Supporting Information

A bis(triazole)benzamide receptor for the complexation of halide anions and neutral carboxylic acid guests. Guest-controlled topicity and self-assembly

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1. Supplementary Figures

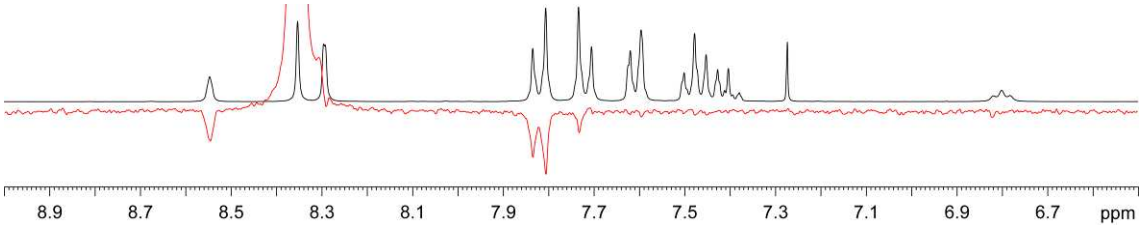


Figure S1. Partial ^{1}H NMR spectra ($CDCl_3$, 300 MHz, 298 K) (black) and NOE experiments (red) of **1** in $CDCl_3$ at 50 mM.

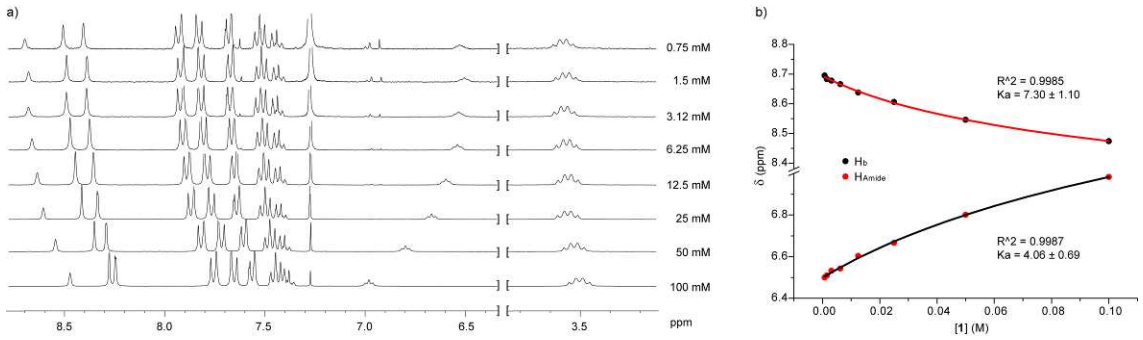


Figure S2. (a) Partial ^{1}H NMR spectra at different concentrations of receptor **1** ($CDCl_3$, 300 MHz, 298 K). (b) Concentration dependence of the chemical shift corresponding to the proton in the 1,2,3-triazole ring (H_b in Scheme 1) and to the amide proton, and fit to the isodesmic model.

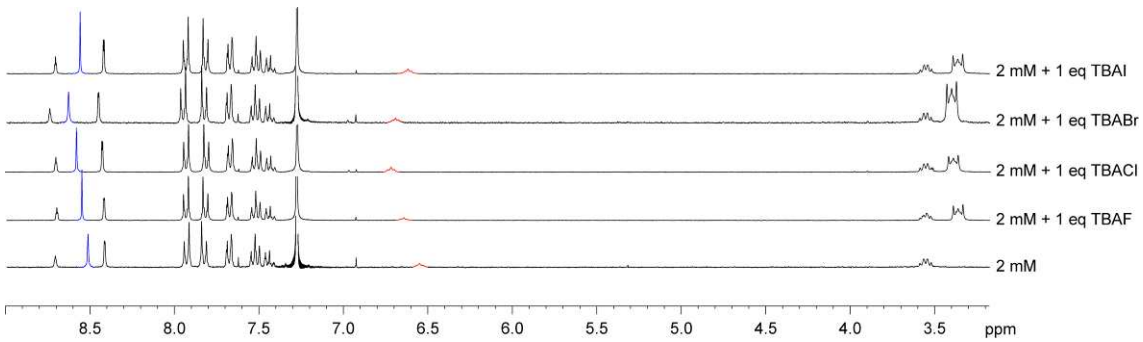


Figure S3. Partial ^{1}H NMR spectra (300 MHz, 298 K, 2 mM, $CDCl_3$) of aryl triazole **1** upon titrational addition of tetrabutylammonium salts of F^-, Cl^-, Br^-, and I^-.

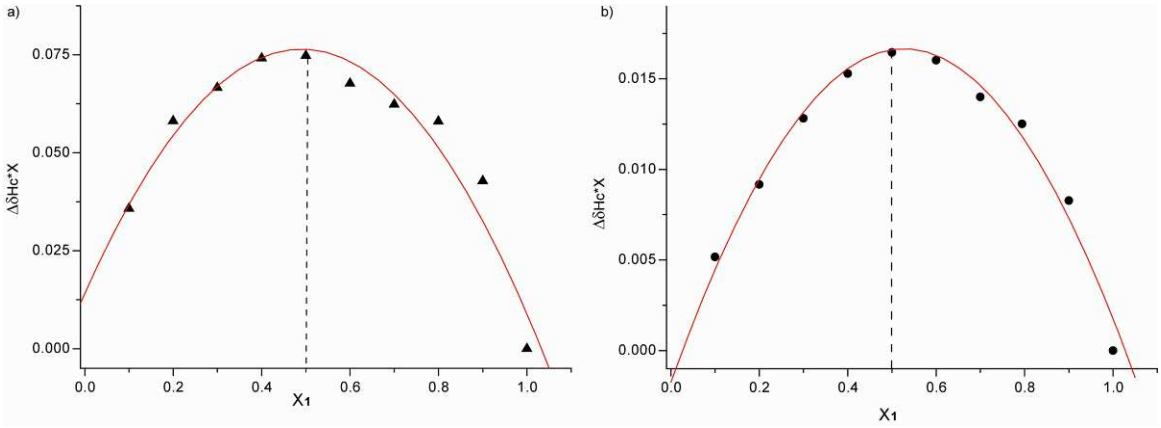


Figure S4. Job plot showing the 1:1 stoichiometry of the complex formed by **1** and TBACl (a) and **1** and TBABr (b) in $CDCl_3$ at a total concentration of 3 mM.

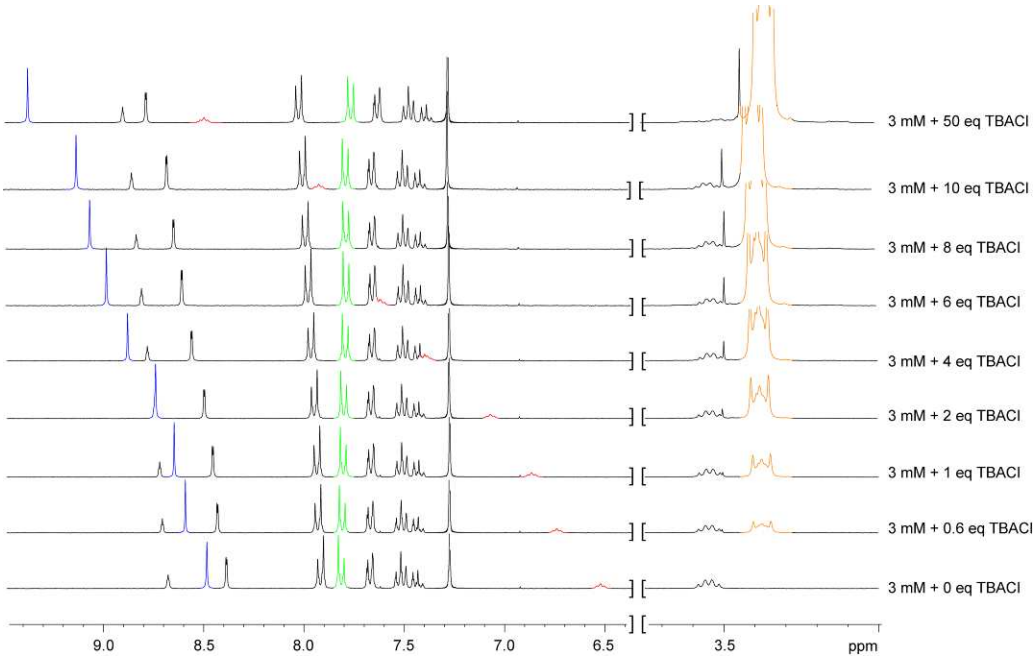


Figure S5. Partial ^{1}H NMR spectra (300 MHz, 298 K, 3 mM, $CDCl_3$) of aryl triazole **1** upon titrational addition of TBACl.

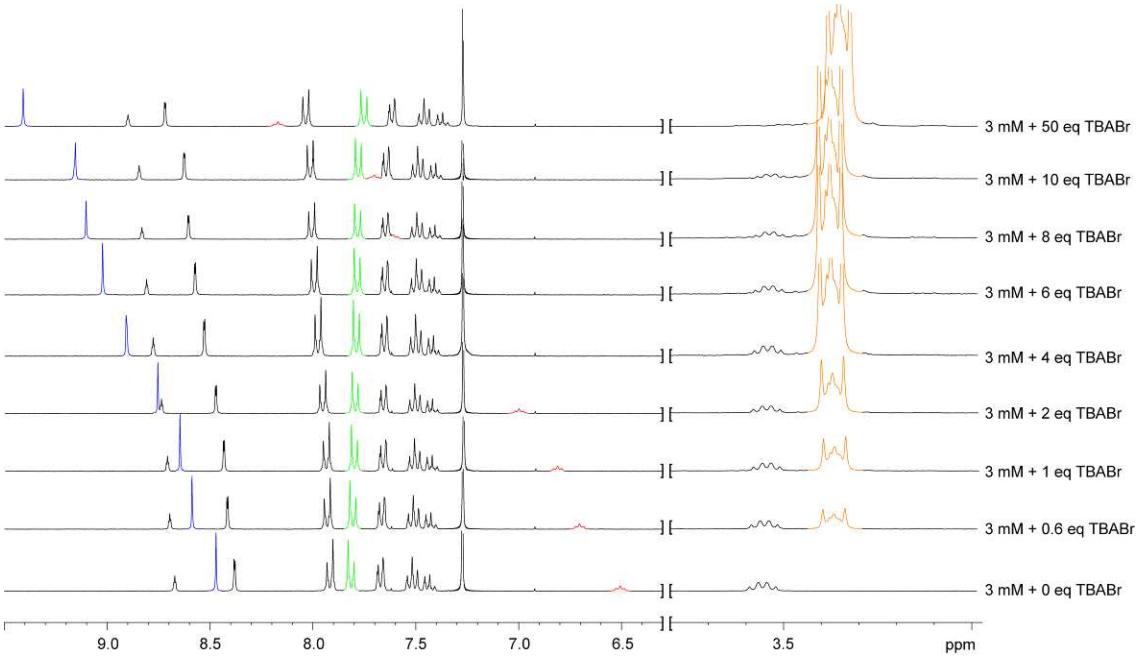


Figure S6. Partial ^{1}H NMR spectra (300 MHz, 298 K, 3 mM, $CDCl_3$) of aryl triazole **1** upon titrational addition of TBABr.

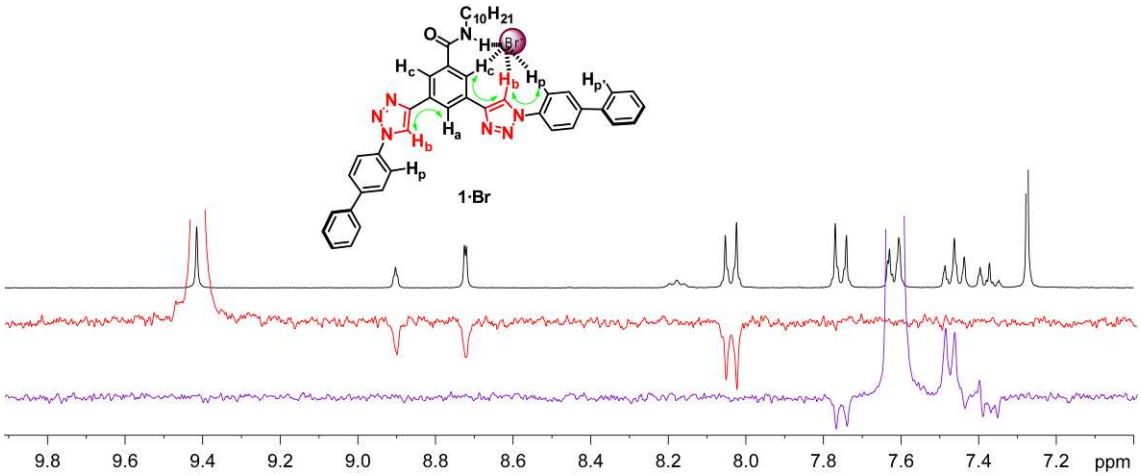


Figure S7. Partial 1H NMR spectra (300 MHz, 298 K) (black) and NOE experiments (red and violet) of aryl triazole **1** in $CDCl_3$ at 3 mM upon addition of TBABr. The NOE contacts are represented by curved green arrows in the drawing of the chemical formula.

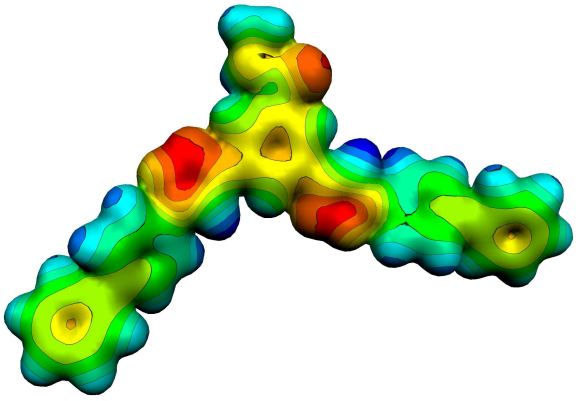


Figure S8. M06-2X/6-311G** molecular electrostatic potential calculated for receptor **1** in conformation A (red and blue are negative and positive potentials, respectively).

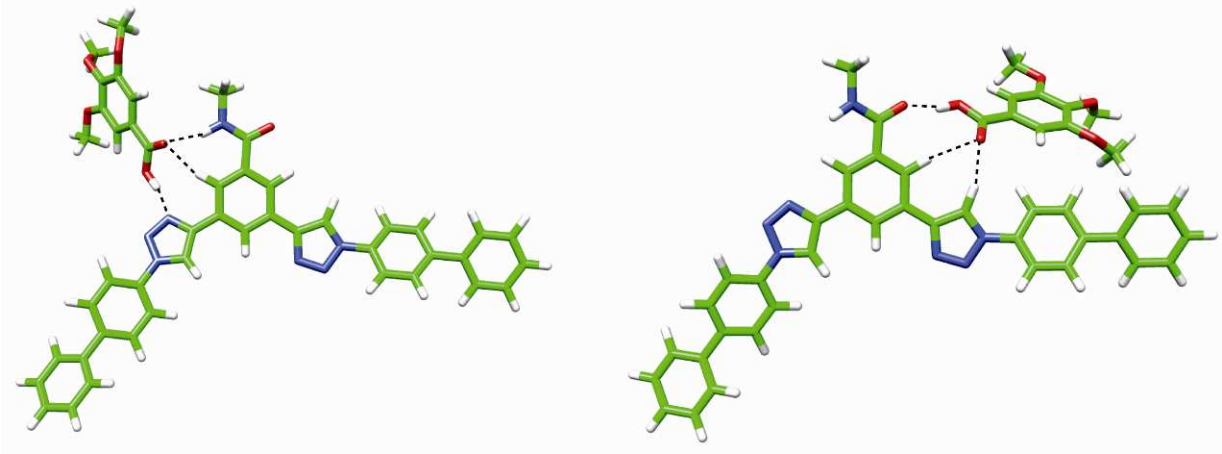


Figure S9. Minimum-energy structures calculated for complexes **1•12GA-l** and **1•12GA-r** at the M06-2X/6-311G** level.

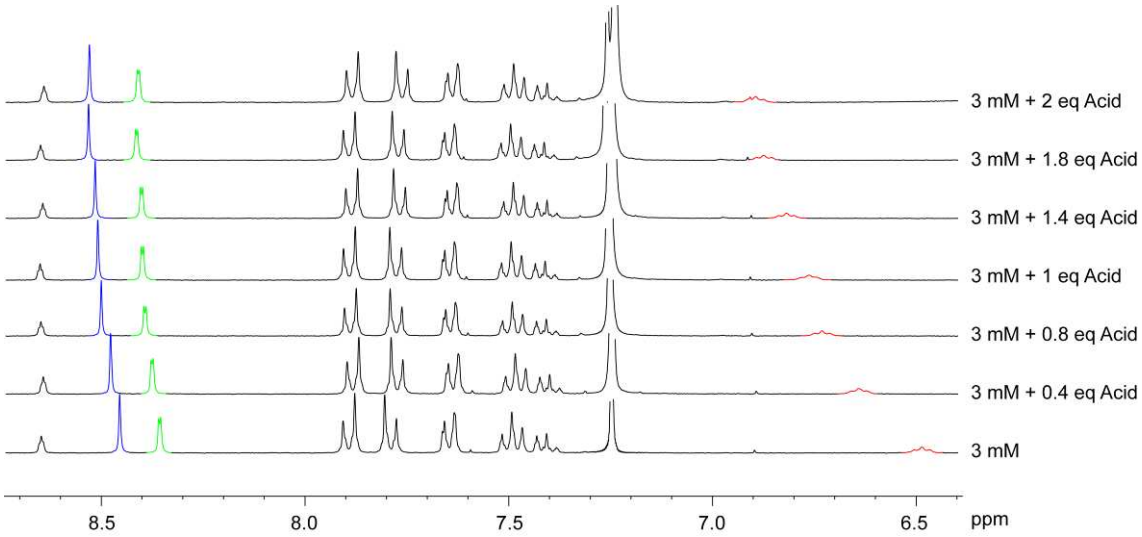


Figure S10. Partial ^{1}H NMR spectra (300 MHz, 298 K, 3 mM, $CDCl_3$) of aryl triazole **1** upon titrational addition of **12GA**.

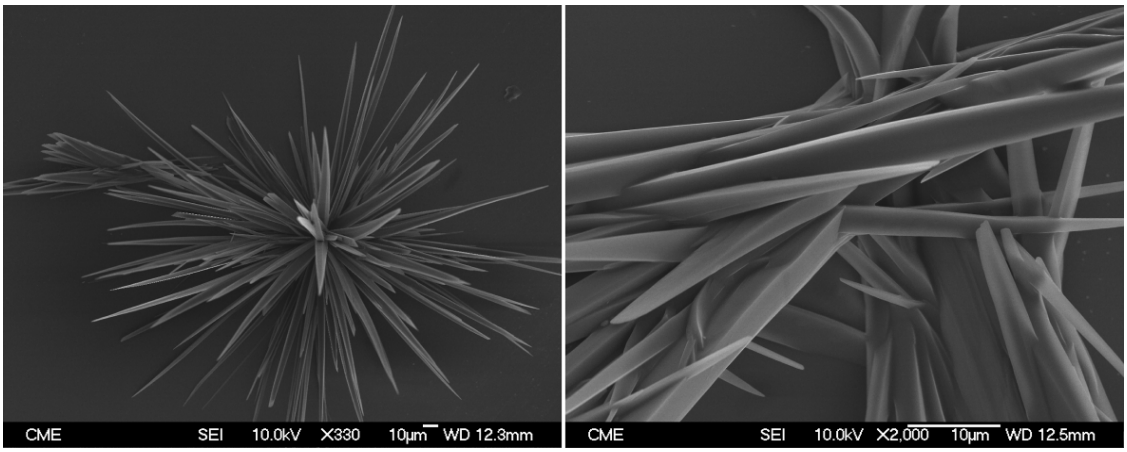


Figure S11. SEM images (298 K, 1×10^{-4} M in chloroform/acetonitrile, glass substrate) of the needle-like objects formed from **1**.

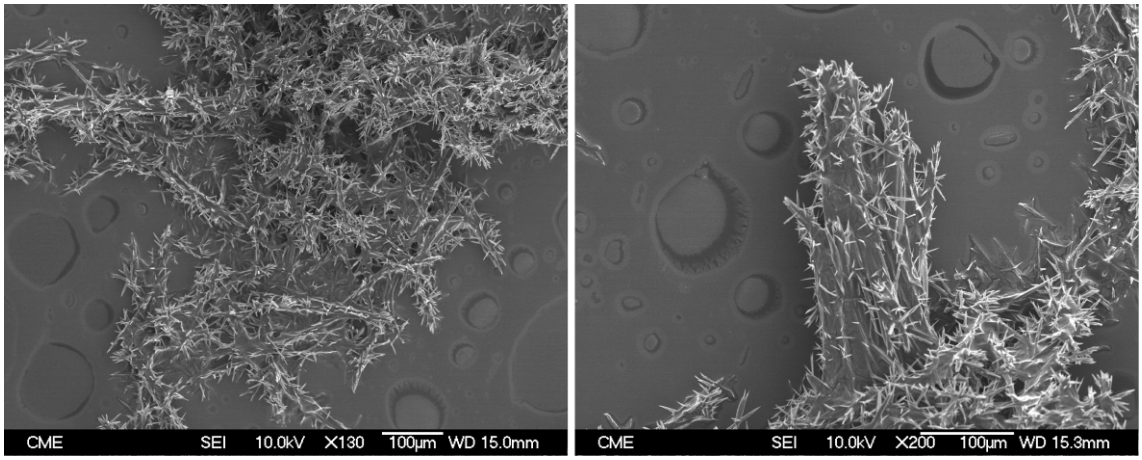


Figure S12. SEM images (298 K, 1×10^{-4} M in chloroform/acetonitrile, glass substrate) of the prickle-like objects formed from complex **1**•$Br^{-}TBA^{+}$.

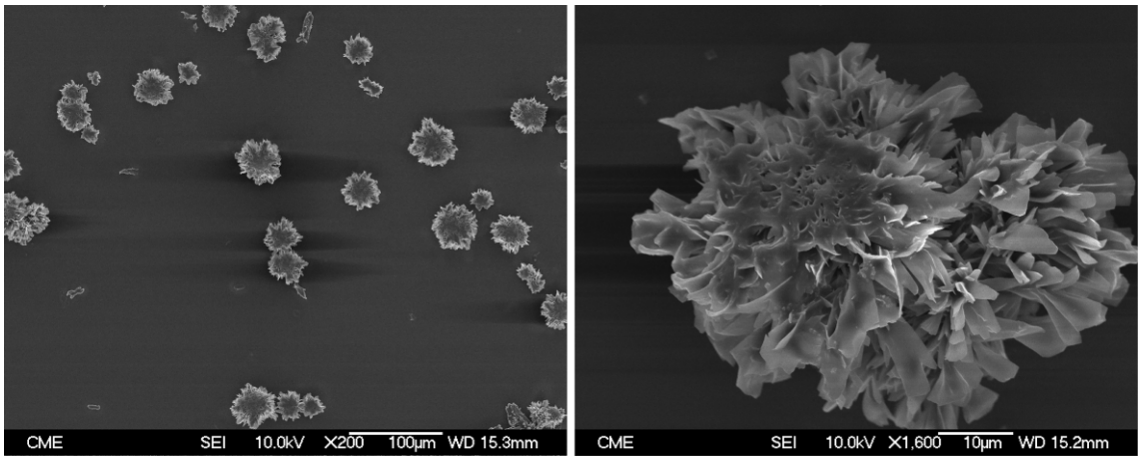
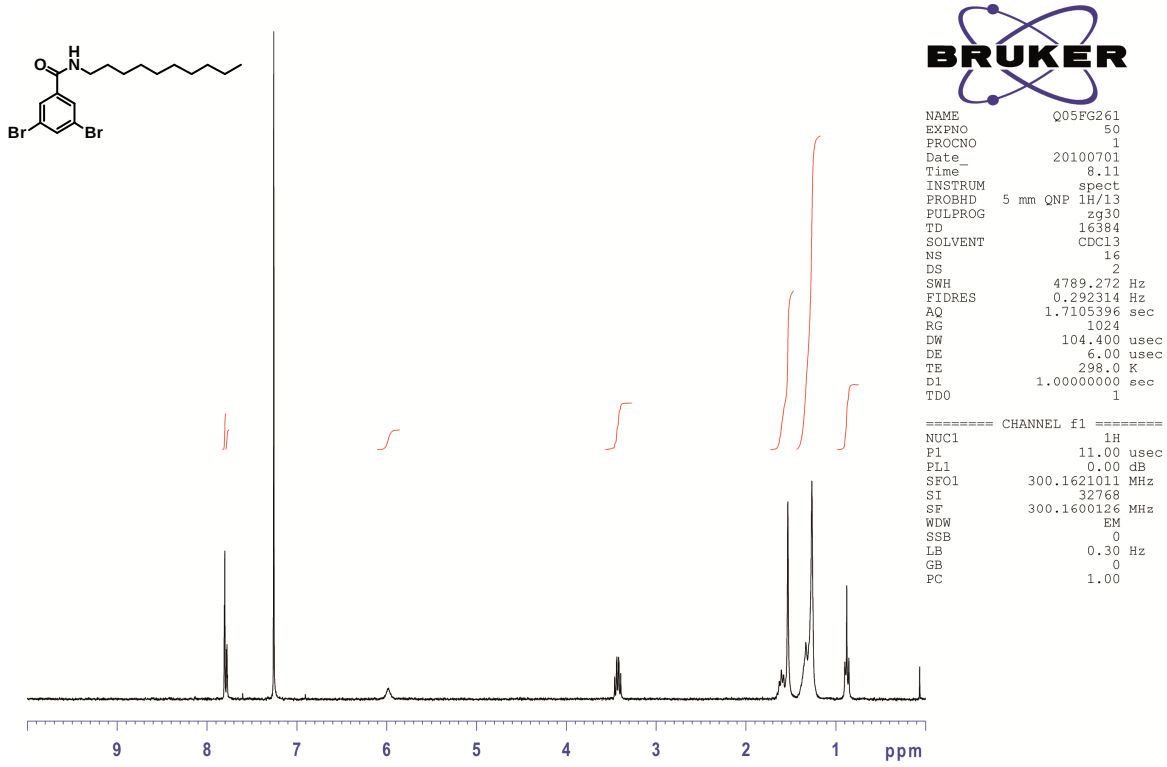


Figure S13. SEM images (298 K, 1×10^{-4} M in chloroform/acetonitrile, glass substrate) of the objects formed from complex **1**•(**12GA**)$_2$.

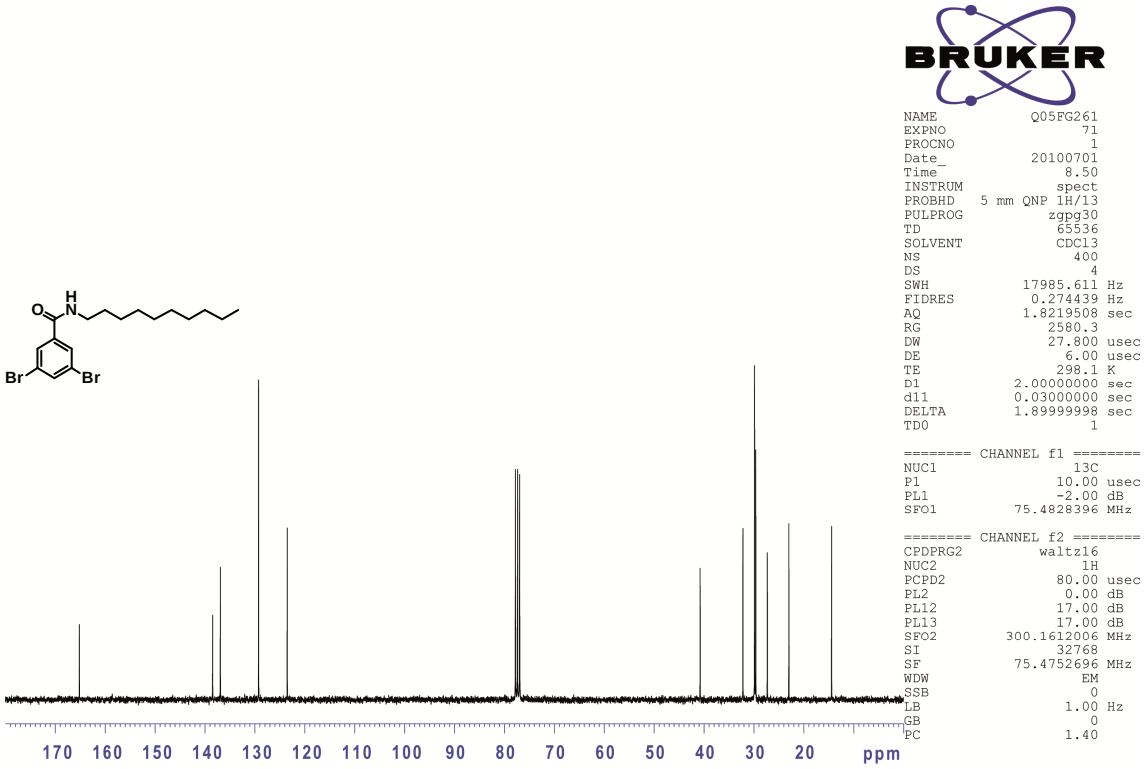
2. Experimental Section

General. All solvents were dried according to standard procedures. Reagents were used as purchased. All air-sensitive reactions were carried out under argon atmosphere. Flash chromatography was performed using silica gel (Merck, Kieselgel 60, 230-240 mesh or Scharlau 60, 230–240 mesh). Analytical thin layer chromatography (TLC) was performed using aluminum coated Merck Kieselgel 60 F254 plates. NMR spectra were recorded on a Bruker Avance 300 (^{1}H: 300 MHz; ^{13}C: 75 MHz) spectrometer at 298 K using partially deuterated solvents as internal standards. Coupling constants (*J*) are denoted in Hz and chemical shifts (δ) in ppm. Multiplicities are denoted as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad. FT-IR spectra were recorded on a Bruker Tensor 27 (ATR device) spectrometer. UV-Vis spectra were recorded on a Varian Cary 50 spectrophotometer. High resolution mass spectra (HRMS) were recorded on a FTMS Bruker APEX Q IV spectrometer (high resolution TOF). SEM images were obtained from on a JEOL JSM 6335F microscope working at 10kV. For the preparation of the samples for SEM imaging, a vial containing a solution of the compound 1 or the mixture of compound 1 and tetrabutylammonium bromide or 3,4,5-tri(dodecyloxy)gallic acid (1:1 or 1:2 respectively) in chloroform (1×10^{-4} M) was introduced in a bigger recipient containing acetonitrile. The slow diffusion of acetonitrile vapours into the chloroform solutions results in the precipitation of a yellowish solid that is deposited onto a glass substrate and the remaining solvent was slowly evaporated. For the titration experiments, the solution of receptor **1** in $CDCl_3$ at 298 K was titrated by adding known aliquots of concentrated solutions of the corresponding tetrabutylammonium salts of each halide or the gallic acid derivative. The guest solutions used to effect the titration contained the receptors at the same concentration as the receptor solution into which they were being titrated so as to obviate the need to account for dilution effects during the titrations.

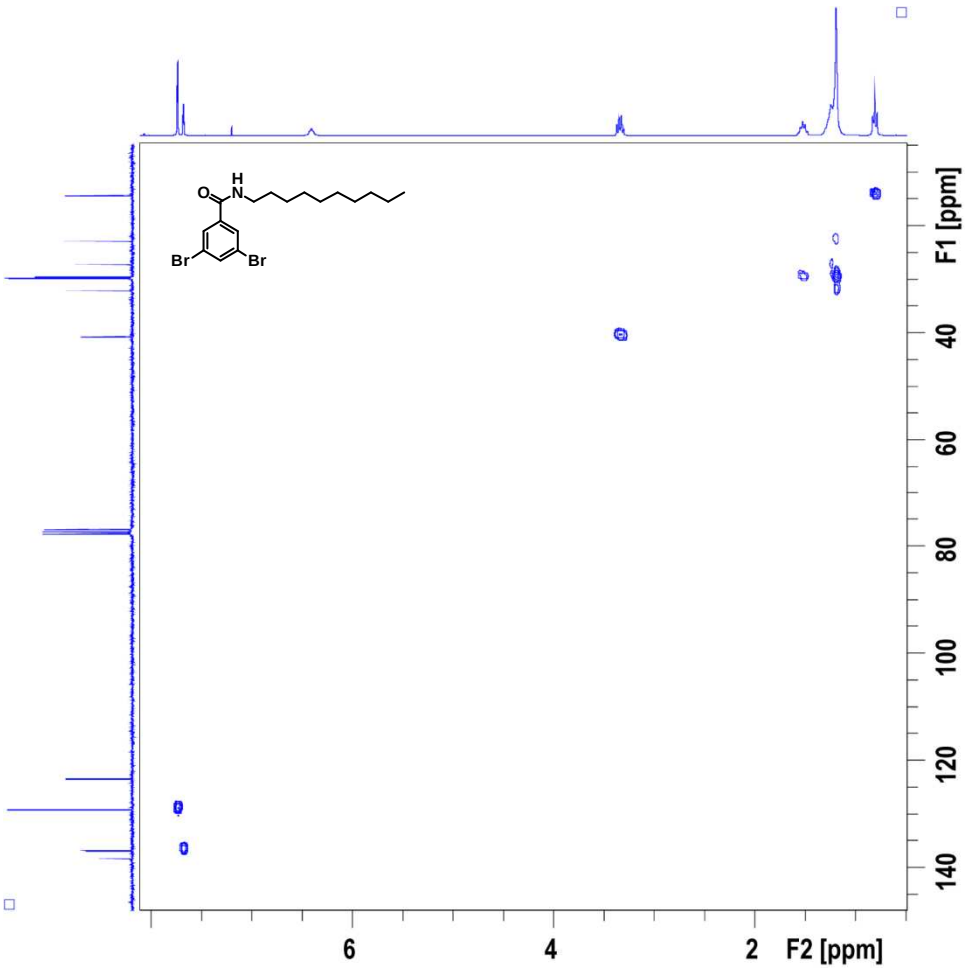
3. Collection of spectra



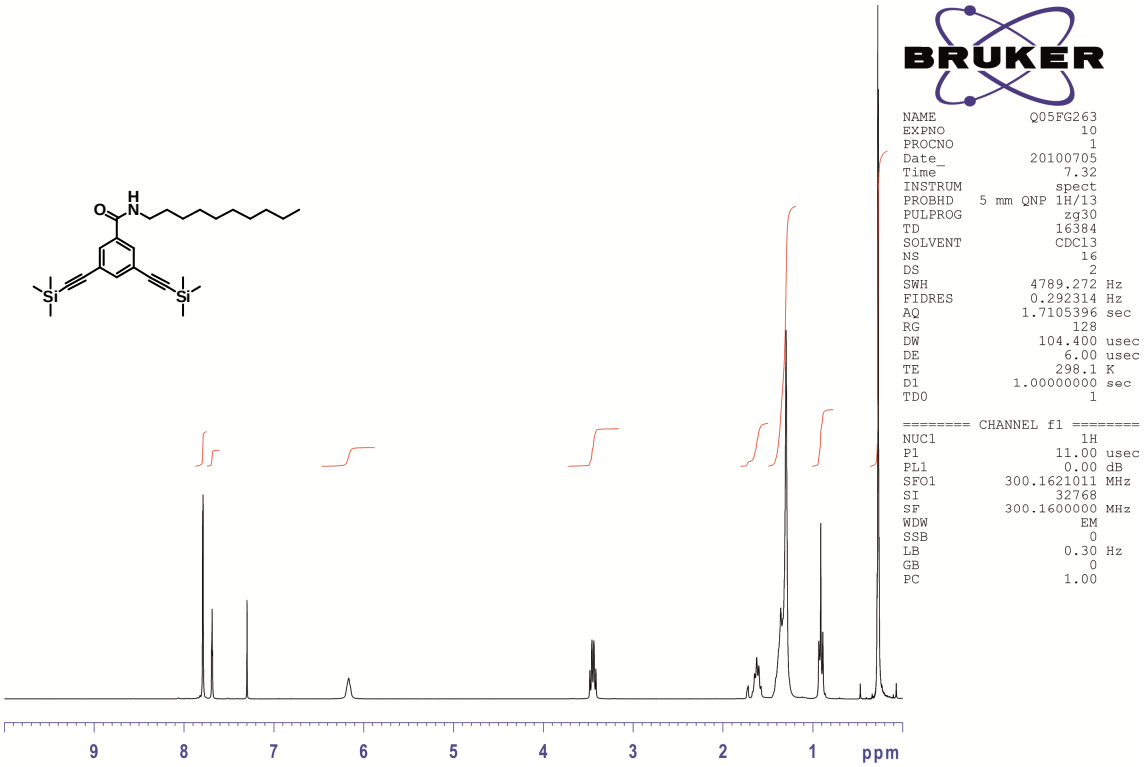
^{1}H NMR ($CDCl_3$, 300 MHz, 298 K) of compound **3**.



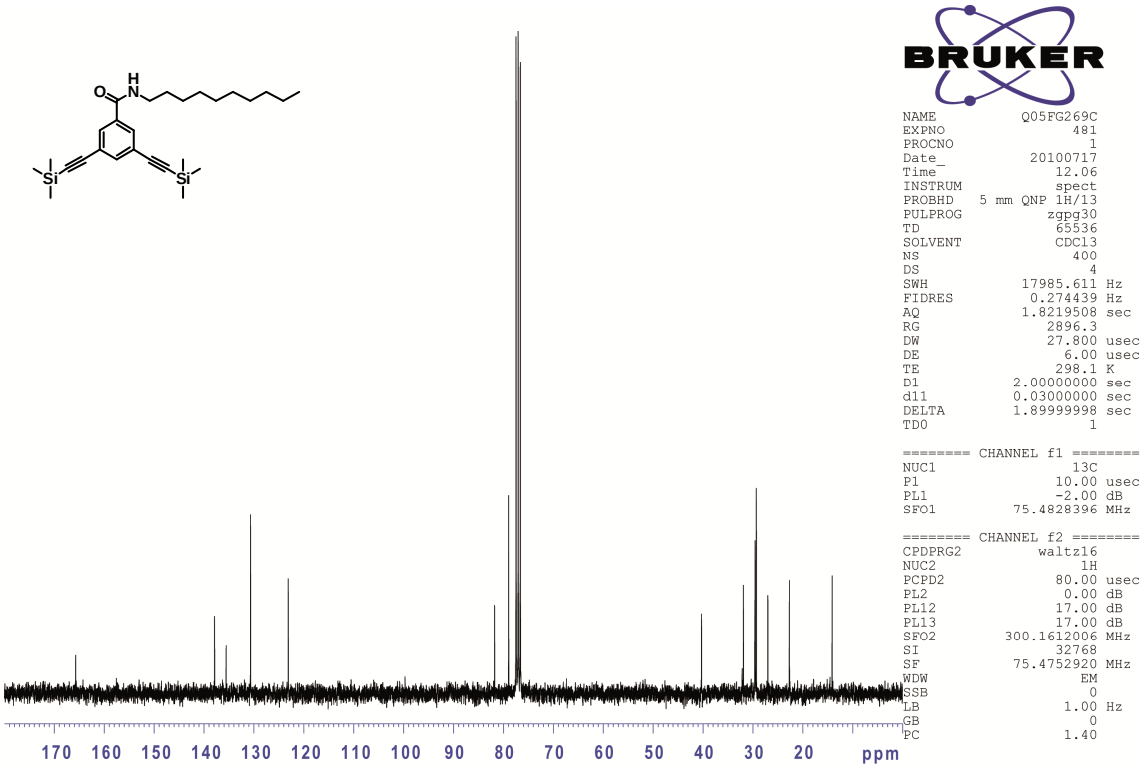
^{13}C NMR ($CDCl_3$, 75 MHz, 298 K) of compound **3**.



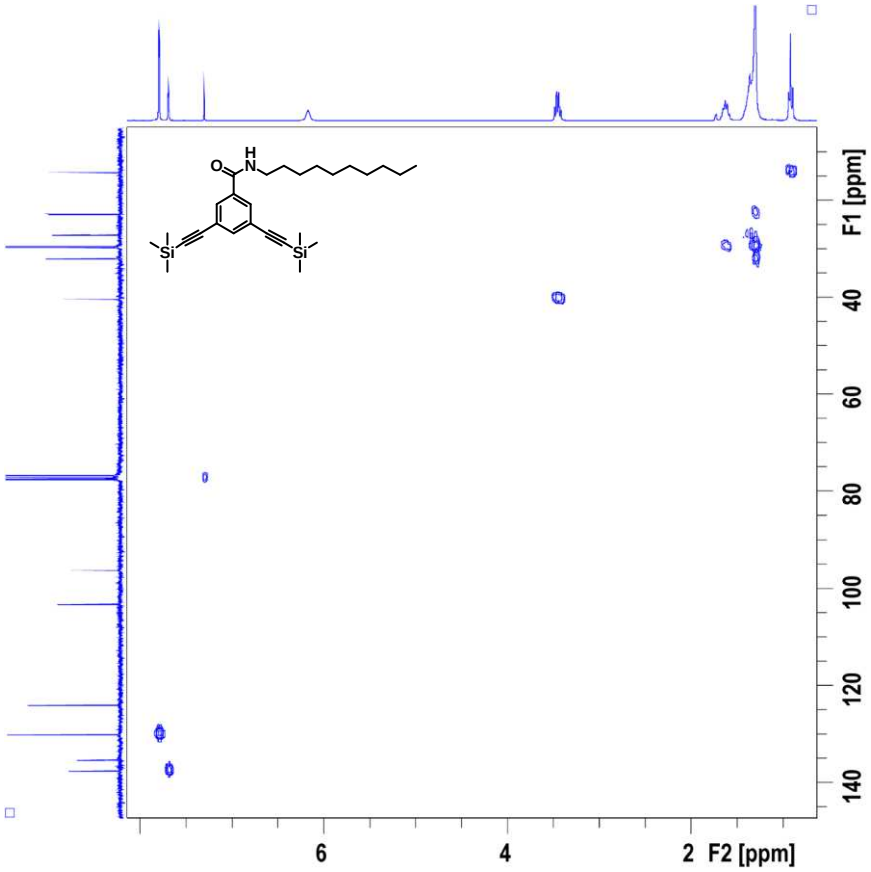
^{1}H, ^{13}C-HMQC spectrum ($CDCl_3$, 298 K) of compound **3**.



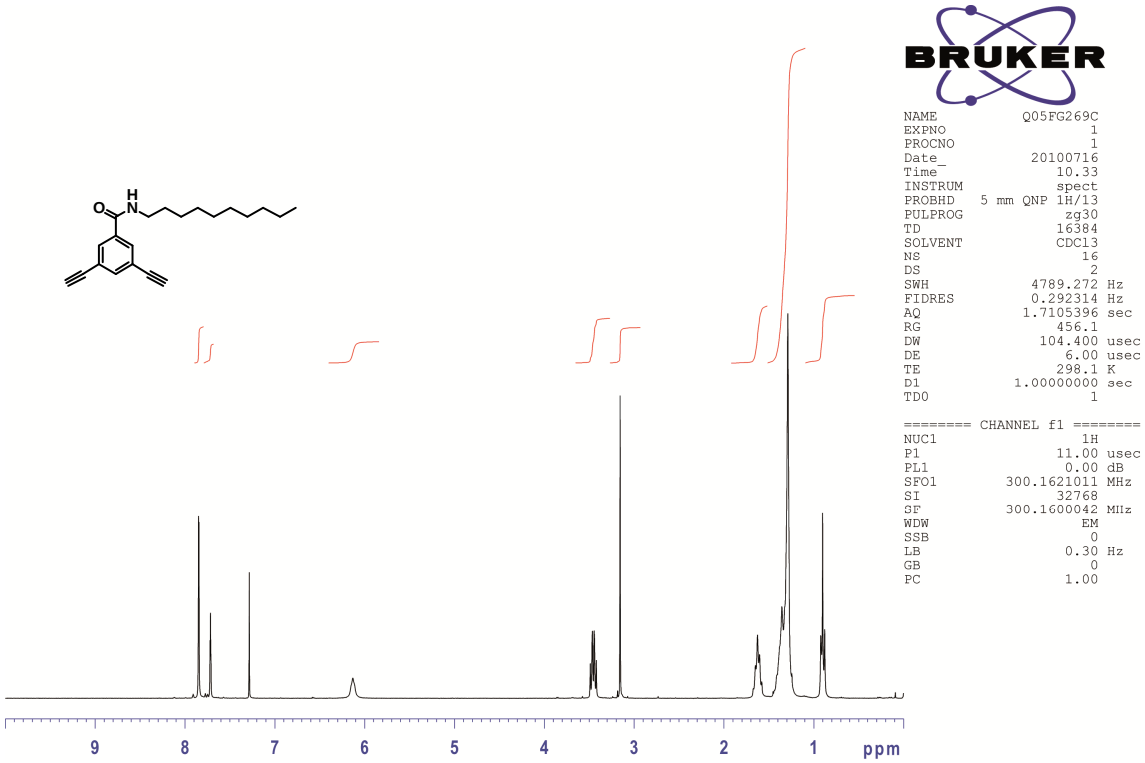
^{1}H NMR ($CDCl_3$, 300 MHz, 298 K) of compound **4**.



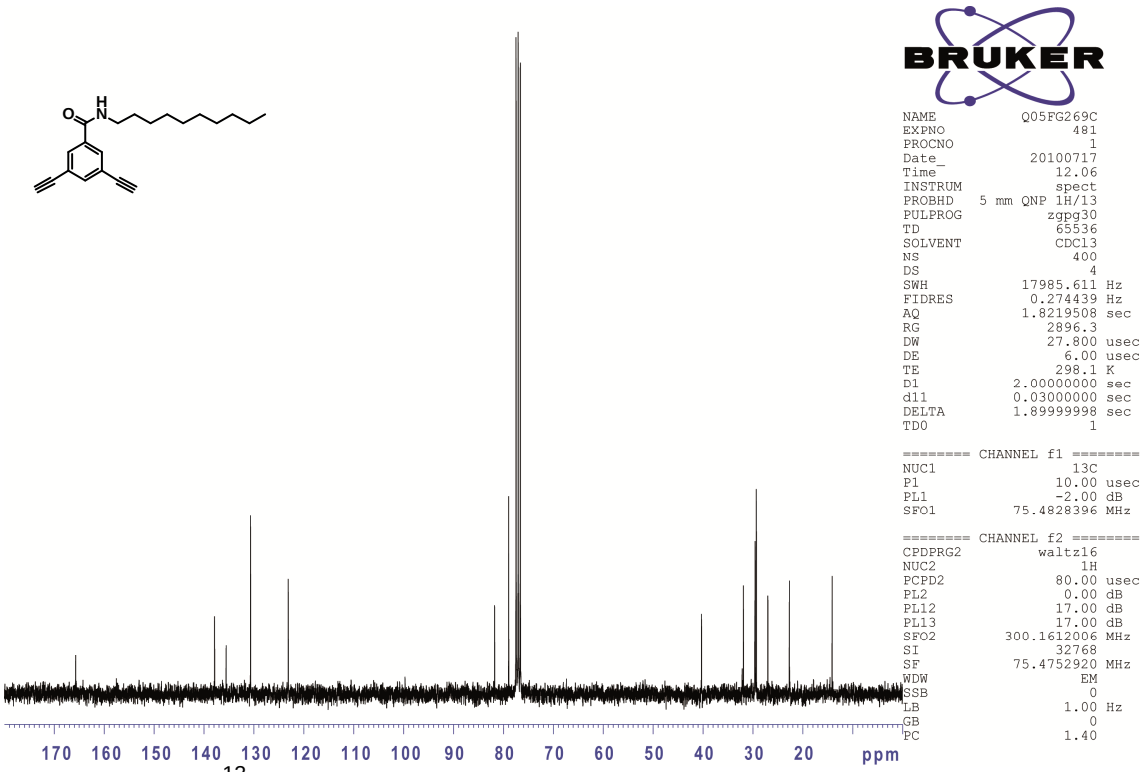
^{13}C NMR ($CDCl_3$, 75 MHz, 298 K) of compound **4**.



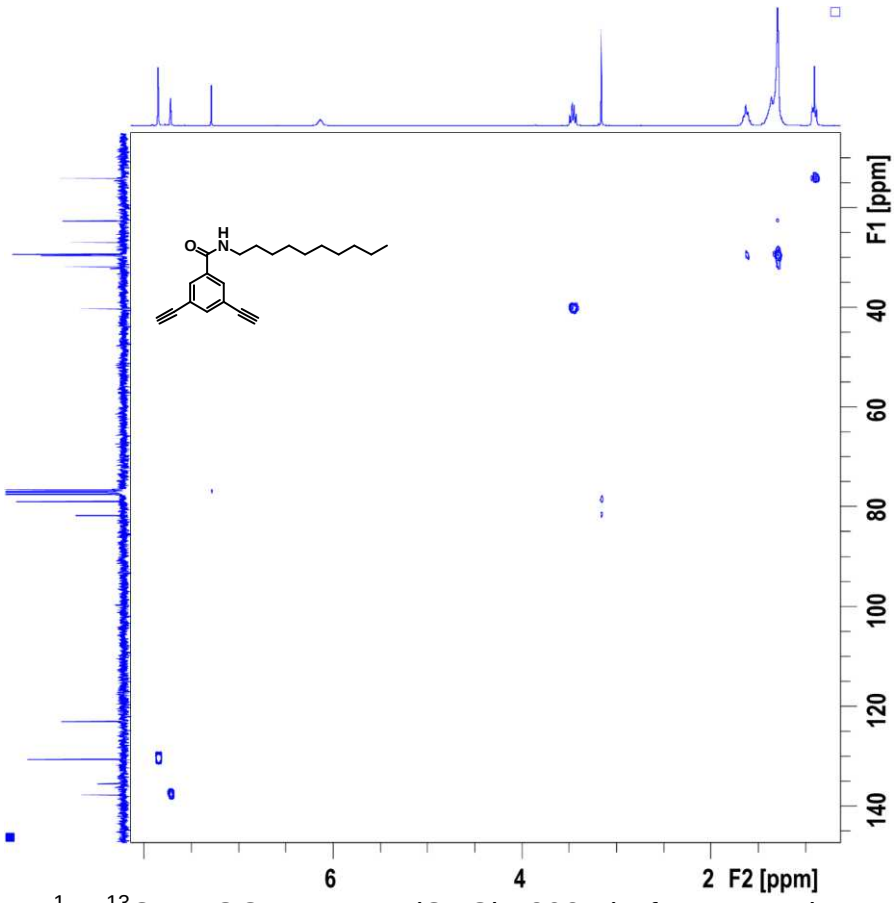
^{1}H, ^{13}C-HMQC spectrum ($CDCl_3$, 298 K) of compound **4**.



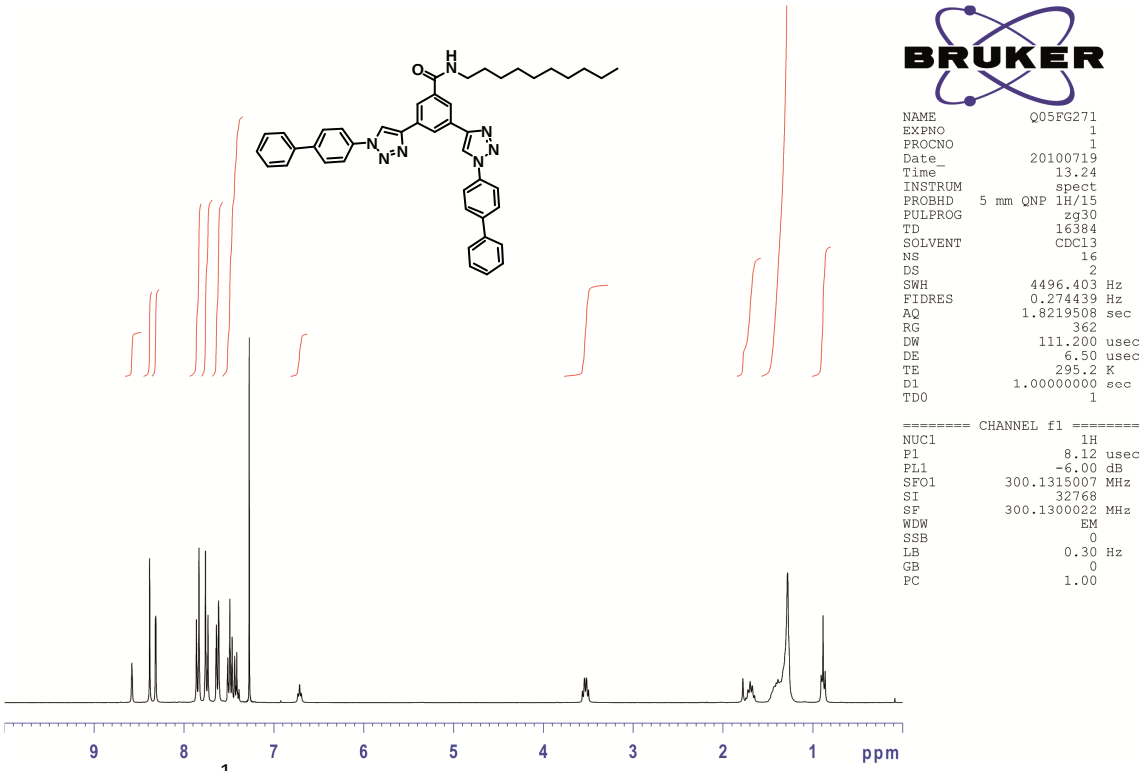
^{1}H NMR ($CDCl_3$, 300 MHz, 298 K) of compound **5**.



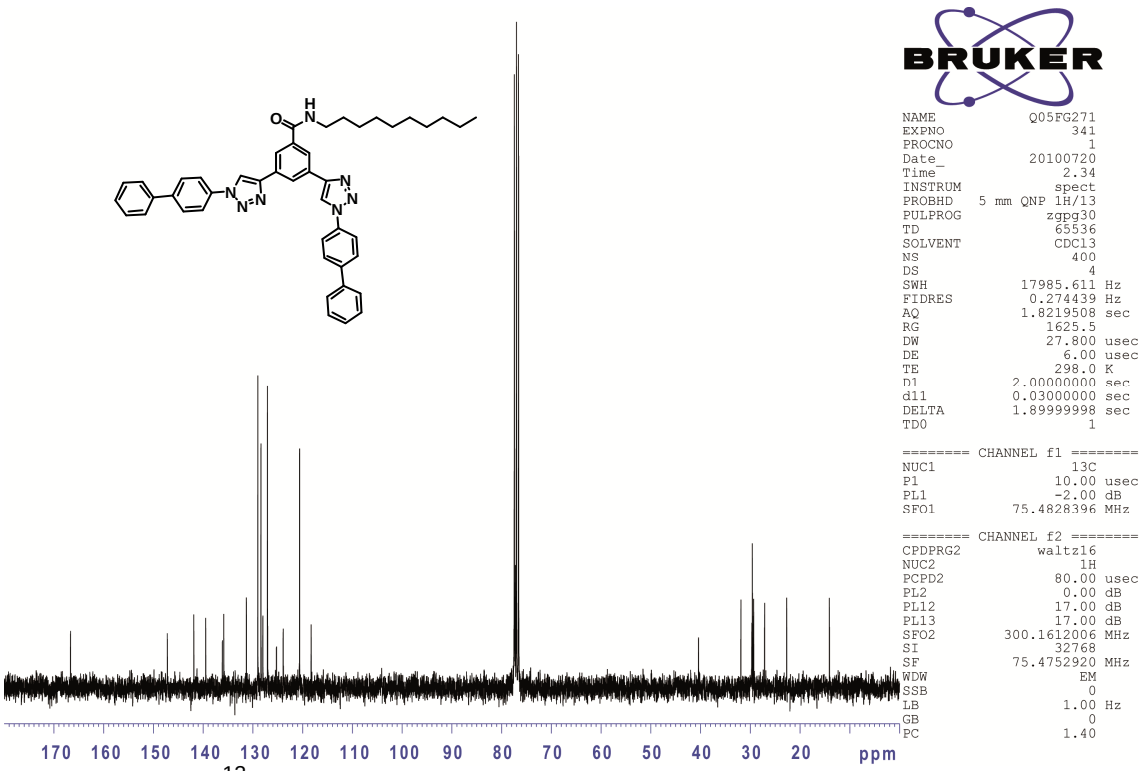
^{13}C NMR ($CDCl_3$, 75 MHz, 298 K) of compound **5**.



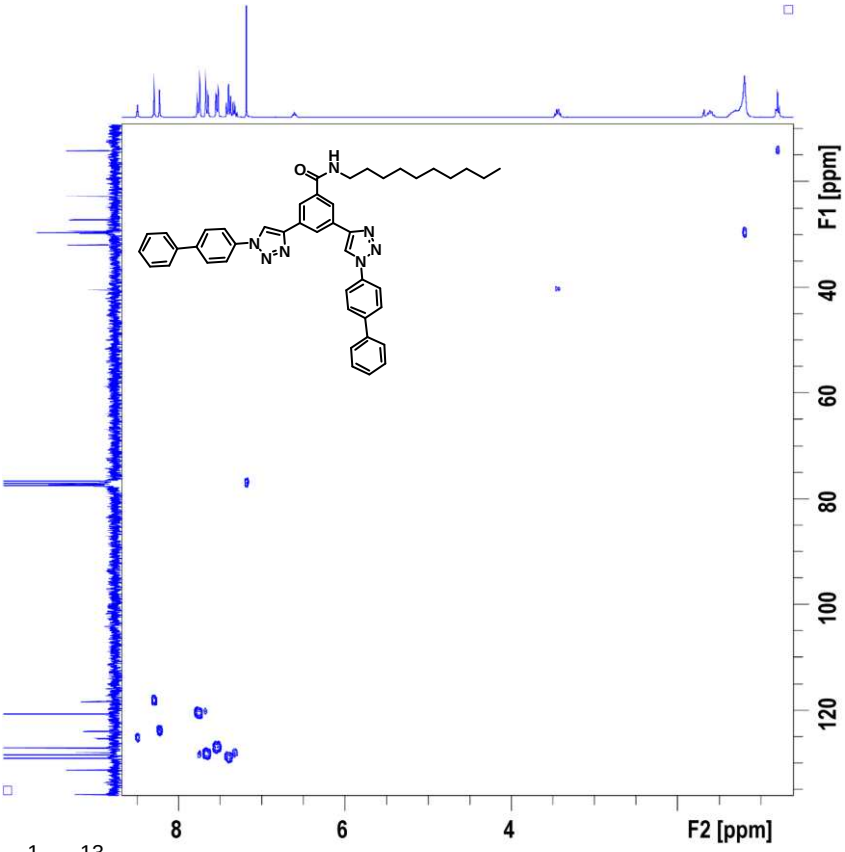
^{1}H, ^{13}C-HMQC spectrum ($CDCl_3$, 298 K) of compound **5**.



^{1}H NMR ($CDCl_3$, 300 MHz, 298 K) of compound **1**.



^{13}C NMR ($CDCl_3$, 75 MHz, 298 K) of compound **1**.



^{1}H, ^{13}C-HMQC spectrum ($CDCl_3$, 298 K) of compound **1**.

4. Atomic coordinates and total energy for all optimized molecular structures at the M06-2X/6-311G level.**

Compound **1** (Conformation A); E(RM062X) = -1846.25957560 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.377832	4.071866	0.069696
2	6	0	-0.961013	3.693185	0.070574
3	1	0	-1.762045	4.416810	0.162995
4	6	0	-1.305629	2.342874	-0.011461
5	6	0	-0.301438	1.381030	-0.081552
6	1	0	-0.541423	0.326587	-0.152901
7	6	0	1.042167	1.753259	-0.059401
8	6	0	1.374475	3.103436	0.017774
9	1	0	2.405053	3.438035	0.041726
10	6	0	-2.720216	1.956146	-0.016812
11	6	0	-3.301067	0.710167	0.007671
12	1	0	-2.898434	-0.285280	0.071292
13	6	0	2.080261	0.718988	-0.117718
14	6	0	3.446615	0.825737	-0.009647
15	1	0	4.104144	1.658103	0.168807
16	6	0	-5.712949	0.038625	-0.003058
17	6	0	-5.541242	-1.236055	-0.530556
18	1	0	-4.600999	-1.517033	-0.988757
19	6	0	-6.599501	-2.132430	-0.503439
20	1	0	-6.472831	-3.117185	-0.938023
21	6	0	-7.838547	-1.768827	0.029217
22	6	0	-7.987911	-0.475591	0.540106
23	1	0	-8.934855	-0.182031	0.978048
24	6	0	-6.935828	0.426352	0.534192
25	1	0	-7.043046	1.423106	0.940368
26	6	0	-8.968432	-2.729072	0.043187
27	6	0	-8.757737	-4.072686	0.364938
28	1	0	-7.762197	-4.406140	0.635977
29	6	0	-9.815145	-4.973240	0.372382
30	1	0	-9.636270	-6.009895	0.631898
31	6	0	-11.100132	-4.544785	0.057473
32	1	0	-11.924957	-5.246899	0.061994
33	6	0	-11.320930	-3.209762	-0.263549
34	1	0	-12.317669	-2.870431	-0.518829
35	6	0	-10.263856	-2.308848	-0.270236
36	1	0	-10.437002	-1.274813	-0.546883
37	6	0	5.226516	-0.935109	-0.085095
38	6	0	6.279571	-0.108920	-0.460339
39	1	0	6.087326	0.892723	-0.824598
40	6	0	7.578552	-0.593219	-0.403630
41	1	0	8.397261	0.042485	-0.719790
42	6	0	7.842495	-1.901452	0.007909
43	6	0	6.763364	-2.715264	0.367086
44	1	0	6.950048	-3.725949	0.710997
45	6	0	5.461667	-2.241379	0.330633
46	1	0	4.625011	-2.862837	0.619650
47	6	0	9.232049	-2.417212	0.052383
48	6	0	9.525059	-3.709194	-0.391924
49	1	0	8.730201	-4.328597	-0.792144
50	6	0	10.827138	-4.191678	-0.356347
51	1	0	11.039185	-5.192454	-0.713271

52	6	0	11.856685	-3.390444	0.125332
53	1	0	12.872001	-3.766891	0.153500
54	6	0	11.575810	-2.103667	0.571193
55	1	0	12.370968	-1.476312	0.955820
56	6	0	10.273923	-1.620413	0.534540
57	1	0	10.056558	-0.625199	0.906311
58	7	0	-4.632119	0.961240	-0.011016
59	7	0	-4.862447	2.282717	-0.041928
60	7	0	-3.723781	2.880206	-0.044706
61	7	0	3.891802	-0.448623	-0.124574
62	7	0	2.863046	-1.294210	-0.291336
63	7	0	1.779875	-0.601096	-0.286352
64	6	0	0.831906	5.505469	0.151984
65	8	0	1.966047	5.790590	0.485322
66	7	0	-0.098588	6.443434	-0.166125
67	1	0	-0.947251	6.147381	-0.618366
68	6	0	0.236430	7.854173	-0.164670
69	1	0	0.997821	8.020068	0.594901
70	1	0	0.635656	8.180328	-1.129383
71	1	0	-0.650781	8.439589	0.075331

Compound **1** (Conformation B); E(RM062X) = -1846.25558023 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.357819	4.133932	-0.063735
2	6	0	-0.983183	3.768510	-0.112818
3	1	0	-1.743689	4.534815	-0.199264
4	6	0	-1.340148	2.421781	-0.053557
5	6	0	-0.343053	1.450444	0.024392
6	1	0	-0.591821	0.396299	0.059606
7	6	0	1.002851	1.808008	0.042546
8	6	0	1.349414	3.158948	0.005779
9	1	0	2.394405	3.450568	-0.006316
10	6	0	-2.754735	2.036308	-0.081765
11	6	0	-3.334211	0.790319	-0.029186
12	1	0	-2.931167	-0.201799	0.072078
13	6	0	2.026655	0.757647	0.085310
14	6	0	3.397275	0.839957	0.010898
15	1	0	4.081371	1.665878	-0.070214
16	6	0	-5.745721	0.115860	-0.069796
17	6	0	-5.555482	-1.189010	-0.509936
18	1	0	-4.597821	-1.499029	-0.909438
19	6	0	-6.615517	-2.082996	-0.471051
20	1	0	-6.472893	-3.092615	-0.838155
21	6	0	-7.874838	-1.688132	-0.013607
22	6	0	-8.042689	-0.365789	0.408674
23	1	0	-9.006733	-0.045825	0.786726
24	6	0	-6.989835	0.534941	0.390802
25	1	0	-7.111697	1.554843	0.729278
26	6	0	-9.006373	-2.646063	0.015489
27	6	0	-8.814027	-3.963830	0.438966
28	1	0	-7.832112	-4.277585	0.775358
29	6	0	-9.873622	-4.861581	0.463081
30	1	0	-9.710124	-5.877347	0.802830
31	6	0	-11.142428	-4.456013	0.063554
32	1	0	-11.968926	-5.155980	0.081707
33	6	0	-11.344904	-3.146747	-0.359306
34	1	0	-12.328569	-2.825631	-0.680401
35	6	0	-10.285687	-2.248617	-0.382617
36	1	0	-10.442549	-1.236434	-0.738405
37	6	0	5.140740	-0.960934	0.062405
38	6	0	6.144053	-0.263215	-0.600109
39	1	0	5.915662	0.653837	-1.129048
40	6	0	7.432791	-0.777451	-0.619145
41	1	0	8.208883	-0.247952	-1.159500
42	6	0	7.732946	-1.992432	0.000985
43	6	0	6.702292	-2.678244	0.651801
44	1	0	6.920864	-3.610796	1.158765
45	6	0	5.414026	-2.170153	0.693306
46	1	0	4.616351	-2.692156	1.204389
47	6	0	9.106126	-2.550331	-0.042594
48	6	0	9.308187	-3.915563	-0.262608
49	1	0	8.453015	-4.562188	-0.424829
50	6	0	10.592450	-4.442252	-0.310204
51	1	0	10.733080	-5.501143	-0.491458
52	6	0	11.694817	-3.612502	-0.137373
53	1	0	12.696548	-4.023013	-0.174717
54	6	0	11.504951	-2.252639	0.083221

55	1	0	12.358540	-1.601193	0.227589
56	6	0	10.220529	-1.725277	0.129478
57	1	0	10.076497	-0.668601	0.326162
58	7	0	-4.664561	1.037301	-0.087665
59	7	0	-4.894580	2.358234	-0.168861
60	7	0	-3.758127	2.957274	-0.164771
61	7	0	3.816310	-0.446352	0.094999
62	7	0	2.768521	-1.275169	0.214995
63	7	0	1.699334	-0.561357	0.210039
64	6	0	0.680632	5.601287	-0.125466
65	8	0	-0.051282	6.399303	-0.669969
66	7	0	1.858305	5.969405	0.463980
67	1	0	2.248190	5.344207	1.150822
68	6	0	2.203063	7.377432	0.543122
69	1	0	2.027456	7.833121	-0.429823
70	1	0	1.593665	7.908026	1.280559
71	1	0	3.256436	7.474299	0.802812

Complex **1**•F^-; E(RM062X) = -1946.18188703 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.634806	-3.426512	0.119101
2	6	0	-9.691222	-2.032350	0.030453
3	6	0	-10.943572	-1.421199	-0.080735
4	6	0	-12.105735	-2.182267	-0.101863
5	6	0	-12.036720	-3.568524	-0.013903
6	6	0	-10.796443	-4.187852	0.095929
7	6	0	-8.448971	-1.223657	0.056126
8	6	0	-7.306133	-1.646249	-0.625982
9	6	0	-6.139061	-0.897083	-0.602977
10	6	0	-6.096672	0.289204	0.123480
11	6	0	-7.225047	0.733062	0.808977
12	6	0	-8.387938	-0.019349	0.764235
13	7	0	-4.906348	1.050088	0.170255
14	7	0	-4.941819	2.361658	0.467757
15	7	0	-3.737208	2.806681	0.430478
16	6	0	-2.876127	1.792218	0.108430
17	6	0	-3.627613	0.655212	-0.063758
18	6	0	-1.425002	1.971245	-0.023857
19	6	0	-0.596955	0.841753	-0.091880
20	6	0	0.771066	0.997704	-0.262201
21	6	0	1.301145	2.284099	-0.387260
22	6	0	0.503758	3.402949	-0.233887
23	6	0	-0.872408	3.252581	-0.067928
24	6	0	1.132637	4.774352	-0.215303
25	7	0	2.474519	4.796741	-0.097640
26	6	0	3.144953	6.076003	-0.095323
27	6	0	1.763896	-0.080566	-0.239661
28	6	0	3.101526	0.150379	-0.022850
29	7	0	3.652662	-1.075249	-0.120362
30	7	0	2.714776	-2.019764	-0.361027
31	7	0	1.573208	-1.418296	-0.427475
32	6	0	5.033529	-1.370589	-0.059893
33	6	0	5.948520	-0.316858	-0.105658
34	6	0	7.302147	-0.608917	-0.036928
35	6	0	7.763628	-1.925446	0.065012
36	6	0	6.821996	-2.957532	0.098273
37	6	0	5.462530	-2.689883	0.040585
38	6	0	9.215111	-2.218157	0.138714
39	6	0	10.075494	-1.391509	0.868559
40	6	0	11.435978	-1.662809	0.938705
41	6	0	11.964826	-2.769777	0.283394
42	6	0	11.120046	-3.600945	-0.444474
43	6	0	9.760173	-3.326412	-0.517669
44	8	0	0.443292	5.786517	-0.283308
45	1	0	2.366588	2.397162	-0.568850
46	1	0	-1.005698	-0.157729	0.015551
47	1	0	-1.500553	4.130840	0.021771
48	1	0	3.642827	1.091497	0.174361
49	1	0	-3.363192	-0.358203	-0.306620
50	1	0	5.602233	0.712034	-0.200962
51	1	0	8.015116	0.205630	-0.094975
52	1	0	7.157369	-3.983339	0.203306
53	1	0	4.724587	-3.479953	0.077792
54	1	0	9.665077	-0.541574	1.402007

55	1	0	12.083239	-1.012398	1.515775
56	1	0	13.025992	-2.982070	0.338466
57	1	0	11.523201	-4.461292	-0.966334
58	1	0	9.112133	-3.961366	-1.111625
59	1	0	-5.275884	-1.219935	-1.171011
60	1	0	-7.338619	-2.557080	-1.212806
61	1	0	-9.256159	0.316007	1.320296
62	1	0	-7.168311	1.657388	1.367493
63	1	0	-11.001481	-0.342609	-0.176398
64	1	0	-13.067353	-1.691584	-0.197366
65	1	0	-12.943120	-4.161971	-0.030394
66	1	0	-10.733013	-5.266973	0.173814
67	1	0	-8.672230	-3.912470	0.233786
68	1	0	3.086654	3.952010	0.005438
69	1	0	2.868578	6.664166	-0.974987
70	1	0	2.880901	6.667967	0.787434
71	1	0	4.218157	5.888537	-0.100705
72	9	0	4.169211	2.713804	-0.018622

Complex **1**•Cl^-; E(RM062X) = -2306.58593432 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.454640	-3.731090	0.234528
2	6	0	-9.574087	-2.350770	0.048750
3	6	0	-10.851034	-1.809357	-0.127538
4	6	0	-11.975827	-2.624436	-0.116747
5	6	0	-11.844494	-3.996380	0.069039
6	6	0	-10.579229	-4.546742	0.243467
7	6	0	-8.374787	-1.479240	0.042804
8	6	0	-7.193416	-1.887087	-0.580221
9	6	0	-6.070281	-1.072601	-0.590221
10	6	0	-6.113263	0.164811	0.044046
11	6	0	-7.280169	0.594084	0.671131
12	6	0	-8.397792	-0.224634	0.660081
13	7	0	-4.970219	0.997808	0.057152
14	7	0	-5.096919	2.328560	0.208084
15	7	0	-3.919660	2.840765	0.182131
16	6	0	-2.986786	1.854401	0.014529
17	6	0	-3.660975	0.659789	-0.068568
18	6	0	-1.544150	2.120423	-0.047834
19	6	0	-0.641781	1.054275	-0.090328
20	6	0	0.724761	1.296895	-0.156616
21	6	0	1.189056	2.613619	-0.186059
22	6	0	0.299819	3.677219	-0.121913
23	6	0	-1.070634	3.431864	-0.058792
24	6	0	0.763647	5.115094	-0.129356
25	7	0	2.090223	5.321287	-0.023281
26	6	0	2.614548	6.668630	-0.047257
27	6	0	1.705169	0.208336	-0.174870
28	6	0	3.071429	0.326431	-0.095165
29	7	0	3.511224	-0.950717	-0.137675
30	7	0	2.479201	-1.812498	-0.235067
31	7	0	1.393569	-1.117943	-0.255954
32	6	0	4.853903	-1.404717	-0.087194
33	6	0	5.893700	-0.477428	-0.048445
34	6	0	7.201060	-0.937448	0.007099
35	6	0	7.495209	-2.303556	0.022302
36	6	0	6.431493	-3.209303	-0.019365
37	6	0	5.117552	-2.771958	-0.072753
38	6	0	8.896606	-2.783317	0.086523
39	6	0	9.841561	-2.132067	0.885298
40	6	0	11.152935	-2.586071	0.949214
41	6	0	11.545596	-3.701750	0.217275
42	6	0	10.615498	-4.357484	-0.582125
43	6	0	9.305077	-3.901320	-0.647838
44	8	0	-0.041396	6.031145	-0.224190
45	1	0	2.257547	2.785602	-0.261983
46	1	0	-0.983136	0.025089	-0.063802
47	1	0	-1.755146	4.270188	-0.022779
48	1	0	3.717551	1.194236	-0.005549
49	1	0	-3.328037	-0.357177	-0.174102
50	1	0	5.700618	0.592086	-0.065868
51	1	0	8.007093	-0.212795	0.013506
52	1	0	6.633571	-4.273829	0.019362
53	1	0	4.289254	-3.466454	-0.093460

54	1	0	9.536380	-1.276134	1.476753
55	1	0	11.868457	-2.070836	1.579416
56	1	0	12.568307	-4.056193	0.268331
57	1	0	10.912904	-5.221599	-1.165295
58	1	0	8.590993	-4.399150	-1.294246
59	1	0	-5.175834	-1.385742	-1.113960
60	1	0	-7.161660	-2.839070	-1.097477
61	1	0	-9.296717	0.101197	1.170882
62	1	0	-7.288153	1.559093	1.159275
63	1	0	-10.957631	-0.744044	-0.299026
64	1	0	-12.956841	-2.187219	-0.262236
65	1	0	-12.721901	-4.632046	0.077168
66	1	0	-10.467118	-5.613618	0.397292
67	1	0	-8.473433	-4.162803	0.398429
68	1	0	2.771872	4.572782	0.087748
69	1	0	2.281530	7.194495	-0.945299
70	1	0	2.272892	7.241241	0.819928
71	1	0	3.701544	6.601455	-0.038589
72	17	0	4.749571	3.310503	0.104711

Complex **1**•Br^-; E(RM062X) = -4420.56649559 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-9.741692	-3.710370	0.212233
2	6	0	-9.851379	-2.325740	0.054649
3	6	0	-11.125238	-1.770034	-0.097194
4	6	0	-12.256768	-2.575937	-0.090570
5	6	0	-12.135178	-3.952270	0.067014
6	6	0	-10.873002	-4.516653	0.217436
7	6	0	-8.643665	-1.465883	0.052141
8	6	0	-7.476818	-1.870543	-0.599643
9	6	0	-6.344226	-1.069487	-0.604568
10	6	0	-6.362500	0.150468	0.063963
11	6	0	-7.514890	0.576988	0.718918
12	6	0	-8.642834	-0.227830	0.702227
13	7	0	-5.206793	0.966024	0.084464
14	7	0	-5.307904	2.293286	0.279236
15	7	0	-4.122214	2.786320	0.249125
16	6	0	-3.210058	1.789952	0.035176
17	6	0	-3.906160	0.610249	-0.073914
18	6	0	-1.763817	2.028804	-0.047783
19	6	0	-0.885143	0.944373	-0.102724
20	6	0	0.485076	1.155819	-0.195946
21	6	0	0.978441	2.461701	-0.240528
22	6	0	0.112416	3.544357	-0.157910
23	6	0	-1.261608	3.329163	-0.069024
24	6	0	0.602352	4.973233	-0.180483
25	7	0	1.930196	5.154867	-0.047480
26	6	0	2.488965	6.487936	-0.090059
27	6	0	1.431156	0.037807	-0.225305
28	6	0	2.798557	0.101151	-0.112505
29	7	0	3.191300	-1.190606	-0.184899
30	7	0	2.129878	-2.008315	-0.329433
31	7	0	1.072006	-1.272956	-0.351524
32	6	0	4.513244	-1.702011	-0.123423
33	6	0	5.593405	-0.822343	-0.096804
34	6	0	6.878376	-1.340385	-0.026767
35	6	0	7.110200	-2.717735	0.012717
36	6	0	6.006737	-3.575238	-0.019223
37	6	0	4.714303	-3.079266	-0.084511
38	6	0	8.489076	-3.256986	0.092427
39	6	0	9.455520	-2.634625	0.888613
40	6	0	10.746607	-3.141262	0.966644
41	6	0	11.096509	-4.282174	0.252095
42	6	0	10.144688	-4.909768	-0.544300
43	6	0	8.854471	-4.400986	-0.624168
44	8	0	-0.182273	5.901956	-0.310523
45	1	0	2.048165	2.611291	-0.350334
46	1	0	-1.247369	-0.077117	-0.065016
47	1	0	-1.927088	4.182372	-0.024850
48	1	0	3.475223	0.938510	0.023280
49	1	0	-3.592764	-0.407923	-0.219370
50	1	0	5.448790	0.254444	-0.134184
51	1	0	7.716066	-0.652562	-0.028494
52	1	0	6.160176	-4.647018	0.038359
53	1	0	3.855835	-3.736281	-0.096356

54	1	0	9.182003	-1.758937	1.466490
55	1	0	11.479396	-2.647781	1.594395
56	1	0	12.103448	-4.677620	0.314311
57	1	0	10.410084	-5.792945	-1.114142
58	1	0	8.124195	-4.877194	-1.268820
59	1	0	-5.461659	-1.379183	-1.150029
60	1	0	-7.464531	-2.808665	-1.142355
61	1	0	-9.530270	0.094509	1.234937
62	1	0	-7.503602	1.528142	1.233491
63	1	0	-11.224274	-0.700612	-0.246520
64	1	0	-13.235528	-2.128102	-0.217728
65	1	0	-13.017845	-4.580663	0.071978
66	1	0	-10.768552	-5.587272	0.349225
67	1	0	-8.762382	-4.153049	0.357306
68	1	0	2.585996	4.393479	0.111038
69	1	0	2.159656	7.009930	-0.991200
70	1	0	2.171546	7.079350	0.773852
71	1	0	3.574004	6.392331	-0.091478
72	35	0	4.738956	3.107020	0.131044

Complex **1**•I^-; E(RM062X) = -8766.32042427 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.092841	-3.551737	0.778505
2	6	0	-10.146986	-2.271524	0.219959
3	6	0	-11.380404	-1.790581	-0.229277
4	6	0	-12.526825	-2.567418	-0.121831
5	6	0	-12.460829	-3.839769	0.435698
6	6	0	-11.239046	-4.329234	0.885085
7	6	0	-8.923238	-1.442326	0.106682
8	6	0	-7.705717	-2.010772	-0.273247
9	6	0	-6.558384	-1.239154	-0.385781
10	6	0	-6.614594	0.121074	-0.098675
11	6	0	-7.817636	0.711149	0.280776
12	6	0	-8.957956	-0.070076	0.373422
13	7	0	-5.447176	0.916060	-0.186594
14	7	0	-5.537932	2.248817	-0.344606
15	7	0	-4.344958	2.722030	-0.390041
16	6	0	-3.437894	1.706456	-0.263650
17	6	0	-4.144789	0.535945	-0.128798
18	6	0	-1.986424	1.925844	-0.265189
19	6	0	-1.118138	0.833880	-0.310380
20	6	0	0.258650	1.028970	-0.304348
21	6	0	0.769032	2.328265	-0.260132
22	6	0	-0.090413	3.419336	-0.199994
23	6	0	-1.468896	3.218896	-0.212121
24	6	0	0.402479	4.846392	-0.138508
25	7	0	1.718000	5.018918	0.090883
26	6	0	2.287086	6.347836	0.133537
27	6	0	1.178777	-0.111213	-0.339770
28	6	0	2.545174	-0.106150	-0.194943
29	7	0	2.890276	-1.410732	-0.298359
30	7	0	1.801660	-2.179024	-0.492213
31	7	0	0.774432	-1.403095	-0.515393
32	6	0	4.186736	-1.985254	-0.225487
33	6	0	5.305521	-1.162548	-0.122040
34	6	0	6.562883	-1.743098	-0.043925
35	6	0	6.729666	-3.129746	-0.069950
36	6	0	5.589037	-3.930320	-0.178440
37	6	0	4.323400	-3.370768	-0.253928
38	6	0	8.079337	-3.735771	0.024495
39	6	0	9.042654	-3.198406	0.884096
40	6	0	10.307321	-3.764785	0.978074
41	6	0	10.633434	-4.881768	0.216001
42	6	0	9.684296	-5.425411	-0.643087
43	6	0	8.420172	-4.857065	-0.738541
44	8	0	-0.369819	5.781536	-0.288182
45	1	0	1.845436	2.466555	-0.290314
46	1	0	-1.493307	-0.182188	-0.361690
47	1	0	-2.125502	4.079531	-0.184188
48	1	0	3.252031	0.694919	-0.017847
49	1	0	-3.839733	-0.481833	0.035868
50	1	0	5.215878	-0.080330	-0.104410
51	1	0	7.429972	-1.095133	0.014080
52	1	0	5.690785	-5.009783	-0.172794
53	1	0	3.437155	-3.985826	-0.323699
54	1	0	8.785859	-2.341919	1.497300

55	1	0	11.037516	-3.337102	1.655313
56	1	0	11.619948	-5.323933	0.290659
57	1	0	9.932431	-6.289642	-1.248632
58	1	0	7.693274	-5.267852	-1.430549
59	1	0	-5.632377	-1.688186	-0.722156
60	1	0	-7.662127	-3.065297	-0.520407
61	1	0	-9.887547	0.387140	0.692847
62	1	0	-7.835985	1.769602	0.501382
63	1	0	-11.433564	-0.809869	-0.688704
64	1	0	-13.472777	-2.181462	-0.483572
65	1	0	-13.355121	-4.445902	0.517423
66	1	0	-11.178351	-5.316497	1.327822
67	1	0	-9.147672	-3.927880	1.154296
68	1	0	2.352581	4.248075	0.270472
69	1	0	1.996981	6.911152	-0.755596
70	1	0	1.939334	6.901161	1.010837
71	1	0	3.370657	6.241851	0.171356
72	53	0	4.785562	2.989295	0.368659

Complex **1•(12GA)$_2$**; E(RM062X) = -3374.89466883 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.628705	3.563964	0.034203
2	6	0	1.685518	2.246563	-0.316284
3	6	0	3.002085	1.913166	-0.513174
4	7	0	3.671162	3.057393	-0.255804
5	7	0	2.823123	4.047314	0.071182
6	6	0	0.514889	1.374890	-0.422211
7	6	0	-0.768367	1.875820	-0.223500
8	6	0	-1.874347	1.030939	-0.308793
9	6	0	-1.696294	-0.323291	-0.585437
10	6	0	-0.412170	-0.827767	-0.782872
11	6	0	0.686331	0.017471	-0.700254
12	6	0	-0.142645	-2.280676	-1.057751
13	7	0	-1.190014	-3.045768	-1.388354
14	6	0	-1.030475	-4.466939	-1.629107
15	6	0	-3.229123	1.557179	-0.108444
16	6	0	-3.676707	2.857271	-0.087440
17	7	0	-5.013920	2.755486	0.111677
18	7	0	-5.383764	1.480726	0.205416
19	7	0	-4.320610	0.759185	0.072690
20	6	0	-5.980451	3.797155	0.208312
21	6	0	-5.611105	5.035699	0.717709
22	6	0	-6.556540	6.048470	0.788923
23	6	0	-7.872789	5.835755	0.371896
24	6	0	-8.218562	4.574214	-0.123011
25	6	0	-7.282736	3.556277	-0.213415
26	6	0	-8.881475	6.919216	0.456700
27	6	0	-8.545242	8.233994	0.123111
28	6	0	-9.492022	9.247459	0.200504
29	6	0	-10.788710	8.962279	0.613939
30	6	0	-11.133287	7.657377	0.949278
31	6	0	-10.187201	6.643537	0.871145
32	6	0	5.078372	3.242177	-0.283013
33	6	0	5.899227	2.129436	-0.131629
34	6	0	7.273730	2.279090	-0.217212
35	6	0	7.845823	3.536543	-0.431466
36	6	0	6.999062	4.643147	-0.548925
37	6	0	5.619612	4.506020	-0.483156
38	6	0	9.317113	3.680646	-0.542924
39	6	0	9.974656	4.787530	0.000946
40	6	0	11.353098	4.918978	-0.109446
41	6	0	12.098592	3.945002	-0.765029
42	6	0	11.455375	2.837586	-1.307933
43	6	0	10.076221	2.705895	-1.198946
44	8	0	0.994224	-2.748070	-0.977396
45	1	0	-2.570565	-0.958962	-0.644584
46	1	0	-0.880492	2.927993	0.013604
47	1	0	1.677323	-0.397705	-0.852572
48	1	0	-3.181571	3.800664	-0.235958
49	1	0	3.484963	0.999382	-0.818601
50	1	0	-4.605353	5.198882	1.085321
51	1	0	-6.277317	7.007378	1.209251
52	1	0	-9.228513	4.398406	-0.474222
53	1	0	-7.541794	2.583582	-0.609659
54	1	0	-7.542685	8.456869	-0.224795

55	1	0	-9.218584	10.260258	-0.070416
56	1	0	-11.526768	9.752815	0.675722
57	1	0	-12.139320	7.429274	1.280412
58	1	0	-10.454167	5.632561	1.158269
59	1	0	5.465382	1.153792	0.055265
60	1	0	7.908163	1.405987	-0.104744
61	1	0	7.424098	5.622457	-0.736671
62	1	0	4.957858	5.354064	-0.598497
63	1	0	9.403044	5.537614	0.536068
64	1	0	11.846773	5.779983	0.325388
65	1	0	13.173578	4.048357	-0.852179
66	1	0	12.026187	2.076361	-1.826812
67	1	0	9.580350	1.845783	-1.637378
68	1	0	-2.113693	-2.650458	-1.507934
69	1	0	-0.352373	-4.888365	-0.887527
70	1	0	-2.008244	-4.939319	-1.546926
71	1	0	-0.614749	-4.658964	-2.621484
72	1	0	2.605826	-2.752451	-0.475484
73	8	0	3.513144	-2.981547	-0.155714
74	6	0	4.369142	-2.009701	-0.400236
75	8	0	4.068459	-0.960431	-0.930173
76	6	0	5.759010	-2.311986	0.055362
77	6	0	6.028142	-3.461731	0.799744
78	6	0	7.325584	-3.703076	1.228402
79	6	0	8.356814	-2.788583	0.936367
80	6	0	8.064017	-1.634991	0.202394
81	6	0	6.766533	-1.413555	-0.255303
82	1	0	5.220888	-4.146361	1.012921
83	8	0	7.710670	-4.807897	1.916021
84	8	0	9.647100	-3.044660	1.286023
85	8	0	9.006548	-0.711635	-0.135412
86	1	0	6.557580	-0.538674	-0.857306
87	6	0	6.723341	-5.786135	2.179974
88	1	0	7.231924	-6.589501	2.707638
89	1	0	5.924492	-5.381889	2.808915
90	1	0	6.296110	-6.172135	1.249899
91	6	0	9.924295	-3.131322	2.682467
92	1	0	11.004976	-3.037609	2.782296
93	1	0	9.435785	-2.313694	3.221873
94	1	0	9.593288	-4.086110	3.087803
95	6	0	9.952700	-0.320214	0.858176
96	1	0	10.255735	0.695537	0.602958
97	1	0	9.488798	-0.319227	1.849328
98	1	0	10.818147	-0.981036	0.857075
99	1	0	-4.819383	-0.945109	0.228968
100	8	0	-5.307448	-1.797494	0.379383
101	6	0	-4.938147	-2.717980	-0.489241
102	8	0	-4.052906	-2.555302	-1.306055
103	6	0	-5.708667	-3.988230	-0.377268
104	6	0	-6.655657	-4.158875	0.635255
105	6	0	-7.361148	-5.351080	0.705313
106	6	0	-7.122274	-6.380285	-0.227886
107	6	0	-6.163595	-6.192609	-1.228941
108	6	0	-5.464045	-4.988577	-1.301418
109	1	0	-6.828776	-3.352463	1.332019
110	8	0	-8.331787	-5.611750	1.617448
111	8	0	-7.870351	-7.518532	-0.221685
112	8	0	-5.901839	-7.104683	-2.198562
113	1	0	-4.737595	-4.846860	-2.090625
114	6	0	-5.836441	-8.482415	-1.852145

115	1	0	-5.204172	-8.947557	-2.607196
116	1	0	-5.374805	-8.612592	-0.868379
117	1	0	-6.824358	-8.941054	-1.857972
118	6	0	-7.732412	-8.357589	0.922977
119	1	0	-8.228720	-9.293795	0.671786
120	1	0	-6.675040	-8.549174	1.132216
121	1	0	-8.203999	-7.909266	1.796279
122	6	0	-8.662400	-4.580451	2.527461
123	1	0	-9.465504	-4.973491	3.146255
124	1	0	-7.807148	-4.320392	3.158275
125	1	0	-9.010380	-3.688228	1.998759

Complex **1•12GA-l**; E(RM062X) = -2610.57328078 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	4.211894	1.292927	0.261557
2	6	0	3.868283	0.002758	-0.021054
3	6	0	5.027721	-0.732766	-0.088665
4	7	0	6.009422	0.166704	0.162213
5	7	0	5.490111	1.386205	0.370762
6	6	0	2.473662	-0.410099	-0.209514
7	6	0	1.452059	0.527706	-0.066018
8	6	0	0.123836	0.150691	-0.245310
9	6	0	-0.191712	-1.170786	-0.562468
10	6	0	0.824632	-2.111583	-0.701255
11	6	0	2.149160	-1.727823	-0.523644
12	6	0	0.586024	-3.567946	-1.028482
13	7	0	-0.687951	-3.935560	-1.273755
14	6	0	-1.001941	-5.316122	-1.581898
15	6	0	-0.951010	1.140648	-0.113567
16	6	0	-0.902965	2.509970	-0.225508
17	7	0	-2.184504	2.913391	-0.042922
18	7	0	-2.984107	1.869940	0.166048
19	7	0	-2.252458	0.806303	0.122730
20	6	0	-2.715942	4.234492	-0.071490
21	6	0	-1.912083	5.311244	0.281914
22	6	0	-2.437483	6.594475	0.232132
23	6	0	-3.762446	6.815916	-0.150826
24	6	0	-4.551680	5.711549	-0.487789
25	6	0	-4.037561	4.425150	-0.458032
26	6	0	-4.320646	8.189006	-0.192185
27	6	0	-3.566067	9.250267	-0.698945
28	6	0	-4.090207	10.536123	-0.735963
29	6	0	-5.375631	10.780723	-0.265490
30	6	0	-6.134491	9.731543	0.241642
31	6	0	-5.611494	8.445284	0.277120
32	6	0	7.414193	-0.039419	0.218077
33	6	0	7.920873	-1.284062	0.573209
34	6	0	9.294500	-1.475678	0.606460
35	6	0	10.175414	-0.434495	0.304528
36	6	0	9.638829	0.811526	-0.034270
37	6	0	8.268997	1.014840	-0.086001
38	6	0	11.642529	-0.645439	0.347693
39	6	0	12.487718	0.331782	0.880617
40	6	0	13.861800	0.133013	0.921613
41	6	0	14.413025	-1.045368	0.430018
42	6	0	13.581153	-2.024201	-0.102802
43	6	0	12.207025	-1.825774	-0.143594
44	8	0	1.516969	-4.356088	-1.052280
45	1	0	-1.233012	-1.428163	-0.712602
46	1	0	1.714005	1.545182	0.200990
47	1	0	2.908861	-2.492593	-0.636660
48	1	0	-0.103854	3.190909	-0.459430
49	1	0	5.227595	-1.765596	-0.313803
50	1	0	-0.897090	5.149389	0.623546
51	1	0	-1.820471	7.433862	0.530522
52	1	0	-5.574498	5.866554	-0.810477
53	1	0	-4.639469	3.569554	-0.733420

54	1	0	-2.572739	9.060545	-1.090505
55	1	0	-3.496476	11.346987	-1.140585
56	1	0	-5.783762	11.783673	-0.294445
57	1	0	-7.133549	9.915679	0.618239
58	1	0	-6.197433	7.635157	0.696749
59	1	0	7.251767	-2.088491	0.852531
60	1	0	9.688724	-2.438886	0.908532
61	1	0	10.305284	1.625721	-0.294017
62	1	0	7.849190	1.972787	-0.361618
63	1	0	12.060936	1.241120	1.288941
64	1	0	14.503229	0.896446	1.345441
65	1	0	15.484667	-1.200120	0.461692
66	1	0	14.003398	-2.941286	-0.496173
67	1	0	11.564816	-2.580528	-0.583679
68	1	0	-1.440006	-3.262143	-1.309336
69	1	0	-0.404502	-5.971692	-0.948657
70	1	0	-2.061134	-5.484339	-1.390848
71	1	0	-0.780476	-5.557625	-2.625486
72	1	0	-3.308379	-0.604099	0.425931
73	8	0	-4.043445	-1.239913	0.632093
74	6	0	-4.036975	-2.247681	-0.218569
75	8	0	-3.195393	-2.390216	-1.083462
76	6	0	-5.160828	-3.206262	-0.024823
77	6	0	-6.070783	-3.041710	1.021930
78	6	0	-7.107146	-3.953022	1.165062
79	6	0	-7.234048	-5.037362	0.273781
80	6	0	-6.306415	-5.189608	-0.761359
81	6	0	-5.275510	-4.263695	-0.910232
82	1	0	-5.956557	-2.199421	1.687868
83	8	0	-8.073406	-3.868403	2.114959
84	8	0	-8.291246	-5.892290	0.353528
85	8	0	-6.379010	-6.177317	-1.689523
86	1	0	-4.572854	-4.381519	-1.724246
87	6	0	-6.681957	-7.498308	-1.257869
88	1	0	-6.250475	-8.162516	-2.005377
89	1	0	-6.219428	-7.702418	-0.287071
90	1	0	-7.757472	-7.658522	-1.193230
91	6	0	-8.375081	-6.683315	1.536995
92	1	0	-9.133935	-7.439580	1.341474
93	1	0	-7.416178	-7.171552	1.738502
94	1	0	-8.665393	-6.077419	2.394130
95	6	0	-8.024430	-2.762288	2.994991
96	1	0	-8.883787	-2.865164	3.653367
97	1	0	-7.105328	-2.769239	3.588507
98	1	0	-8.096229	-1.819533	2.444777

Complex **1•12GA-r**; E(RM062X) = -2610.57986701 au

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.675096	1.929423	-0.375185
2	6	0	-0.212403	0.705107	-0.759187
3	6	0	1.145897	0.797176	-0.934300
4	7	0	1.427783	2.082641	-0.631122
5	7	0	0.312581	2.753827	-0.297750
6	6	0	-1.060496	-0.478528	-0.903971
7	6	0	-2.436974	-0.396993	-0.710203
8	6	0	-3.237745	-1.533419	-0.815254
9	6	0	-2.652650	-2.761922	-1.122790
10	6	0	-1.277184	-2.842511	-1.330848
11	6	0	-0.482189	-1.709645	-1.213726
12	6	0	-0.587691	-4.130338	-1.659811
13	7	0	-1.338988	-5.084731	-2.244041
14	6	0	-0.761359	-6.358573	-2.632663
15	6	0	-4.685874	-1.459354	-0.594169
16	6	0	-5.483600	-0.385778	-0.276117
17	7	0	-6.731901	-0.906966	-0.201117
18	7	0	-6.709234	-2.223488	-0.459660
19	7	0	-5.490018	-2.556896	-0.696014
20	6	0	-7.956927	-0.250328	0.096615
21	6	0	-7.955429	0.912071	0.859266
22	6	0	-9.156562	1.552095	1.128266
23	6	0	-10.367992	1.038082	0.659563
24	6	0	-10.341590	-0.139734	-0.093955
25	6	0	-9.148849	-0.782644	-0.383968
26	6	0	-11.650473	1.717961	0.962058
27	6	0	-11.748673	3.111270	0.917168
28	6	0	-12.950887	3.745752	1.202723
29	6	0	-14.074190	2.997371	1.538042
30	6	0	-13.987282	1.610261	1.586260
31	6	0	-12.785445	0.975603	1.300395
32	6	0	2.711456	2.688189	-0.607697
33	6	0	3.826664	1.876948	-0.430288
34	6	0	5.092075	2.439989	-0.460002
35	6	0	5.259330	3.815744	-0.643058
36	6	0	4.119763	4.612809	-0.790295
37	6	0	2.846891	4.059721	-0.781239
38	6	0	6.619417	4.404903	-0.683218
39	6	0	6.885568	5.640456	-0.086619
40	6	0	8.162711	6.185825	-0.123296
41	6	0	9.196476	5.504435	-0.756893
42	6	0	8.943702	4.273614	-1.353686
43	6	0	7.666363	3.727997	-1.317922
44	8	0	0.601932	-4.317623	-1.420486
45	1	0	-3.289378	-3.638291	-1.155019
46	1	0	-2.864120	0.569052	-0.465541
47	1	0	0.588243	-1.797839	-1.369790
48	1	0	-5.280300	0.660638	-0.132591
49	1	0	1.891668	0.085322	-1.249346
50	1	0	-7.029749	1.298850	1.267494
51	1	0	-9.157101	2.443811	1.744230
52	1	0	-11.268618	-0.541153	-0.486712
53	1	0	-9.124319	-1.685940	-0.978194

54	1	0	-10.882659	3.698083	0.631299
55	1	0	-13.012777	4.826442	1.154978
56	1	0	-15.011584	3.492707	1.760106
57	1	0	-14.855695	1.020803	1.855608
58	1	0	-12.716277	-0.104634	1.365217
59	1	0	3.705788	0.813515	-0.260741
60	1	0	5.955528	1.797379	-0.322808
61	1	0	4.231819	5.678217	-0.955374
62	1	0	1.962428	4.667565	-0.918713
63	1	0	6.089948	6.164067	0.431913
64	1	0	8.352353	7.141293	0.351411
65	1	0	10.192271	5.929901	-0.786722
66	1	0	9.741238	3.739662	-1.857127
67	1	0	7.472896	2.774880	-1.799198
68	1	0	-2.257058	-4.837739	-2.575046
69	1	0	-0.086481	-6.692601	-1.846570
70	1	0	-1.560027	-7.087059	-2.760995
71	1	0	-0.191991	-6.273751	-3.561740
72	1	0	2.006957	-3.729723	-0.635349
73	8	0	2.861542	-3.622294	-0.152558
74	6	0	3.466746	-2.498736	-0.488679
75	8	0	3.003448	-1.687589	-1.263308
76	6	0	4.780294	-2.305847	0.194259
77	6	0	5.182958	-3.169298	1.214896
78	6	0	6.397755	-2.949063	1.848153
79	6	0	7.209854	-1.859020	1.477951
80	6	0	6.782132	-0.995319	0.465219
81	6	0	5.574910	-1.237417	-0.189015
82	1	0	4.544700	-3.998785	1.480386
83	8	0	6.907893	-3.742282	2.823404
84	8	0	8.436622	-1.674079	2.035408
85	8	0	7.511678	0.071438	0.039424
86	1	0	5.270658	-0.585730	-0.998300
87	6	0	6.146423	-4.870780	3.208287
88	1	0	6.722021	-5.370012	3.984027
89	1	0	5.173279	-4.571689	3.609103
90	1	0	6.000550	-5.552401	2.365261
91	6	0	8.474993	-1.433779	3.441050
92	1	0	9.413531	-0.915249	3.635203
93	1	0	7.637421	-0.798652	3.745464
94	1	0	8.443353	-2.369977	3.995844
95	6	0	8.179749	0.872271	1.014194
96	1	0	8.258044	1.870168	0.581835
97	1	0	7.593296	0.923928	1.936672
98	1	0	9.171353	0.477984	1.229991
