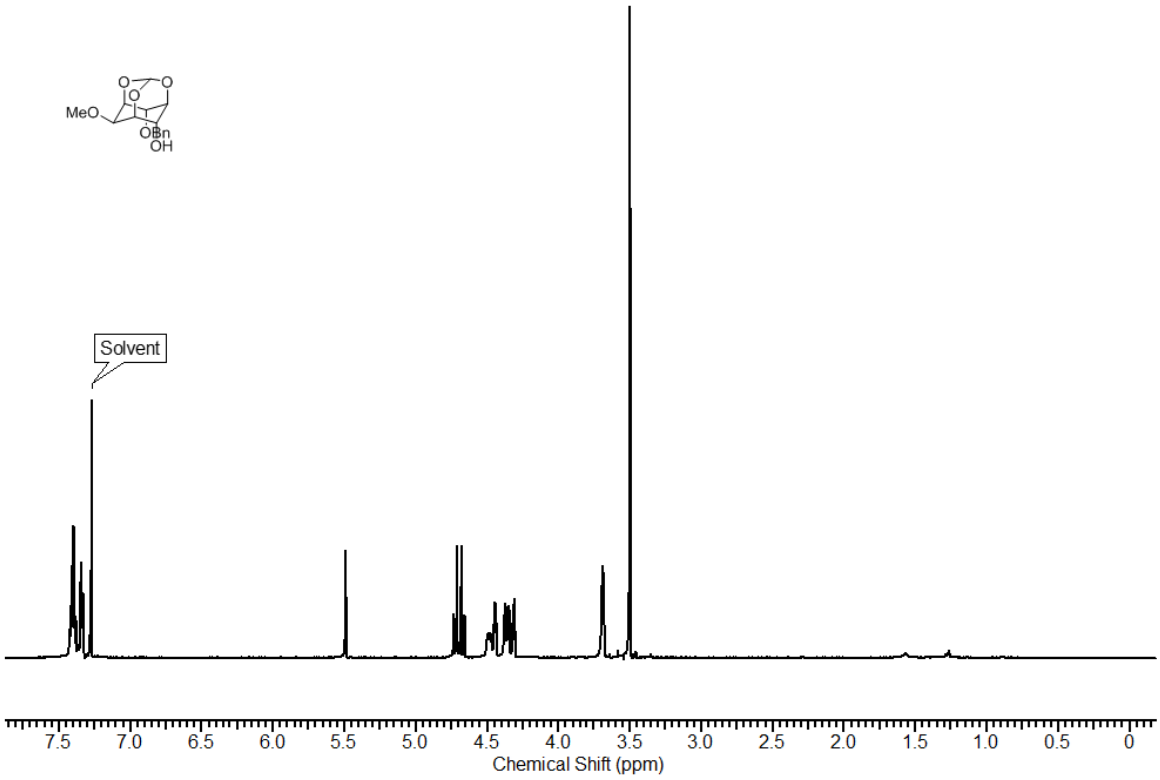
Figures S1 NMR (^{1}H and ^{13}C) spectra of title compounds.



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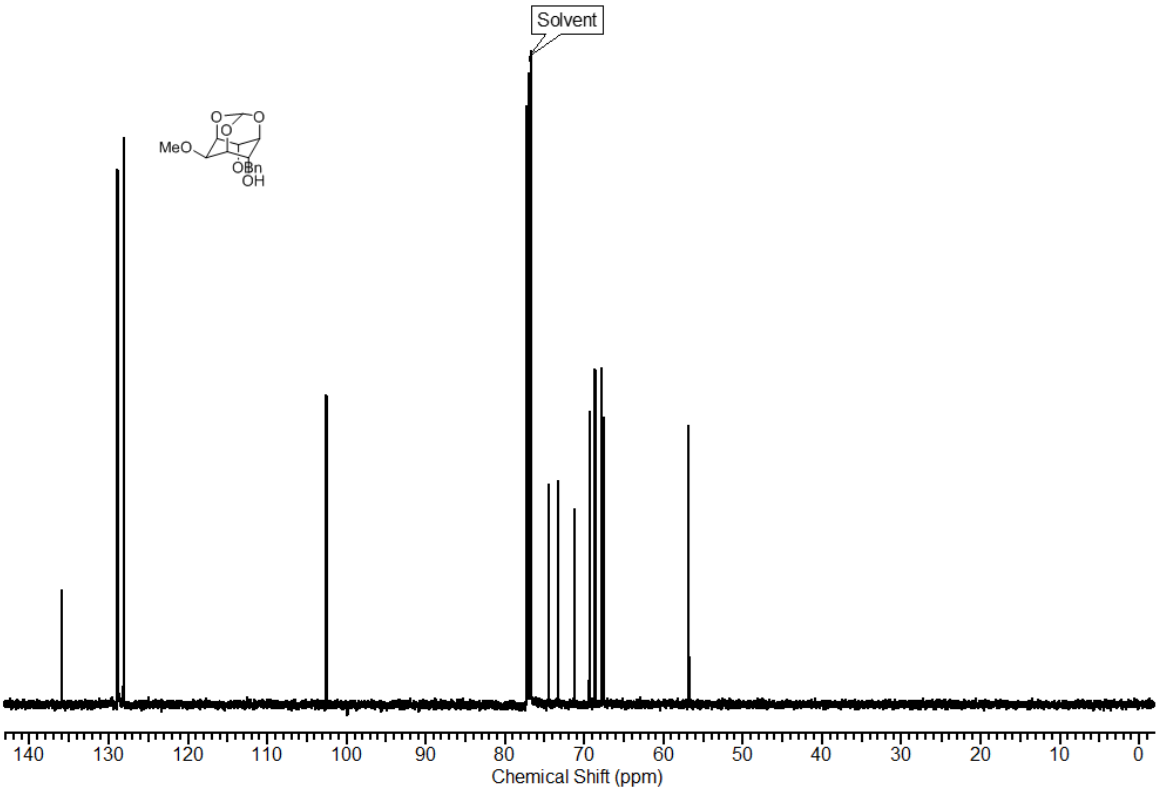
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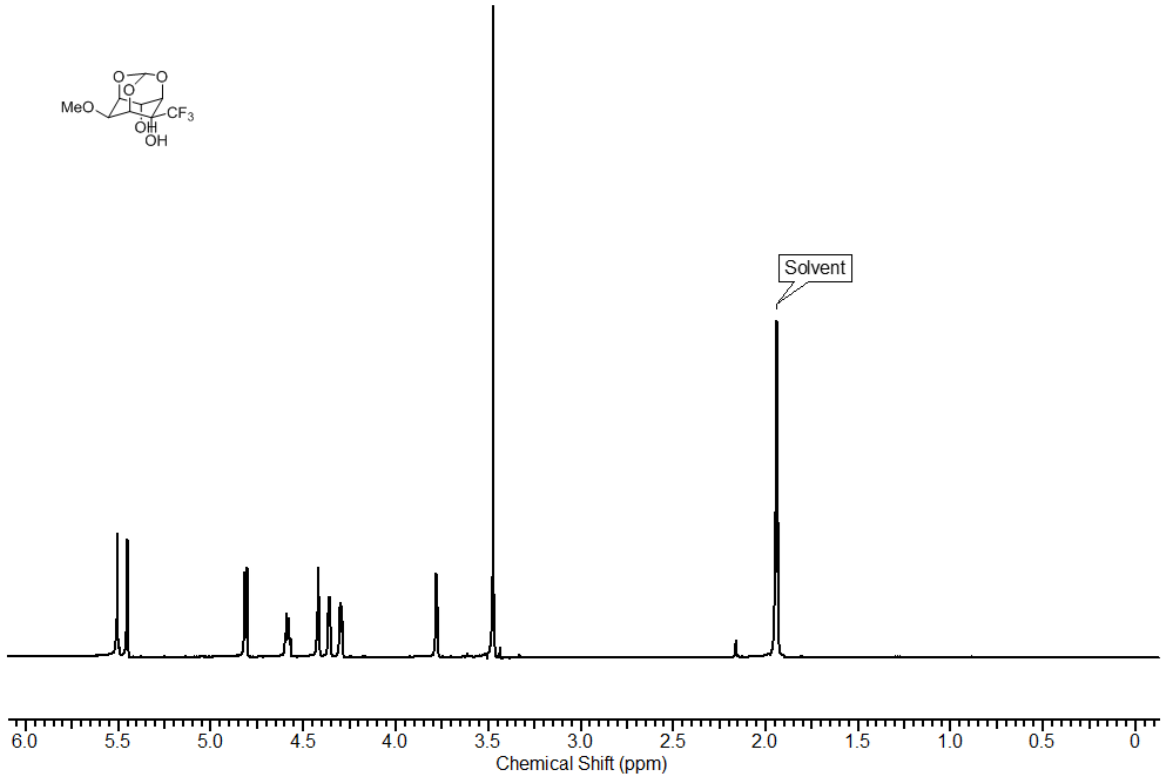
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1.0
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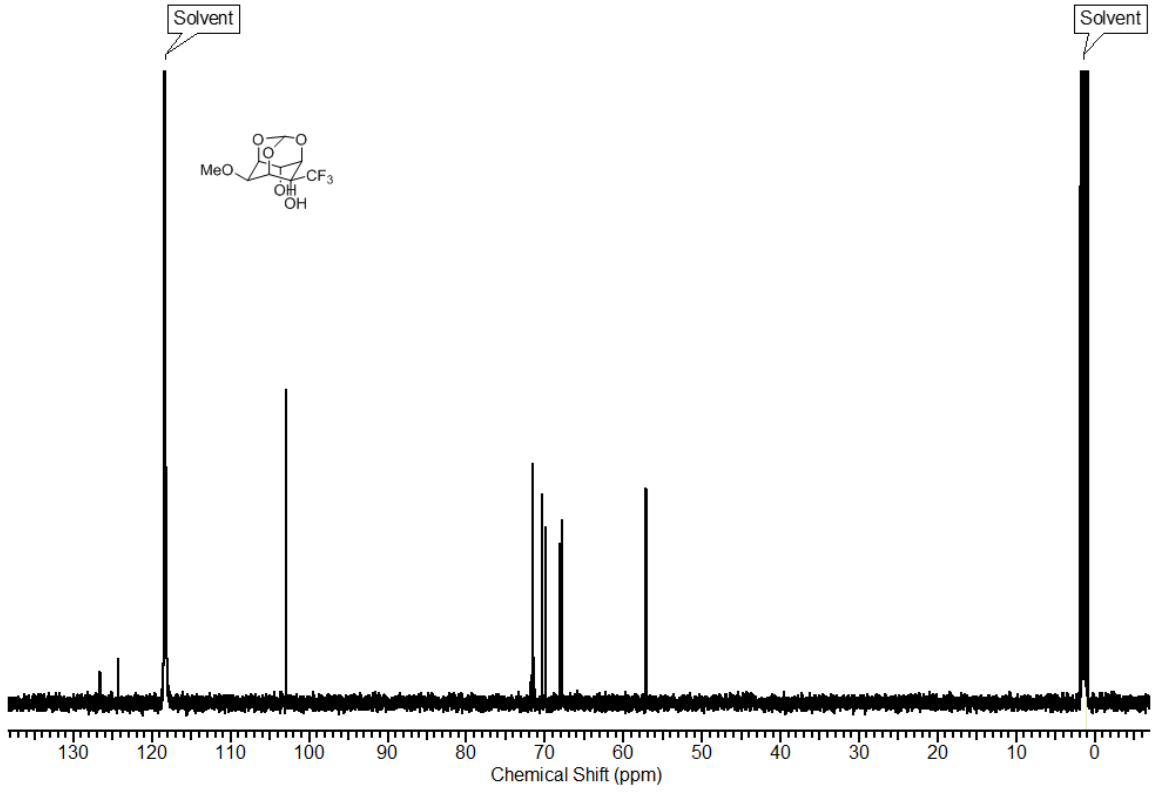
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50
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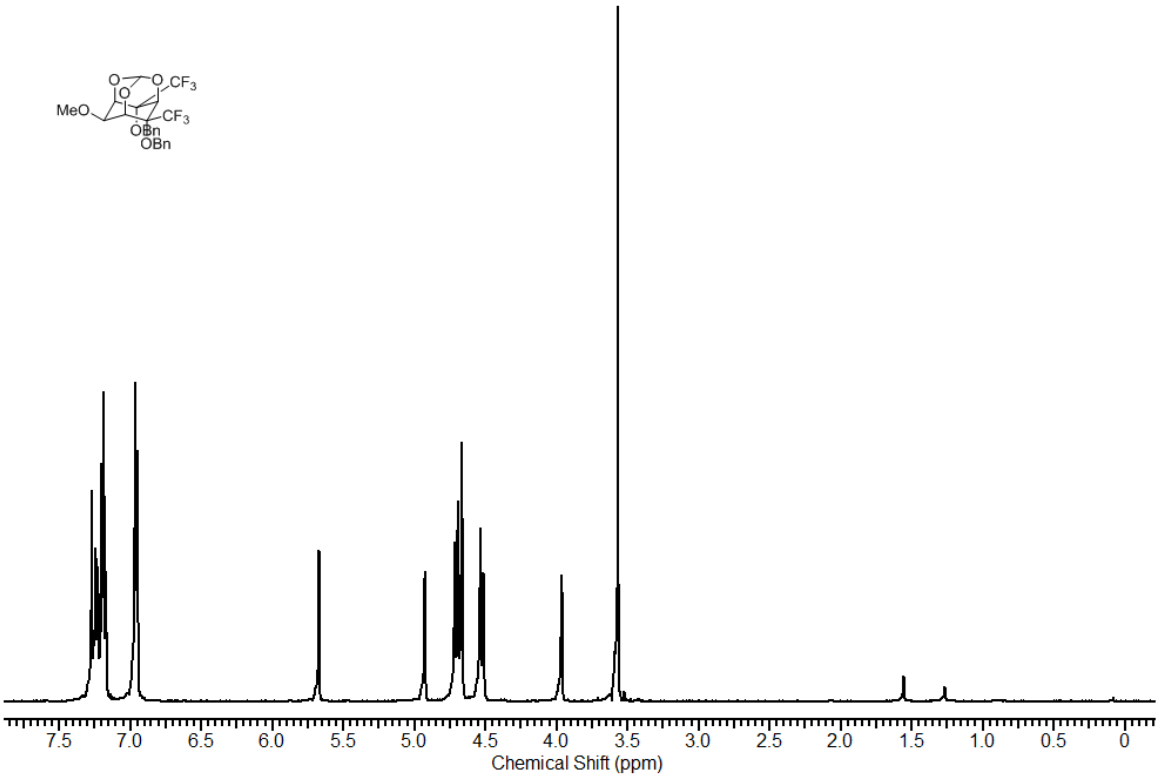
Chemical Shift (ppm)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CF3
OBn
OBn
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6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
1.0
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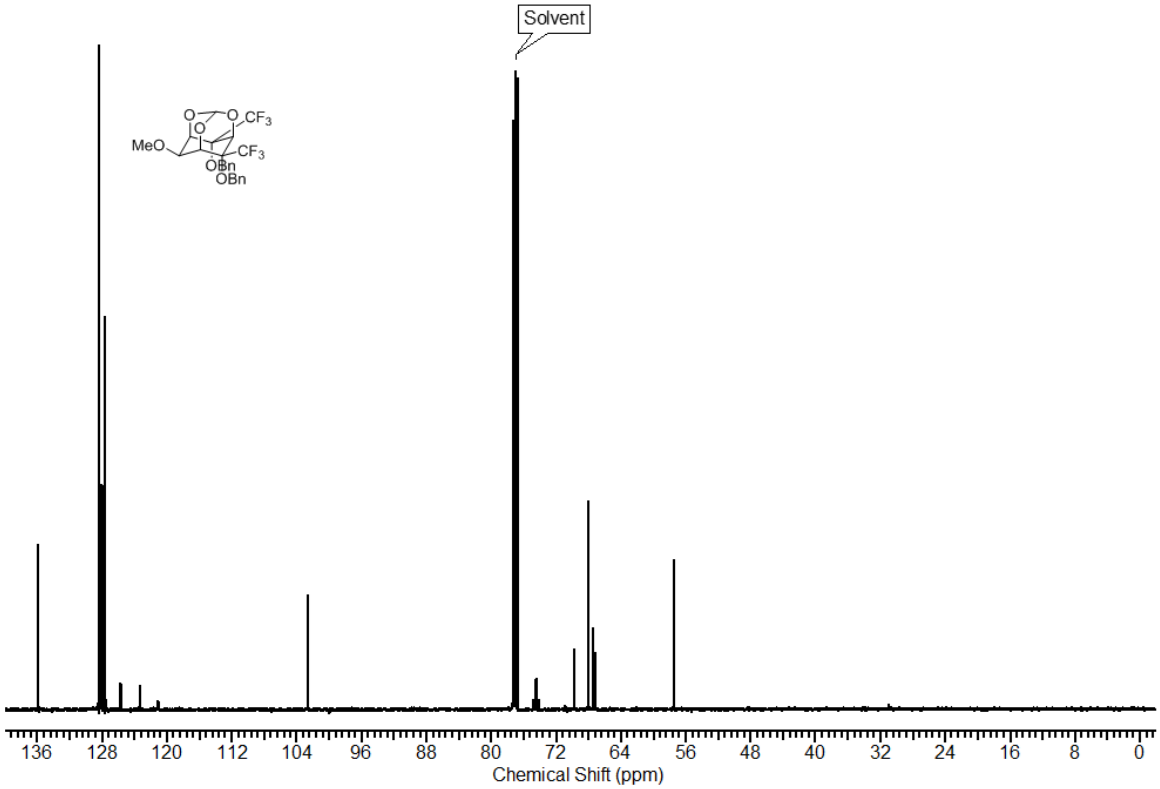
Chemical Shift (ppm)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CF3
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OBn
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80
72
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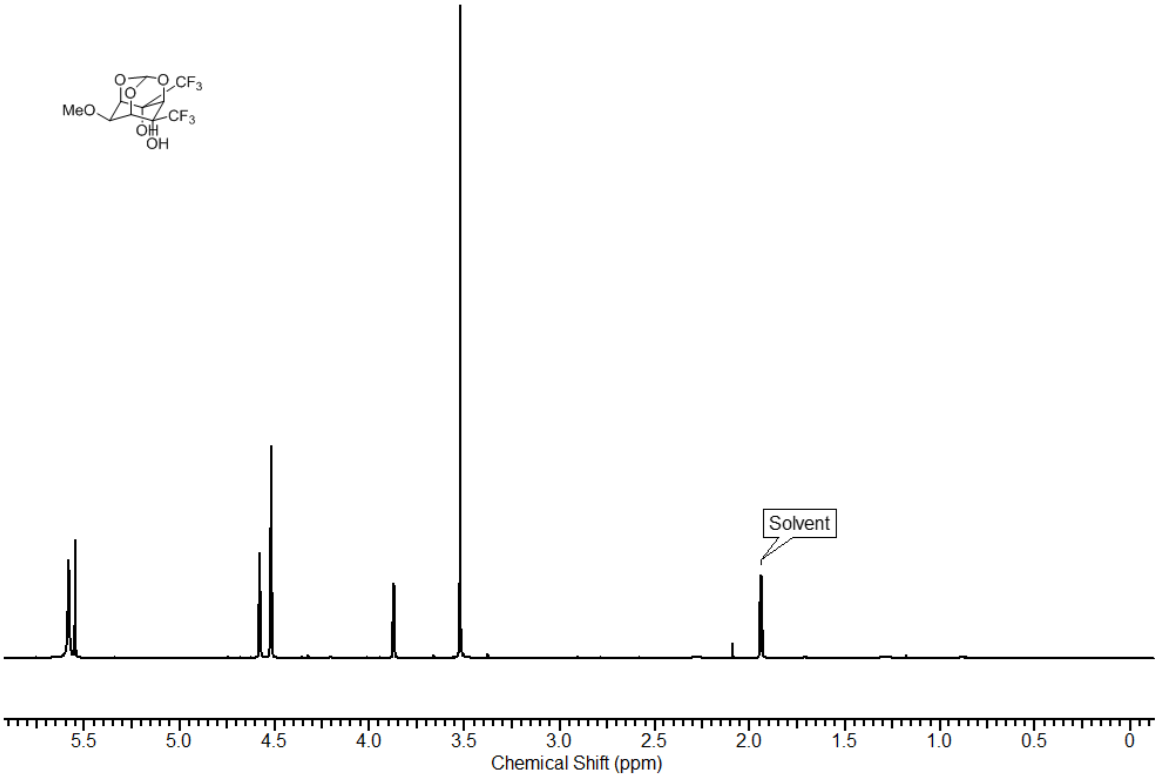
40
32
24
16
8
0
Chemical Shift (ppm)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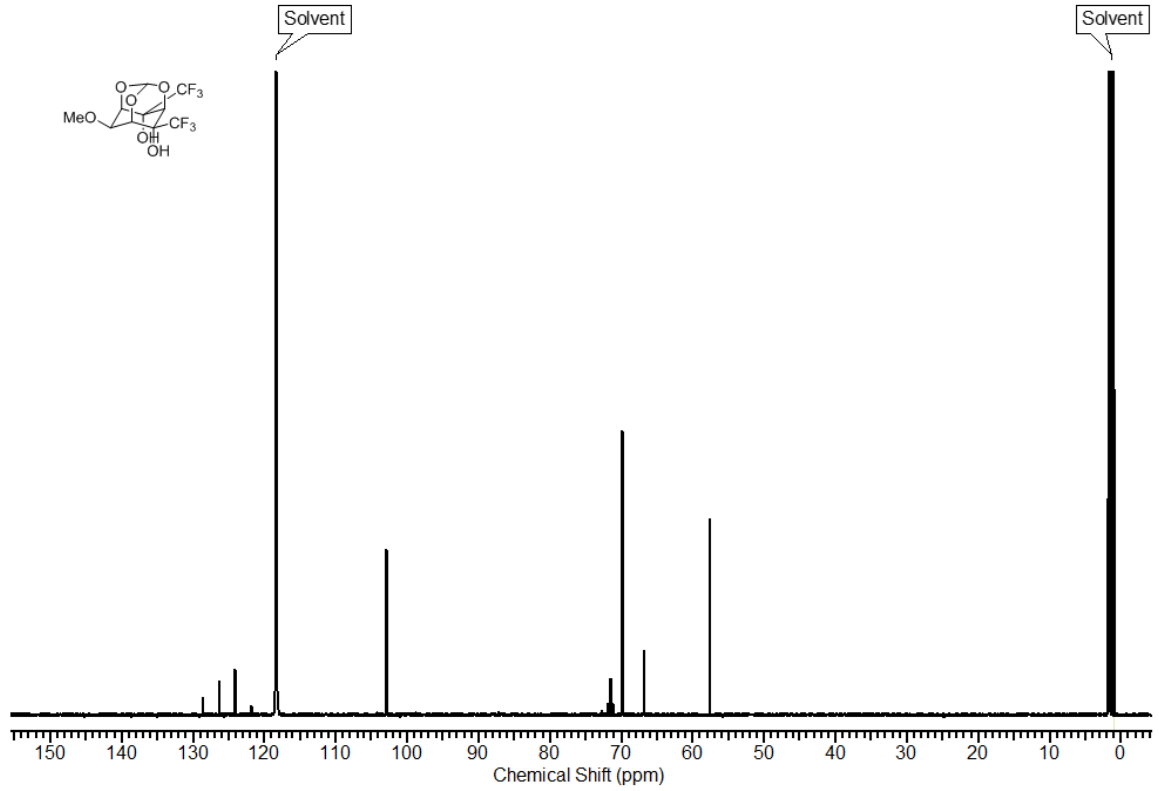
2.5
2.0
1.5
1.0
0.5
0
Chemical Shift (ppm)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CF3
OH
OH
Solvent
Solvent
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140
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120
110
100
90
80
70
60
50
40
30
20
10
0
Chemical Shift (ppm)

Figure S2 Experimental IR spectrum of **5(1)** • Cl^- (solid line) and the B3LYP/6-31+G(d,p) prediction (dotted line) for the less stable conformer with 2 primary hydrogen bonds to chloride ion.

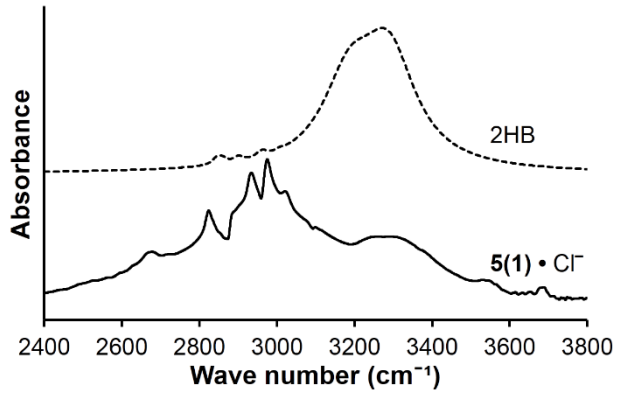

Figure S3 Experimental IR spectrum of **5(2)** • Cl^- (solid line) and the B3LYP/6-31+G(d,p) computed (dotted line) for the less stable conformer with 1 primary and 1 secondary hydrogen bonds to chloride ion.

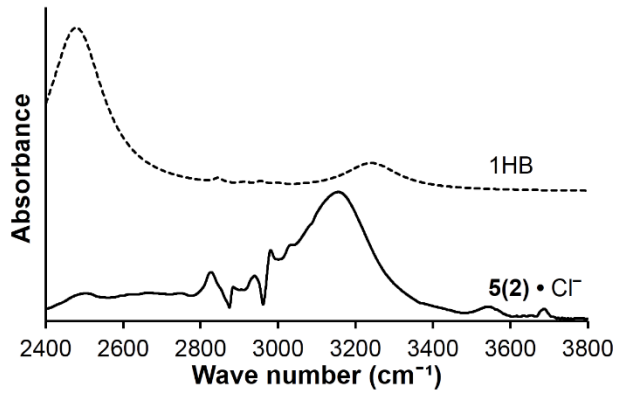

Table S1 Titration data for chloride binding to **5(1)** in CD_3CN

V (μL of Cl^- added)	[Cl^-] mM[a]	[**5(1)**] mM	δ (C−H) in ppm[b]	Δδ (ppm)	%bound[c]
0	0.00	0.45[d]	4.3587	0.0000	0.0
1.00	0.13	0.45	4.3705	0.0118	7.2
3.00	0.38	0.45	4.3959	0.0372	22.8
6.00	0.77	0.45	4.4125	0.0538	32.9
10.0	1.28	0.45	4.4349	0.0762	46.6
15.0	1.92	0.45	4.4535	0.0948	58.0
22.0	2.82	0.45	4.4691	0.1104	67.5
32.0	4.10	0.45	4.4828	0.1241	75.9
50.0	6.41	0.45	4.4945	0.1358	83.1
90.0	11.5	0.45	4.5053	0.1466	89.7
170	21.8	0.45	4.5101	0.1514	92.6

[a]A 75.62 mM TBACl and 0.45 mM **5(1)** stock solution was used. [b]NMR spectra were recorded with a Varian VI–500 spectrometer and the chemical shifts are referenced to the residual solvent signal at 1.94 δ. [c]Bound (%) = 100 × $\Delta\delta/\Delta\delta_{max}$, where $\Delta\delta_{max}$ = 0.1635 ppm. [d]The initial volume was 590 μL.

Figure S4 Non-linear 1:1 chloride binding isotherm for **5(1)** in CD_3CN, where the dashed line represents the fit to the experimental data (i.e., the squares).

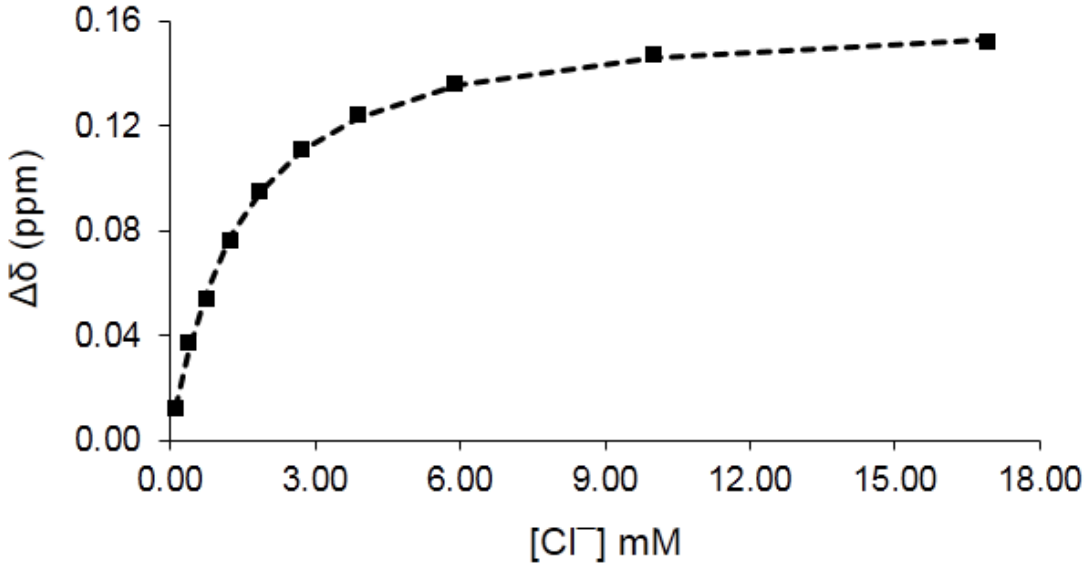

Table S2 Titration data for chloride binding to **5(2)** in CD_3CN

V (μL of Cl^- added)	[Cl^-] mM[a]	[**5(2)**] mM	δ (C−H) in ppm[b]	Δδ (ppm)	%bound[c]
0	0.00	0.47[d]	4.5990	0.0000	0.0
2.00	0.027	0.47	4.6166	0.0176	4.5
6.00	0.082	0.47	4.6616	0.0626	16.2
12.0	0.16	0.47	4.7212	0.1222	31.5
22.0	0.30	0.47	4.8130	0.2140	55.2
32.0	0.43	0.47	4.8745	0.2755	71.1
42.0	0.57	0.47	4.9136	0.3146	81.2
54.0	0.73	0.47	4.9409	0.3419	88.3
66.0	0.90	0.47	4.9536	0.3546	91.5
80.0	1.09	0.47	4.9634	0.3644	94.1
100	1.36	0.47	4.9712	0.3722	96.1

[a]A 8.01 mM TBACl and 0.47 mM **5(2)** stock solution was used. [b]NMR spectra were recorded with a Varian VI–500 spectrometer and the chemical shifts are referenced to the residual solvent signal at 1.94 δ. [c]Bound (%) = 100 × $\Delta\delta/\Delta\delta_{max}$, where $\Delta\delta_{max}$ = 0.3873 ppm. [d]The initial volume was 590 μL.

Figure S5 Non-linear 1:1 chloride binding isotherm for **5(2)** in CD_3CN, where the dashed line represents the fit to the experimental data (i.e., the squares).

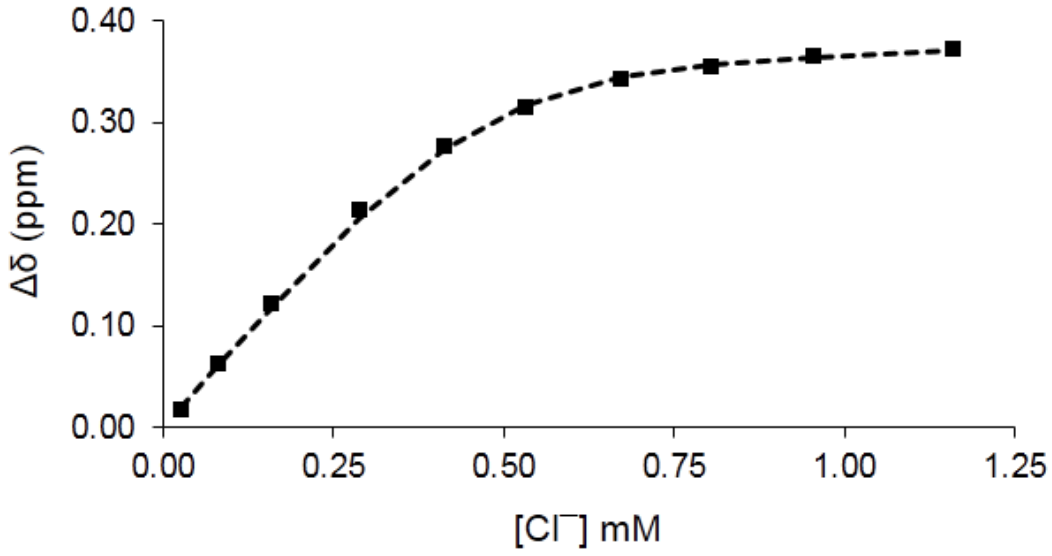

Table S3 Optimized computed geometries and energies for **5(1)**, **5(2)** and their Cl^- complexes

5(1)

B3LYP/6-31+G(d,p) = -1100.463878, zpe = 0.216430, tc = 0.230577

B3LYP/6-31+G(d,p)/CPCM = -1100.479393

1	1	0	-0.893091	-2.901989	-0.403042
2	6	0	-0.740465	-1.873369	-0.739863
3	6	0	-1.652730	0.480642	-0.422386
4	6	0	0.854713	0.109306	-0.430484
5	6	0	-0.309671	0.893519	0.230142
6	6	0	0.601020	-1.397307	-0.125724
7	6	0	-1.855779	-1.007508	-0.110386
8	1	0	-0.137035	1.968344	0.160903
9	1	0	1.432153	-2.019892	-0.467724
10	1	0	-2.845447	-1.337727	-0.429414
11	8	0	0.804163	0.372011	-1.836672
12	1	0	1.646743	0.112091	-2.240332
13	8	0	-0.770700	-1.906879	-2.154527
14	1	0	-0.422549	-1.065101	-2.486376
15	8	0	-1.795983	-1.209328	1.318326
16	8	0	0.500167	-1.571955	1.295539
17	8	0	-0.330348	0.570306	1.623884
18	6	0	-0.562251	-0.805783	1.837515
19	1	0	-0.570364	-0.975668	2.911437
20	6	0	2.242353	0.598586	0.054728
21	9	0	2.366301	1.936616	-0.100350
22	9	0	3.206021	0.025291	-0.737681
23	9	0	2.545249	0.300995	1.319266
24	1	0	-1.593341	0.626233	-1.509443
25	8	0	-2.748668	1.202332	0.098256
26	6	0	-2.913329	2.505693	-0.442974
27	1	0	-2.082031	3.174237	-0.180233
28	1	0	-3.832088	2.906093	-0.010690
29	1	0	-3.013303	2.472701	-1.538045

5(1) • Cl^- (1HB)

B3LYP/6-31+G(d,p) = -1560.795467, zpe = 0.216197, tc = 0.231344

B3LYP/6-31+G(d,p)/CPCM = -1560.876171

1	1	0	-1.071160	-1.121217	2.185682
2	6	0	-0.794813	-0.922319	1.141556
3	6	0	-0.929785	0.851877	-0.669832
4	6	0	1.201699	-0.463661	-0.374630
5	6	0	0.604390	0.947660	-0.671694
6	6	0	0.745909	-0.822152	1.071894
7	6	0	-1.356641	0.467863	0.758589
8	1	0	0.968157	1.345883	-1.620432
9	1	0	1.214750	-1.749520	1.407831
10	1	0	-2.439519	0.491573	0.877329
11	8	0	0.764351	-1.414407	-1.321946
12	1	0	-0.055417	-1.830582	-0.958881
13	8	0	-1.225172	-1.969490	0.291863
14	1	0	-2.231526	-1.913190	0.164480
15	8	0	-0.806269	1.422350	1.702458
16	8	0	1.161653	0.215671	1.977246
17	8	0	1.030373	1.869447	0.350650
18	6	0	0.587920	1.464930	1.623034
19	1	0	0.947453	2.197108	2.344118
20	6	0	2.742027	-0.484434	-0.523151
21	9	0	3.101545	-0.223950	-1.807829
22	9	0	3.242626	-1.709831	-0.215373
23	9	0	3.403417	0.404325	0.247649
24	1	0	-1.247653	0.063687	-1.360950
25	8	0	-1.459675	2.100459	-1.088622
26	6	0	-2.776464	1.996665	-1.625325
27	1	0	-2.769859	1.445286	-2.577325
28	1	0	-3.119634	3.019573	-1.801790
29	1	0	-3.466444	1.486032	-0.943271
30	17	0	-4.136764	-1.510609	-0.083097

5(1) • Cl^- (1HB) (The less stable conformer with 1 direct hydrogen bond to chloride ion)

B3LYP/6-31+G(d,p) = -1560.793779, zpe = 0.215934 , tc = 0.231129

B3LYP/6-31+G(d,p)/CPCM = -1560.874964

1	6	0	0.824276	0.267983	0.242083
2	6	0	-1.602849	-0.414197	-0.029609
3	6	0	-0.140534	-1.615261	1.676146
4	6	0	-1.282176	-1.753044	0.642533
5	6	0	1.103224	-1.111165	0.903983
6	6	0	-0.326293	0.028193	-0.783695
7	1	0	-2.178414	-2.184503	1.092657
8	1	0	1.974758	-1.056475	1.559330
9	1	0	-0.510488	0.916589	-1.388094
10	8	0	-0.484168	-0.835338	2.803787
11	1	0	-0.315828	0.097357	2.559874
12	8	0	0.463832	1.161223	1.267621
13	1	0	-0.104023	1.943268	0.926958
14	8	0	0.067460	-1.023379	-1.690575
15	8	0	1.397933	-2.089076	-0.112468
16	8	0	-0.831045	-2.703377	-0.356340
17	6	0	0.313262	-2.226707	-1.015818
18	1	0	0.605216	-2.969505	-1.756387
19	1	0	-1.855323	0.334982	0.728273
20	8	0	-2.697926	-0.603378	-0.912411
21	6	0	-3.459558	0.579362	-1.149343
22	1	0	-3.952838	0.922840	-0.229803
23	1	0	-4.213996	0.310805	-1.894212
24	1	0	-2.843166	1.405511	-1.520383
25	17	0	-1.379847	3.272543	0.375388
26	1	0	0.094162	-2.622681	2.036590
27	6	0	2.102933	0.846782	-0.425821
28	9	0	1.867601	2.077358	-0.931060
29	9	0	3.100582	0.976622	0.492815
30	9	0	2.613477	0.101963	-1.434652

5(1) • Cl^- (2HB)

B3LYP/6-31+G(d,p) = -1560.793624, zpe = 0.215882, tc = 0.231127

B3LYP/6-31+G(d,p)/CPCM = -1560.874543

1	6	0	-0.503775	0.479201	-0.307320
2	6	0	1.715837	-0.674569	-0.625447
3	6	0	0.138802	-1.626365	1.085308
4	6	0	1.614412	-1.323997	0.757976
5	6	0	-0.611016	-0.261099	1.059093
6	6	0	1.016124	0.699517	-0.540848
7	1	0	2.221248	-2.230283	0.803888
8	1	0	-1.651455	-0.373114	1.366713
9	1	0	1.182743	1.295543	-1.439777
10	8	0	-0.300214	-2.639699	0.220771
11	1	0	-1.282249	-2.593805	0.084902
12	8	0	-1.001433	-0.244319	-1.397329
13	1	0	-1.809977	-0.773019	-1.143886
14	8	0	1.563134	1.456327	0.553721
15	8	0	0.043599	0.552308	2.068085
16	8	0	2.130534	-0.432453	1.771668
17	6	0	1.405074	0.769761	1.774357
18	1	0	1.810025	1.403952	2.561439
19	1	0	1.179763	-1.307551	-1.340647
20	8	0	3.089617	-0.560792	-0.989952
21	6	0	3.301763	-0.444249	-2.383926
22	1	0	2.886349	-1.306627	-2.927912
23	1	0	4.383999	-0.410500	-2.537297
24	1	0	2.860789	0.473608	-2.800361
25	17	0	-3.247718	-2.082323	-0.395284
26	1	0	0.093009	-1.952389	2.136352
27	6	0	-1.276509	1.834395	-0.302076
28	9	0	-1.076670	2.492164	-1.480000
29	9	0	-2.607820	1.620565	-0.191201
30	9	0	-0.945421	2.710287	0.675422

5(2)

B3LYP/6-31+G(d,p) = -1437.510002, zpe = 0.219404, tc = 0.236608

B3LYP/6-31+G(d,p)/CPCM = -1437.527091

1	1	0	-1.939536	1.946640	-0.172450
2	6	0	-1.115157	1.272816	0.074012
3	6	0	-0.169111	-1.033116	0.036355
4	6	0	1.346724	0.938496	0.101005
5	6	0	1.201356	-0.495256	-0.484474
6	6	0	0.216680	1.834259	-0.465292
7	6	0	-1.347992	-0.161331	-0.485423
8	1	0	-0.309707	-2.080754	-0.234704
9	1	0	2.335444	1.339629	-0.124320
10	8	0	1.236948	0.888138	1.530914
11	8	0	-0.185266	-0.951474	1.462998
12	8	0	-1.061629	1.198830	1.501541
13	6	0	-0.002907	0.378943	1.930571
14	1	0	-0.024793	0.342978	3.016702
15	8	0	1.324823	-0.468574	-1.892148
16	1	0	0.442422	-0.448564	-2.296637
17	8	0	-1.324723	-0.187632	-1.910975
18	1	0	-2.115859	0.242219	-2.269460
19	1	0	0.230889	1.788185	-1.561355
20	8	0	0.297869	3.175660	-0.036001
21	6	0	1.300174	3.950302	-0.683286
22	1	0	2.313277	3.619690	-0.420308
23	1	0	1.166141	4.976313	-0.336545
24	1	0	1.184242	3.918533	-1.776596
25	6	0	2.363933	-1.433433	-0.051479
26	6	0	-2.727263	-0.750123	-0.077292
27	9	0	-3.027882	-0.688241	1.220034
28	9	0	-3.697680	-0.052814	-0.750712
29	9	0	-2.830750	-2.038526	-0.469060
30	9	0	2.173479	-2.672895	-0.562517
31	9	0	3.534442	-0.964080	-0.541347
32	9	0	2.516688	-1.571645	1.276585

CPCM optimized structure

1	1	0	-1.967335	1.920390	-0.139890
2	6	0	-1.132375	1.257353	0.094363
3	6	0	-0.155658	-1.037902	0.024699
4	6	0	1.335378	0.955735	0.110742
5	6	0	1.208631	-0.474943	-0.488738
6	6	0	0.191481	1.847724	-0.430244
7	6	0	-1.342459	-0.170155	-0.489952
8	1	0	-0.283298	-2.083130	-0.259754
9	1	0	2.314758	1.382237	-0.108002
10	8	0	1.227676	0.881101	1.545336
11	8	0	-0.165708	-0.977832	1.455458
12	8	0	-1.076419	1.157904	1.526192
13	6	0	-0.005505	0.346676	1.942814
14	1	0	-0.023108	0.296053	3.028476
15	8	0	1.331227	-0.445613	-1.895845
16	1	0	0.443648	-0.359562	-2.290317
17	8	0	-1.306137	-0.185097	-1.910043
18	1	0	-1.947542	0.438515	-2.287596
19	1	0	0.197318	1.840421	-1.525559
20	8	0	0.282442	3.175193	0.045847
21	6	0	1.152065	4.015101	-0.719119
22	1	0	2.192200	3.669975	-0.678436
23	1	0	1.090414	5.008687	-0.273127
24	1	0	0.826711	4.063326	-1.766155
25	6	0	2.383571	-1.399041	-0.063915
26	6	0	-2.715876	-0.785797	-0.097680
27	9	0	-2.984216	-0.814710	1.216441
28	9	0	-3.705838	-0.067224	-0.693400
29	9	0	-2.814205	-2.054312	-0.558103
30	9	0	2.212566	-2.644091	-0.572558
31	9	0	3.550099	-0.919949	-0.560311
32	9	0	2.552269	-1.538678	1.264262

5(2) • Cl^- (1HB)

B3LYP/6-31+G(d,p) = -1897.847303, zpe = 0.219304, tc = 0.237355

B3LYP/6-31+G(d,p)/CPCM = -1897.923511

1	1	0	-2.168407	0.482132	0.938004
2	6	0	-1.094994	0.333259	0.821827
3	6	0	0.756786	-1.034622	-0.129479
4	6	0	1.114946	1.376787	0.373696
5	6	0	1.482314	0.251615	-0.639676
6	6	0	-0.402152	1.629162	0.333379
7	6	0	-0.789624	-0.830467	-0.170031
8	1	0	1.047205	-1.904878	-0.719848
9	1	0	1.663266	2.295975	0.162394
10	8	0	1.493660	0.964852	1.701607
11	8	0	1.158565	-1.283038	1.223999
12	8	0	-0.570905	-0.015205	2.119495
13	6	0	0.815177	-0.203649	2.080152
14	1	0	1.146828	-0.473083	3.080923
15	8	0	1.125175	0.611345	-1.953874
16	1	0	0.209383	0.276968	-2.101896
17	8	0	-1.166723	-0.537297	-1.493348
18	1	0	-2.045271	0.002576	-1.544056
19	1	0	-0.723342	1.854154	-0.687782
20	8	0	-0.684175	2.723260	1.188956
21	6	0	-1.843099	3.466687	0.809815
22	1	0	-1.681997	3.984602	-0.145847
23	1	0	-2.004134	4.202233	1.602524
24	1	0	-2.727732	2.830338	0.698824
25	6	0	3.014775	0.029973	-0.736514
26	6	0	-1.528685	-2.148798	0.207243
27	9	0	-1.305923	-2.606728	1.459906
28	9	0	-2.863329	-1.993383	0.080483
29	9	0	-1.158201	-3.150304	-0.637670
30	9	0	3.298542	-0.989545	-1.588191
31	9	0	3.619058	1.140453	-1.231943
32	9	0	3.634688	-0.257600	0.426253
33	17	0	-3.513927	1.190114	-1.638820

CPCM optimized structure

1	1	0	-2.080460	0.606979	1.042874
2	6	0	-1.018195	0.422128	0.878375
3	6	0	0.740705	-1.038255	-0.114662
4	6	0	1.205737	1.373236	0.304564
5	6	0	1.489135	0.207608	-0.687705
6	6	0	-0.302119	1.680787	0.326180
7	6	0	-0.797249	-0.780928	-0.085505
8	1	0	0.974487	-1.935427	-0.689471
9	1	0	1.775725	2.265740	0.044158
10	8	0	1.623350	0.983967	1.628369
11	8	0	1.187628	-1.261943	1.228418
12	8	0	-0.454119	0.092735	2.161007
13	6	0	0.927353	-0.151290	2.071777
14	1	0	1.289820	-0.405951	3.064681
15	8	0	1.095387	0.550942	-1.999188
16	1	0	0.171906	0.242633	-2.121600
17	8	0	-1.224028	-0.512388	-1.404339
18	1	0	-2.110923	-0.034681	-1.450408
19	1	0	-0.652507	1.901846	-0.687124
20	8	0	-0.496547	2.803370	1.165337
21	6	0	-1.702725	3.529274	0.914133
22	1	0	-1.734340	3.889597	-0.121858
23	1	0	-1.695484	4.381430	1.595570
24	1	0	-2.593777	2.921641	1.111284
25	6	0	3.008031	-0.073774	-0.841987
26	6	0	-1.568428	-2.056901	0.363151
27	9	0	-1.291069	-2.499183	1.604837
28	9	0	-2.904512	-1.828187	0.316451
29	9	0	-1.310902	-3.082992	-0.485985
30	9	0	3.213619	-1.122376	-1.677355
31	9	0	3.625084	1.001379	-1.392015
32	9	0	3.661274	-0.353555	0.302337
33	17	0	-3.766631	1.012096	-1.812312

5(2) • Cl^- (2HB)

B3LYP/6-31+G(d,p) = -1897.846742, zpe = 0.219300, tc = 0.237429

B3LYP/6-31+G(d,p)/CPCM = -1897.924294

1	1	0	2.503658	1.185455	0.583412
2	6	0	1.502042	1.029414	0.179965
3	6	0	-0.207396	-0.592164	-0.610387
4	6	0	-0.907799	1.618742	0.289072
5	6	0	-1.336645	0.127781	0.205905
6	6	0	0.422431	1.707614	1.051512
7	6	0	1.191342	-0.489509	0.091123
8	1	0	-0.470349	-1.630405	-0.818363
9	1	0	-1.672904	2.219276	0.782288
10	8	0	-0.752722	2.151669	-1.037496
11	8	0	-0.098333	0.085427	-1.880893
12	8	0	1.496773	1.605769	-1.136538
13	6	0	0.237397	1.448125	-1.743601
14	1	0	0.296019	1.869257	-2.745373
15	8	0	-1.527938	-0.320356	1.513120
16	1	0	-1.404290	-1.310350	1.591886
17	8	0	1.269408	-0.999434	1.387491
18	1	0	0.713210	-1.824595	1.499717
19	1	0	0.324881	1.161836	1.994551
20	8	0	0.707349	3.081774	1.292160
21	6	0	1.596732	3.298079	2.372495
22	1	0	1.202118	2.874661	3.308678
23	1	0	1.700131	4.380817	2.482850
24	1	0	2.591978	2.867809	2.187856
25	6	0	-2.722372	-0.023957	-0.502494
26	6	0	2.286225	-1.246424	-0.729663
27	9	0	2.428865	-0.891822	-2.027103
28	9	0	3.505470	-1.058673	-0.152295
29	9	0	2.042494	-2.577292	-0.719103
30	9	0	-3.114122	-1.319464	-0.488141
31	9	0	-3.665740	0.686725	0.173649
32	9	0	-2.796192	0.385037	-1.789733
33	17	0	-0.736439	-3.230550	1.731219

CPCM optimized structure

1	1	0	-2.584495	-1.004704	0.630557
2	6	0	-1.578345	-0.926722	0.217477
3	6	0	0.235809	0.543182	-0.640368
4	6	0	0.786839	-1.683984	0.323138
5	6	0	1.315243	-0.230432	0.188914
6	6	0	-0.545567	-1.676571	1.090302
7	6	0	-1.155479	0.560210	0.077636
8	1	0	0.570162	1.553704	-0.881696
9	1	0	1.513804	-2.324654	0.823297
10	8	0	0.585020	-2.232660	-0.992539
11	8	0	0.069866	-0.151349	-1.889053
12	8	0	-1.623439	-1.527666	-1.089887
13	6	0	-0.364445	-1.487462	-1.713490
14	1	0	-0.461896	-1.929883	-2.701988
15	8	0	1.543785	0.256573	1.484377
16	1	0	1.512795	1.244830	1.514886
17	8	0	-1.164512	1.121938	1.363263
18	1	0	-0.570694	1.910921	1.421932
19	1	0	-0.412672	-1.148105	2.038294
20	8	0	-0.925304	-3.023875	1.313813
21	6	0	-1.804293	-3.204823	2.425515
22	1	0	-1.343821	-2.839702	3.352755
23	1	0	-1.983576	-4.278105	2.507705
24	1	0	-2.764133	-2.694885	2.275626
25	6	0	2.704589	-0.183946	-0.521698
26	6	0	-2.196562	1.385549	-0.742218
27	9	0	-2.390296	1.012960	-2.023018
28	9	0	-3.409291	1.333220	-0.135941
29	9	0	-1.824581	2.693356	-0.771059
30	9	0	3.163369	1.096006	-0.545346
31	9	0	3.607705	-0.914437	0.179309
32	9	0	2.750196	-0.631613	-1.792196
33	17	0	1.010620	3.299499	1.709521

5(2)H [OCH_3 has been replaced by a H]

B3LYP/6-31+G(d,p) = -1322.992824, zpe = 0.187508, tc = 0.202576

1	6	0	-0.008659	1.453802	1.765078
2	6	0	-1.293628	-0.293998	0.462272
3	6	0	1.279778	-0.281665	0.431682
4	6	0	-0.012521	-0.523571	-0.401033
5	6	0	1.233745	1.204740	0.893095
6	6	0	-1.251685	1.197472	0.897660
7	1	0	-0.010285	-1.520275	-0.845230
8	1	0	2.158166	1.482271	1.406993
9	1	0	-2.173692	1.469864	1.412938
10	8	0	1.270136	-1.174674	1.543025
11	1	0	2.113401	-1.131025	2.018387
12	8	0	-1.392847	-1.132647	1.594121
13	1	0	-0.504704	-1.412418	1.869238
14	8	0	-0.000906	0.422971	-1.473451
15	8	0	1.153729	2.040098	-0.271052
16	8	0	-1.169588	2.035668	-0.272063
17	6	0	-0.013663	1.764370	-1.012571
18	1	0	-0.010476	2.406201	-1.889972
19	6	0	-2.574200	-0.646304	-0.345160
20	6	0	2.560769	-0.629408	-0.374895
21	1	0	-0.005473	2.500732	2.079604
22	9	0	-2.540821	-1.944778	-0.728693
23	9	0	-3.666946	-0.477175	0.433638
24	9	0	-2.760670	0.089368	-1.455284
25	9	0	3.626721	-0.584715	0.488231
26	9	0	2.846655	0.183254	-1.393244
27	9	0	2.499753	-1.890897	-0.852563
28	1	0	-0.012954	0.825182	2.657872

5(2)H • Cl^- (1HB) [OCH_3 has been replaced by a H]

B3LYP/6-31+G(d,p) = -1783.308238, zpe = 0.187645, tc = 0.203538

1	1	0	-2.146829	0.291989	1.499486
2	6	0	-1.108879	0.119814	1.214621
3	6	0	0.500271	-0.654999	-0.521094
4	6	0	1.222248	0.978172	1.210851
5	6	0	1.403420	0.598665	-0.288307
6	6	0	-0.238733	1.355055	1.487646
7	6	0	-0.999414	-0.293898	-0.282973
8	1	0	0.648079	-1.063095	-1.522324
9	1	0	1.914408	1.775464	1.489225
10	8	0	1.562082	-0.160831	2.037540
11	8	0	0.886773	-1.675327	0.411080
12	8	0	-0.619710	-0.970984	2.033563
13	6	0	0.723410	-1.253199	1.753290
14	1	0	1.031706	-2.081585	2.387447
15	8	0	1.083615	1.686719	-1.123756
16	1	0	0.118021	1.617805	-1.325251
17	8	0	-1.355660	0.746833	-1.160267
18	1	0	-2.111305	1.342363	-0.777876
19	1	0	-0.576197	2.208493	0.896251
20	6	0	2.881994	0.299786	-0.649205
21	6	0	-1.921891	-1.493946	-0.645344
22	9	0	-1.732444	-2.617336	0.084726
23	9	0	-3.219905	-1.150750	-0.503038
24	9	0	-1.740575	-1.851005	-1.946540
25	9	0	2.995750	-0.073907	-1.949983
26	9	0	3.639635	1.416105	-0.490161
27	9	0	3.472285	-0.669460	0.081098
28	17	0	-3.323631	2.580119	0.003571
29	1	0	-0.340232	1.619736	2.545222

5(2)H • Cl^- (2HB) [OCH_3 has been replaced by a H]

B3LYP/6-31+G(d,p) = -1783.307771, zpe = 0.187559, tc = 0.203581

1	1	0	-2.162797	-1.393146	1.749028
2	6	0	-1.242436	-1.265562	1.176346
3	6	0	-0.000031	0.059374	-0.519983
4	6	0	1.241915	-1.266409	1.176028
5	6	0	1.302885	0.046787	0.351558
6	6	0	-0.000127	-1.257920	2.077732
7	6	0	-1.302863	0.047553	0.351685
8	1	0	0.000139	0.893907	-1.223090
9	1	0	2.162307	-1.394559	1.748532
10	8	0	1.160280	-2.396428	0.280931
11	8	0	-0.000489	-1.153806	-1.305110
12	8	0	-1.161808	-2.395621	0.281203
13	6	0	-0.000847	-2.315784	-0.511088
14	1	0	-0.001214	-3.168921	-1.186200
15	8	0	1.441560	1.092504	1.265394
16	1	0	1.092785	1.957656	0.897532
17	8	0	-1.441120	1.093634	1.265146
18	1	0	-1.092233	1.958624	0.896900
19	1	0	0.000225	-0.377097	2.722308
20	6	0	2.578905	0.099777	-0.550374
21	6	0	-2.578770	0.100632	-0.550339
22	9	0	-2.691486	-0.854514	-1.502826
23	9	0	-3.695110	-0.006730	0.222203
24	9	0	-2.652057	1.290772	-1.190688
25	9	0	2.652376	1.289953	-1.190595
26	9	0	3.695155	-0.007655	0.222334
27	9	0	2.691796	-0.855266	-1.502930
28	17	0	0.000935	3.562725	0.227933
29	1	0	-0.000340	-2.164787	2.692751