Electronic Supplementary Information for:

Synthesis of Chiral Large-ring Triangular Salen Ligands and Structural Characterization of Their Complexes

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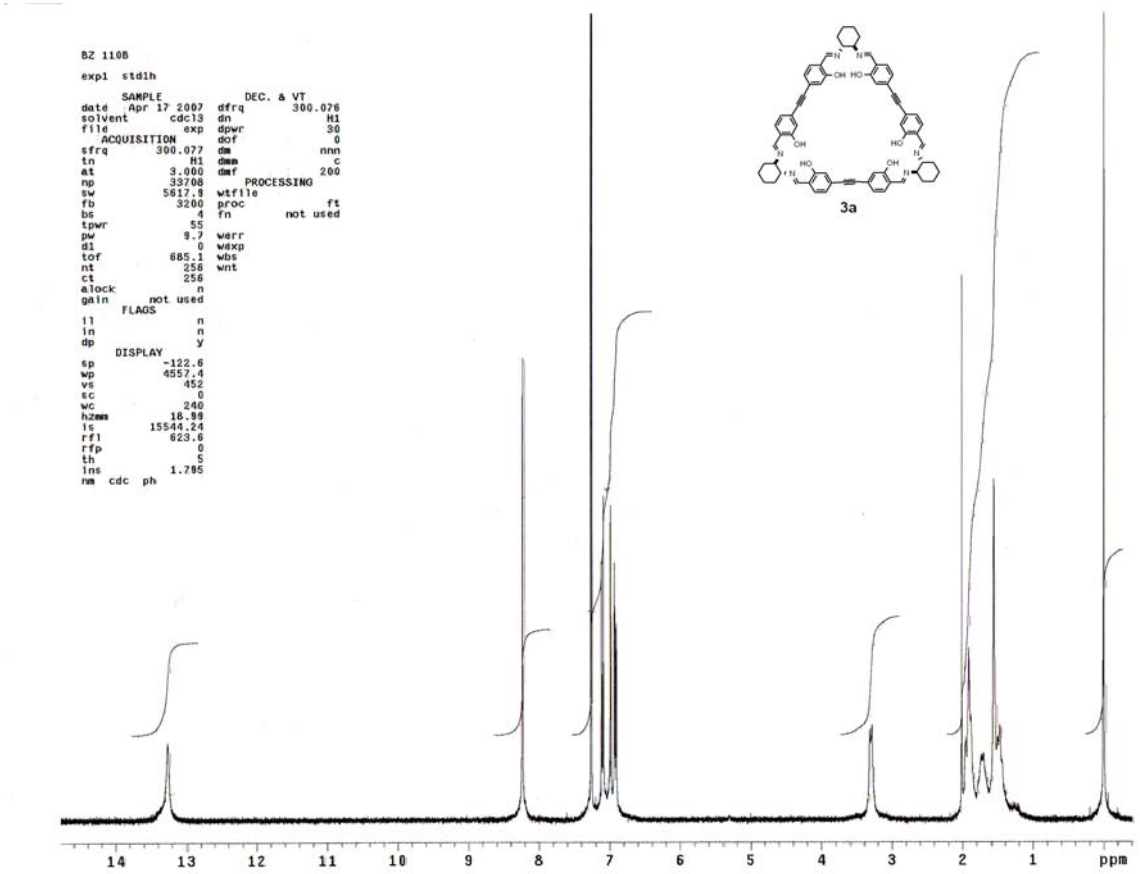


Figure S1. The ^{1}H NMR spectrum of macrocycle **3a**

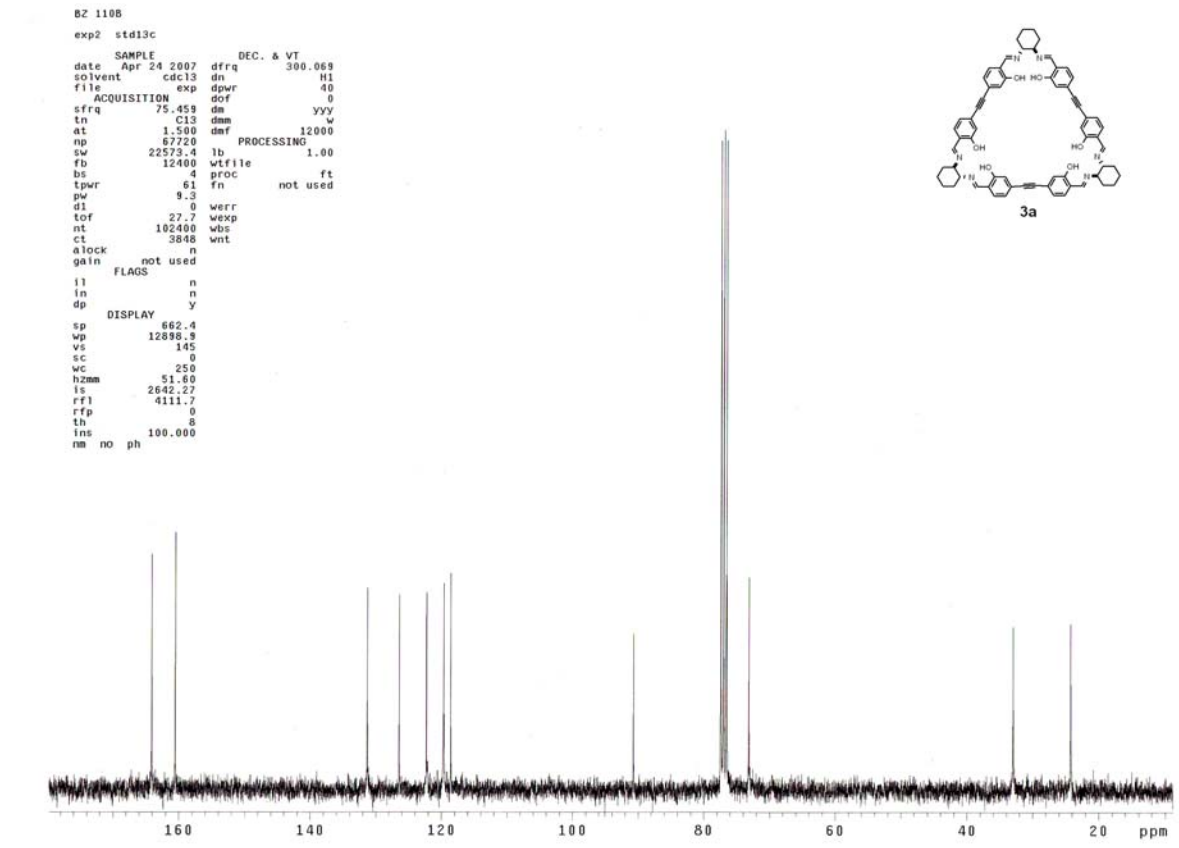


Figure S2. The ^{13}C NMR spectrum of macrocycle **3a**

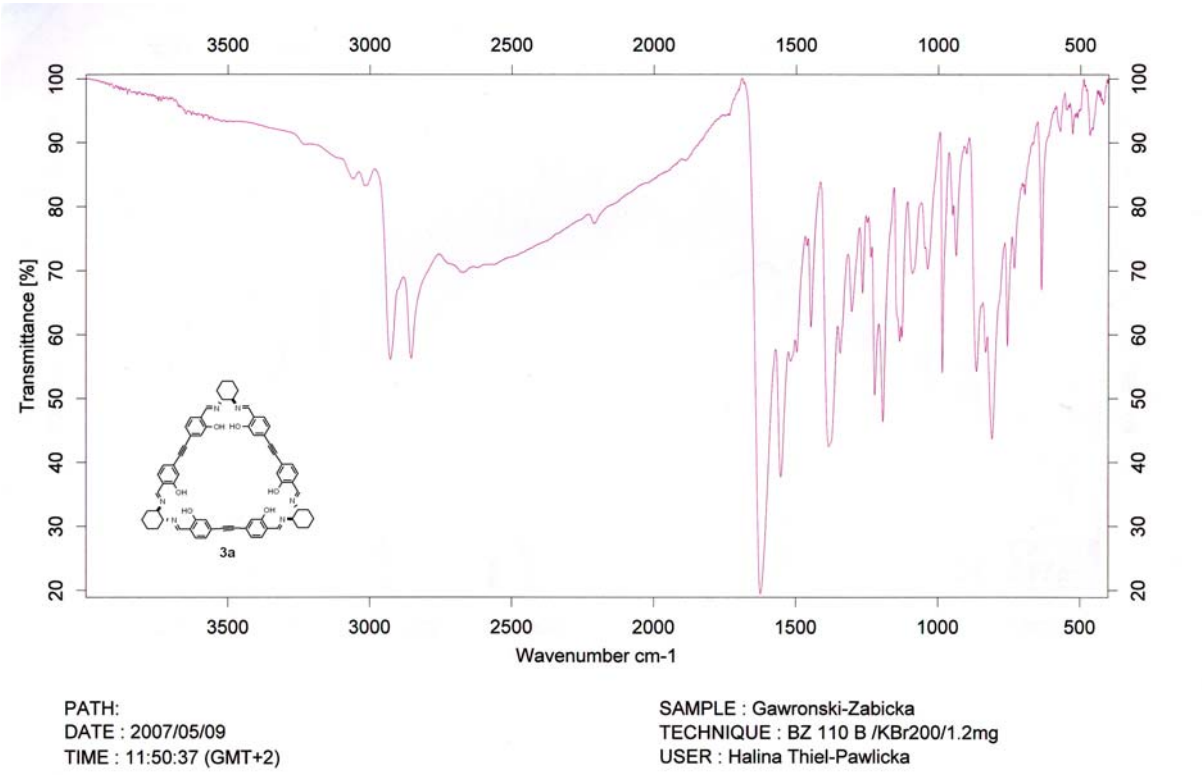


Figure S3. The IR spectrum of macrocycle **3a**

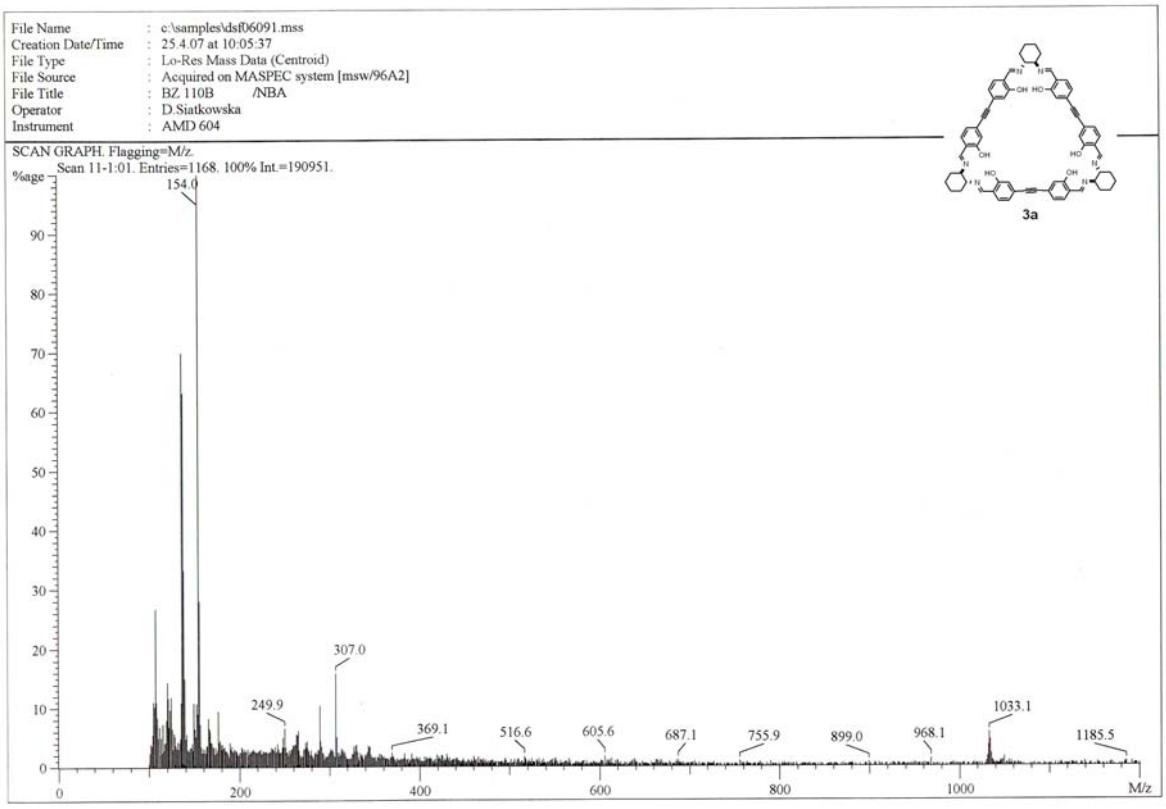


Figure S4. The MS spectrum of macrocycle **3a**

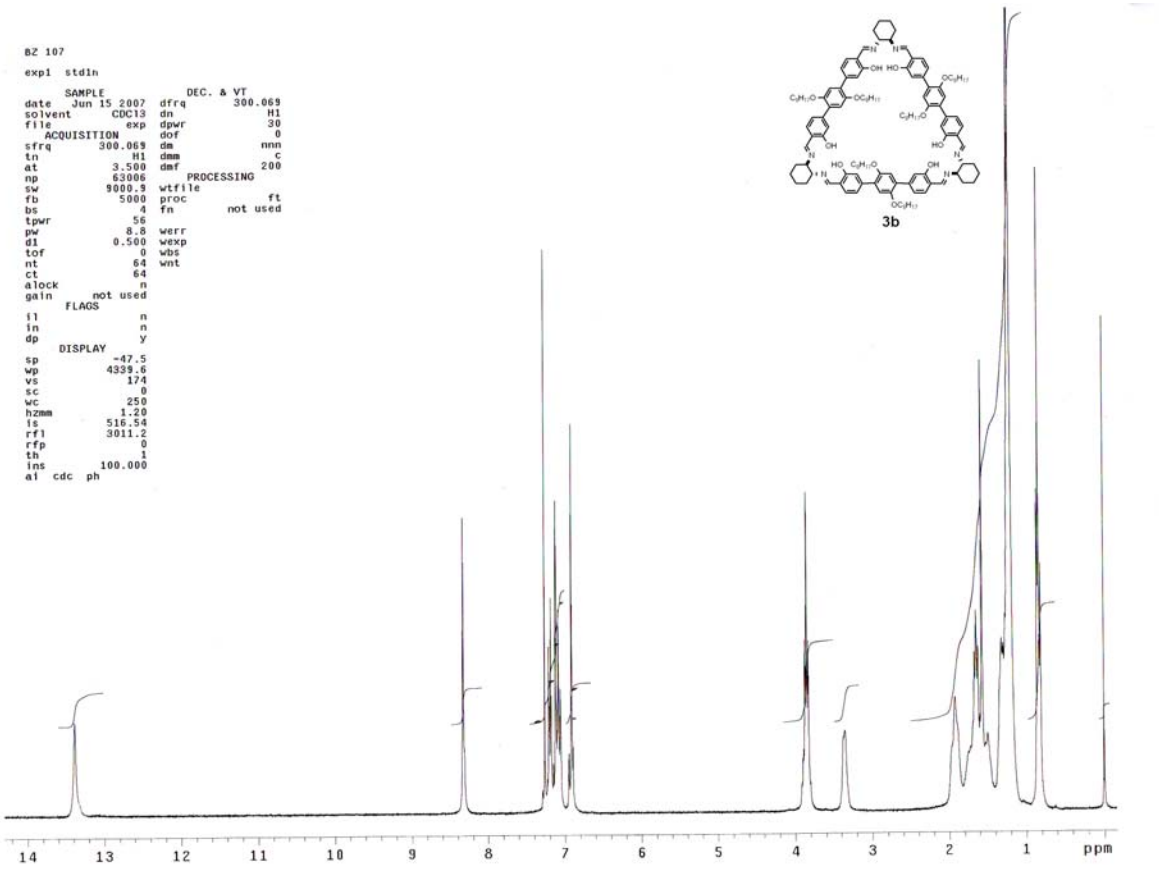


Figure S5. The ^{1}H NMR spectrum of macrocycle **3b**

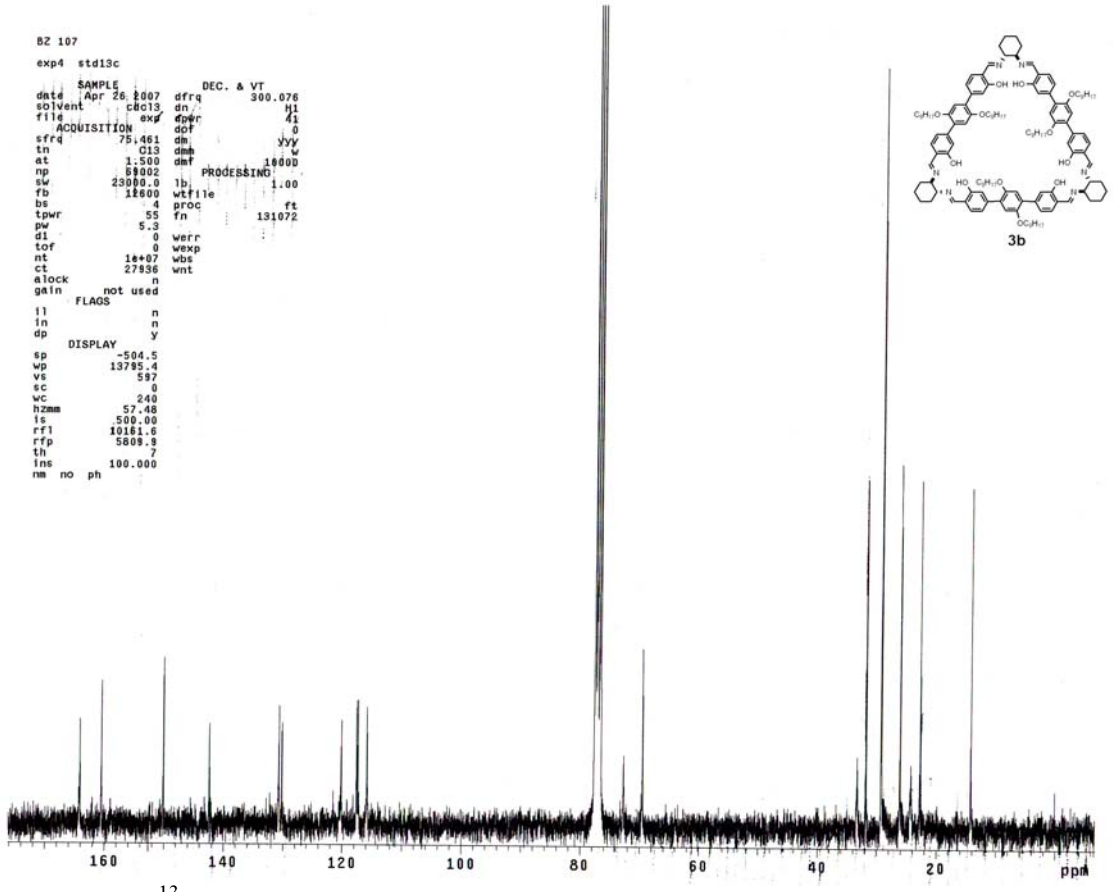


Figure S6. The ^{13}C NMR spectrum of macrocycle **3b**

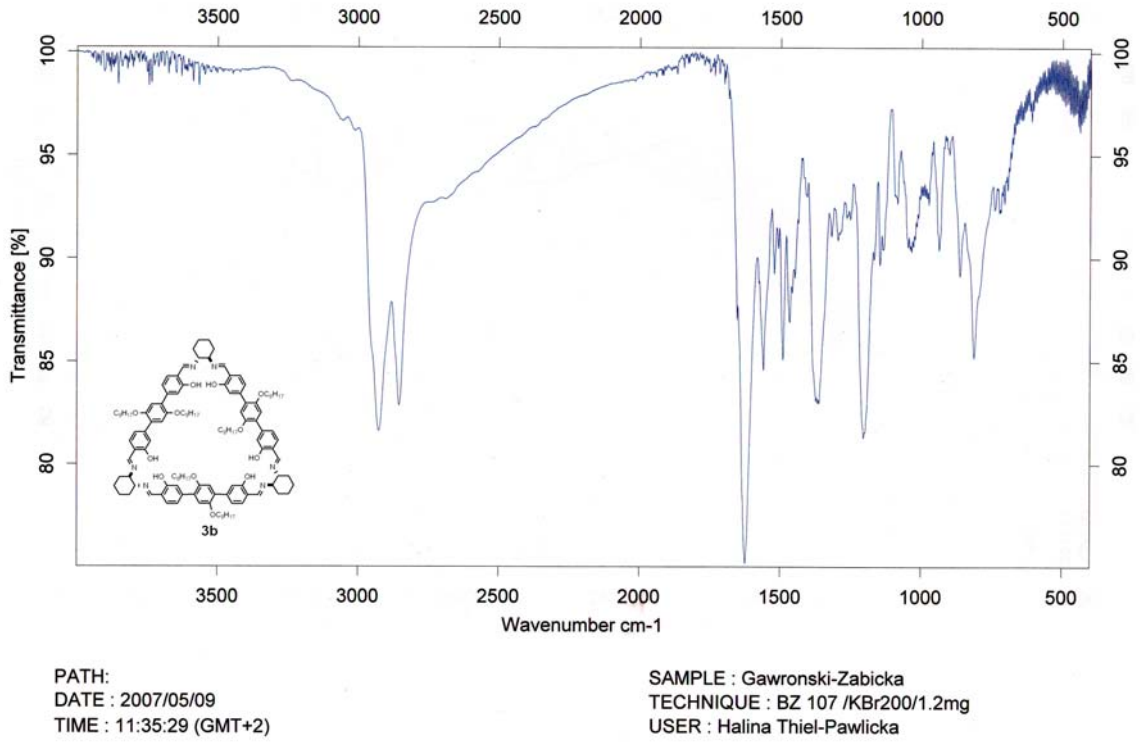


Figure S7. The IR spectrum of macrocycle **3b**

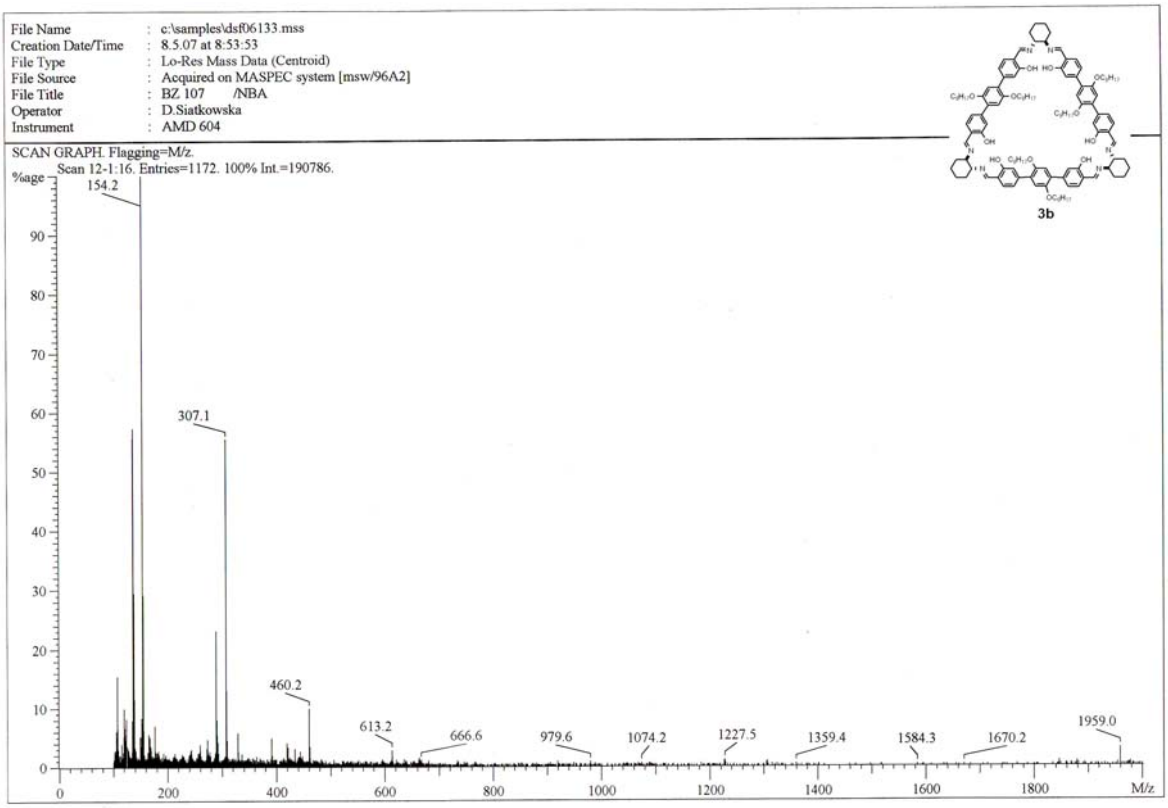


Figure S8. The MS spectrum of macrocycle **3b**

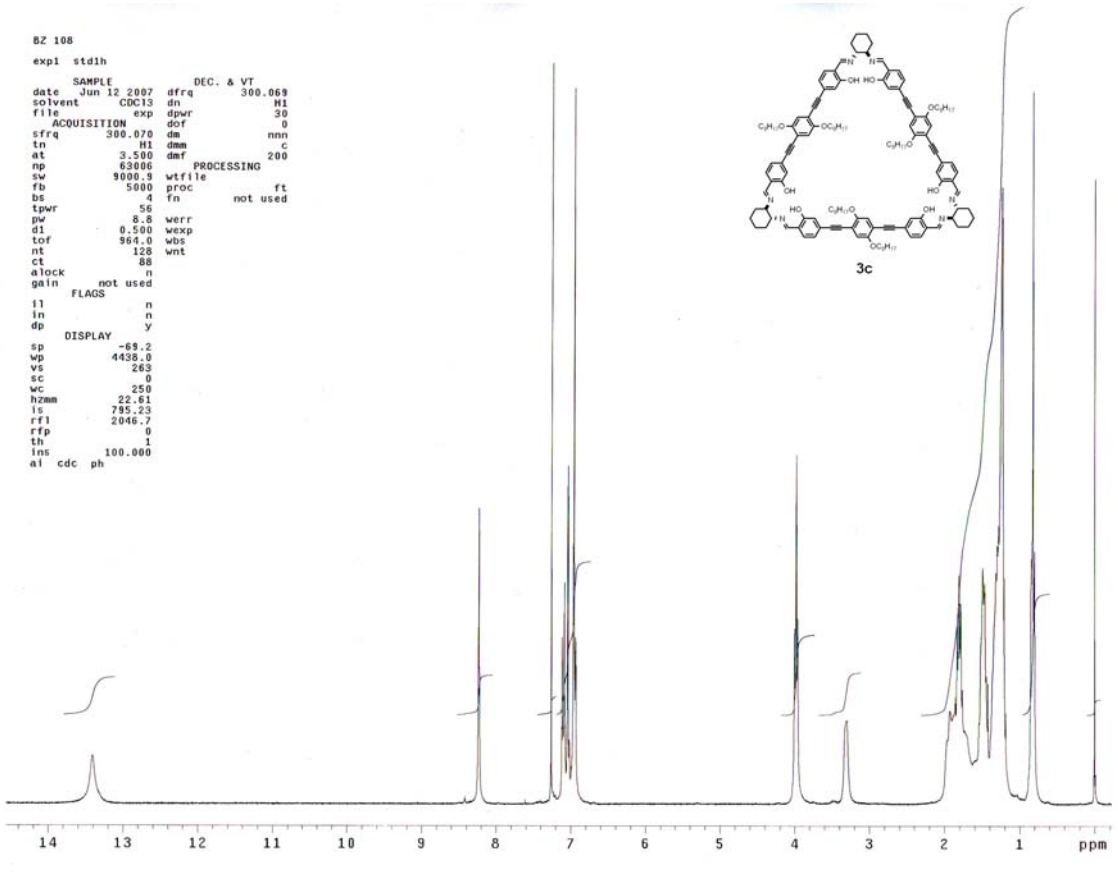


Figure S9. The ^{1}H NMR spectrum of macrocycle **3c**

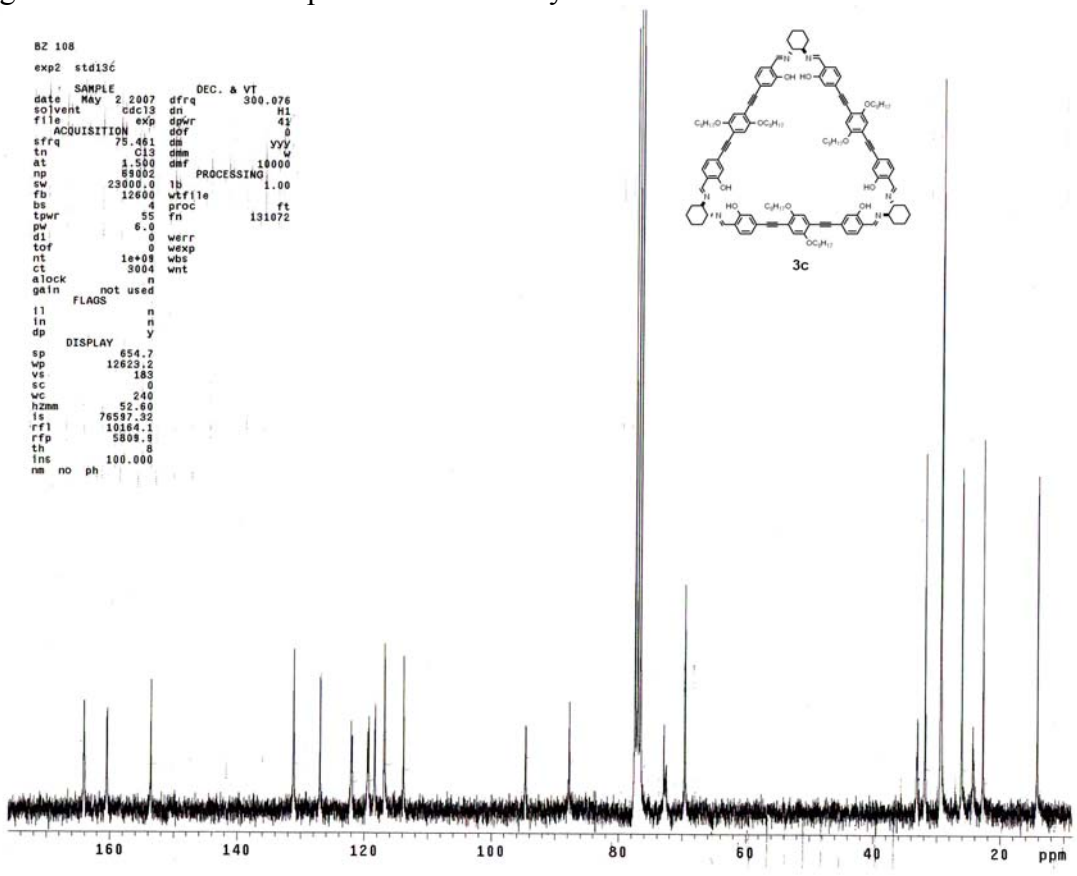


Figure S10. The ^{13}C NMR spectrum of macrocycle **3c**

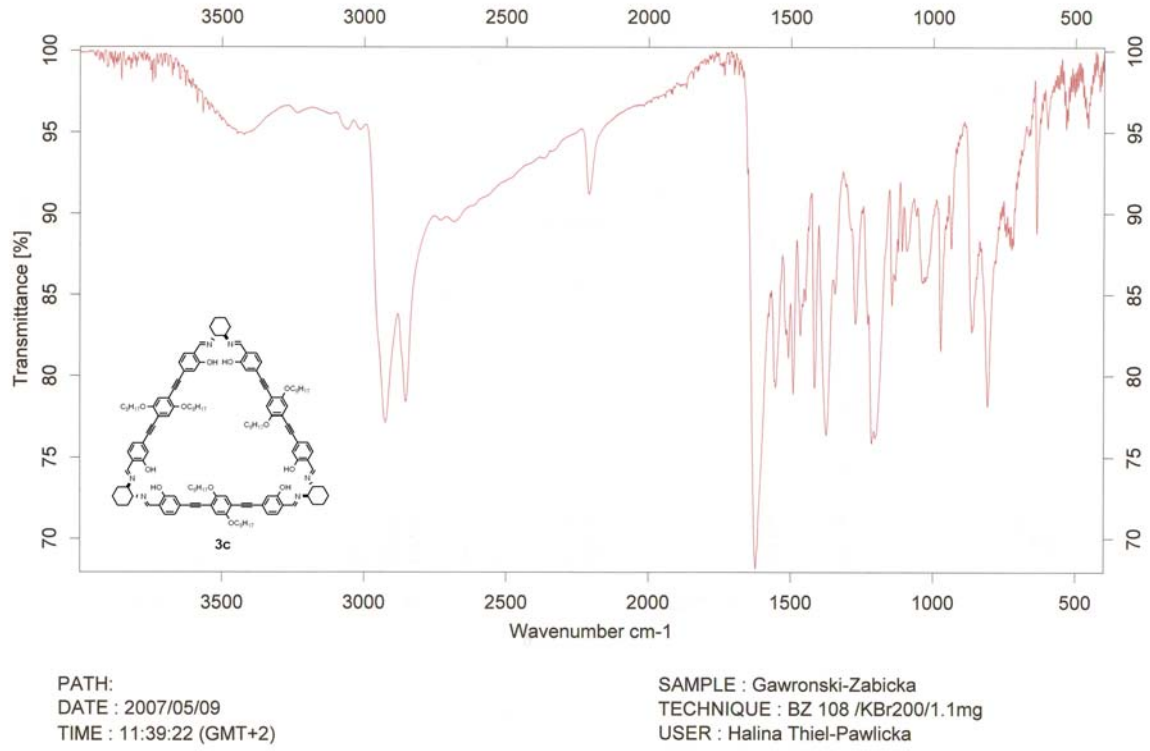


Figure S11. The IR spectrum of macrocycle **3c**

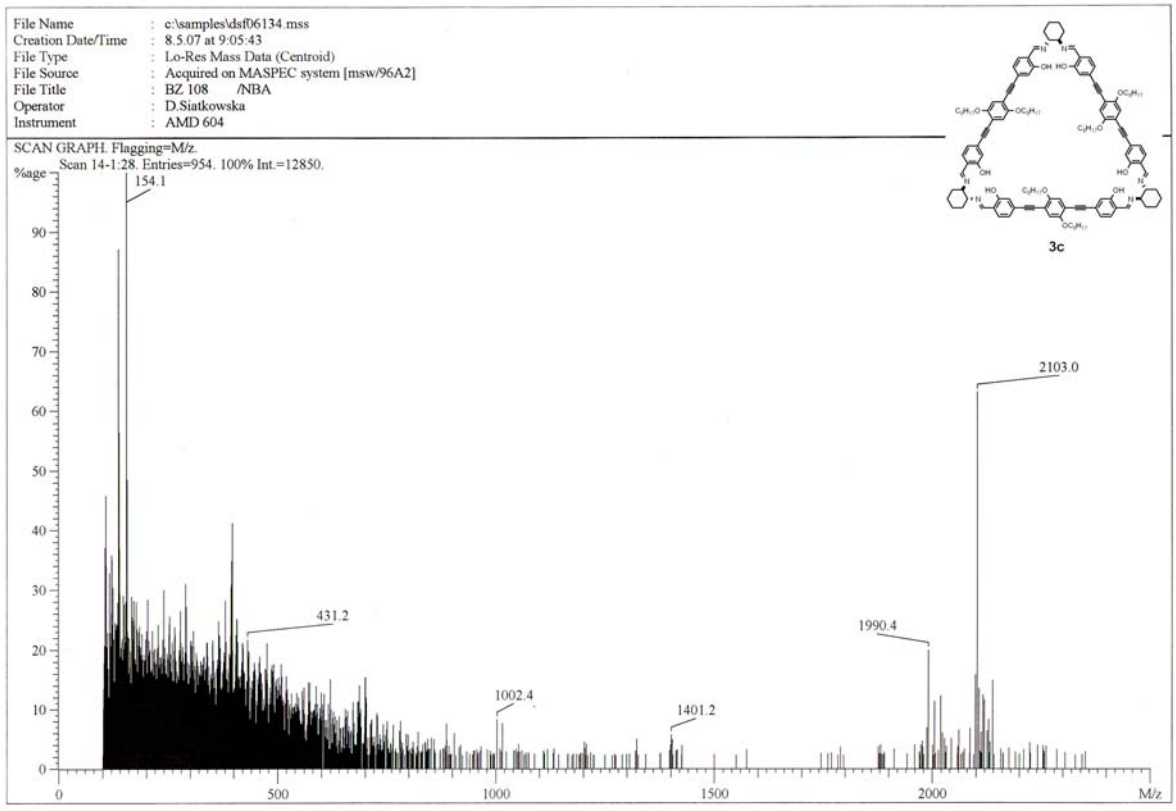


Figure S12. The MS spectrum of macrocycle **3c**

Computational details

Our computational studies were performed as follows: (i) conformational searches for all investigated molecules **3a-3c** and complexes of **3a** with the use CONFLEX[1] software and MM3 force field which allowed of construction of PES for these molecules (ii) full structure optimizations at the B3LYP/6-31g*[2] level were performed for the energy minima found on the PES; (iii) oscillator and rotatory strengths for thermally accessible conformers of **3a-3c** were calculated with the use ZINDO method; (iv) for all optimized structures, frequency calculations were carried out at the B3LYP/6-31g* level of theory to confirm that the conformers are stable. For simplification of structure optimization, the octyl groups were replaced by the methyl groups in the cases of **3b** and **3c**.

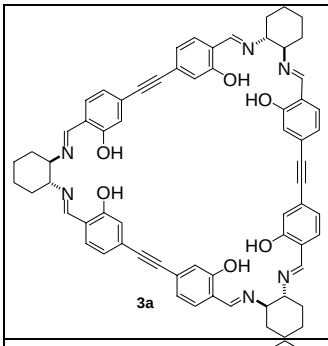
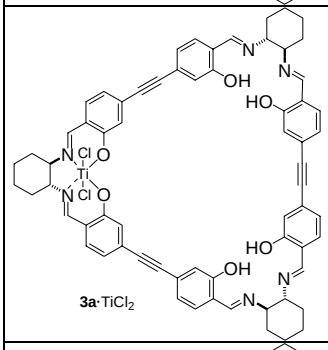
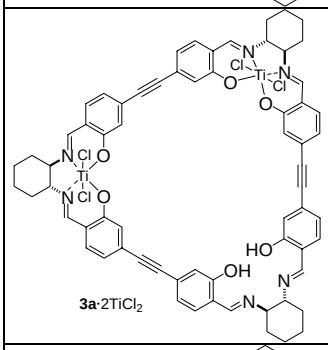
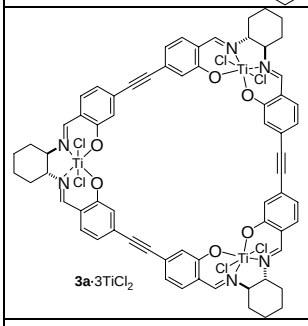
Calculations for simple compounds ($TiCl_4$, HCl, $ZnEt_2$, ethane) were performed at B3LYP/6-31g* level for the structures of the highest symmetry available.

Note, that in the case of **3a**·nZn there are two different coordination pattern possible: square planar and tetrahedral. However, the square planar complexes of **3a**·nZn are not stable and during energy optimization process they change their conformation to tetrahedral complexes.

Rotatory strengths were calculated using both length and velocity representations. In the present study the differences between the values of rotatory strengths calculated in length and velocity representations were quite small, and for this reason only velocity representations were taken into account. The computed oscillator strengths and rotational strengths were converted to the UV and CD spectra by broadening to gaussian shape absorption curves, according to the procedure described by Grimme et al.[3]

1. CAChe WS Pro ver. 4.5, Fujitsu Ltd. 2001
2. Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.
3. Diedrich, C.; Grimme, S. *J. Phys. Chem. A* **2003**, *107*, 2524.

Table A. B3LYP/6-31g* computed total electronic energies (HF, Hartree) zero-point energies (ZPE, kcal mol^{-1}), thermal correction to Gibbs free energy (G, Hartree) and the sum of electronic and thermal free energies (G_{tot}, Hartree) for **3a**, **3a**·n$TiCl_2$, $TiCl_4$ and HCl.

 **3a**	HF = -3330.917517 ZPE = 707.94 G = 1.01722 G_{tot} = -3329.90030
 **3a**·$TiCl_2$	HF = -5099.708625 ZPE = 697.47 G = 0.99758 G_{tot} = -5098.81305
 **3a**·$2TiCl_2$	HF = -6868.708625 ZPE = 687.04 G = 0.98008 G_{tot} = -6867.72854
 **3a**·$3TiCl_2$	HF = -8637.608771 ZPE = 661.23 G = 0.948761 G_{tot} = -8636.66001
$TiCl_4$	HF = -2690.478512 ZPE = 3.62 G = 0.02604 G_{tot} = -2690.50456
HCl	HF = -460.795694 ZPE = 4.19 G = -0.01122 G_{tot} = -460.80691

Scheme A. Thermodynamics of complexation reactions

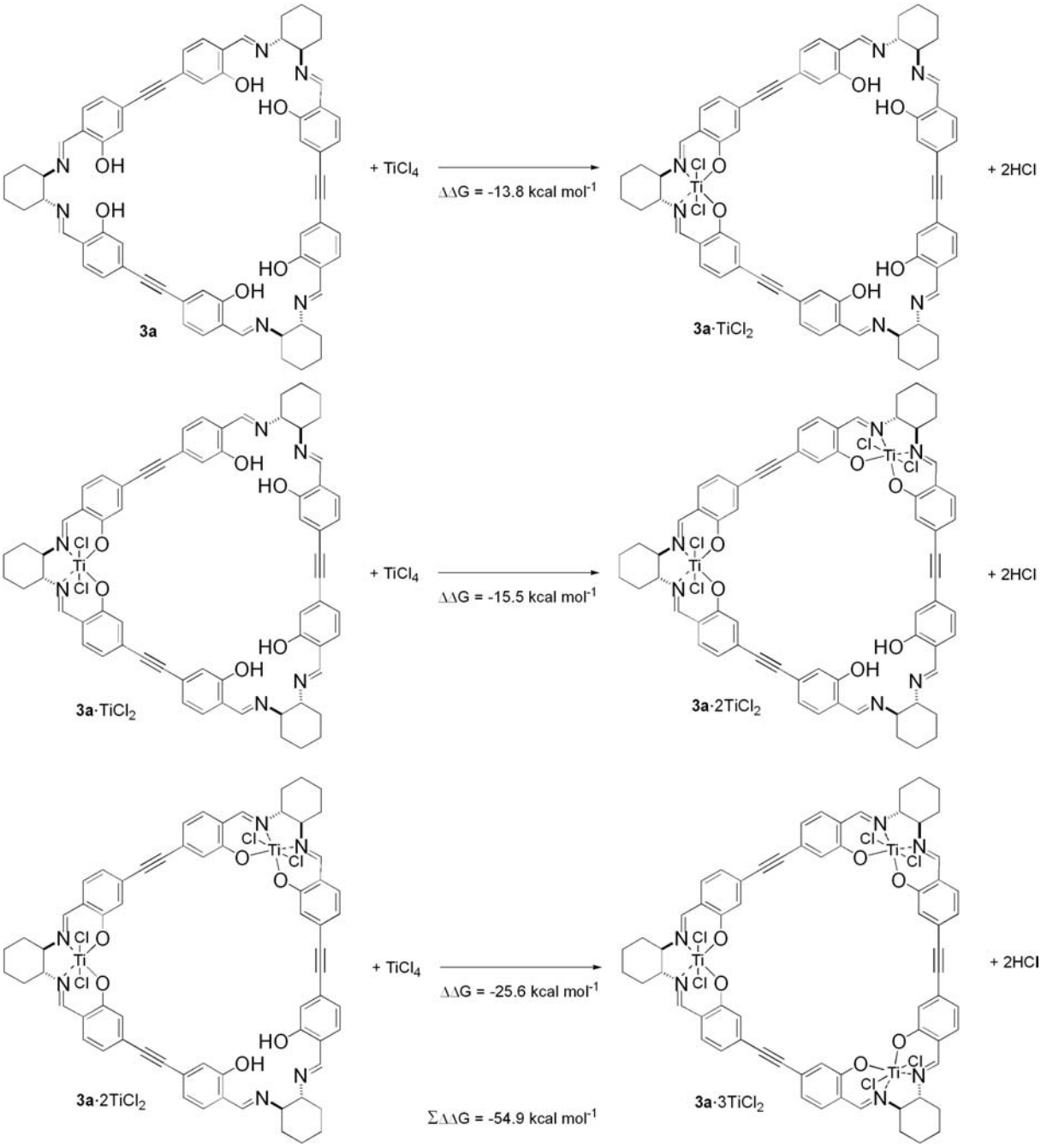
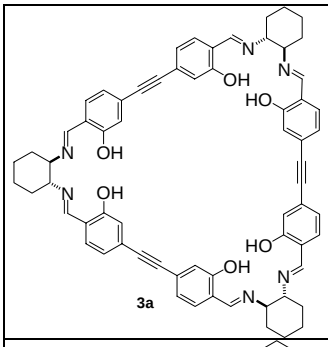
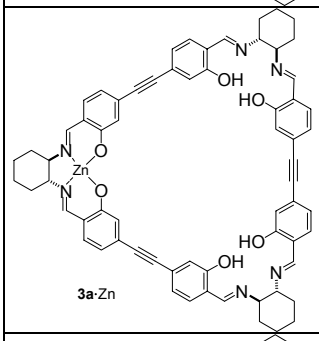
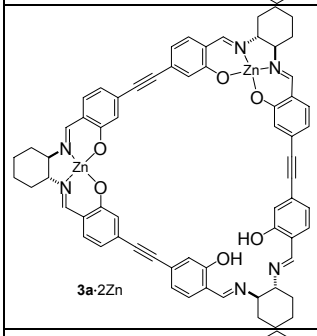
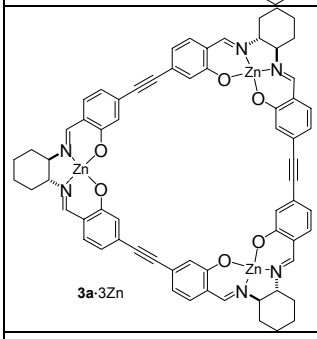
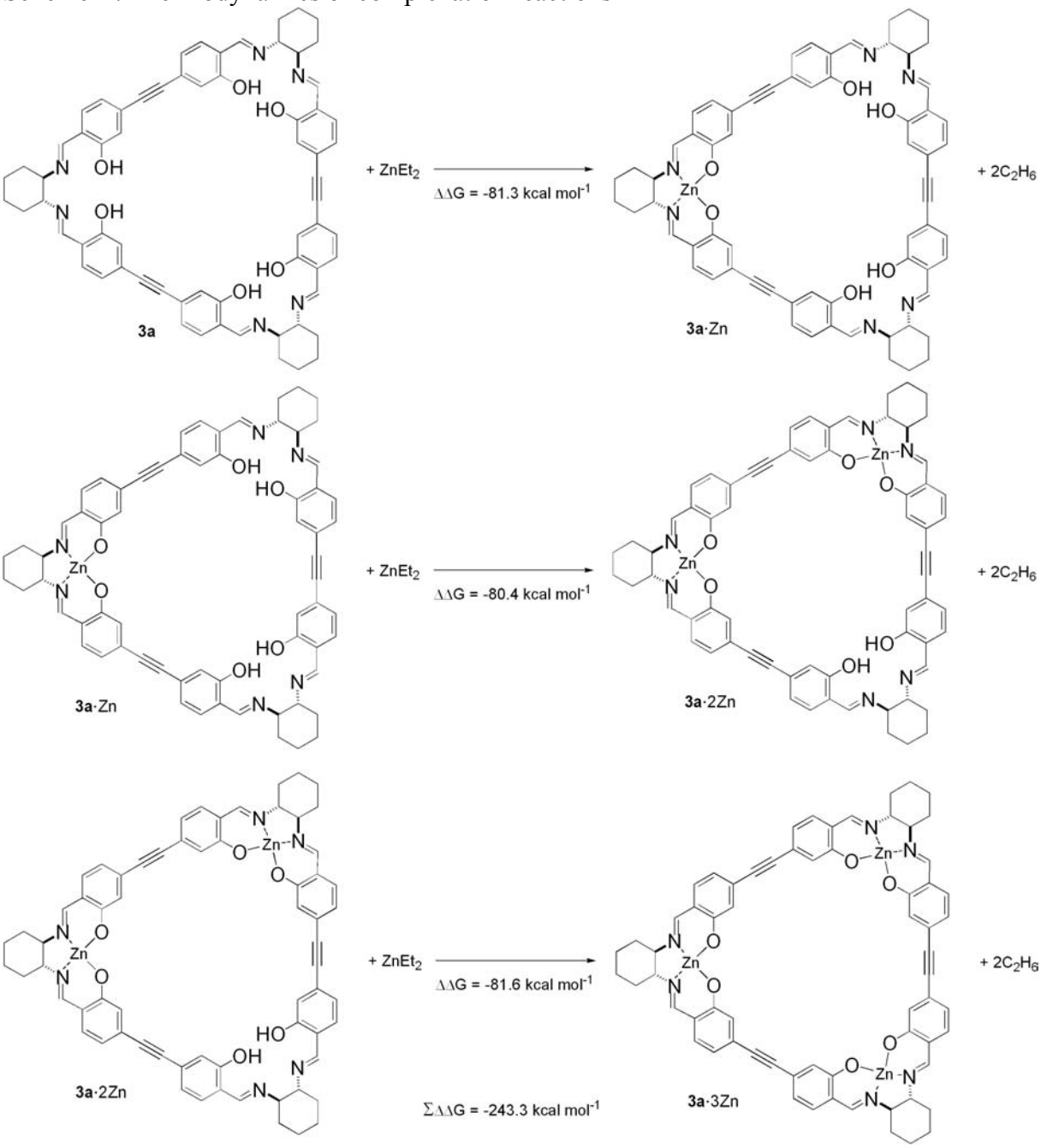


Table B. B3LYP/6-31g* computed total electronic energies (HF, Hartree) zero-point energies (ZPE, kcal mol^{-1}), thermal correction to Gibbs free energy (G, Hartree) and the sum of electronic and thermal free energies (G_{tot}, Hartree) for **3a**, **3a**·nZn, $ZnEt_2$ and C_2H_6.

 **3a**	HF = -3330.917517 ZPE = 707.94 G = 1.01722 G_{tot} = -3329.90030
 **3a**·Zn	HF = -5108.933799 ZPE = 694.41 G = 0.99547 G_{tot} = -5107.93833
 **3a**·2Zn	HF = -6886.952502 ZPE = 680.87 G = 0.97753 G_{tot} = -6885.97497
 **3a**·3Zn	HF = -8664.969798 ZPE = 667.30 G = 0.95754 G_{tot} = -8664.01226
$ZnEt_2$	HF = -1937.555801 ZPE = 81.34 G = 0.09533 G_{tot} = -1937.46047
C_2H_6	HF = -79.830417 ZPE = 47.21 G = 0.05381 G_{tot} = -79.77661

Scheme B. Thermodynamics of complexation reactions



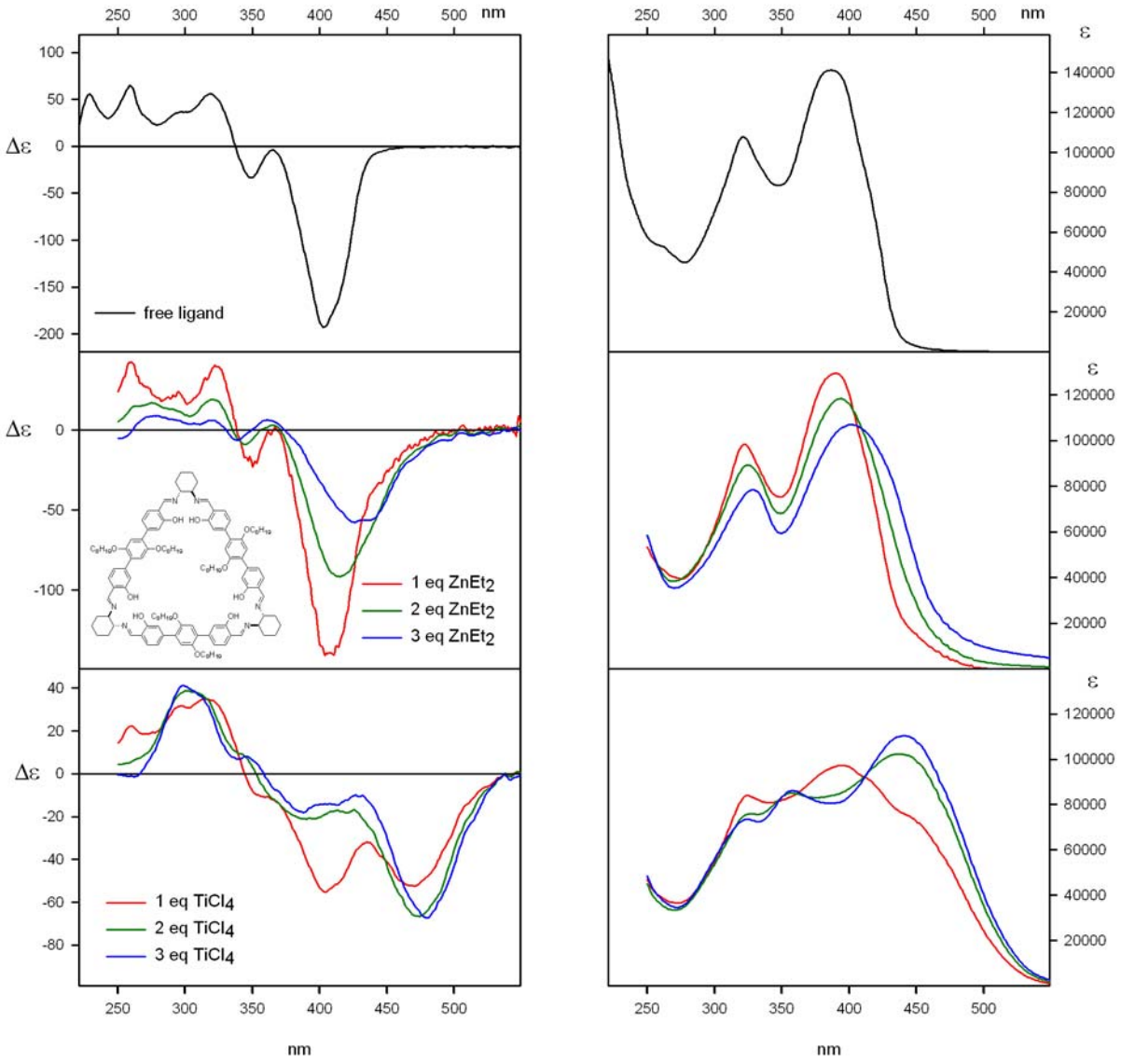


Figure S13. Changes in the UV/VIS (upper panels) and CD (lower panels) spectra of **3b** upon addition of aliquots of $ZnEt_2$ and $TiCl_4$ (solvent CH_2Cl_2).

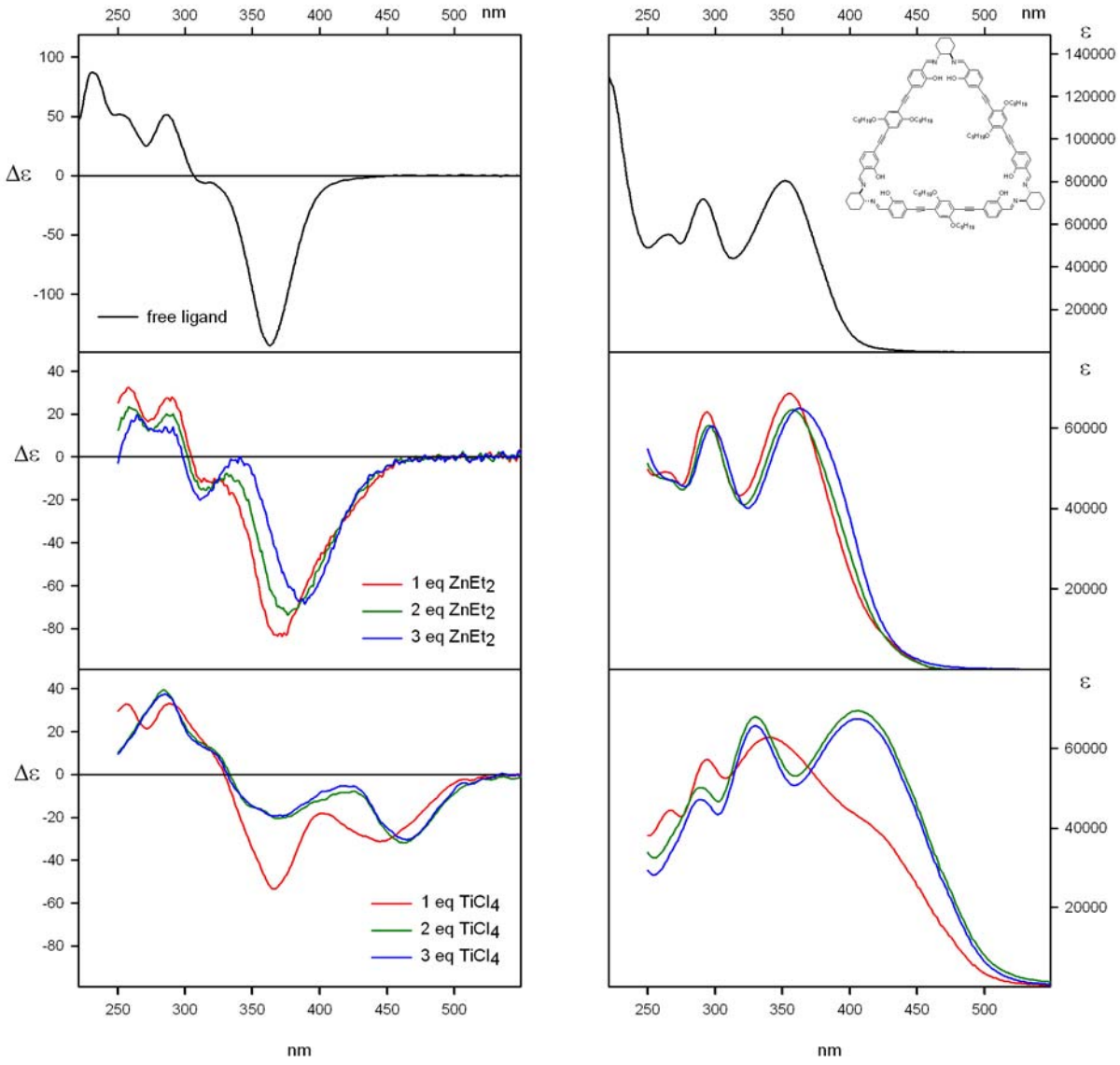


Figure S14. Changes in the UV/VIS (upper panels) and CD (lower panels) spectra of **3c** upon addition of aliquots of $ZnEt_2$ and $TiCl_4$ (solvent CH_2Cl_2).

Table C1. Cartesian coordinates for **3a**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.697875	6.867381	0.487588
2	6	0	11.296264	5.830941	-0.487588
3	6	0	10.620686	4.455178	-0.300593
4	6	0	9.091167	4.557106	-0.489761
5	6	0	8.492153	5.594628	0.489761
6	6	0	9.168640	6.970194	0.300593
7	7	0	8.479645	3.241390	-0.211284
8	6	0	7.801260	2.625961	-1.129520
9	6	0	7.173478	1.346382	-0.880049
10	6	0	6.457127	0.682476	-1.893050
11	6	0	5.838018	-0.528700	-1.654409
12	6	0	5.915786	-1.109461	-0.360763
13	6	0	6.627980	-0.462892	0.655001
14	6	0	7.269081	0.761302	0.416494
15	1	0	10.920724	6.564196	1.519493
16	1	0	11.156118	7.849737	0.325293
17	1	0	11.145123	6.175526	-1.519493
18	1	0	12.376131	5.736613	-0.325293
19	1	0	11.017586	3.725036	-1.014661
20	1	0	10.816546	4.074112	0.709500
21	1	0	8.855894	4.880509	-1.515312
22	7	0	7.046949	5.722893	0.211284
23	1	0	8.654591	5.229175	1.515312
24	1	0	8.936557	7.330347	-0.709500
25	1	0	8.734768	7.678991	1.014661
26	1	0	7.670808	3.054794	-2.129460
27	1	0	6.390777	1.141263	-2.874500
28	1	0	5.282759	-1.037285	-2.430538
29	6	0	5.247549	-2.338683	-0.101176
30	1	0	6.697343	-0.893930	1.643741
31	8	0	7.954388	1.365273	1.412340
32	6	0	6.174779	5.443109	1.129520
33	6	0	4.752740	5.539223	0.880049
34	6	0	4.293847	5.914558	-0.416494
35	6	0	3.819606	5.250798	1.893050
36	6	0	2.461141	5.320222	1.654409
37	6	0	1.997072	5.677951	0.360763
38	6	0	2.913114	5.971445	-0.655001
39	1	0	6.480933	5.115718	2.129460
40	8	0	5.159555	6.206065	-1.412340
41	1	0	4.183751	4.963944	2.874500
42	1	0	1.743065	5.093646	2.430538
43	6	0	0.598416	5.713852	0.101176
44	1	0	2.574505	6.247034	-1.643741
45	1	0	8.346937	2.263239	1.009363
46	1	0	6.133491	6.097040	-1.009363
47	6	0	-0.598416	5.713852	-0.101176
48	6	0	-1.997072	5.677951	-0.360763
49	6	0	-2.461141	5.320222	-1.654409
50	6	0	-3.819606	5.250798	-1.893050
51	6	0	-4.752740	5.539223	-0.880049
52	6	0	-4.293847	5.914558	0.416494
53	6	0	-2.913114	5.971445	0.655001
54	6	0	-6.174779	5.443109	-1.129520
55	7	0	-7.046949	5.722893	-0.211284
56	6	0	-8.492153	5.594628	-0.489761
57	6	0	-9.168640	6.970194	-0.300593
58	6	0	-10.697875	6.867381	-0.487588
59	6	0	-11.296264	5.830941	0.487588
60	6	0	-10.620686	4.455178	0.300593
61	6	0	-9.091167	4.557106	0.489761
62	1	0	-1.743065	5.093646	-2.430538
63	1	0	-4.183751	4.963944	-2.874500
64	8	0	-5.159555	6.206065	1.412340
65	1	0	-2.574505	6.247034	1.643741
66	1	0	-6.480933	5.115718	-2.129460
67	1	0	-8.654591	5.229175	-1.515312
68	1	0	-8.734768	7.678991	-1.014661
69	1	0	-8.936557	7.330347	0.709500
70	1	0	-10.920724	6.564196	-1.519493

71	1	0	-11.156118	7.849737	-0.325293
72	1	0	-12.376131	5.736613	0.325293
73	1	0	-11.145123	6.175526	1.519493
74	1	0	-10.816546	4.074112	-0.709500
75	1	0	-11.017586	3.725036	1.014661
76	7	0	-8.479645	3.241390	0.211284
77	1	0	-8.855894	4.880509	1.515312
78	1	0	-6.133491	6.097040	1.009363
79	6	0	-7.801260	2.625961	1.129520
80	6	0	-7.173478	1.346382	0.880049
81	6	0	-7.269081	0.761302	-0.416494
82	6	0	-6.627980	-0.462892	-0.655001
83	6	0	-5.915786	-1.109461	0.360763
84	6	0	-5.838018	-0.528700	1.654409
85	6	0	-6.457127	0.682476	1.893050
86	1	0	-7.670808	3.054794	2.129460
87	8	0	-7.954388	1.365273	-1.412340
88	1	0	-6.697343	-0.893930	-1.643741
89	6	0	-5.247549	-2.338683	0.101176
90	1	0	-5.282759	-1.037285	2.430538
91	1	0	-6.390777	1.141263	2.874500
92	1	0	-8.346937	2.263239	-1.009363
93	6	0	-4.649133	-3.375169	-0.101176
94	6	0	-3.918714	-4.568490	-0.360763
95	6	0	-3.714866	-5.508553	0.655001
96	6	0	-2.975234	-6.675860	0.416494
97	6	0	-2.420738	-6.885605	-0.880049
98	6	0	-2.637522	-5.933275	-1.893050
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102	6	0	0.599014	-10.151735	0.489761
103	1	0	-4.122838	-5.353104	1.643741
104	1	0	-2.207026	-6.105206	-2.874500
105	1	0	-3.539694	-4.056361	-2.430538
106	1	0	-1.189875	-8.170512	-2.129460
107	7	0	1.432696	-8.964284	0.211284
108	6	0	4.649133	-3.375169	0.101176
109	6	0	3.918714	-4.568490	0.360763
110	6	0	3.714866	-5.508553	-0.655001
111	6	0	2.975234	-6.675860	-0.416494
112	6	0	2.420738	-6.885605	0.880049
113	6	0	2.637522	-5.933275	1.893050
114	6	0	3.376877	-4.791521	1.654409
115	1	0	4.122838	-5.353104	-1.643741
116	8	0	2.794833	-7.571339	-1.412340
117	6	0	1.626481	-8.069070	1.129520
118	1	0	2.207026	-6.105206	2.874500
119	1	0	3.539694	-4.056361	2.430538
120	1	0	1.189875	-8.170512	2.129460
121	6	0	1.452045	-11.425372	0.300593
122	6	0	-1.452045	-11.425372	-0.300593
123	6	0	0.598389	-12.698322	0.487588
124	6	0	-0.598389	-12.698322	-0.487588
125	1	0	2.282817	-11.404027	1.014661
126	1	0	1.879988	-11.404459	-0.709500
127	1	0	-2.282817	-11.404027	-1.014661
128	1	0	-1.879988	-11.404459	0.709500
129	1	0	0.224399	-12.739723	1.519493
130	1	0	1.220013	-13.586350	0.325293
131	1	0	-0.224399	-12.739723	-1.519493
132	1	0	-1.220013	-13.586350	-0.325293
133	6	0	-0.599014	-10.151735	-0.489761
134	1	0	0.201303	-10.109684	1.515312
135	1	0	-0.201303	-10.109684	-1.515312
136	8	0	-2.794833	-7.571339	1.412340
137	1	0	2.213446	-8.360279	-1.009363
138	1	0	-2.213446	-8.360279	1.009363

Table C2. Cartesian coordinates for **3b**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.586597	-13.703633	0.483021
2	6	0	-0.586597	-13.703633	-0.483021
3	6	0	-1.436831	-12.456390	-0.304744
4	6	0	-0.588934	-11.192307	-0.504290
5	6	0	0.588934	-11.192307	0.504290
6	6	0	1.436831	-12.456390	0.304744
7	7	0	-1.438170	-10.008918	-0.258392
8	6	0	-1.693342	-9.150077	-1.197117
9	6	0	-2.516843	-7.981711	-0.896184
10	6	0	-2.759626	-7.050893	-1.917136
11	6	0	-3.500195	-5.911312	-1.678564
12	6	0	-4.029962	-5.646769	-0.400628
13	6	0	-3.813840	-6.565948	0.619091
14	6	0	-3.061570	-7.731580	0.380001
15	1	0	0.217666	-13.767009	1.526439
16	1	0	1.207375	-14.606791	0.327024
17	1	0	-0.217666	-13.767009	-1.526439
18	1	0	-1.207375	-14.606791	-0.327024
19	1	0	-2.278075	-12.469542	-1.025229
20	1	0	-1.901156	-12.456830	0.702574
21	1	0	-0.178196	-11.190616	-1.549518
22	7	0	1.438170	-10.008918	0.258392
23	1	0	0.178196	-11.190616	1.549518
24	1	0	1.901156	-12.456830	-0.702574
25	1	0	2.278075	-12.469542	1.025229
26	1	0	-1.305432	-9.245719	-2.225546
27	1	0	-2.348595	-7.231091	-2.917687
28	1	0	-3.682904	-5.197417	-2.495087
29	1	0	-4.217382	-6.356596	1.627789
30	8	0	-2.902873	-8.559181	1.442521
31	6	0	1.693342	-9.150077	1.197117
32	6	0	2.516843	-7.981711	0.896184
33	6	0	3.061570	-7.731580	-0.380001
34	6	0	2.759626	-7.050893	1.917136
35	6	0	3.500195	-5.911312	1.678564
36	6	0	4.029962	-5.646769	0.400628
37	6	0	3.813840	-6.565948	-0.619091
38	1	0	1.305432	-9.245719	2.225546
39	8	0	2.902873	-8.559181	-1.442521
40	1	0	2.348595	-7.231091	2.917687
41	1	0	3.682904	-5.197417	2.495087
42	1	0	4.217382	-6.356596	-1.627789
43	1	0	-2.361630	-9.307544	1.154093
44	1	0	2.361630	-9.307544	-1.154093
45	6	0	6.905226	-0.666665	-0.400628
46	6	0	6.869444	-0.075602	-1.678564
47	6	0	7.486066	1.135540	-1.917136
48	6	0	8.170786	1.811206	-0.896184
49	6	0	8.226530	1.214393	0.380001
50	6	0	7.593198	-0.019908	0.619091
51	6	0	8.770870	3.108561	-1.197117
52	7	0	9.387063	3.758967	-0.258392
53	6	0	9.987290	5.086122	-0.504290
54	6	0	11.505966	4.983863	-0.304744
55	6	0	12.160992	6.343809	-0.483021
56	6	0	11.574396	7.359824	0.483021
57	6	0	10.069135	7.472527	0.304744
58	6	0	9.398355	6.106186	0.504290
59	1	0	6.342547	-0.590780	-2.495087
60	1	0	7.436606	1.581603	-2.917687
61	8	0	8.863905	1.765629	1.442521
62	1	0	7.613665	-0.474062	1.627789
63	1	0	8.659743	3.492322	-2.225546
64	1	0	9.780456	5.440986	-1.549518
65	1	0	11.937978	4.261900	-1.025229
66	1	0	11.738509	4.581966	0.702574
67	1	0	12.031413	6.695000	-1.526439
68	1	0	13.253540	6.257778	-0.327024
69	1	0	12.046165	8.349013	0.327024
70	1	0	11.813746	7.072009	1.526439
71	1	0	9.837353	7.874864	-0.702574
72	1	0	9.659902	8.207642	1.025229
73	7	0	7.948892	6.249951	0.258392
74	1	0	9.602260	5.749631	1.549518
75	1	0	9.241384	2.608541	1.154093
76	6	0	7.077528	6.041516	1.197117

77	6	0	5.653943	6.170505	0.896184
78	6	0	5.164960	6.517187	-0.380001
79	6	0	3.779358	6.585856	-0.619091
80	6	0	2.875264	6.313434	0.400628
81	6	0	3.369248	5.986914	1.678564
82	6	0	4.726439	5.915353	1.917136
83	1	0	7.354311	5.753397	2.225546
84	8	0	5.961032	6.793552	-1.442521
85	1	0	3.396283	6.830658	-1.627789
86	1	0	2.659643	5.788197	2.495087
87	1	0	5.088011	5.649489	2.917687
88	1	0	6.879755	6.699003	-1.154093
89	6	0	-2.875264	6.313434	-0.400628
90	6	0	-3.779358	6.585856	0.619091
91	6	0	-5.164960	6.517187	0.380001
92	6	0	-5.653943	6.170505	-0.896184
93	6	0	-4.726439	5.915353	-1.917136
94	6	0	-3.369248	5.986914	-1.678564
95	6	0	-7.077528	6.041516	-1.197117
96	7	0	-7.948892	6.249951	-0.258392
97	6	0	-9.987290	5.086122	0.504290
98	1	0	-3.396283	6.830658	1.627789
99	1	0	-5.088011	5.649489	-2.917687
100	1	0	-2.659643	5.788197	-2.495087
101	1	0	-7.354311	5.753397	-2.225546
102	7	0	-9.387063	3.758967	0.258392
103	6	0	-6.905226	-0.666665	0.400628
104	6	0	-7.593198	-0.019908	-0.619091
105	6	0	-8.226530	1.214393	-0.380001
106	6	0	-8.170786	1.811206	0.896184
107	6	0	-7.486066	1.135540	1.917136
108	6	0	-6.869444	-0.075602	1.678564
109	1	0	-7.613665	-0.474062	-1.627789
110	8	0	-8.863905	1.765629	-1.442521
111	6	0	-8.770870	3.108561	1.197117
112	1	0	-7.436606	1.581603	2.917687
113	1	0	-6.342547	-0.590780	2.495087
114	1	0	-8.659743	3.492322	2.225546
115	6	0	-11.505966	4.983863	0.304744
116	6	0	-10.069135	7.472527	-0.304744
117	6	0	-12.160992	6.343809	0.483021
118	6	0	-11.574396	7.359824	-0.483021
119	1	0	-11.937978	4.261900	1.025229
120	1	0	-11.738509	4.581966	-0.702574
121	1	0	-9.659902	8.207642	-1.025229
122	1	0	-9.837353	7.874864	0.702574
123	1	0	-12.031413	6.695000	1.526439
124	1	0	-13.253540	6.257778	0.327024
125	1	0	-11.813746	7.072009	-1.526439
126	1	0	-12.046165	8.349013	-0.327024
127	6	0	-9.398355	6.106186	-0.504290
128	1	0	-9.780456	5.440986	1.549518
129	1	0	-9.602260	5.749631	-1.549518
130	8	0	-5.961032	6.793552	1.442521
131	1	0	-9.241384	2.608541	-1.154093
132	1	0	-6.879755	6.699003	1.154093
133	6	0	1.423574	6.351454	0.163919
134	6	0	0.559587	6.365557	1.261690
135	6	0	0.829985	6.365262	-1.117412
136	6	0	-0.829985	6.365262	1.117412
137	1	0	0.991118	6.364079	2.281585
138	6	0	-0.559587	6.365557	-1.261690
139	6	0	-1.423574	6.351454	-0.163919
140	1	0	-0.991118	6.364079	-2.281585
141	6	0	6.212308	-1.942876	-0.163919
142	6	0	5.927471	-2.463843	1.117412
143	6	0	5.792527	-2.698162	-1.261690
144	6	0	5.232940	-3.667395	1.261690
145	6	0	5.097487	-3.901419	-1.117412
146	1	0	6.007013	-2.323706	-2.281585
147	6	0	4.788734	-4.408578	0.163919
148	1	0	5.015895	-4.040373	2.281585
149	6	0	-6.212308	-1.942876	0.163919
150	6	0	-5.792527	-2.698162	1.261690
151	6	0	-5.927471	-2.463843	-1.117412
152	6	0	-5.097487	-3.901419	1.117412
153	1	0	-6.007013	-2.323706	2.281585

154	6	0	-5.232940	-3.667395	-1.261690
155	6	0	-4.788734	-4.408578	-0.163919
156	1	0	-5.015895	-4.040373	-2.281585
157	8	0	-1.672615	6.436032	2.216965
158	8	0	1.672615	6.436032	-2.216965
159	8	0	6.410075	-1.769489	2.216965
160	8	0	4.737460	-4.666543	-2.216965
161	8	0	-4.737460	-4.666543	2.216965
162	8	0	-6.410075	-1.769489	-2.216965
163	6	0	-4.535367	-3.973331	3.427368
164	1	0	-3.599421	-3.405088	3.402836
165	1	0	-5.365304	-3.294247	3.674205
166	1	0	-4.471739	-4.782747	4.158404
167	6	0	-5.708689	-1.941077	-3.427368
168	1	0	-4.748604	-1.414646	-3.402836
169	1	0	-5.535553	-2.999366	-3.674205
170	1	0	-6.377850	-1.481266	-4.158404
171	6	0	4.535367	-3.973331	-3.427368
172	1	0	3.599421	-3.405088	-3.402836
173	1	0	5.365304	-3.294247	-3.674205
174	1	0	4.471739	-4.782747	-4.158404
175	6	0	5.708689	-1.941077	3.427368
176	1	0	4.748604	-1.414646	3.402836
177	1	0	5.535553	-2.999366	3.674205
178	1	0	6.377850	-1.481266	4.158404
179	6	0	-1.173322	5.914408	3.427368
180	1	0	-1.149182	4.819734	3.402836
181	1	0	-0.170249	6.293613	3.674205
182	1	0	-1.906111	6.264013	4.158404
183	6	0	1.173322	5.914408	-3.427368
184	1	0	1.149182	4.819734	-3.402836
185	1	0	0.170249	6.293613	-3.674205
186	1	0	1.906111	6.264013	-4.158404

Table C2. Cartesian coordinates for **3c**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.544556	16.543076	0.529835
2	6	0	0.544556	16.543076	-0.529835
3	6	0	1.407131	15.296587	-0.420011
4	6	0	0.547714	14.030698	-0.548566
5	6	0	-0.547714	14.030698	0.548566
6	6	0	-1.407131	15.296587	0.420011
7	7	0	1.417785	12.851288	-0.364583
8	6	0	1.629682	12.004469	-1.324222
9	6	0	2.493824	10.849923	-1.084087
10	6	0	2.692948	9.937903	-2.131012
11	6	0	3.482172	8.816448	-1.958826
12	6	0	4.095453	8.577504	-0.717175
13	6	0	3.925659	9.465790	0.339287
14	6	0	3.122323	10.607851	0.156531
15	1	0	-1.175621	17.446685	0.426561
16	1	0	-0.090942	16.604932	1.539429
17	1	0	1.175621	17.446685	-0.426561
18	1	0	0.090942	16.604932	-1.539429
19	1	0	1.951675	15.298896	0.546360
20	1	0	2.187018	15.309607	-1.206547
21	1	0	0.057312	14.023746	-1.558760
22	7	0	-1.417785	12.851288	0.364583
23	1	0	-0.057312	14.023746	1.558760
24	1	0	-1.951675	15.298896	-0.546360
25	1	0	-2.187018	15.309607	1.206547
26	1	0	1.180304	12.101838	-2.327173
27	1	0	2.209595	10.116497	-3.099200
28	1	0	3.625985	8.108248	-2.781700
29	1	0	4.405516	9.281139	1.307638
30	8	0	3.005595	11.423119	1.233408
31	6	0	-1.629682	12.004469	1.324222
32	6	0	-2.493824	10.849923	1.084087
33	6	0	-3.122323	10.607851	-0.156531
34	6	0	-2.692948	9.937903	2.131012

35	6	0	-3.482172	8.816448	1.958826
36	6	0	-4.095453	8.577504	0.717175
37	6	0	-3.925659	9.465790	-0.339287
38	1	0	-1.180304	12.101838	2.327173
39	8	0	-3.005595	11.423119	-1.233408
40	1	0	-2.209595	10.116497	3.099200
41	1	0	-3.625985	8.108248	2.781700
42	1	0	-4.405516	9.281139	-1.307638
43	1	0	2.428863	12.159744	0.985818
44	1	0	-2.428863	12.159744	-0.985818
45	6	0	-9.476063	-0.741985	-0.717175
46	6	0	-9.376354	-1.392575	-1.958826
47	6	0	-9.952950	-2.636790	-2.131012
48	6	0	-10.643221	-3.265247	-1.084087
49	6	0	-10.747830	-2.599914	0.156531
50	6	0	-10.160444	-1.333175	0.339287
51	6	0	-11.211016	-4.590888	-1.324222
52	7	0	-11.838434	-5.197806	-0.364583
53	6	0	-12.424798	-6.541014	-0.548566
54	6	0	-13.950798	-6.429682	-0.420011
55	6	0	-14.599002	-7.799939	-0.529835
56	6	0	-14.054446	-8.743137	0.529835
57	6	0	-12.543667	-8.866905	0.420011
58	6	0	-11.877084	-7.489684	0.548566
59	1	0	-8.834941	-0.913929	-2.781700
60	1	0	-9.865941	-3.144683	-3.099200
61	8	0	-11.395509	-3.108638	1.233408
62	1	0	-10.240460	-0.825281	1.307638
63	1	0	-11.070651	-5.028745	-2.327173
64	1	0	-12.173576	-6.962239	-1.558760
65	1	0	-14.352018	-5.760791	-1.206547
66	1	0	-14.225070	-5.959248	0.546360
67	1	0	-14.425764	-8.223708	-1.539429
68	1	0	-15.697084	-7.705225	-0.426561
69	1	0	-14.521462	-9.741461	0.426561
70	1	0	-14.334822	-8.381224	1.539429
71	1	0	-12.273396	-9.339648	-0.546360
72	1	0	-12.165000	-9.548817	1.206547
73	7	0	-10.420649	-7.653482	0.364583
74	1	0	-12.116264	-7.061507	1.558760
75	1	0	-11.745078	-3.976415	0.985818
76	6	0	-9.581334	-7.413580	1.324222
77	6	0	-8.149397	-7.584677	1.084087
78	6	0	-7.625506	-8.007937	-0.156531
79	6	0	-6.234785	-8.132615	-0.339287
80	6	0	-5.380609	-7.835518	0.717175
81	6	0	-5.894182	-7.423873	1.958826
82	6	0	-7.260002	-7.301113	2.131012
83	1	0	-9.890347	-7.073092	2.327173
84	8	0	-8.389914	-8.314481	-1.233408
85	1	0	-5.834944	-8.455858	-1.307638
86	1	0	-5.208957	-7.194319	2.781700
87	1	0	-7.656346	-6.971814	3.099200
88	1	0	-9.316215	-8.183329	-0.985818
89	6	0	5.380609	-7.835518	-0.717175
90	6	0	6.234785	-8.132615	0.339287
91	6	0	7.625506	-8.007937	0.156531
92	6	0	8.149397	-7.584677	-1.084087
93	6	0	7.260002	-7.301113	-2.131012
94	6	0	5.894182	-7.423873	-1.958826
95	6	0	9.581334	-7.413580	-1.324222
96	7	0	10.420649	-7.653482	-0.364583
97	6	0	12.424798	-6.541014	0.548566
98	1	0	5.834944	-8.455858	1.307638
99	1	0	7.656346	-6.971814	-3.099200
100	1	0	5.208957	-7.194319	-2.781700
101	1	0	9.890347	-7.073092	-2.327173
102	7	0	11.838434	-5.197806	0.364583
103	6	0	9.476063	-0.741985	0.717175
104	6	0	10.160444	-1.333175	-0.339287
105	6	0	10.747830	-2.599914	-0.156531
106	6	0	10.643221	-3.265247	1.084087
107	6	0	9.952950	-2.636790	2.131012
108	6	0	9.376354	-1.392575	1.958826
109	1	0	10.240460	-0.825281	-1.307638
110	8	0	11.395509	-3.108638	-1.233408
111	6	0	11.211016	-4.590888	1.324222

112	1	0	9.865941	-3.144683	3.099200
113	1	0	8.834941	-0.913929	2.781700
114	1	0	11.070651	-5.028745	2.327173
115	6	0	13.950798	-6.429682	0.420011
116	6	0	12.543667	-8.866905	-0.420011
117	6	0	14.599002	-7.799939	0.529835
118	6	0	14.054446	-8.743137	-0.529835
119	1	0	14.352018	-5.760791	1.206547
120	1	0	14.225070	-5.959248	-0.546360
121	1	0	12.273396	-9.339648	0.546360
122	1	0	12.165000	-9.548817	-1.206547
123	1	0	14.425764	-8.223708	1.539429
124	1	0	15.697084	-7.705225	0.426561
125	1	0	14.334822	-8.381224	-1.539429
126	1	0	14.521462	-9.741461	-0.426561
127	6	0	11.877084	-7.489684	-0.548566
128	1	0	12.173576	-6.962239	1.558760
129	1	0	12.116264	-7.061507	-1.558760
130	8	0	8.389914	-8.314481	1.233408
131	1	0	11.745078	-3.976415	-0.985818
132	1	0	9.316215	-8.183329	0.985818
133	6	0	-1.391556	-8.045369	0.219055
134	6	0	-0.887571	-8.058603	-1.085628
135	6	0	-0.492831	-8.059931	1.303701
136	6	0	0.492831	-8.059931	-1.303701
137	1	0	-1.578108	-8.048459	-1.938094
138	6	0	0.887571	-8.058603	1.085628
139	6	0	1.391556	-8.045369	-0.219055
140	1	0	1.578108	-8.048459	1.938094
141	6	0	-7.663272	2.817562	-0.219055
142	6	0	-7.422740	3.260643	1.085628
143	6	0	-7.226520	3.603162	-1.303701
144	6	0	-6.733690	4.456769	1.303701
145	6	0	-6.535170	4.797960	-1.085628
146	6	0	-6.271716	5.227807	0.219055
147	6	0	7.663272	2.817562	0.219055
148	6	0	7.422740	3.260643	-1.085628
149	6	0	7.226520	3.603162	1.303701
150	6	0	6.733690	4.456769	-1.303701
151	1	0	7.759224	2.657548	-1.938094
152	6	0	6.535170	4.797960	1.085628
153	6	0	6.271716	5.227807	-0.219055
154	1	0	6.181116	5.390911	1.938094
155	8	0	0.914654	-7.956505	-2.625539
156	8	0	-0.914654	-7.956505	2.625539
157	8	0	6.433208	4.770366	-2.625539
158	8	0	7.347862	3.186138	2.625539
159	6	0	7.126535	5.893293	-3.123599
160	1	0	6.756602	5.966996	-4.149211
161	1	0	6.885986	6.806709	-2.566318
162	1	0	8.210557	5.735270	-3.122223
163	6	0	8.667009	3.225114	3.123599
164	1	0	8.545871	2.867891	4.149211
165	1	0	9.337775	2.560084	2.566318
166	1	0	9.072168	4.242916	3.122223
167	6	0	1.540474	-9.118407	-3.123599
168	1	0	1.789269	-8.834887	-4.149211
169	1	0	2.451790	-9.366793	-2.566318
170	1	0	0.861611	-9.978186	-3.122223
171	6	0	-1.540474	-9.118407	3.123599
172	1	0	-1.789269	-8.834887	4.149211
173	1	0	-2.451790	-9.366793	2.566318
174	1	0	-0.861611	-9.978186	3.122223
175	6	0	-4.881571	7.412533	0.544737
176	6	0	-5.531467	6.418759	0.405005
177	6	0	-8.324542	1.581011	-0.405005
178	6	0	-8.860228	0.521298	-0.544737
179	6	0	-3.978656	-7.933831	0.544737
180	6	0	-2.793075	-7.999770	0.405005
181	6	0	2.793075	-7.999770	-0.405005
182	6	0	3.978656	-7.933831	-0.544737
183	6	0	8.860228	0.521298	0.544737
184	6	0	8.324542	1.581011	0.405005
185	6	0	5.531467	6.418759	-0.405005
186	6	0	4.881571	7.412533	-0.544737
187	8	0	-6.433208	4.770366	2.625539
188	8	0	-7.347862	3.186138	-2.625539

189	1	0	-6.181116	5.390911	-1.938094
190	1	0	-7.759224	2.657548	1.938094
191	6	0	-8.667009	3.225114	-3.123599
192	1	0	-9.072168	4.242916	-3.122223
193	1	0	-8.545871	2.867891	-4.149211
194	1	0	-9.337775	2.560084	-2.566318
195	6	0	-7.126535	5.893293	3.123599
196	1	0	-8.210557	5.735270	3.122223
197	1	0	-6.756602	5.966996	4.149211
198	1	0	-6.885986	6.806709	2.566318

Table D1. Cartesian coordinates for **3a**·$TiCl_2$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742735	10.520602	-7.870416
2	6	0	0.142718	11.326775	-6.910971
3	6	0	-0.000000	10.817642	-5.470520
4	6	0	0.297519	9.310711	-5.353887
5	6	0	-0.597567	8.496109	-6.322230
6	6	0	-0.447788	9.018370	-7.765646
7	7	0	0.064153	8.879449	-3.985315
8	6	0	1.015925	8.323366	-3.324323
9	6	0	0.856546	7.864861	-1.952894
10	6	0	1.930643	7.237700	-1.294800
11	6	0	1.810187	6.757824	-0.003408
12	6	0	0.578339	6.900679	0.677496
13	6	0	-0.498262	7.540625	0.050168
14	6	0	-0.375150	8.020548	-1.259269
15	1	0	-1.800110	10.704317	-7.631105
16	1	0	-0.593984	10.855672	-8.904139
17	1	0	1.192377	11.244830	-7.228149
18	1	0	-0.113968	12.392200	-6.954840
19	1	0	0.670804	11.362689	-4.795700
20	1	0	-1.021601	10.998632	-5.109148
21	1	0	1.346649	9.125406	-5.643223
22	7	0	-0.224004	7.091169	-6.276021
23	1	0	-1.644944	8.627634	-5.999418
24	1	0	0.576458	8.812033	-8.105196
25	1	0	-1.115139	8.443406	-8.418798
26	1	0	2.004701	8.165601	-3.779199
27	1	0	2.871207	7.120773	-1.828526
28	1	0	2.639562	6.261731	0.488114
29	6	0	0.427484	6.337407	1.980345
30	1	0	-1.449350	7.653681	0.558485
31	8	0	-1.440405	8.609653	-1.825984
32	6	0	-1.115119	6.207401	-5.995086
33	6	0	-0.830868	4.781171	-5.965989
34	6	0	0.473708	4.280177	-6.231518
35	6	0	-1.862011	3.864954	-5.683093
36	6	0	-1.637617	2.500688	-5.664180
37	6	0	-0.337834	2.004706	-5.927236
38	6	0	0.705592	2.900605	-6.203299
39	1	0	-2.150710	6.501524	-5.768718
40	8	0	1.503109	5.096196	-6.514078
41	1	0	-2.858352	4.250554	-5.478178
42	1	0	-2.441296	1.805707	-5.447821
43	6	0	-0.095333	0.600918	-5.918760
44	1	0	1.706394	2.537414	-6.408773
45	1	0	-1.175574	8.865584	-2.754531
46	1	0	1.148094	6.029257	-6.511791
47	6	0	0.095333	-0.600918	-5.918760
48	6	0	0.337834	-2.004706	-5.927236
49	6	0	1.637617	-2.500688	-5.664180
50	6	0	1.862011	-3.864954	-5.683093
51	6	0	0.830868	-4.781171	-5.965989
52	6	0	-0.473708	-4.280177	-6.231518
53	6	0	-0.705592	-2.900605	-6.203299
54	6	0	1.115119	-6.207401	-5.995086
55	7	0	0.224004	-7.091169	-6.276021
56	6	0	0.597567	-8.496109	-6.322230
57	6	0	0.447788	-9.018370	-7.765646

58	6	0	0.742735	-10.520602	-7.870416
59	6	0	-0.142718	-11.326775	-6.910971
60	6	0	0.000000	-10.817642	-5.470520
61	6	0	-0.297519	-9.310711	-5.353887
62	1	0	2.441296	-1.805707	-5.447821
63	1	0	2.858352	-4.250554	-5.478178
64	8	0	-1.503109	-5.096196	-6.514078
65	1	0	-1.706394	-2.537414	-6.408773
66	1	0	2.150710	-6.501524	-5.768718
67	1	0	1.644944	-8.627634	-5.999418
68	1	0	1.115139	-8.443406	-8.418798
69	1	0	-0.576458	-8.812033	-8.105196
70	1	0	1.800110	-10.704317	-7.631105
71	1	0	0.593984	-10.855672	-8.904139
72	1	0	0.113968	-12.392200	-6.954840
73	1	0	-1.192377	-11.244830	-7.228149
74	1	0	1.021601	-10.998632	-5.109148
75	1	0	-0.670804	-11.362689	-4.795700
76	7	0	-0.064153	-8.879449	-3.985315
77	1	0	-1.346649	-9.125406	-5.643223
78	1	0	-1.148094	-6.029257	-6.511791
79	6	0	-1.015925	-8.323366	-3.324323
80	6	0	-0.856546	-7.864861	-1.952894
81	6	0	0.375150	-8.020548	-1.259269
82	6	0	0.498262	-7.540625	0.050168
83	6	0	-0.578339	-6.900679	0.677496
84	6	0	-1.810187	-6.757824	-0.003408
85	6	0	-1.930643	-7.237700	-1.294800
86	1	0	-2.004701	-8.165601	-3.779199
87	8	0	1.440405	-8.609653	-1.825984
88	1	0	1.449350	-7.653681	0.558485
89	6	0	-0.427484	-6.337407	1.980345
90	1	0	-2.639562	-6.261731	0.488114
91	1	0	-2.871207	-7.120773	-1.828526
92	1	0	1.175574	-8.865584	-2.754531
93	6	0	-0.322368	-5.793273	3.062765
94	6	0	-0.194116	-5.018918	4.253917
95	6	0	-0.081797	-3.627529	4.131973
96	6	0	0.031322	-2.815401	5.263901
97	6	0	0.035513	-3.400146	6.559692
98	6	0	-0.066097	-4.803784	6.659135
99	6	0	-0.181899	-5.608913	5.538987
100	6	0	0.174903	-2.620325	7.773578
101	7	0	0.217136	-1.332496	7.857904
102	6	0	-0.444721	0.635288	9.140516
103	1	0	-0.083516	-3.156905	3.155714
104	1	0	-0.057108	-5.259294	7.646738
105	1	0	-0.265357	-6.685753	5.635940
106	1	0	0.258901	-3.216863	8.683789
107	7	0	-0.217136	1.332496	7.857904
108	6	0	0.322368	5.793273	3.062765
109	6	0	0.194116	5.018918	4.253917
110	6	0	0.081797	3.627529	4.131973
111	6	0	-0.031322	2.815401	5.263901
112	6	0	-0.035513	3.400146	6.559692
113	6	0	0.066097	4.803784	6.659135
114	6	0	0.181899	5.608913	5.538987
115	1	0	0.083516	3.156905	3.155714
116	8	0	-0.147090	1.505334	5.102319
117	6	0	-0.174903	2.620325	7.773578
118	1	0	0.057108	5.259294	7.646738
119	1	0	0.265357	6.685753	5.635940
120	1	0	-0.258901	3.216863	8.683789
121	6	0	-0.233617	1.468454	10.412742
122	6	0	0.233617	-1.468454	10.412742
123	6	0	-0.450817	0.618683	11.674354
124	6	0	0.450817	-0.618683	11.674354
125	1	0	-0.927478	2.317027	10.428307
126	1	0	0.785253	1.881576	10.415930
127	1	0	0.927478	-2.317027	10.428307
128	1	0	-0.785253	-1.881576	10.415930
129	1	0	-1.503093	0.305594	11.726326
130	1	0	-0.262033	1.230186	12.564509
131	1	0	1.503093	-0.305594	11.726326
132	1	0	0.262033	-1.230186	12.564509
133	6	0	0.444721	-0.635288	9.140516
134	1	0	-1.489121	0.297313	9.103287

135	1	0	1.489121	-0.297313	9.103287
136	8	0	0.147090	-1.505334	5.102319
137	22	0	-0.000000	0.000000	6.141432
138	17	0	-2.322039	-0.317956	6.421062
139	17	0	2.322039	0.317956	6.421062

Table D2. Cartesian coordinates for **3a**·2$TiCl_2$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.824148	11.033550	-4.796770
2	6	0	-1.667612	10.479608	-5.948753
3	6	0	-1.360443	8.996104	-6.201712
4	6	0	-1.559925	8.165920	-4.926823
5	6	0	-0.721689	8.728059	-3.749352
6	6	0	-1.021648	10.214717	-3.512211
7	7	0	-1.258155	6.724844	-5.030366
8	6	0	-1.128070	6.129393	-6.168754
9	6	0	-0.885754	4.715163	-6.373388
10	6	0	-0.655038	4.245152	-7.683689
11	6	0	-0.409980	2.909196	-7.948637
12	6	0	-0.394834	1.980210	-6.882376
13	6	0	-0.646521	2.422877	-5.575209
14	6	0	-0.888776	3.772478	-5.308966
15	1	0	0.237093	11.014853	-5.079035
16	1	0	-1.077926	12.081832	-4.605444
17	1	0	-2.733556	10.594612	-5.710668
18	1	0	-1.488447	11.052873	-6.864811
19	1	0	-2.013871	8.624765	-6.998565
20	1	0	-0.325053	8.887160	-6.552565
21	1	0	-2.615046	8.219310	-4.627357
22	7	0	-0.920206	7.831045	-2.591492
23	1	0	0.335545	8.614379	-4.025456
24	1	0	-2.054533	10.325243	-3.154796
25	1	0	-0.364577	10.613710	-2.732146
26	1	0	-1.201038	6.711753	-7.088829
27	1	0	-0.660593	4.960162	-8.502450
28	1	0	-0.222138	2.569458	-8.960517
29	6	0	-0.117650	0.596986	-7.068443
30	1	0	-0.646937	1.724938	-4.746863
31	8	0	-1.127870	4.146690	-4.060105
32	6	0	-0.952011	8.278887	-1.380528
33	6	0	-1.046256	7.489532	-0.169410
34	6	0	-1.033324	6.067585	-0.167970
35	6	0	-1.111211	8.158940	1.070754
36	6	0	-1.168362	7.470514	2.268676
37	6	0	-1.162998	6.055245	2.263307
38	6	0	-1.096556	5.369595	1.042548
39	1	0	-0.890820	9.354810	-1.208909
40	8	0	-0.944642	5.384562	-1.300111
41	1	0	-1.115099	9.245954	1.077659
42	1	0	-1.218045	8.001454	3.212154
43	6	0	-1.214227	5.312678	3.478340
44	1	0	-1.083697	4.286675	1.016117
45	6	0	-1.245053	4.631778	4.485781
46	6	0	-1.280442	3.801710	5.645048
47	6	0	-2.202926	2.730340	5.715230
48	6	0	-2.216749	1.918552	6.834638
49	6	0	-1.325555	2.121989	7.904853
50	6	0	-0.396186	3.197136	7.829000
51	6	0	-0.391548	4.030012	6.703846
52	6	0	-1.360443	1.244647	9.064325
53	7	0	-0.538227	1.373475	10.045675
54	6	0	-0.615400	0.474841	11.186937
55	6	0	-0.667506	1.314132	12.477722
56	6	0	-0.619721	0.451701	13.744246
57	6	0	0.619721	-0.451701	13.744246
58	6	0	0.667506	-1.314132	12.477722
59	6	0	0.615400	-0.474841	11.186937
60	1	0	-2.886824	2.558460	4.892448
61	1	0	-2.923842	1.094996	6.895220

62	8	0	0.484593	3.439069	8.810196
63	1	0	0.322964	4.843787	6.662548
64	1	0	-2.130215	0.460184	9.066533
65	1	0	-1.516151	-0.158697	11.123786
66	1	0	-1.572553	1.931178	12.457691
67	1	0	0.183024	2.008286	12.469379
68	1	0	-1.523802	-0.170089	13.803103
69	1	0	-0.627140	1.096120	14.630494
70	1	0	0.627140	-1.096120	14.630494
71	1	0	1.523802	0.170089	13.803103
72	1	0	-0.183024	-2.008286	12.469379
73	1	0	1.572553	-1.931178	12.457691
74	7	0	0.538227	-1.373475	10.045675
75	1	0	1.516151	0.158697	11.123786
76	1	0	0.332973	2.744358	9.513110
77	6	0	1.360443	-1.244647	9.064325
78	6	0	1.325555	-2.121989	7.904853
79	6	0	0.396186	-3.197136	7.829000
80	6	0	0.391548	-4.030012	6.703846
81	6	0	1.280442	-3.801710	5.645048
82	6	0	2.202926	-2.730340	5.715230
83	6	0	2.216749	-1.918552	6.834638
84	1	0	2.130215	-0.460184	9.066533
85	8	0	-0.484593	-3.439069	8.810196
86	1	0	-0.322964	-4.843787	6.662548
87	6	0	1.245053	-4.631778	4.485781
88	1	0	2.886824	-2.558460	4.892448
89	1	0	2.923842	-1.094996	6.895220
90	1	0	-0.332973	-2.744358	9.513110
91	6	0	1.214227	-5.312678	3.478340
92	6	0	1.162998	-6.055245	2.263307
93	6	0	1.096556	-5.369595	1.042548
94	6	0	1.033324	-6.067585	-0.167970
95	6	0	1.046256	-7.489532	-0.169410
96	6	0	1.111211	-8.158940	1.070754
97	6	0	1.168362	-7.470514	2.268676
98	6	0	0.952011	-8.278887	-1.380528
99	7	0	0.920206	-7.831045	-2.591492
100	6	0	1.559925	-8.165920	-4.926823
101	1	0	1.083697	-4.286675	1.016117
102	1	0	1.115099	-9.245954	1.077659
103	1	0	1.218045	-8.001454	3.212154
104	1	0	0.890820	-9.354810	-1.208909
105	7	0	1.258155	-6.724844	-5.030366
106	6	0	0.117650	-0.596986	-7.068443
107	6	0	0.394834	-1.980210	-6.882376
108	6	0	0.646521	-2.422877	-5.575209
109	6	0	0.888776	-3.772478	-5.308966
110	6	0	0.885754	-4.715163	-6.373388
111	6	0	0.655038	-4.245152	-7.683689
112	6	0	0.409980	-2.909196	-7.948637
113	1	0	0.646937	-1.724938	-4.746863
114	8	0	1.127870	-4.146690	-4.060105
115	6	0	1.128070	-6.129393	-6.168754
116	1	0	0.660593	-4.960162	-8.502450
117	1	0	0.222138	-2.569458	-8.960517
118	1	0	1.201038	-6.711753	-7.088829
119	6	0	1.360443	-8.996104	-6.201712
120	6	0	1.021648	-10.214717	-3.512211
121	6	0	1.667612	-10.479608	-5.948753
122	6	0	0.824148	-11.033550	-4.796770
123	1	0	2.013871	-8.624765	-6.998565
124	1	0	0.325053	-8.887160	-6.552565
125	1	0	0.364577	-10.613710	-2.732146
126	1	0	2.054533	-10.325243	-3.154796
127	1	0	2.733556	-10.594612	-5.710668
128	1	0	1.488447	-11.052873	-6.864811
129	1	0	-0.237093	-11.014853	-5.079035
130	1	0	1.077926	-12.081832	-4.605444
131	6	0	0.721689	-8.728059	-3.749352
132	1	0	2.615046	-8.219310	-4.627357
133	1	0	-0.335545	-8.614379	-4.025456
134	8	0	0.944642	-5.384562	-1.300111
135	22	0	-1.069088	5.713623	-3.102225
136	22	0	1.069088	-5.713623	-3.102225
137	17	0	1.258154	5.914223	-3.452640
138	17	0	3.400581	-6.028459	-2.982242

139	17	0	-3.400581	6.028459	-2.982242
140	17	0	-1.258154	-5.914223	-3.452640

Table D3. Cartesian coordinates for **3a**·3$TiCl_2$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.656739	-6.845079	0.475845
2	6	0	-11.256382	-5.806467	-0.475845
3	6	0	-10.592270	-4.433206	-0.295082
4	6	0	-9.070407	-4.526603	-0.471013
5	6	0	-8.455357	-5.591901	0.471013
6	6	0	-9.135404	-6.956572	0.295082
7	7	0	-8.311549	-3.274818	-0.273648
8	6	0	-8.886384	-2.118814	-0.283256
9	6	0	-8.231350	-0.830370	-0.185785
10	6	0	-9.028412	0.333192	-0.148685
11	6	0	-8.471043	1.597195	-0.089959
12	6	0	-7.062925	1.738686	-0.075764
13	6	0	-6.251545	0.595355	-0.119173
14	6	0	-6.816870	-0.682563	-0.169865
15	1	0	-10.880654	-6.562898	1.513329
16	1	0	-11.117889	-7.825117	0.312458
17	1	0	-11.123963	-6.141474	-1.513329
18	1	0	-12.335695	-5.715816	-0.312458
19	1	0	-11.014267	-3.732492	-1.023597
20	1	0	-10.821689	-4.040224	0.704927
21	1	0	-8.847762	-4.839877	-1.499814
22	7	0	-6.991850	-5.560604	0.273648
23	1	0	-8.615337	-5.242448	1.499814
24	1	0	-8.909781	-7.351746	-0.704927
25	1	0	-8.739566	-7.672389	1.023597
26	1	0	-9.971198	-2.063617	-0.387097
27	1	0	-10.109864	0.225204	-0.165067
28	1	0	-9.098759	2.480065	-0.058014
29	6	0	-6.441495	3.016938	-0.022064
30	1	0	-5.171901	0.683411	-0.112495
31	8	0	-6.017652	-1.738095	-0.219714
32	6	0	-6.278139	-6.636427	0.283256
33	6	0	-4.834796	-6.713373	0.185785
34	6	0	-3.999552	-5.562301	0.169865
35	6	0	-4.225653	-7.985430	0.148685
36	6	0	-2.852310	-8.134736	0.089959
37	6	0	-2.025716	-6.986016	0.075764
38	6	0	-2.610180	-5.711674	0.119173
39	1	0	-6.772744	-7.603502	0.387097
40	8	0	-4.514060	-4.342392	0.219714
41	1	0	-4.859900	-8.868001	0.165067
42	1	0	-2.401580	-9.119789	0.058014
43	6	0	-0.608002	-7.086967	0.022064
44	1	0	-1.994099	-4.820703	0.112495
45	6	0	0.608002	-7.086967	-0.022064
46	6	0	2.025716	-6.986016	-0.075764
47	6	0	2.852310	-8.134736	-0.089959
48	6	0	4.225653	-7.985430	-0.148685
49	6	0	4.834796	-6.713373	-0.185785
50	6	0	3.999552	-5.562301	-0.169865
51	6	0	2.610180	-5.711674	-0.119173
52	6	0	6.278139	-6.636427	-0.283256
53	7	0	6.991850	-5.560604	-0.273648
54	6	0	8.455357	-5.591901	-0.471013
55	6	0	9.135404	-6.956572	-0.295082
56	6	0	10.656739	-6.845079	-0.475845
57	6	0	11.256382	-5.806467	0.475845
58	6	0	10.592270	-4.433206	0.295082
59	6	0	9.070407	-4.526603	0.471013
60	1	0	2.401580	-9.119789	-0.058014
61	1	0	4.859900	-8.868001	-0.165067
62	8	0	4.514060	-4.342392	-0.219714

63	1	0	1.994099	-4.820703	-0.112495
64	1	0	6.772744	-7.603502	-0.387097
65	1	0	8.615337	-5.242448	-1.499814
66	1	0	8.739566	-7.672389	-1.023597
67	1	0	8.909781	-7.351746	0.704927
68	1	0	10.880654	-6.562898	-1.513329
69	1	0	11.117889	-7.825117	-0.312458
70	1	0	12.335695	-5.715816	0.312458
71	1	0	11.123963	-6.141474	1.513329
72	1	0	10.821689	-4.040224	-0.704927
73	1	0	11.014267	-3.732492	1.023597
74	7	0	8.311549	-3.274818	0.273648
75	1	0	8.847762	-4.839877	1.499814
76	6	0	8.886384	-2.118814	0.283256
77	6	0	8.231350	-0.830370	0.185785
78	6	0	6.816870	-0.682563	0.169865
79	6	0	6.251545	0.595355	0.119173
80	6	0	7.062925	1.738686	0.075764
81	6	0	8.471043	1.597195	0.089959
82	6	0	9.028412	0.333192	0.148685
83	1	0	9.971198	-2.063617	0.387097
84	8	0	6.017652	-1.738095	0.219714
85	1	0	5.171901	0.683411	0.112495
86	6	0	6.441495	3.016938	0.022064
87	1	0	9.098759	2.480065	0.058014
88	1	0	10.109864	0.225204	0.165067
89	6	0	5.833493	4.070029	-0.022064
90	6	0	5.037209	5.247329	-0.075764
91	6	0	3.641365	5.116319	-0.119173
92	6	0	2.817318	6.244864	-0.169865
93	6	0	3.396554	7.543743	-0.185785
94	6	0	4.802759	7.652238	-0.148685
95	6	0	5.618733	6.537541	-0.089959
96	6	0	2.608245	8.755241	-0.283256
97	7	0	1.319699	8.835422	-0.273648
98	6	0	-0.615050	10.118504	0.471013
99	1	0	3.177802	4.137292	-0.112495
100	1	0	5.249964	8.642797	-0.165067
101	1	0	6.697179	6.639724	-0.058014
102	1	0	3.198454	9.667119	-0.387097
103	7	0	-1.319699	8.835422	0.273648
104	6	0	-5.833493	4.070029	0.022064
105	6	0	-5.037209	5.247329	0.075764
106	6	0	-3.641365	5.116319	0.119173
107	6	0	-2.817318	6.244864	0.169865
108	6	0	-3.396554	7.543743	0.185785
109	6	0	-4.802759	7.652238	0.148685
110	6	0	-5.618733	6.537541	0.089959
111	1	0	-3.177802	4.137292	0.112495
112	8	0	-1.503592	6.080487	0.219714
113	6	0	-2.608245	8.755241	0.283256
114	1	0	-5.249964	8.642797	0.165067
115	1	0	-6.697179	6.639724	0.058014
116	1	0	-3.198454	9.667119	0.387097
117	6	0	-1.456866	11.389778	0.295082
118	6	0	1.456866	11.389778	-0.295082
119	6	0	-0.599643	12.651546	0.475845
120	6	0	0.599643	12.651546	-0.475845
121	1	0	-2.274701	11.404881	1.023597
122	1	0	-1.911908	11.391970	-0.704927
123	1	0	2.274701	11.404881	-1.023597
124	1	0	1.911908	11.391970	0.704927
125	1	0	-0.243309	12.704372	1.513329
126	1	0	-1.217806	13.540933	0.312458
127	1	0	0.243309	12.704372	-1.513329
128	1	0	1.217806	13.540933	-0.312458
129	6	0	0.615050	10.118504	-0.471013
130	1	0	-0.232425	10.082325	1.499814
131	1	0	0.232425	10.082325	-1.499814
132	8	0	1.503592	6.080487	-0.219714
133	22	0	0.000000	7.115397	-0.000000
134	22	0	6.162115	-3.557699	-0.000000
135	22	0	-6.162115	-3.557699	-0.000000
136	17	0	-6.615966	-3.331893	2.302118
137	17	0	0.422479	7.395541	2.302118
138	17	0	6.193487	-4.063648	2.302118
139	17	0	-0.422479	7.395541	-2.302118

140	17	0	-6.193487	-4.063648	-2.302118
141	17	0	6.615966	-3.331893	-2.302118

Table D4. Cartesian coordinates for **3a**·Zn.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.947781	-7.004467	0.440989
2	6	0	-11.653866	-5.984410	-0.461854
3	6	0	-11.074896	-4.578004	-0.260356
4	6	0	-9.552070	-4.536882	-0.481744
5	6	0	-8.831920	-5.573127	0.421524
6	6	0	-9.429721	-6.980314	0.218940
7	7	0	-9.059065	-3.200755	-0.189540
8	6	0	-8.296490	-2.606208	-1.037634
9	6	0	-7.750390	-1.278810	-0.807058
10	6	0	-6.881913	-0.705089	-1.754922
11	6	0	-6.316499	0.540779	-1.559641
12	6	0	-6.620918	1.267927	-0.383097
13	6	0	-7.500184	0.724465	0.563847
14	6	0	-8.060540	-0.543305	0.370533
15	1	0	-11.169093	-6.773828	1.493124
16	1	0	-11.332465	-8.014663	0.255113
17	1	0	-11.535297	-6.284726	-1.513002
18	1	0	-12.731941	-5.974416	-0.260292
19	1	0	-11.549122	-3.859042	-0.939009
20	1	0	-11.285977	-4.230100	0.760206
21	1	0	-9.329318	-4.811065	-1.527563
22	7	0	-7.415476	-5.603291	0.093438
23	1	0	-8.980505	-5.264405	1.470676
24	1	0	-9.195458	-7.312135	-0.801837
25	1	0	-8.924718	-7.678193	0.897581
26	1	0	-8.018603	-3.089211	-1.985522
27	1	0	-6.645792	-1.270926	-2.653449
28	1	0	-5.635912	0.966329	-2.288549
29	6	0	-5.989461	2.524910	-0.158876
30	1	0	-7.740075	1.266398	1.471912
31	8	0	-8.876741	-1.033383	1.318567
32	6	0	-6.541072	-5.373468	1.008021
33	6	0	-5.109143	-5.413977	0.754096
34	6	0	-4.595317	-5.696378	-0.542211
35	6	0	-4.200976	-5.177993	1.803969
36	6	0	-2.833069	-5.220205	1.605713
37	6	0	-2.324540	-5.500517	0.314429
38	6	0	-3.211819	-5.731663	-0.747042
39	1	0	-6.847708	-5.137789	2.037793
40	8	0	-5.402740	-5.934903	-1.589431
41	1	0	-4.595979	-4.959166	2.793634
42	1	0	-2.144668	-5.038566	2.423536
43	6	0	-0.917920	-5.555819	0.096737
44	1	0	-2.839079	-5.949651	-1.741665
45	1	0	-9.155680	-1.945631	1.022798
46	1	0	-6.341757	-5.891535	-1.251725
47	6	0	0.285080	-5.612741	-0.077312
48	6	0	1.690244	-5.691981	-0.296975
49	6	0	2.219405	-5.478811	-1.592824
50	6	0	3.584293	-5.571995	-1.794497
51	6	0	4.468771	-5.880837	-0.743303
52	6	0	3.934409	-6.092880	0.558100
53	6	0	2.554647	-5.991517	0.766205
54	6	0	5.895652	-5.994979	-1.002770
55	7	0	6.745989	-6.301939	-0.088108
56	6	0	8.153084	-6.446057	-0.427598
57	6	0	8.566612	-7.919258	-0.237318
58	6	0	10.068100	-8.137902	-0.464702
59	6	0	10.901701	-7.222620	0.441555
60	6	0	10.510350	-5.752444	0.246738
61	6	0	9.006052	-5.514464	0.473976
62	1	0	1.548934	-5.243606	-2.411894
63	1	0	3.995166	-5.407595	-2.788262
64	8	0	4.718306	-6.394079	1.606997

65	1	0	2.165996	-6.159063	1.764502
66	1	0	6.219838	-5.813570	-2.038257
67	1	0	8.330411	-6.152751	-1.476649
68	1	0	7.973719	-8.541158	-0.918854
69	1	0	8.294520	-8.226234	0.781899
70	1	0	10.315637	-7.932357	-1.516319
71	1	0	10.319619	-9.190339	-0.285122
72	1	0	11.971810	-7.352223	0.239036
73	1	0	10.745160	-7.509586	1.491554
74	1	0	10.762299	-5.430656	-0.773198
75	1	0	11.075891	-5.103881	0.926410
76	7	0	8.685040	-4.125610	0.186131
77	1	0	8.753428	-5.758957	1.520578
78	1	0	5.655478	-6.449605	1.266101
79	6	0	8.005500	-3.444592	1.039766
80	6	0	7.615477	-2.062896	0.812250
81	6	0	7.989160	-1.372425	-0.373980
82	6	0	7.569530	-0.051584	-0.569007
83	6	0	6.769104	0.590945	0.385761
84	6	0	6.404793	-0.090760	1.572408
85	6	0	6.830902	-1.390738	1.768542
86	1	0	7.678905	-3.892556	1.989407
87	8	0	8.732371	-1.955152	-1.329703
88	1	0	7.853834	0.454816	-1.484722
89	6	0	6.271782	1.906515	0.158804
90	1	0	5.786272	0.411807	2.307568
91	1	0	6.545971	-1.921894	2.674067
92	1	0	8.912238	-2.891441	-1.032627
93	6	0	5.771063	3.003317	-0.004516
94	6	0	5.071126	4.234747	-0.166338
95	6	0	3.765769	4.324191	0.311113
96	6	0	2.963760	5.478528	0.126806
97	6	0	3.573457	6.602399	-0.545350
98	6	0	4.921509	6.498313	-0.977285
99	6	0	5.664235	5.350288	-0.818764
100	6	0	2.906009	7.861575	-0.749394
101	7	0	1.632132	8.057857	-0.605946
102	6	0	0.021719	9.419551	0.621221
103	1	0	3.306746	3.479862	0.813317
104	1	0	5.370346	7.360799	-1.467130
105	1	0	6.685278	5.286151	-1.178135
106	1	0	3.554976	8.696839	-1.034757
107	7	0	-0.753404	8.176734	0.603017
108	6	0	-5.379570	3.565003	0.004236
109	6	0	-4.559615	4.719620	0.167018
110	6	0	-3.257114	4.684466	-0.325224
111	6	0	-2.342689	5.751649	-0.139550
112	6	0	-2.830724	6.923631	0.549521
113	6	0	-4.177832	6.949317	0.995837
114	6	0	-5.032243	5.881999	0.835948
115	1	0	-2.889254	3.804004	-0.840257
116	8	0	-1.139467	5.610965	-0.620778
117	6	0	-2.039189	8.108188	0.757122
118	1	0	-4.533760	7.847066	1.498470
119	1	0	-6.050649	5.915584	1.206798
120	1	0	-2.598809	9.001928	1.054646
121	6	0	-0.774202	10.729684	0.645274
122	6	0	1.909565	10.596608	-0.640292
123	6	0	0.160387	11.949124	0.607600
124	6	0	1.100002	11.902289	-0.604080
125	1	0	-1.400467	10.772517	1.544900
126	1	0	-1.454547	10.757437	-0.218116
127	1	0	2.539059	10.577464	-1.538415
128	1	0	2.586948	10.557411	0.224924
129	1	0	0.756750	11.978551	1.530629
130	1	0	-0.435028	12.869696	0.592278
131	1	0	0.509391	11.989681	-1.527146
132	1	0	1.783240	12.759684	-0.589131
133	6	0	0.986700	9.372713	-0.619097
134	1	0	0.667637	9.382887	1.512672
135	1	0	0.340251	9.404077	-1.510350
136	8	0	1.747159	5.453457	0.593837
137	30	0	0.360690	6.608052	-0.009433

Table D5. Cartesian coordinates for **3a**·2Zn.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.351075	10.974506	-5.202607
2	6	0	-0.803913	10.589215	-6.135680
3	6	0	-0.832578	9.075470	-6.398264
4	6	0	-0.913881	8.289563	-5.084764
5	6	0	0.266182	8.680345	-4.124690
6	6	0	0.294957	10.194072	-3.880162
7	7	0	-0.913497	6.827676	-5.181417
8	6	0	-0.909813	6.174553	-6.303113
9	6	0	-0.696982	4.758877	-6.439289
10	6	0	-0.917783	4.184242	-7.719127
11	6	0	-0.720693	2.846583	-7.976192
12	6	0	-0.266182	2.006074	-6.922939
13	6	0	-0.004527	2.549340	-5.667025
14	6	0	-0.206890	3.920659	-5.370543
15	1	0	1.307613	10.771542	-5.705133
16	1	0	0.330811	12.051097	-4.995771
17	1	0	-1.757405	10.898897	-5.684545
18	1	0	-0.720188	11.127563	-7.087195
19	1	0	-1.687599	8.825590	-7.038590
20	1	0	0.073814	8.781181	-6.946844
21	1	0	-1.841026	8.574500	-4.563024
22	7	0	0.149236	7.826829	-2.940085
23	1	0	1.192812	8.387853	-4.643959
24	1	0	-0.602208	10.485790	-3.315316
25	1	0	1.160449	10.459348	-3.260804
26	1	0	-1.062217	6.715952	-7.243063
27	1	0	-1.267673	4.835409	-8.518480
28	1	0	-0.912735	2.427760	-8.957857
29	6	0	-0.085785	0.602452	-7.094576
30	1	0	0.351607	1.917694	-4.860859
31	8	0	0.080488	4.330952	-4.168325
32	6	0	0.277094	8.246756	-1.720313
33	6	0	0.001466	7.462464	-0.546330
34	6	0	-0.725052	6.214179	-0.573627
35	6	0	0.433381	7.985127	0.699951
36	6	0	0.228978	7.324149	1.888504
37	6	0	-0.469135	6.084253	1.874321
38	6	0	-0.952183	5.572566	0.671905
39	1	0	0.611513	9.272660	-1.530966
40	8	0	-1.201520	5.652403	-1.649300
41	1	0	0.962725	8.936518	0.701122
42	1	0	0.589718	7.728098	2.827853
43	6	0	-0.649777	5.349515	3.081847
44	1	0	-1.490253	4.631214	0.651925
45	6	0	-0.770248	4.693113	4.099349
46	6	0	-0.893553	3.891285	5.269824
47	6	0	-1.950688	2.956253	5.384361
48	6	0	-2.041191	2.166680	6.515945
49	6	0	-1.101123	2.258981	7.560472
50	6	0	-0.039145	3.198801	7.441988
51	6	0	0.046548	4.007699	6.304036
52	6	0	-1.224841	1.403215	8.729817
53	7	0	-0.374215	1.423796	9.694905
54	6	0	-0.552669	0.546666	10.840429
55	6	0	-0.493749	1.388780	12.129358
56	6	0	-0.556182	0.528422	13.397253
57	6	0	0.556182	-0.528422	13.397253
58	6	0	0.493749	-1.388780	12.129358
59	6	0	0.552669	-0.546666	10.840429
60	1	0	-2.674734	2.867610	4.582122
61	1	0	-2.850853	1.445966	6.607521
62	8	0	0.897627	3.336579	8.395145
63	1	0	0.864267	4.715955	6.230295
64	1	0	-2.092357	0.727854	8.753561
65	1	0	-1.525499	0.028293	10.785678
66	1	0	-1.313084	2.117321	12.110340
67	1	0	0.439412	1.968605	12.119100
68	1	0	-1.533776	0.028330	13.457219
69	1	0	-0.478928	1.169633	14.283810
70	1	0	0.478928	-1.169633	14.283810

71	1	0	1.533776	-0.028330	13.457219
72	1	0	-0.439412	-1.968605	12.119100
73	1	0	1.313084	-2.117321	12.110340
74	7	0	0.374215	-1.423796	9.694905
75	1	0	1.525499	-0.028293	10.785678
76	1	0	0.680592	2.679273	9.116022
77	6	0	1.224841	-1.403215	8.729817
78	6	0	1.101123	-2.258981	7.560472
79	6	0	0.039145	-3.198801	7.441988
80	6	0	-0.046548	-4.007699	6.304036
81	6	0	0.893553	-3.891285	5.269824
82	6	0	1.950688	-2.956253	5.384361
83	6	0	2.041191	-2.166680	6.515945
84	1	0	2.092357	-0.727854	8.753561
85	8	0	-0.897627	-3.336579	8.395145
86	1	0	-0.864267	-4.715955	6.230295
87	6	0	0.770248	-4.693113	4.099349
88	1	0	2.674734	-2.867610	4.582122
89	1	0	2.850853	-1.445966	6.607521
90	1	0	-0.680592	-2.679273	9.116022
91	6	0	0.649777	-5.349515	3.081847
92	6	0	0.469135	-6.084253	1.874321
93	6	0	0.952183	-5.572566	0.671905
94	6	0	0.725052	-6.214179	-0.573627
95	6	0	-0.001466	-7.462464	-0.546330
96	6	0	-0.433381	-7.985127	0.699951
97	6	0	-0.228978	-7.324149	1.888504
98	6	0	-0.277094	-8.246756	-1.720313
99	7	0	-0.149236	-7.826829	-2.940085
100	6	0	0.913881	-8.289563	-5.084764
101	1	0	1.490253	-4.631214	0.651925
102	1	0	-0.962725	-8.936518	0.701122
103	1	0	-0.589718	-7.728098	2.827853
104	1	0	-0.611513	-9.272660	-1.530966
105	7	0	0.913497	-6.827676	-5.181417
106	6	0	0.085785	-0.602452	-7.094576
107	6	0	0.266182	-2.006074	-6.922939
108	6	0	0.004527	-2.549340	-5.667025
109	6	0	0.206890	-3.920659	-5.370543
110	6	0	0.696982	-4.758877	-6.439289
111	6	0	0.917783	-4.184242	-7.719127
112	6	0	0.720693	-2.846583	-7.976192
113	1	0	-0.351607	-1.917694	-4.860859
114	8	0	-0.080488	-4.330952	-4.168325
115	6	0	0.909813	-6.174553	-6.303113
116	1	0	1.267673	-4.835409	-8.518480
117	1	0	0.912735	-2.427760	-8.957857
118	1	0	1.062217	-6.715952	-7.243063
119	6	0	0.832578	-9.075470	-6.398264
120	6	0	-0.294957	-10.194072	-3.880162
121	6	0	0.803913	-10.589215	-6.135680
122	6	0	-0.351075	-10.974506	-5.202607
123	1	0	1.687599	-8.825590	-7.038590
124	1	0	-0.073814	-8.781181	-6.946844
125	1	0	-1.160449	-10.459348	-3.260804
126	1	0	0.602208	-10.485790	-3.315316
127	1	0	1.757405	-10.898897	-5.684545
128	1	0	0.720188	-11.127563	-7.087195
129	1	0	-1.307613	-10.771542	-5.705133
130	1	0	-0.330811	-12.051097	-4.995771
131	6	0	-0.266182	-8.680345	-4.124690
132	1	0	1.841026	-8.574500	-4.563024
133	1	0	-1.192812	-8.387853	-4.643959
134	8	0	1.201520	-5.652403	-1.649300
135	30	0	-0.504698	5.966457	-3.396295
136	30	0	0.504698	-5.966457	-3.396295

Table D6. Cartesian coordinates for **3a**·3Zn.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-10.643168	-6.685524	0.607247
2	6	0	-11.111418	-5.874492	-0.607247
3	6	0	-10.453155	-4.487114	-0.644684
4	6	0	-8.924288	-4.595609	-0.619427
5	6	0	-8.442058	-5.430856	0.619427
6	6	0	-9.112532	-6.809141	0.644684
7	7	0	-8.172257	-3.338723	-0.600034
8	6	0	-8.715966	-2.167638	-0.728969
9	6	0	-8.042174	-0.913938	-0.529290
10	6	0	-8.735754	0.264884	-0.908960
11	6	0	-8.198451	1.521513	-0.755059
12	6	0	-6.901495	1.648460	-0.184647
13	6	0	-6.214251	0.512894	0.236655
14	6	0	-6.740749	-0.796079	0.085142
15	1	0	-10.991428	-6.197215	1.527586
16	1	0	-11.093917	-7.684009	0.595525
17	1	0	-10.862660	-6.420249	-1.527586
18	1	0	-12.201505	-5.765609	-0.595525
19	1	0	-10.776483	-3.948909	-1.543170
20	1	0	-10.789966	-3.896556	0.218560
21	1	0	-8.597109	-5.154635	-1.510058
22	7	0	-6.977548	-5.408021	0.600034
23	1	0	-8.762599	-4.867997	1.510058
24	1	0	-8.769499	-7.396107	-0.218560
25	1	0	-8.808097	-7.358254	1.543170
26	1	0	-9.774187	-2.088849	-0.999819
27	1	0	-9.724719	0.157201	-1.350004
28	1	0	-8.738200	2.407145	-1.069351
29	6	0	-6.276293	2.924107	-0.055599
30	1	0	-5.230208	0.600684	0.682372
31	8	0	-6.030471	-1.795242	0.525316
32	6	0	-6.235213	-6.464429	0.728969
33	6	0	-4.812581	-6.507758	0.529290
34	6	0	-4.059799	-5.439621	-0.085142
35	6	0	-4.138481	-7.697827	0.908960
36	6	0	-2.781556	-7.860823	0.755059
37	6	0	-2.023139	-6.801100	0.184647
38	6	0	-2.662946	-5.638146	-0.236655
39	1	0	-6.696090	-7.420270	0.999819
40	8	0	-4.569961	-4.324920	-0.525316
41	1	0	-4.726220	-8.500454	1.350004
42	1	0	-2.284451	-8.771076	1.069351
43	6	0	-0.605795	-6.897483	0.055599
44	1	0	-2.094896	-4.829835	-0.682372
45	6	0	0.605795	-6.897483	-0.055599
46	6	0	2.023139	-6.801100	-0.184647
47	6	0	2.781556	-7.860823	-0.755059
48	6	0	4.138481	-7.697827	-0.908960
49	6	0	4.812581	-6.507758	-0.529290
50	6	0	4.059799	-5.439621	0.085142
51	6	0	2.662946	-5.638146	0.236655
52	6	0	6.235213	-6.464429	-0.728969
53	7	0	6.977548	-5.408021	-0.600034
54	6	0	8.442058	-5.430856	-0.619427
55	6	0	9.112532	-6.809141	-0.644684
56	6	0	10.643168	-6.685524	-0.607247
57	6	0	11.111418	-5.874492	0.607247
58	6	0	10.453155	-4.487114	0.644684
59	6	0	8.924288	-4.595609	0.619427
60	1	0	2.284451	-8.771076	-1.069351
61	1	0	4.726220	-8.500454	-1.350004
62	8	0	4.569961	-4.324920	0.525316
63	1	0	2.094896	-4.829835	0.682372
64	1	0	6.696090	-7.420270	-0.999819
65	1	0	8.762599	-4.867997	-1.510058
66	1	0	8.808097	-7.358254	-1.543170
67	1	0	8.769499	-7.396107	0.218560
68	1	0	10.991428	-6.197215	-1.527586
69	1	0	11.093917	-7.684009	-0.595525
70	1	0	12.201505	-5.765609	0.595525
71	1	0	10.862660	-6.420249	1.527586
72	1	0	10.789966	-3.896556	-0.218560
73	1	0	10.776483	-3.948909	1.543170
74	7	0	8.172257	-3.338723	0.600034
75	1	0	8.597109	-5.154635	1.510058
76	6	0	8.715966	-2.167638	0.728969
77	6	0	8.042174	-0.913938	0.529290

78	6	0	6.740749	-0.796079	-0.085142
79	6	0	6.214251	0.512894	-0.236655
80	6	0	6.901495	1.648460	0.184647
81	6	0	8.198451	1.521513	0.755059
82	6	0	8.735754	0.264884	0.908960
83	1	0	9.774187	-2.088849	0.999819
84	8	0	6.030471	-1.795242	-0.525316
85	1	0	5.230208	0.600684	-0.682372
86	6	0	6.276293	2.924107	0.055599
87	1	0	8.738200	2.407145	1.069351
88	1	0	9.724719	0.157201	1.350004
89	6	0	5.670498	3.973376	-0.055599
90	6	0	4.878355	5.152640	-0.184647
91	6	0	3.551305	5.125252	0.236655
92	6	0	2.680950	6.235700	0.085142
93	6	0	3.229594	7.421696	-0.529290
94	6	0	4.597273	7.432943	-0.908960
95	6	0	5.416895	6.339310	-0.755059
96	6	0	2.480753	8.632067	-0.728969
97	7	0	1.194709	8.746744	-0.600034
98	6	0	-0.482230	10.026464	0.619427
99	1	0	3.135312	4.229151	0.682372
100	1	0	4.998499	8.343254	-1.350004
101	1	0	6.453749	6.363931	-1.069351
102	1	0	3.078097	9.509119	-0.999819
103	7	0	-1.194709	8.746744	0.600034
104	6	0	-5.670498	3.973376	0.055599
105	6	0	-4.878355	5.152640	0.184647
106	6	0	-3.551305	5.125252	-0.236655
107	6	0	-2.680950	6.235700	-0.085142
108	6	0	-3.229594	7.421696	0.529290
109	6	0	-4.597273	7.432943	0.908960
110	6	0	-5.416895	6.339310	0.755059
111	1	0	-3.135312	4.229151	-0.682372
112	8	0	-1.460510	6.120162	-0.525316
113	6	0	-2.480753	8.632067	0.728969
114	1	0	-4.998499	8.343254	1.350004
115	1	0	-6.453749	6.363931	1.069351
116	1	0	-3.078097	9.509119	0.999819
117	6	0	-1.340623	11.296255	0.644684
118	6	0	1.340623	11.296255	-0.644684
119	6	0	-0.468250	12.560016	0.607247
120	6	0	0.468250	12.560016	-0.607247
121	1	0	-1.968386	11.307162	1.543170
122	1	0	-2.020467	11.292663	-0.218560
123	1	0	1.968386	11.307162	-1.543170
124	1	0	2.020467	11.292663	0.218560
125	1	0	0.128768	12.617464	1.527586
126	1	0	-1.107588	13.449618	0.595525
127	1	0	-0.128768	12.617464	-1.527586
128	1	0	1.107588	13.449618	-0.595525
129	6	0	0.482230	10.026464	-0.619427
130	1	0	0.165491	10.022632	1.510058
131	1	0	-0.165491	10.022632	-1.510058
132	8	0	1.460510	6.120162	0.525316
133	30	0	0.000000	7.224378	-0.000000
134	30	0	-6.256495	-3.612189	-0.000000
135	30	0	6.256495	-3.612189	-0.000000