Supplementary Information

β-Arylethynyl Substituted Silver Corrole Complexes

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Mass Spectra

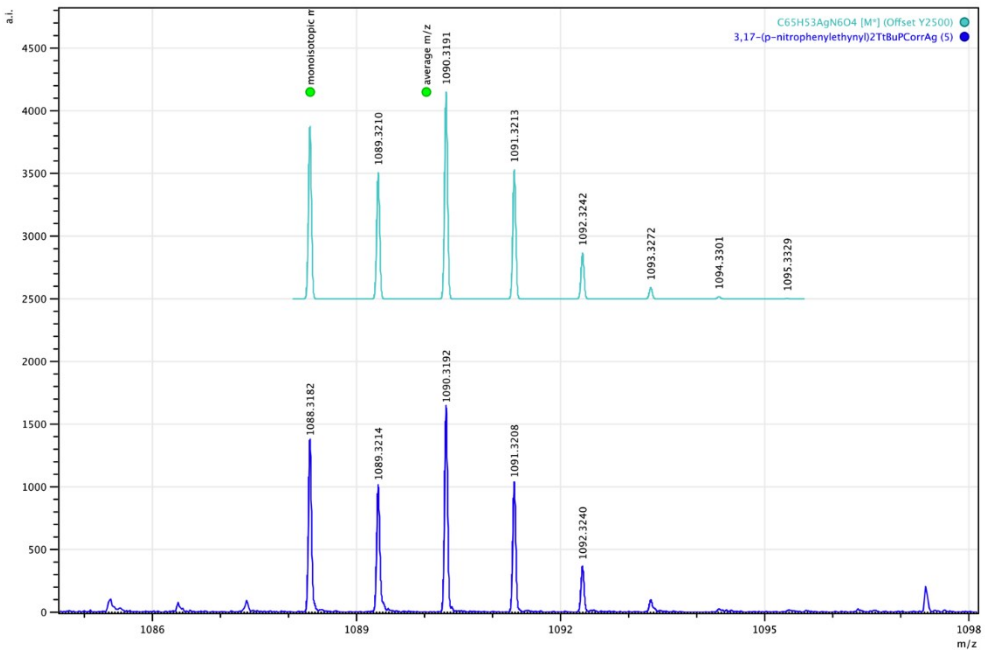


Figure S1: MALDI-TOF mass spectrum of Ag Corrole **5** (Top: simulated; Bottom: observed).

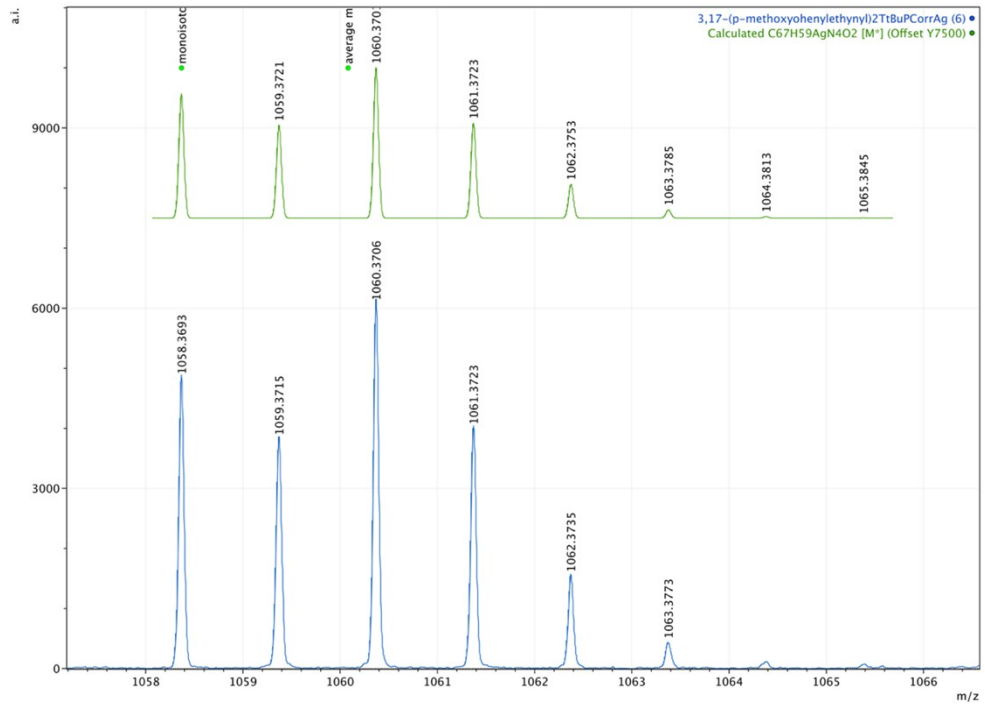


Figure S2: MALDI-TOF mass spectrum of Ag Corrole **6** (Top: simulated; Bottom: observed).

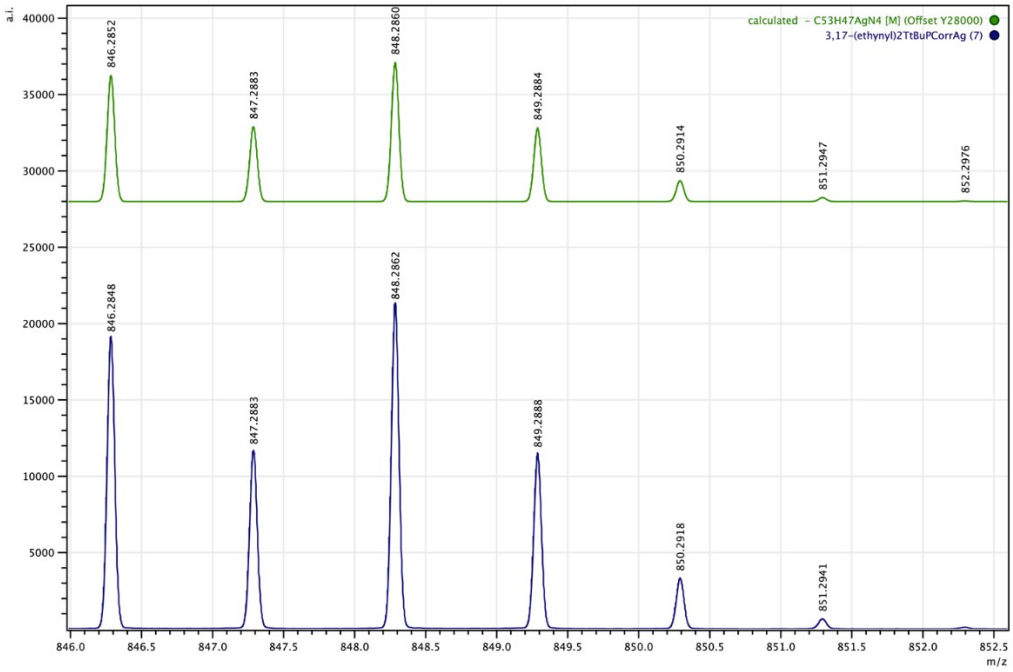


Figure S3: MALDI-TOF mass spectrum of Ag Corrole **7** (Top: simulated; Bottom: observed).

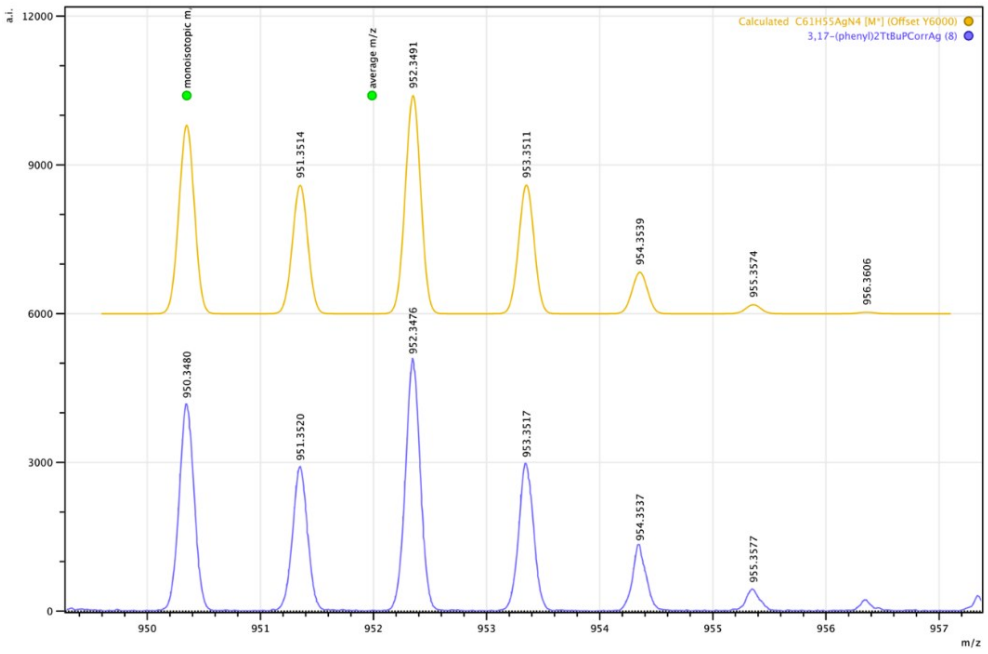


Figure S4: MALDI-TOF mass spectrum of Ag Corrole **3** (Top: simulated; Bottom: observed).

[1]H NMR Spectra

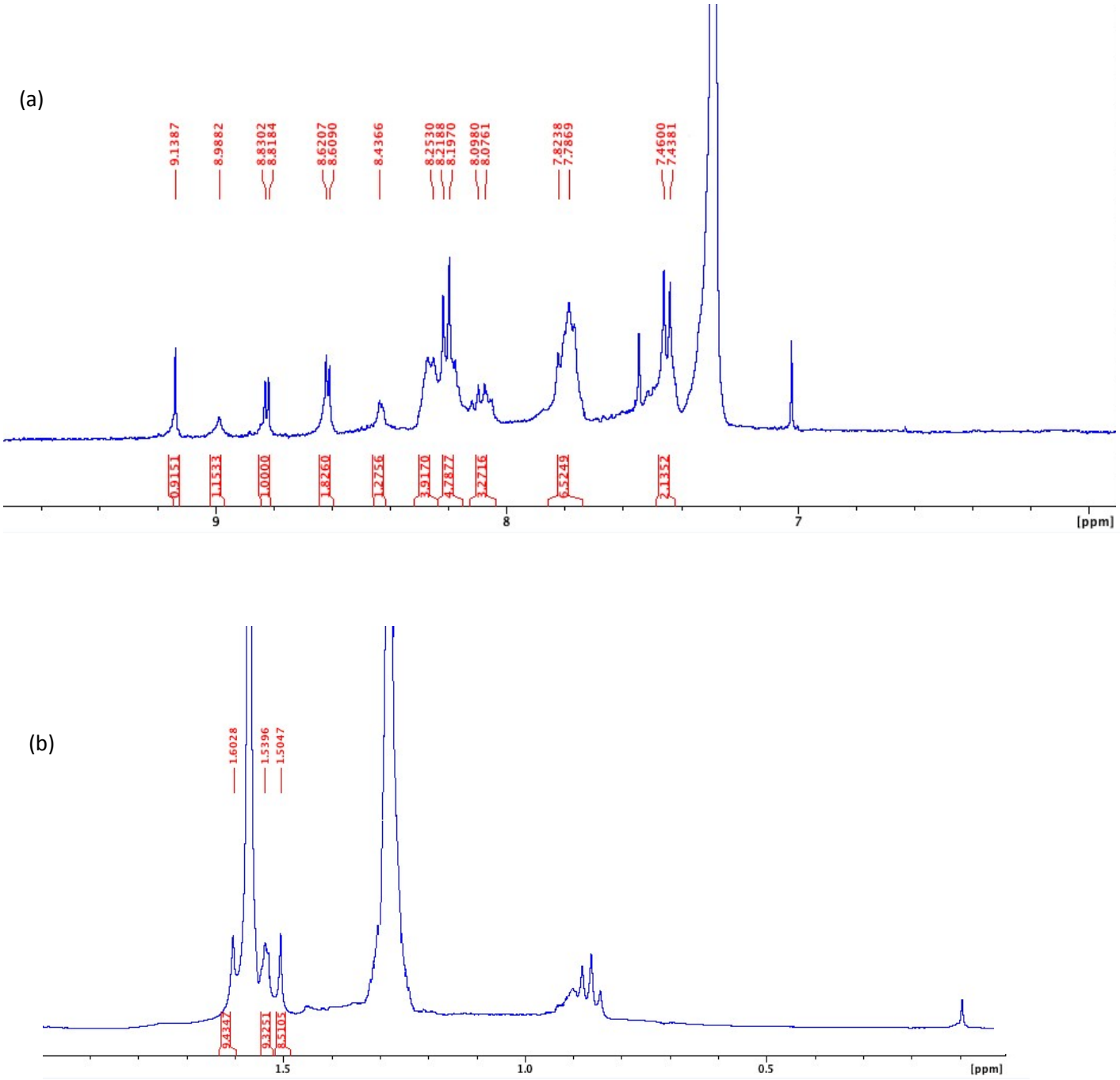


Figure S5: ^{1}H NMR spectrum of Ag Corrole **5** in $CDCl_3$, at 298 K. (a) Aromatic region; (b) Aliphatic region.

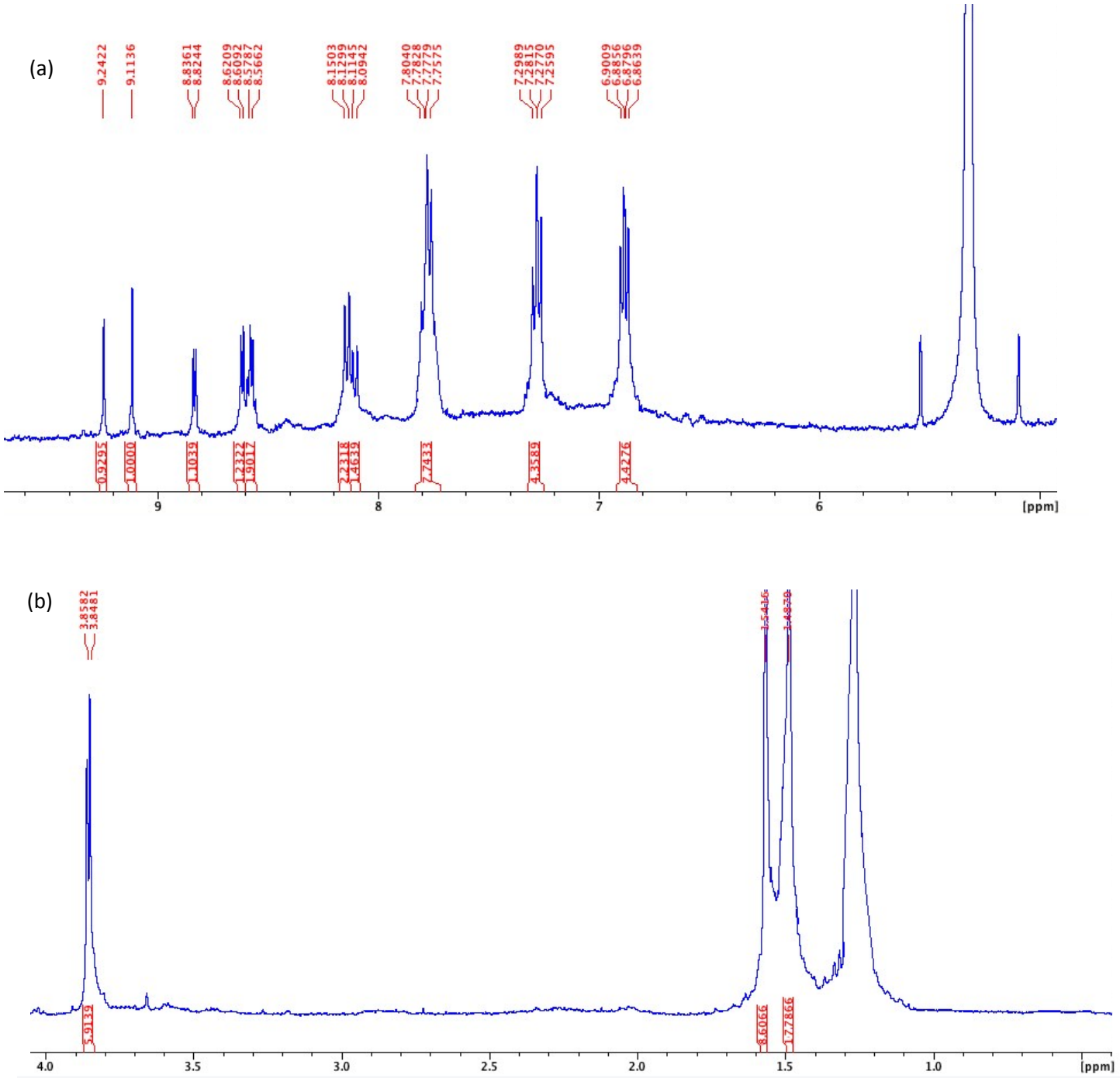


Figure S6: ^{1}H NMR spectrum of Ag Corrole **6** in CD_2Cl_2, at 298 K. (a) Aromatic region; (b) Aliphatic region.

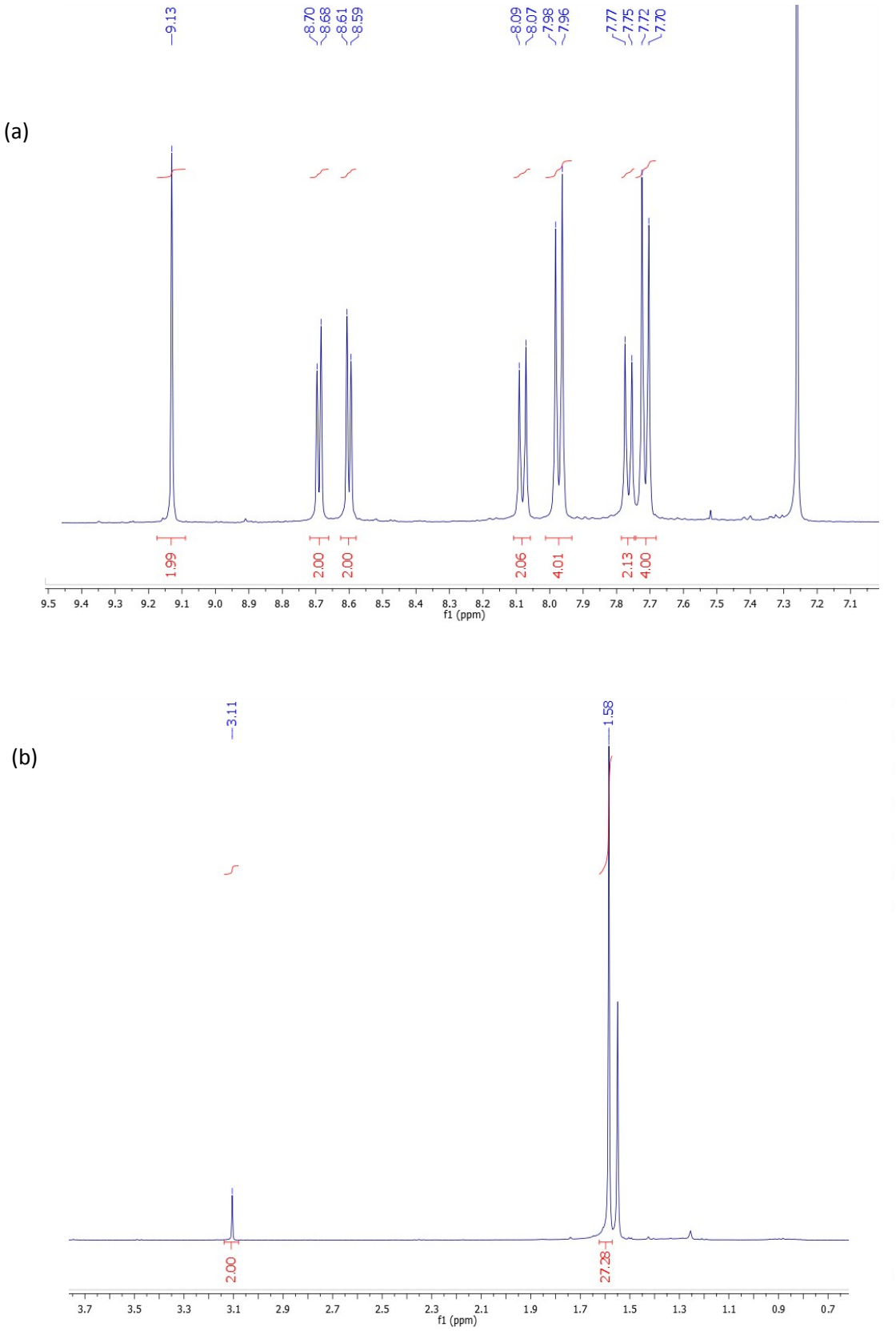


Figure S7: ^{1}H NMR spectrum of Ag Corrole **7** in $CDCl_3$, at 298 K. (a) Aromatic region; (b) Aliphatic region.

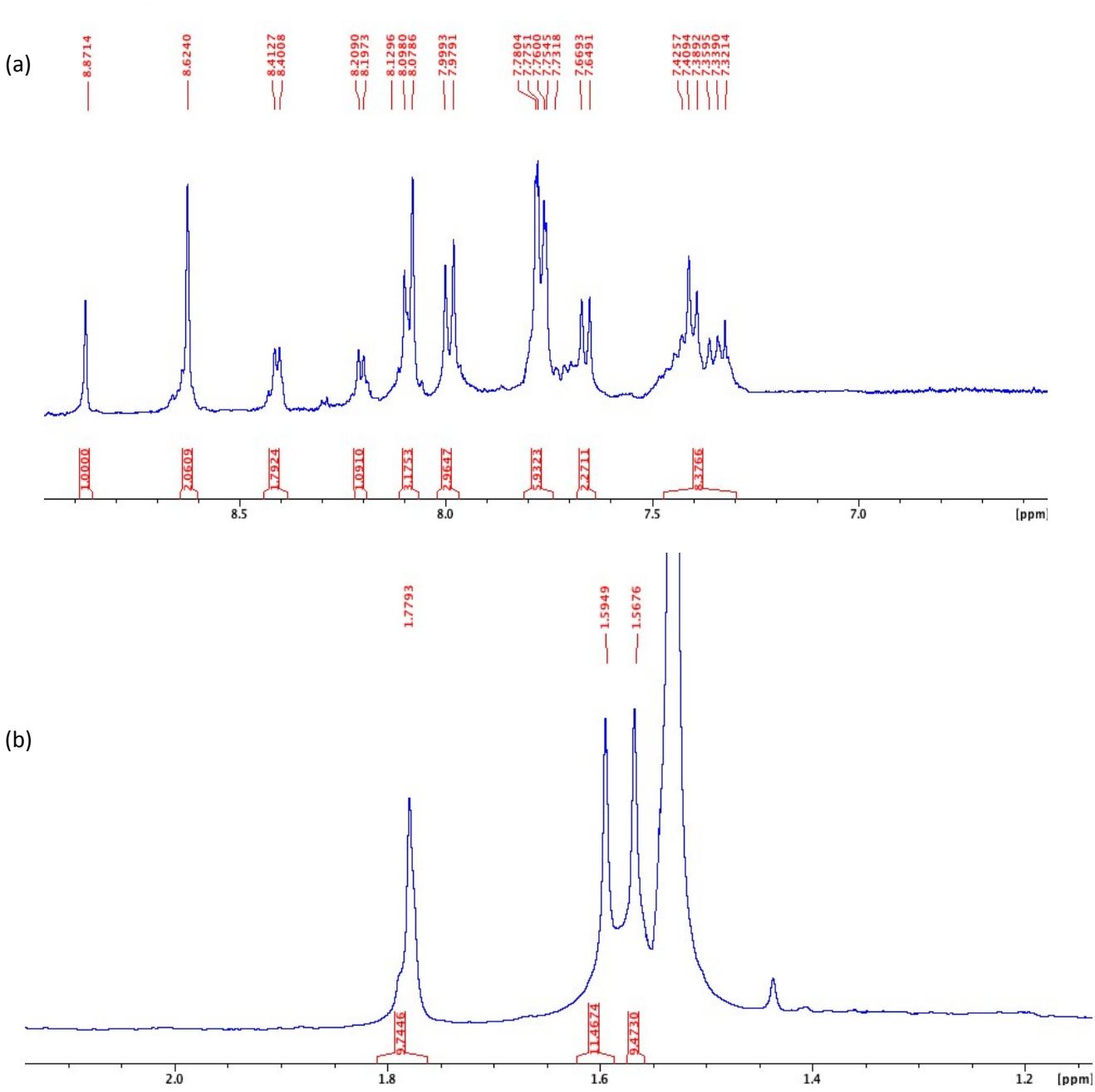
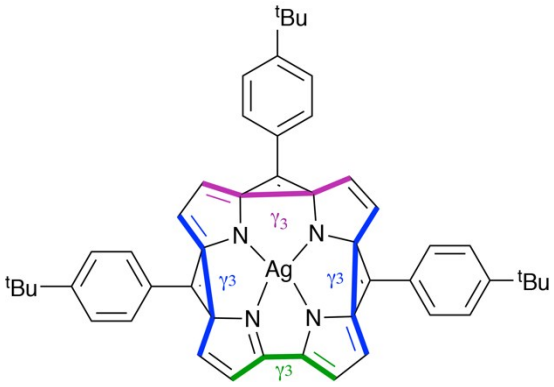


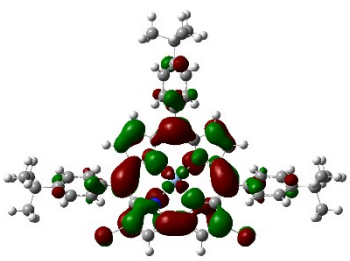
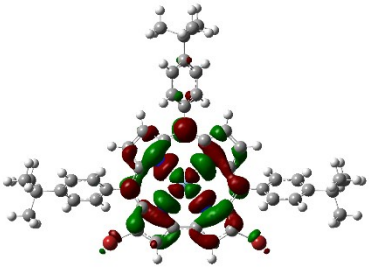
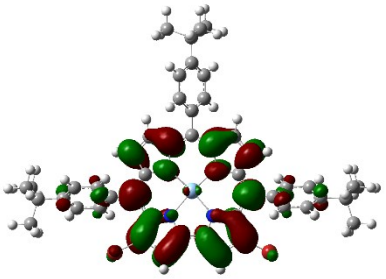
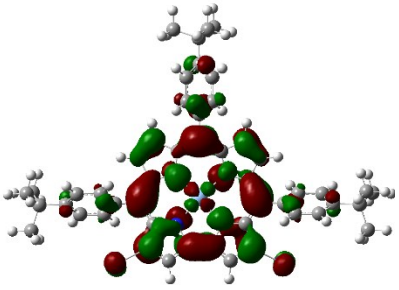
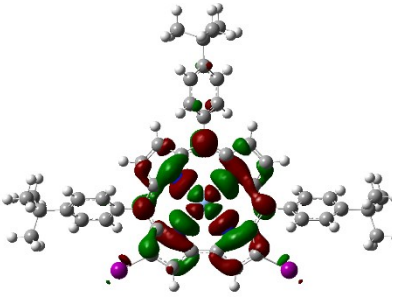
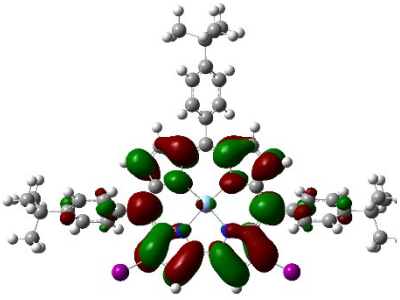
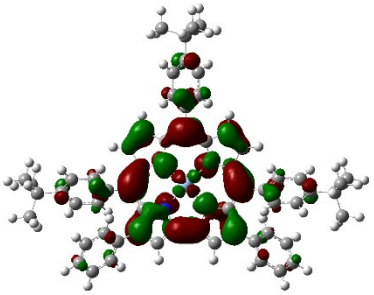
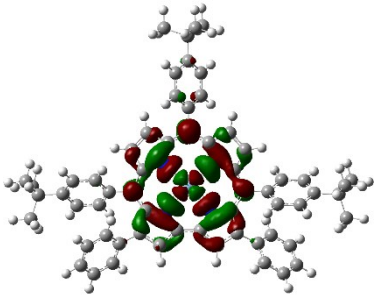
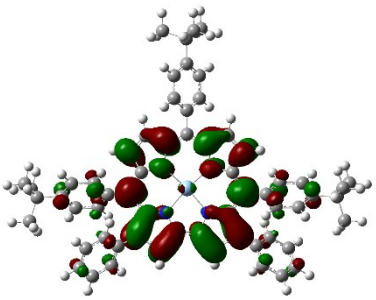
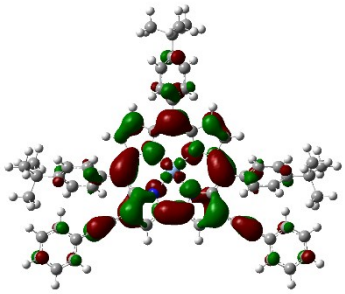
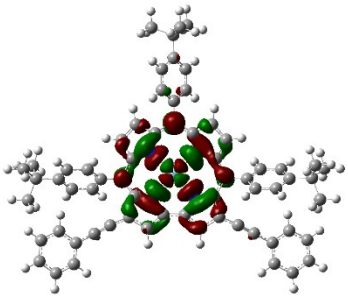
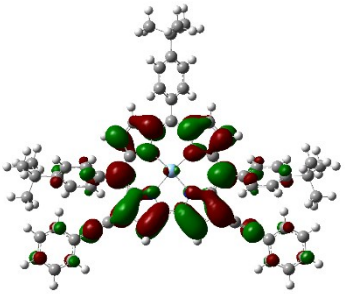
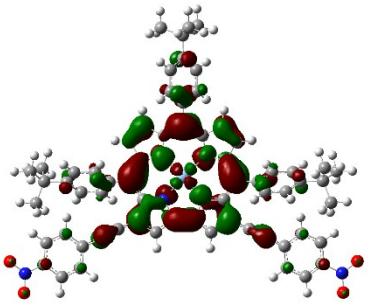
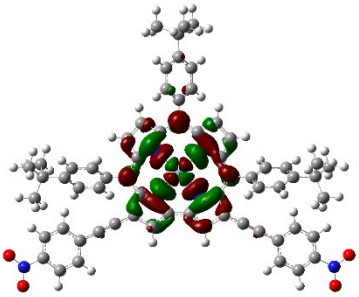
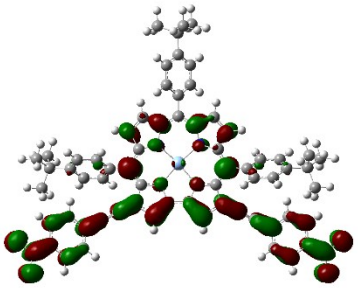
Figure S8: ^{1}H NMR spectrum of Ag Corrole **3** in CD_2Cl_2, at 298 K. (a) Aromatic region; (b) Aliphatic region.

DTF Calculations

Table S1. Calculated dihedral values of compounds **1-8** using B3LYP LANL2DZ.[1]



Corrole	γ1	γ2	γ3
1	23,2	-44,7	43,8
2	23,1	-44,3	44,1
3	21,4	-40,8	47,4
4	21,3	-42,7	43,2
5	22,3	-43,9	43,8
6	21,2	-42,7	43,1
7	19,7	-40,3	40,5
8	19,1	-38,2	38,8

	HOMO	LUMO	LUMO+1
1			
2			
3			
4			
5			

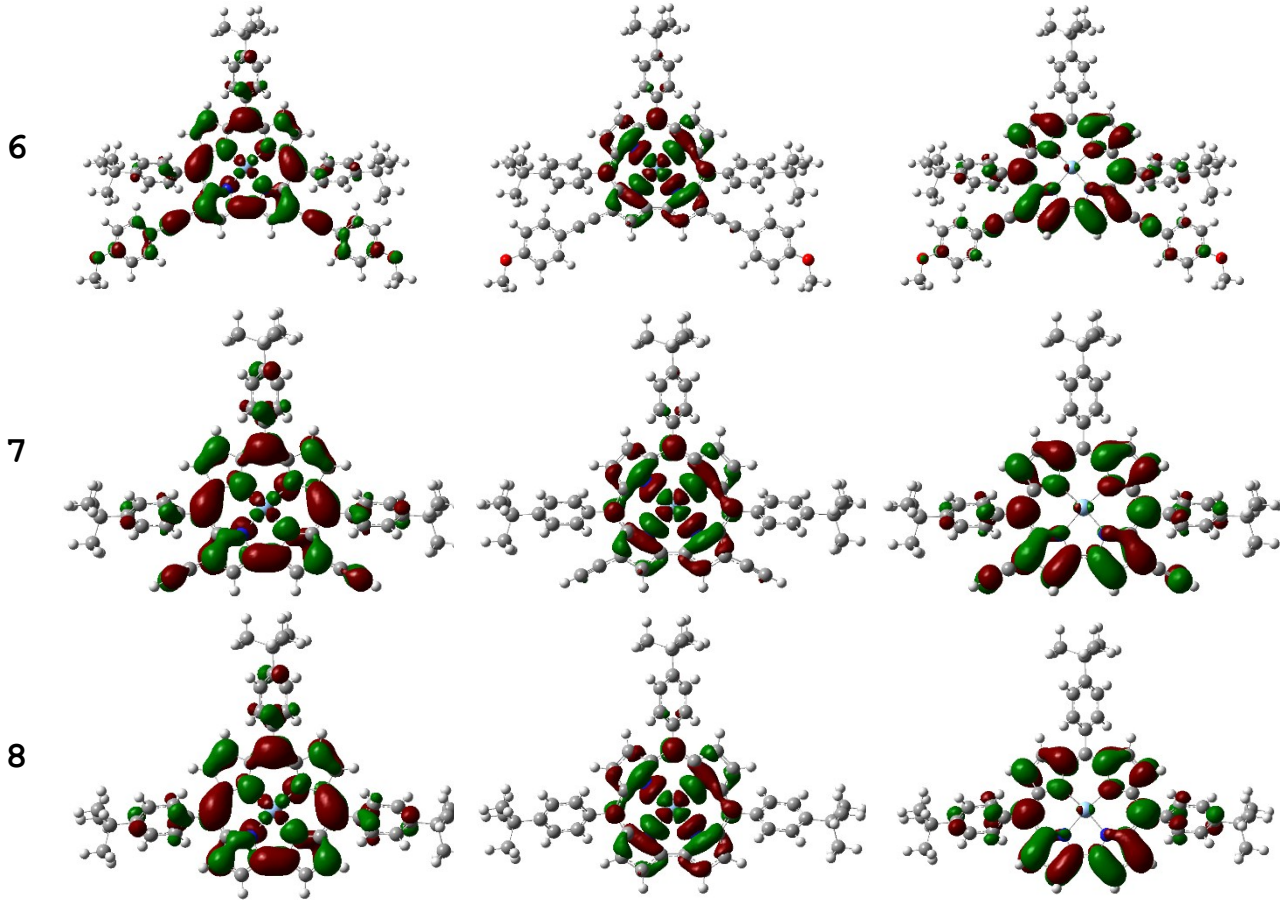


Figure S9. Representation of HOMO, LUMO and LUMO+1 frontier orbitals of compounds **1-8** calculated with B3LYP functional and LANL2DZ basis set.

Table S2. HOMO-1, HOMO, LUMO and LUMO+1 energy levels for **1-8**.

Corrole	HOMO-1 (eV)	HOMO-1 (eV)	LUMO (eV)	LUMO+1 (eV)	HOMO-LUMO gap (eV)
1	-5,43	-5,10	-3,11	-2,53	1,99
2	-5,39	-5,07	-3,10	-2,50	1,97
3	-5,16	-4,85	-2,85	-2,33	2,00
4	-5,21	-4,91	-2,99	-2,57	1,92
5	-5,73	-5,42	-3,47	-3,35	1,95
6	-5,07	-4,79	-2,91	-2,66	1,88
7	-5,33	-4,99	-3,03	-2,55	1,96
8	-5,17	-4,84	-2,81	-2,27	2,03

Table S3. Optimized cartesian coordinates (in Angstroms) of **1-8**

- **1**

Total Energies: -2285,055061 Hartrees
Stoichiometry C49H45AgBr2N4
Framework group C1[X(C49H45AgBr2N4)]
Deg. of freedom 297
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.831406	0.497941	-0.007973
2	6	0	3.510949	1.754979	0.262971
3	6	0	2.571499	2.771986	0.274194
4	6	0	1.266754	2.187489	0.016138
5	7	0	1.478127	0.823522	-0.179186
6	1	0	4.569870	1.849646	0.454084
7	1	0	2.747923	3.816570	0.484773
8	6	0	-0.003100	2.843093	-0.010570
9	6	0	-0.710687	-3.276331	0.041684
10	7	0	-1.282763	-2.022538	-0.097915
11	6	0	-2.659822	-2.031758	0.095202
12	6	0	-2.965731	-3.436578	0.325868
13	6	0	-1.780850	-4.190003	0.287702
14	1	0	-1.700177	-5.255973	0.444370
15	6	0	-3.416074	-0.817887	0.054905
16	6	0	-2.827638	0.485948	-0.001483
17	7	0	-1.475757	0.818035	0.168193
18	6	0	-1.270154	2.181928	-0.033632
19	6	0	-2.577325	2.759734	-0.294275
20	6	0	-3.512502	1.738825	-0.278190
21	1	0	-2.758305	3.802542	-0.509844
22	1	0	-4.571827	1.828124	-0.469663
23	6	0	3.425382	-0.803597	-0.058415
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26	6	0	0.730458	-3.273449	-0.034031
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28	6	0	2.986182	-3.425401	-0.317364
29	1	0	1.728377	-5.250688	-0.427588
30	6	0	-0.006438	4.339198	-0.014253
31	6	0	-0.012630	7.216600	-0.022142
32	6	0	-0.754898	5.073763	0.937197
33	6	0	0.736264	5.071928	-0.965946
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42	6	0	5.567963	-1.482487	1.100297
43	6	0	5.722603	-0.254361	-0.978161
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52	6	0	-5.555727	-1.511147	-1.100670
53	6	0	-5.715611	-0.274438	0.972301
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55	6	0	-6.953715	-1.535833	-1.189039
56	1	0	-4.956622	-1.978729	-1.878038
57	1	0	-5.242546	0.211054	1.822685
58	1	0	-7.697392	0.148517	1.678938
59	1	0	-7.409471	-2.028928	-2.044287
60	6	0	9.321812	-0.967178	0.324925
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63	1	0	9.781522	0.796105	-0.919094
64	1	0	9.802489	-0.741475	-1.816131
65	6	0	9.754477	-0.262531	1.644994
66	1	0	10.846141	-0.307240	1.758656
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72	1	0	9.331361	-2.997871	1.202574
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76	1	0	-1.914549	8.925978	-1.138133
77	1	0	-1.545931	10.352123	-0.140276
78	6	0	0.822109	9.390331	-1.113320
79	1	0	1.878108	9.104128	-1.023291
80	1	0	0.768681	10.484574	-1.048648
81	1	0	0.468999	9.099521	-2.111261
82	6	0	0.502458	9.261203	1.379669
83	1	0	1.540065	8.936307	1.530204
84	1	0	-0.093654	8.879567	2.217285
85	1	0	0.476555	10.358534	1.421000
86	6	0	-9.311743	-1.008926	-0.327249
87	6	0	-9.747609	-0.311893	-1.650303
88	1	0	-9.296751	-0.788861	-2.528790
89	1	0	-9.450280	0.744829	-1.651841
90	1	0	-10.839069	-0.361946	-1.763696
91	6	0	-9.764323	-2.499052	-0.358419
92	1	0	-9.312405	-3.043389	-1.196175
93	1	0	-10.855826	-2.561943	-0.465195
94	1	0	-9.479013	-3.013052	0.568414
95	6	0	-10.035223	-0.308306	0.849736
96	1	0	-9.793208	-0.776133	1.812864
97	1	0	-11.121277	-0.381293	0.709336
98	1	0	-9.779189	0.757646	0.909205
99	47	0	0.004002	-0.507265	-0.002533
100	35	0	-4.665012	-4.238453	0.817351
101	35	0	4.688885	-4.222267	-0.805152

Rotational constants (GHZ): 0.0390404 0.0221552 0.0145282

- **2**

Total Energies: -2281,495338 Hartrees
Stoichiometry C49H45AgI2N4
Framework group C1[X(C49H45AgI2N4)]
Deg. of freedom 297
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.829410	0.799767	0.017418
2	6	0	3.506729	2.056508	0.295897
3	6	0	2.567580	3.073829	0.298463
4	6	0	1.265233	2.489834	0.027619
5	7	0	1.478251	1.126015	-0.167227
6	1	0	4.563859	2.151022	0.496686
7	1	0	2.742334	4.118302	0.511009
8	6	0	-0.004265	3.145470	-0.009827
9	6	0	-0.711203	-2.971946	0.036750
10	7	0	-1.284569	-1.719555	-0.104974
11	6	0	-2.663416	-1.733039	0.077377
12	6	0	-2.975108	-3.140154	0.307755
13	6	0	-1.781783	-3.885881	0.274897
14	1	0	-1.695469	-4.951288	0.432044
15	6	0	-3.416331	-0.516983	0.024594
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28	6	0	2.994983	-3.127789	-0.301156
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32	6	0	-0.766116	5.376021	0.930277
33	6	0	0.744350	5.374512	-0.957507
34	6	0	0.736723	6.781033	-0.962646
35	6	0	-0.763645	6.777811	0.926000
36	1	0	-1.341197	4.841121	1.681920
37	1	0	1.322544	4.839614	-1.706896
38	1	0	1.322985	7.295758	-1.716648
39	1	0	-1.352221	7.298172	1.677884
40	6	0	4.917027	-0.547000	0.070226
41	6	0	7.775931	-0.565969	0.321485
42	6	0	5.545543	-1.137871	1.190384
43	6	0	5.738060	0.038198	-0.914978
44	6	0	7.139556	0.018890	-0.795798
45	6	0	6.941450	-1.138423	1.313172
46	1	0	4.933905	-1.590089	1.967129

47	1	0	5.278458	0.493200	-1.789258
48	1	0	7.730280	0.467529	-1.587555
49	1	0	7.383289	-1.597569	2.194229
50	6	0	-4.908773	-0.569566	-0.073946
51	6	0	-7.767508	-0.602390	-0.325445
52	6	0	-5.534434	-1.166905	-1.192265
53	6	0	-5.732565	0.015070	0.909271
54	6	0	-7.133949	-0.011047	0.790020
55	6	0	-6.930308	-1.174196	-1.315214
56	1	0	-4.920639	-1.618833	-1.967476
57	1	0	-5.275136	0.475012	1.782106
58	1	0	-7.726817	0.437423	1.580271
59	1	0	-7.369950	-1.638182	-2.194834
60	6	0	9.311775	-0.601178	0.492597
61	6	0	10.053324	0.072229	-0.689027
62	1	0	11.136592	0.020902	-0.520371
63	1	0	9.783004	1.131539	-0.789485
64	1	0	9.841822	-0.430237	-1.641842
65	6	0	9.703428	0.146035	1.802036
66	1	0	10.792383	0.118130	1.943608
67	1	0	9.238441	-0.309420	2.684557
68	1	0	9.389240	1.197067	1.761265
69	6	0	9.786960	-2.081687	0.584325
70	1	0	10.876273	-2.122900	0.720059
71	1	0	9.533436	-2.630146	-0.331970
72	1	0	9.322756	-2.605923	1.428172
73	6	0	-0.045002	9.064027	0.008200
74	6	0	-1.509572	9.556399	-0.188779
75	1	0	-2.175722	9.174117	0.593978
76	1	0	-1.905553	9.226901	-1.158073
77	1	0	-1.548445	10.653678	-0.156892
78	6	0	0.830475	9.692976	-1.104269
79	1	0	1.885571	9.407215	-1.002951
80	1	0	0.775866	10.787218	-1.040390
81	1	0	0.488142	9.401805	-2.105853
82	6	0	0.484329	9.564379	1.385157
83	1	0	1.520528	9.240276	1.546715
84	1	0	-0.120298	9.182464	2.216519
85	1	0	0.457170	10.661709	1.425982
86	6	0	-9.303151	-0.645094	-0.496653
87	6	0	-9.697974	0.096610	-1.808275
88	1	0	-9.230718	-0.359209	-2.689411
89	1	0	-9.388616	1.149183	-1.770425
90	1	0	-10.786761	0.063302	-1.949971
91	6	0	-9.771635	-2.127987	-0.584257
92	1	0	-9.304905	-2.652542	-1.426509
93	1	0	-10.860721	-2.174473	-0.720105
94	1	0	-9.515864	-2.672697	0.333649
95	6	0	-10.047927	0.028287	0.682953
96	1	0	-9.834185	-0.470448	1.637229
97	1	0	-11.130929	-0.028539	0.514354
98	1	0	-9.782528	1.089123	0.780380
99	47	0	0.003323	-0.205076	-0.002385
100	53	0	4.829212	-4.025760	-0.847829
101	53	0	-4.805386	-4.044291	0.857458

Rotational constants (GHZ): 0.0344376 0.0199546 0.0130176

- **3**

Total Energies: -2721,988849 Hartrees
Stoichiometry C61H55AgN4
Framework group C1[X(C61H55AgN4)]
Deg. of freedom 357
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.832094	0.700891	0.045549
2	6	0	3.497721	1.952716	0.367752
3	6	0	2.557167	2.969623	0.364861
4	6	0	1.264082	2.390076	0.052127
5	7	0	1.483030	1.028428	-0.159695
6	1	0	4.547410	2.046930	0.603140
7	1	0	2.725675	4.009883	0.602072
8	6	0	-0.004320	3.045590	-0.008822
9	6	0	-0.708337	-3.063894	0.038227
10	7	0	-1.283120	-1.809928	-0.083522
11	6	0	-2.658486	-1.832596	0.106083
12	6	0	-2.987060	-3.245001	0.332705
13	6	0	-1.780950	-3.976491	0.264868
14	1	0	-1.688575	-5.041220	0.429663
15	6	0	-3.417999	-0.619730	0.018278
16	6	0	-2.828658	0.686102	-0.053507
17	7	0	-1.481334	1.021356	0.150646
18	6	0	-1.269330	2.383226	-0.066699
19	6	0	-2.565290	2.954914	-0.381822
20	6	0	-3.500665	1.933203	-0.380653
21	1	0	-2.739231	3.993295	-0.623392
22	1	0	-4.550801	2.021105	-0.616501
23	6	0	3.428129	-0.602116	-0.021476
24	6	0	2.674844	-1.819216	-0.104803
25	7	0	1.299420	-1.802980	0.084969
26	6	0	0.731090	-3.060321	-0.032399
27	6	0	1.808358	-3.968138	-0.256035
28	6	0	3.010674	-3.230662	-0.326599
29	1	0	1.721468	-5.033896	-0.417132
30	6	0	-0.008506	4.541511	-0.012187
31	6	0	-0.017739	7.420057	-0.020484
32	6	0	-0.799775	5.276123	0.904243
33	6	0	0.775602	5.276055	-0.928925
34	6	0	0.767377	6.682589	-0.934077
35	6	0	-0.798919	6.677917	0.899848
36	1	0	-1.400393	4.740591	1.635122
37	1	0	1.380189	4.741651	-1.657494
38	1	0	1.379716	7.197733	-1.666871
39	1	0	-1.414435	7.197598	1.630436
40	6	0	4.917173	-0.660825	0.103313
41	6	0	7.774673	-0.741507	0.399161
42	6	0	5.525431	-1.433520	1.119860
43	6	0	5.762761	0.070936	-0.757060
44	6	0	7.161246	0.025873	-0.615487
45	6	0	6.918312	-1.467011	1.263771
46	1	0	4.899008	-1.999283	1.804250
47	1	0	5.323967	0.664535	-1.555674
48	1	0	7.768323	0.597320	-1.310081

49	1	0	7.340994	-2.071529	2.062542
50	6	0	-4.906710	-0.686496	-0.106432
51	6	0	-7.763722	-0.782755	-0.402253
52	6	0	-5.510903	-1.465787	-1.120360
53	6	0	-5.756101	0.043904	0.751343
54	6	0	-7.154324	-0.008785	0.609814
55	6	0	-6.903581	-1.506847	-1.264298
56	1	0	-4.881523	-2.030718	-1.802720
57	1	0	-5.320412	0.642496	1.547930
58	1	0	-7.764382	0.561929	1.302393
59	1	0	-7.323087	-2.116218	-2.061052
60	6	0	9.306273	-0.812207	0.593381
61	6	0	10.073948	0.033917	-0.452801
62	1	0	11.153440	-0.049339	-0.272719
63	1	0	9.808523	1.097440	-0.391258
64	1	0	9.880422	-0.311685	-1.476715
65	6	0	9.671496	-0.280524	2.011341
66	1	0	10.756920	-0.337999	2.170806
67	1	0	9.184286	-0.864557	2.801308
68	1	0	9.362001	0.766207	2.128082
69	6	0	9.776690	-2.291129	0.462726
70	1	0	10.864136	-2.357189	0.604590
71	1	0	9.531731	-2.692073	-0.529072
72	1	0	9.299421	-2.936763	1.209346
73	6	0	-0.051788	8.965066	0.007178
74	6	0	-1.508571	9.454416	-0.247005
75	1	0	-2.203604	9.070777	0.509548
76	1	0	-1.865839	9.123099	-1.230621
77	1	0	-1.551263	10.551699	-0.217527
78	6	0	0.864978	9.595032	-1.070947
79	1	0	1.915651	9.310213	-0.929084
80	1	0	0.806677	10.689286	-1.009508
81	1	0	0.561754	9.303104	-2.084838
82	6	0	0.422503	9.468008	1.403050
83	1	0	1.452309	9.146169	1.605009
84	1	0	-0.213087	9.085338	2.210622
85	1	0	0.391367	10.565379	1.441844
86	6	0	-9.294918	-0.861827	-0.596452
87	6	0	-9.662567	-0.336280	-2.016078
88	1	0	-9.172262	-0.920237	-2.804188
89	1	0	-9.358333	0.711639	-2.135932
90	1	0	-10.747658	-0.399705	-2.175556
91	6	0	-9.757866	-2.342703	-0.461393
92	1	0	-9.277374	-2.988130	-1.206119
93	1	0	-10.844966	-2.414679	-0.603024
94	1	0	-9.510870	-2.739471	0.531581
95	6	0	-10.067036	-0.016434	0.447047
96	1	0	-9.871794	-0.357839	1.472044
97	1	0	-11.146070	-0.105841	0.267161
98	1	0	-9.807134	1.048255	0.382204
99	47	0	0.004268	-0.299671	-0.002001
100	6	0	4.302707	-3.859139	-0.693632
101	6	0	4.708288	-5.056496	-0.055463
102	6	0	5.112923	-3.345971	-1.733863
103	6	0	5.890029	-5.715623	-0.437761
104	1	0	4.100371	-5.459881	0.751399
105	6	0	6.294928	-4.002221	-2.115534
106	1	0	4.806247	-2.442121	-2.252095
107	6	0	6.691117	-5.190281	-1.469936
108	1	0	6.185195	-6.631923	0.068869

109	1	0	6.901171	-3.591523	-2.919809
110	1	0	7.605415	-5.698499	-1.767809
111	6	0	-4.275929	-3.878878	0.701561
112	6	0	-4.675086	-5.080557	0.067475
113	6	0	-5.089160	-3.366238	1.739697
114	6	0	-5.853553	-5.744418	0.451679
115	1	0	-4.064806	-5.483632	-0.737754
116	6	0	-6.267909	-4.027221	2.123255
117	1	0	-4.787341	-2.458997	2.254845
118	6	0	-6.657727	-5.219575	1.481706
119	1	0	-6.143807	-6.664003	-0.051826
120	1	0	-6.876564	-3.616825	2.925861
121	1	0	-7.569507	-5.731446	1.781039

Rotational constants (GHZ): 0.0362518 0.0207835 0.0136993

- **4**

Total Energies: -2874,285638 Hartrees
Stoichiometry C65H55AgN4
Framework group C1[X(C65H55AgN4)]
Deg. of freedom 369
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.828154	1.013408	0.148120
2	6	0	3.490885	2.270667	0.454644
3	6	0	2.551591	3.287678	0.414942
4	6	0	1.262855	2.703131	0.088350
5	7	0	1.485028	1.338561	-0.092508
6	1	0	4.537682	2.366959	0.702697
7	1	0	2.716767	4.332512	0.633358
8	6	0	-0.003576	3.358406	-0.008321
9	6	0	-0.713107	-2.762884	0.004177
10	7	0	-1.273458	-1.503176	-0.156832
11	6	0	-2.651924	-1.514156	-0.048724
12	6	0	-3.002950	-2.922359	0.163182
13	6	0	-1.795024	-3.669007	0.177376
14	1	0	-1.726855	-4.736785	0.330558
15	6	0	-3.411036	-0.306460	-0.131188
16	6	0	-2.825387	1.000847	-0.155826
17	7	0	-1.483700	1.332531	0.083867
18	6	0	-1.267234	2.697318	-0.102118
19	6	0	-2.558328	3.275244	-0.431023
20	6	0	-3.493364	2.254152	-0.467027
21	1	0	-2.727998	4.318514	-0.653523
22	1	0	-4.540519	2.345123	-0.715582
23	6	0	3.419316	-0.291460	0.127838
24	6	0	2.665297	-1.502666	0.049596
25	7	0	1.286835	-1.497223	0.158140
26	6	0	0.731818	-2.759824	0.001135
27	6	0	1.817532	-3.661842	-0.169550
28	6	0	3.022270	-2.909992	-0.158083
29	1	0	1.753882	-4.730370	-0.319415
30	6	0	-0.007143	4.854689	-0.011411

31	6	0	-0.015573	7.732553	-0.019379
32	6	0	-0.807114	5.588742	0.897567
33	6	0	0.786113	5.588526	-0.920494
34	6	0	0.778103	6.995117	-0.925582
35	6	0	-0.805702	6.990578	0.893422
36	1	0	-1.414950	5.053322	1.622599
37	1	0	1.397616	5.054132	-1.643340
38	1	0	1.397565	7.510244	-1.652320
39	1	0	-1.428100	7.510289	1.618051
40	6	0	4.903733	-0.357861	0.303428
41	6	0	7.739082	-0.346642	0.770840
42	6	0	5.462158	-1.015856	1.424187
43	6	0	5.787316	0.284522	-0.588342
44	6	0	7.176758	0.281087	-0.363389
45	6	0	6.844250	-1.000165	1.654109
46	1	0	4.804476	-1.519966	2.127610
47	1	0	5.386606	0.782817	-1.467979
48	1	0	7.815461	0.786163	-1.080787
49	1	0	7.226373	-1.501486	2.539767
50	6	0	-4.895124	-0.379628	-0.306931
51	6	0	-7.730338	-0.381299	-0.775253
52	6	0	-5.450505	-1.043218	-1.425896
53	6	0	-5.781592	0.261773	0.582676
54	6	0	-7.170939	0.252022	0.357312
55	6	0	-6.832578	-1.033809	-1.656297
56	1	0	-4.790557	-1.546721	-2.127631
57	1	0	-5.383181	0.764333	1.460931
58	1	0	-7.811921	0.756616	1.073015
59	1	0	-7.212375	-1.539272	-2.540598
60	6	0	9.250480	-0.302203	1.094448
61	6	0	10.079826	0.333048	-0.049766
62	1	0	11.144210	0.322257	0.217594
63	1	0	9.796322	1.378030	-0.229986
64	1	0	9.966083	-0.221861	-0.990557
65	6	0	9.459022	0.551547	2.381990
66	1	0	10.525349	0.592317	2.643352
67	1	0	8.916884	0.127886	3.236175
68	1	0	9.101736	1.578746	2.232820
69	6	0	9.791546	-1.739735	1.345265
70	1	0	10.864126	-1.702072	1.579334
71	1	0	9.653552	-2.375096	0.462089
72	1	0	9.285454	-2.227460	2.186565
73	6	0	-0.049876	9.277537	0.007842
74	6	0	-1.503946	9.766534	-0.262231
75	1	0	-2.207160	9.383033	0.486805
76	1	0	-1.850487	9.435196	-1.249666
77	1	0	-1.547009	10.863776	-0.233334
78	6	0	0.878507	9.907378	-1.060349
79	1	0	1.927593	9.622511	-0.907265
80	1	0	0.819699	11.001594	-0.999403
81	1	0	0.586132	9.615778	-2.077516
82	6	0	0.409123	9.780569	1.408768
83	1	0	1.436685	9.458909	1.622103
84	1	0	-0.235289	9.398284	2.209499
85	1	0	0.377550	10.877904	1.446903
86	6	0	-9.241778	-0.343778	-1.099550
87	6	0	-9.453199	0.505758	-2.389406
88	1	0	-8.909052	0.082005	-3.242270
89	1	0	-9.100035	1.534749	-2.242799
90	1	0	-10.519577	0.541623	-2.651278

91	6	0	-9.777021	-1.784099	-1.346813
92	1	0	-9.268690	-2.271993	-2.186662
93	1	0	-10.849656	-1.751311	-1.581362
94	1	0	-9.636828	-2.416606	-0.461938
95	6	0	-10.074100	0.291160	0.042677
96	1	0	-9.958444	-0.260774	0.984985
97	1	0	-11.138335	0.275350	-0.225025
98	1	0	-9.794897	1.337758	0.220206
99	47	0	0.003491	0.009163	-0.001978
100	6	0	-4.276895	-3.479568	0.438208
101	6	0	-5.335941	-4.029829	0.729925
102	6	0	4.298456	-3.462602	-0.432015
103	6	0	5.359666	-4.009241	-0.722679
104	6	0	6.599434	-4.625745	-1.086513
105	6	0	6.729986	-6.040021	-1.095409
106	6	0	7.717720	-3.833695	-1.459562
107	6	0	7.942873	-6.641312	-1.467412
108	1	0	5.877932	-6.652064	-0.811731
109	6	0	8.926228	-4.442617	-1.833545
110	1	0	7.620991	-2.751521	-1.452936
111	6	0	9.046216	-5.847059	-1.839589
112	1	0	8.028725	-7.725400	-1.469875
113	1	0	9.773719	-3.825566	-2.123561
114	1	0	9.983710	-6.315013	-2.130185
115	6	0	-6.573309	-4.650521	1.094805
116	6	0	-6.697733	-6.065314	1.108175
117	6	0	-7.695325	-3.862123	1.464373
118	6	0	-7.908317	-6.670652	1.481113
119	1	0	-5.842795	-6.674569	0.827186
120	6	0	-8.901500	-4.475068	1.839315
121	1	0	-7.603277	-2.779568	1.454344
122	6	0	-9.015407	-5.879989	1.849794
123	1	0	-7.989475	-7.755088	1.487014
124	1	0	-9.751904	-3.860766	2.126627
125	1	0	-9.951114	-6.351064	2.141105

Rotational constants (GHZ): 0.0307393 0.0166592 0.0112529

- **5**

Total Energies: -3283,234352 Hartrees
Stoichiometry C65H53AgN6O4
Framework group C1[X(C65H53AgN6O4)]
Deg. of freedom 381
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.813837	1.509835	0.308014
2	6	0	3.457195	2.767291	0.657133
3	6	0	2.521959	3.783134	0.563686
4	6	0	1.254846	3.198099	0.158970
5	7	0	1.487182	1.834807	-0.012372
6	1	0	4.486767	2.862983	0.968990
7	1	0	2.672292	4.827542	0.794080
8	6	0	-0.003427	3.854546	-0.010039

9	6	0	-0.715070	-2.268816	-0.038604
10	7	0	-1.264220	-1.008203	-0.237674
11	6	0	-2.644791	-1.015586	-0.200485
12	6	0	-3.008506	-2.420613	0.001652
13	6	0	-1.803039	-3.171628	0.083565
14	1	0	-1.745235	-4.238629	0.246298
15	6	0	-3.398938	0.193249	-0.329915
16	6	0	-2.812323	1.498787	-0.321030
17	7	0	-1.486825	1.829394	-0.001676
18	6	0	-1.259332	3.192938	-0.176991
19	6	0	-2.528452	3.772320	-0.583427
20	6	0	-3.460103	2.752886	-0.673940
21	1	0	-2.682596	4.815498	-0.816958
22	1	0	-4.489984	2.844011	-0.986149
23	6	0	3.405087	0.206431	0.321148
24	6	0	2.655265	-1.005536	0.195760
25	7	0	1.274688	-1.002891	0.232567
26	6	0	0.730001	-2.266136	0.037988
27	6	0	1.821156	-3.165546	-0.080656
28	6	0	3.023970	-2.410003	-0.001151
29	1	0	1.767158	-4.233344	-0.239421
30	6	0	-0.006759	5.350262	-0.011420
31	6	0	-0.014443	8.227020	-0.015084
32	6	0	-0.857297	6.082156	0.852280
33	6	0	0.837100	6.084598	-0.873345
34	6	0	0.828692	7.491027	-0.876956
35	6	0	-0.854699	7.483784	0.850940
36	1	0	-1.504943	5.546180	1.541630
37	1	0	1.488168	5.551767	-1.562077
38	1	0	1.487345	8.007593	-1.567112
39	1	0	-1.516124	8.002538	1.540519
40	6	0	4.875627	0.137071	0.586121
41	6	0	7.675252	0.154096	1.235449
42	6	0	5.362629	-0.525491	1.737611
43	6	0	5.812998	0.784184	-0.245689
44	6	0	7.185133	0.782774	0.068192
45	6	0	6.727102	-0.506735	2.056149
46	1	0	4.662566	-1.031144	2.397862
47	1	0	5.468959	1.285711	-1.147212
48	1	0	7.867391	1.293085	-0.603777
49	1	0	7.052504	-1.007263	2.964451
50	6	0	-4.869216	0.117755	-0.594587
51	6	0	-7.668916	0.122382	-1.243801
52	6	0	-5.353890	-0.550677	-1.743664
53	6	0	-5.808866	0.764516	0.234931
54	6	0	-7.180998	0.757051	-0.078864
55	6	0	-6.718431	-0.537954	-2.062191
56	1	0	-4.652037	-1.056142	-2.402154
57	1	0	-5.466589	1.270548	1.134606
58	1	0	-7.865049	1.267354	0.591288
59	1	0	-7.042069	-1.042872	-2.968690
60	6	0	9.160861	0.211276	1.660630
61	6	0	10.060916	0.852511	0.574746
62	1	0	11.104640	0.848079	0.912945
63	1	0	9.784233	1.895973	0.376281
64	1	0	10.016298	0.297908	-0.372083
65	6	0	9.271682	1.069126	2.957835
66	1	0	10.317548	1.122983	3.288872
67	1	0	8.679655	0.639978	3.775396
68	1	0	8.913499	2.091928	2.783216

69	6	0	9.697352	-1.220149	1.952410
70	1	0	10.747786	-1.170338	2.267967
71	1	0	9.639653	-1.855320	1.060027
72	1	0	9.134471	-1.715900	2.751945
73	6	0	-0.049252	9.771761	0.013474
74	6	0	-1.486499	10.262178	-0.333423
75	1	0	-2.229837	9.878064	0.375494
76	1	0	-1.779523	9.934530	-1.339230
77	1	0	-1.529770	11.359206	-0.303700
78	6	0	0.935842	10.403058	-1.001679
79	1	0	1.975243	10.118290	-0.792555
80	1	0	0.873938	11.497003	-0.941799
81	1	0	0.698923	10.114033	-2.033907
82	6	0	0.333898	10.270516	1.438627
83	1	0	1.348072	9.947440	1.706763
84	1	0	-0.353582	9.888102	2.202646
85	1	0	0.301741	11.367643	1.477073
86	6	0	-9.154756	0.172619	-1.669039
87	6	0	-9.268784	1.025336	-2.969355
88	1	0	-8.675141	0.595425	-3.785344
89	1	0	-8.914430	2.050096	-2.798458
90	1	0	-10.314842	1.074069	-3.300583
91	6	0	-9.686100	-1.261783	-1.955564
92	1	0	-9.121620	-1.758351	-2.753463
93	1	0	-10.736773	-1.216902	-2.271058
94	1	0	-9.625902	-1.893554	-1.060933
95	6	0	-10.057041	0.814539	-0.585411
96	1	0	-10.010239	0.263622	0.363463
97	1	0	-11.100780	0.804988	-0.923451
98	1	0	-9.784213	1.859751	-0.390863
99	47	0	0.002566	0.504917	-0.005038
100	6	0	-4.293135	-2.970224	0.220074
101	6	0	-5.370935	-3.509070	0.464161
102	6	0	4.310553	-2.956046	-0.216982
103	6	0	5.390185	-3.492396	-0.458450
104	6	0	6.649338	-4.084706	-0.765027
105	6	0	6.783530	-5.498620	-0.858909
106	6	0	7.792526	-3.268475	-0.995390
107	6	0	8.014815	-6.081456	-1.172064
108	1	0	5.914200	-6.125172	-0.684614
109	6	0	9.026543	-3.842865	-1.312134
110	1	0	7.690661	-2.190246	-0.922871
111	6	0	9.125472	-5.245247	-1.396728
112	1	0	8.132427	-7.156688	-1.246628
113	1	0	9.905910	-3.235938	-1.496542
114	6	0	-6.628114	-4.103942	0.773878
115	6	0	-6.757905	-5.517825	0.874083
116	6	0	-7.773724	-3.290223	1.001116
117	6	0	-7.987238	-6.103056	1.190444
118	1	0	-5.886738	-6.142470	0.702129
119	6	0	-9.005809	-3.866999	1.321016
120	1	0	-7.675238	-2.212022	0.923701
121	6	0	-9.100359	-5.269288	1.411943
122	1	0	-8.101493	-7.178303	1.269855
123	1	0	-9.886959	-3.261968	1.503133
124	7	0	10.421853	-5.850735	-1.727075
125	8	0	11.422660	-5.073233	-1.924621
126	8	0	10.494348	-7.128680	-1.802203
127	7	0	-10.394697	-5.877290	1.745677
128	8	0	-11.397810	-5.102002	1.940214

129	8	0	-10.463211	-7.155103	1.826547

Rotational constants (GHZ): 0.0249012 0.0122764 0.0086037

- **6**

Total Energies: -3103,301555 Hartrees
Stoichiometry C67H59AgN4O2
Framework group C1[X(C67H59AgN4O2)]
Deg. of freedom 393
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.819311	1.423855	0.259800
2	6	0	3.469528	2.680907	0.591807
3	6	0	2.532662	3.698299	0.514428
4	6	0	1.257860	3.114070	0.137308
5	7	0	1.486926	1.749216	-0.034227
6	1	0	4.505810	2.777147	0.880754
7	1	0	2.689486	4.743208	0.738656
8	6	0	-0.003811	3.769212	-0.009318
9	6	0	-0.713645	-2.351952	-0.025899
10	7	0	-1.266783	-1.092136	-0.208842
11	6	0	-2.648773	-1.103136	-0.156900
12	6	0	-3.008522	-2.511683	0.041163
13	6	0	-1.802054	-3.258067	0.103762
14	1	0	-1.739839	-4.325732	0.260188
15	6	0	-3.403737	0.104128	-0.269811
16	6	0	-2.817704	1.411817	-0.270535
17	7	0	-1.486658	1.743348	0.022592
18	6	0	-1.262872	3.108447	-0.153580
19	6	0	-2.539839	3.686460	-0.532823
20	6	0	-3.472764	2.665170	-0.606872
21	1	0	-2.700815	4.729963	-0.760727
22	1	0	-4.509359	2.756407	-0.896323
23	6	0	3.410473	0.118499	0.263516
24	6	0	2.660253	-1.092169	0.155043
25	7	0	1.278241	-1.086424	0.207244
26	6	0	0.730017	-2.349030	0.028657
27	6	0	1.821947	-3.251284	-0.098074
28	6	0	3.025496	-2.499948	-0.038236
29	1	0	1.763920	-4.319723	-0.250784
30	6	0	-0.007412	5.265568	-0.011219
31	6	0	-0.015893	8.143640	-0.016061
32	6	0	-0.841891	5.998610	0.867022
33	6	0	0.820115	6.000670	-0.888148
34	6	0	0.812116	7.407318	-0.891930
35	6	0	-0.840493	7.400466	0.864660
36	1	0	-1.477352	5.462211	1.567213
37	1	0	1.459283	5.467124	-1.587300
38	1	0	1.459130	7.923290	-1.593680
39	1	0	-1.490519	7.919146	1.565374
40	6	0	4.886430	0.052272	0.501572
41	6	0	7.699260	0.066564	1.091042

42	6	0	5.396150	-0.600075	1.648508
43	6	0	5.807736	0.690137	-0.354424
44	6	0	7.186287	0.688157	-0.069700
45	6	0	6.767054	-0.582877	1.937952
46	1	0	4.708589	-1.101075	2.325083
47	1	0	5.445337	1.184308	-1.252814
48	1	0	7.855335	1.189860	-0.761381
49	1	0	7.110530	-1.079386	2.841968
50	6	0	-4.879337	0.031302	-0.508147
51	6	0	-7.691914	0.032791	-1.099008
52	6	0	-5.385996	-0.626948	-1.653076
53	6	0	-5.803490	0.668569	0.345202
54	6	0	-7.181889	0.660335	0.059823
55	6	0	-6.756809	-0.615994	-1.943231
56	1	0	-4.696181	-1.127619	-2.327598
57	1	0	-5.443434	1.167248	1.242042
58	1	0	-7.853180	1.161884	0.749440
59	1	0	-7.097933	-1.116902	-2.845709
60	6	0	9.194995	0.115624	1.480590
61	6	0	10.073905	0.738883	0.367156
62	1	0	11.125632	0.730357	0.680662
63	1	0	9.799364	1.782066	0.164019
64	1	0	10.000991	0.174238	-0.571847
65	6	0	9.345383	0.984167	2.766418
66	1	0	10.399139	1.030014	3.073933
67	1	0	8.766649	0.568839	3.600492
68	1	0	8.993403	2.008913	2.590154
69	6	0	9.726144	-1.318009	1.771601
70	1	0	10.786829	-1.275544	2.053914
71	1	0	9.630733	-1.963304	0.890082
72	1	0	9.182961	-1.797506	2.594370
73	6	0	-0.051347	9.688611	0.011884
74	6	0	-1.493939	10.178156	-0.313175
75	1	0	-2.225536	9.793213	0.407401
76	1	0	-1.802047	9.848511	-1.313827
77	1	0	-1.538211	11.275375	-0.283965
78	6	0	0.917312	10.319894	-1.019060
79	1	0	1.959728	10.034622	-0.826319
80	1	0	0.856277	11.414060	-0.958931
81	1	0	0.664107	10.029592	-2.047047
82	6	0	0.353528	10.189871	1.430021
83	1	0	1.371954	9.867406	1.682379
84	1	0	-0.321391	9.806839	2.204838
85	1	0	0.320943	11.287204	1.468285
86	6	0	-9.187622	0.074830	-1.489474
87	6	0	-9.340637	0.938249	-2.778436
88	1	0	-8.759871	0.522208	-3.610741
89	1	0	-8.992682	1.964953	-2.605610
90	1	0	-10.394396	0.978962	-3.086662
91	6	0	-9.713228	-1.361811	-1.775694
92	1	0	-9.167800	-1.842171	-2.596468
93	1	0	-10.773908	-1.324309	-2.058726
94	1	0	-9.615899	-2.003623	-0.891845
95	6	0	-10.069442	0.698708	-0.378694
96	1	0	-9.994820	0.137727	0.562369
97	1	0	-11.120979	0.685028	-0.692655
98	1	0	-9.798993	1.743659	-0.179188
99	47	0	0.002777	0.420047	-0.003459
100	6	0	-4.293282	-3.066594	0.265085
101	6	0	-5.365540	-3.611112	0.517821

102	6	0	4.312333	-3.050765	-0.260365
103	6	0	5.386499	-3.592377	-0.511228
104	6	0	6.642423	-4.199270	-0.827333
105	6	0	6.785418	-5.607889	-0.864968
106	6	0	7.780953	-3.400164	-1.128610
107	6	0	8.012858	-6.208810	-1.189987
108	1	0	5.925571	-6.232621	-0.638527
109	6	0	9.004287	-3.989918	-1.456025
110	1	0	7.685402	-2.318458	-1.102900
111	6	0	9.127339	-5.396717	-1.488463
112	1	0	8.086838	-7.291538	-1.209342
113	1	0	9.877139	-3.389295	-1.693978
114	6	0	-6.619419	-4.221166	0.835949
115	6	0	-6.757385	-5.630099	0.879714
116	6	0	-7.760970	-3.424810	1.133110
117	6	0	-7.982857	-6.233976	1.206699
118	1	0	-5.895179	-6.252743	0.656511
119	6	0	-8.982368	-4.017491	1.462428
120	1	0	-7.669249	-2.342896	1.102717
121	6	0	-9.100406	-5.424570	1.500952
122	1	0	-8.052966	-7.316864	1.230842
123	1	0	-9.857498	-3.418965	1.697278
124	8	0	10.391696	-5.881469	-1.826852
125	8	0	-10.363232	-5.912347	1.840710
126	6	0	10.595292	-7.322326	-1.889202
127	1	0	11.641698	-7.453017	-2.171799
128	1	0	10.414364	-7.792672	-0.912604
129	1	0	9.946946	-7.783366	-2.647309
130	6	0	-10.561712	-7.353633	1.909276
131	1	0	-11.607851	-7.486830	2.191693
132	1	0	-10.378419	-7.827622	0.934877
133	1	0	-9.912253	-7.809007	2.669846

Rotational constants (GHZ): 0.0259458 0.0135836 0.0093090

- **7**

Total Energies: -2412,224465 Hartrees
Stoichiometry C53H47AgN4
Framework group C1[X(C53H47AgN4)]
Deg. of freedom 309
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.832397	0.091207	-0.035131
2	6	0	3.516958	1.351247	0.205724
3	6	0	2.577930	2.368763	0.224985
4	6	0	1.267709	1.782484	0.000601
5	7	0	1.475542	0.416260	-0.179505
6	1	0	4.579808	1.447622	0.372773
7	1	0	2.759047	3.415911	0.418109
8	6	0	-0.001577	2.438492	-0.011619
9	6	0	-0.710832	-3.683479	0.045480
10	7	0	-1.279312	-2.423702	-0.076426

11	6	0	-2.650250	-2.435865	0.101515
12	6	0	-2.988680	-3.844945	0.311746
13	6	0	-1.784077	-4.591566	0.265219
14	1	0	-1.710728	-5.661572	0.399232
15	6	0	-3.410323	-1.224674	0.079925
16	6	0	-2.826560	0.080562	0.025447
17	7	0	-1.470953	0.411539	0.167911
18	6	0	-1.268325	1.777505	-0.019759
19	6	0	-2.580729	2.357612	-0.247140
20	6	0	-3.515927	1.336651	-0.222161
21	1	0	-2.765963	3.402977	-0.446075
22	1	0	-4.579158	1.428080	-0.389597
23	6	0	3.421164	-1.212030	-0.082419
24	6	0	2.665735	-2.426250	-0.097440
25	7	0	1.294749	-2.418343	0.080232
26	6	0	0.731103	-3.680952	-0.034706
27	6	0	1.807838	-4.586124	-0.249268
28	6	0	3.009592	-3.835161	-0.299783
29	1	0	1.738616	-5.657137	-0.377302
30	6	0	-0.004643	3.935083	-0.015491
31	6	0	-0.010034	6.812678	-0.023089
32	6	0	-0.727228	4.669896	0.955351
33	6	0	0.712573	4.667620	-0.986454
34	6	0	0.705875	6.074297	-0.991149
35	6	0	-0.724254	6.071817	0.951045
36	1	0	-1.274923	4.135170	1.727356
37	1	0	1.262784	4.132323	-1.756406
38	1	0	1.264601	6.588698	-1.766035
39	1	0	-1.284780	6.592435	1.723911
40	6	0	4.915217	-1.278603	-0.046648
41	6	0	7.782917	-1.355014	0.065553
42	6	0	5.585830	-1.919844	1.019755
43	6	0	5.700458	-0.676121	-1.051353
44	6	0	7.105453	-0.721605	-0.999747
45	6	0	6.985448	-1.948794	1.075014
46	1	0	5.004937	-2.388033	1.810218
47	1	0	5.208701	-0.186100	-1.888421
48	1	0	7.666011	-0.255570	-1.803359
49	1	0	7.459408	-2.445748	1.918143
50	6	0	-4.904108	-1.297224	0.044826
51	6	0	-7.771496	-1.385838	-0.066065
52	6	0	-5.572423	-1.946928	-1.017891
53	6	0	-5.691483	-0.692415	1.046458
54	6	0	-7.096295	-0.743866	0.995539
55	6	0	-6.971928	-1.981819	-1.072566
56	1	0	-4.989859	-2.417073	-1.805958
57	1	0	-5.201469	-0.195868	1.880699
58	1	0	-7.658506	-0.275744	1.796780
59	1	0	-7.444130	-2.485218	-1.912853
60	6	0	9.324281	-1.420526	0.162635
61	6	0	10.022002	-0.712564	-1.025507
62	1	0	11.110940	-0.785910	-0.909373
63	1	0	9.764249	0.353537	-1.072551
64	1	0	9.758949	-1.174086	-1.986184
65	6	0	9.789986	-0.732060	1.479978
66	1	0	10.883828	-0.781679	1.568277
67	1	0	9.359388	-1.215008	2.365309
68	1	0	9.491774	0.324260	1.495124
69	6	0	9.777921	-2.910597	0.174640
70	1	0	10.871254	-2.974489	0.260307

71	1	0	9.475755	-3.416933	-0.751351
72	1	0	9.341477	-3.460775	1.016819
73	6	0	-0.037847	8.357742	0.008199
74	6	0	-1.508087	8.851768	-0.135046
75	1	0	-2.145762	8.469636	0.671172
76	1	0	-1.939379	8.523214	-1.089482
77	1	0	-1.544685	9.949089	-0.101103
78	6	0	0.796963	8.986207	-1.135388
79	1	0	1.854755	8.699288	-1.072895
80	1	0	0.745868	10.080503	-1.069285
81	1	0	0.417853	8.695575	-2.123799
82	6	0	0.541898	8.857284	1.364970
83	1	0	1.582706	8.531368	1.488873
84	1	0	-0.032859	8.476275	2.217659
85	1	0	0.518093	9.954676	1.406785
86	6	0	-9.312608	-1.458235	-0.162241
87	6	0	-9.781603	-0.778841	-1.483117
88	1	0	-9.349330	-1.264806	-2.365978
89	1	0	-9.487749	0.278599	-1.504099
90	1	0	-10.875261	-0.833427	-1.570741
91	6	0	-9.760067	-2.950222	-0.166029
92	1	0	-9.321675	-3.503107	-1.005420
93	1	0	-10.853159	-3.019117	-0.250894
94	1	0	-9.455434	-3.450312	0.762545
95	6	0	-10.012846	-0.746760	1.022317
96	1	0	-9.747577	-1.202018	1.985371
97	1	0	-11.101511	-0.825212	0.906962
98	1	0	-9.759473	0.320631	1.063531
99	47	0	0.004834	-0.912801	-0.002215
100	6	0	-4.259571	-4.412840	0.606224
101	6	0	-5.323398	-4.957396	0.874269
102	1	0	-6.263179	-5.405207	1.102179
103	6	0	4.282693	-4.399810	-0.590938
104	6	0	5.348637	-4.941778	-0.855807
105	1	0	6.290095	-5.387371	-1.081127

Rotational constants (GHZ): 0.0462682 0.0246859 0.0165149

- **8**

Total Energies: -2259,960894 Hartrees
Stoichiometry C49H47AgN4
Framework group C1[X(C49H47AgN4)]
Deg. of freedom 297
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.839740	-0.101801	0.052584
2	6	0	3.513011	1.159336	0.311676
3	6	0	2.570263	2.175266	0.306882
4	6	0	1.268706	1.586572	0.046215
5	7	0	1.485270	0.219562	-0.122364
6	1	0	4.569917	1.260354	0.511925
7	1	0	2.744451	3.222448	0.506534

8	6	0	-0.001326	2.240066	-0.010123
9	6	0	-0.709269	-3.884722	0.011607
10	7	0	-1.263843	-2.619429	-0.121788
11	6	0	-2.640189	-2.628719	0.003573
12	6	0	-2.994266	-4.024948	0.172002
13	6	0	-1.813568	-4.787835	0.173280
14	1	0	-1.743620	-5.860723	0.291753
15	6	0	-3.410243	-1.424144	-0.016046
16	6	0	-2.832352	-0.114256	-0.059552
17	7	0	-1.479289	0.213806	0.113765
18	6	0	-1.268539	1.580774	-0.062338
19	6	0	-2.572533	2.162531	-0.326145
20	6	0	-3.510987	1.142580	-0.325377
21	1	0	-2.751301	3.207835	-0.531633
22	1	0	-4.568316	1.238032	-0.526134
23	6	0	3.423250	-1.409364	0.015801
24	6	0	2.658363	-2.617352	0.002588
25	7	0	1.282011	-2.613316	0.128105
26	6	0	0.732857	-3.881664	0.001239
27	6	0	1.840992	-4.780831	-0.155946
28	6	0	3.018414	-4.012879	-0.158737
29	1	0	1.775646	-5.854605	-0.268898
30	6	0	-0.004718	3.737218	-0.014441
31	6	0	-0.011057	6.615595	-0.023414
32	6	0	-0.756589	4.472661	0.933432
33	6	0	0.741307	4.470211	-0.963105
34	6	0	0.734558	5.877002	-0.968509
35	6	0	-0.754407	5.874713	0.928572
36	1	0	-1.327459	3.937786	1.688324
37	1	0	1.315074	3.934620	-1.715420
38	1	0	1.316804	6.391162	-1.726134
39	1	0	-1.338733	6.395337	1.683750
40	6	0	4.911714	-1.523600	0.010382
41	6	0	7.779850	-1.767638	-0.015234
42	6	0	5.585184	-2.369279	0.925816
43	6	0	5.702037	-0.806640	-0.915539
44	6	0	7.102929	-0.929299	-0.928487
45	6	0	6.982290	-2.482064	0.912770
46	1	0	5.007887	-2.918048	1.665304
47	1	0	5.213827	-0.167627	-1.647020
48	1	0	7.661617	-0.364938	-1.667895
49	1	0	7.454797	-3.134377	1.643445
50	6	0	-4.898202	-1.544786	-0.010445
51	6	0	-7.765253	-1.801047	0.015463
52	6	0	-5.567707	-2.397853	-0.921925
53	6	0	-5.691904	-0.826702	0.911702
54	6	0	-7.092260	-0.955356	0.924832
55	6	0	-6.964317	-2.516570	-0.908779
56	1	0	-4.987800	-2.947752	-1.658525
57	1	0	-5.206686	-0.181980	1.640159
58	1	0	-7.653629	-0.389806	1.661293
59	1	0	-7.433770	-3.174471	-1.636404
60	6	0	9.317122	-1.926607	0.003991
61	6	0	10.012650	-1.068452	-1.082061
62	1	0	11.098951	-1.214821	-1.026638
63	1	0	9.814590	0.002432	-0.943597
64	1	0	9.690891	-1.351459	-2.092753
65	6	0	9.865008	-1.488346	1.394747
66	1	0	10.956737	-1.605844	1.426846
67	1	0	9.438725	-2.088843	2.207315

68	1	0	9.626665	-0.435641	1.594450
69	6	0	9.685672	-3.419288	-0.245683
70	1	0	10.776030	-3.550608	-0.220651
71	1	0	9.321851	-3.752693	-1.226173
72	1	0	9.250493	-4.077741	0.515688
73	6	0	-0.040652	8.160750	0.006258
74	6	0	-1.506032	8.654108	-0.181664
75	1	0	-2.167363	8.271902	0.605212
76	1	0	-1.908096	8.324334	-1.148371
77	1	0	-1.544458	9.751495	-0.149712
78	6	0	0.828026	8.789218	-1.111842
79	1	0	1.883566	8.502871	-1.016998
80	1	0	0.774203	9.883589	-1.048118
81	1	0	0.479379	8.497429	-2.111067
82	6	0	0.497540	8.661573	1.379557
83	1	0	1.534561	8.336833	1.534514
84	1	0	-0.101883	8.279634	2.214674
85	1	0	0.471083	9.759009	1.420590
86	6	0	-9.301834	-1.966604	-0.003620
87	6	0	-9.850928	-1.536801	-1.396544
88	1	0	-9.421884	-2.139227	-2.206227
89	1	0	-9.616740	-0.484054	-1.600883
90	1	0	-10.942162	-1.658836	-1.428546
91	6	0	-9.664248	-3.459687	0.252512
92	1	0	-9.225896	-4.119715	-0.505668
93	1	0	-10.754032	-3.595685	0.227467
94	1	0	-9.299593	-3.787184	1.234681
95	6	0	-10.001412	-1.106576	1.078338
96	1	0	-9.678789	-1.383671	2.090394
97	1	0	-11.087057	-1.257846	1.023211
98	1	0	-9.807909	-0.035481	0.935142
99	47	0	0.005841	-1.107955	-0.000848
100	1	0	-3.997326	-4.400163	0.318956
101	1	0	4.023054	-4.384539	-0.303921
Rotational constants (GHZ):			0.0506358	0.0262995	0.0177146

References

[1] K. E. Thomas, H. Vazquez-Lima, Y. Fang, Y. Song, K. J. Gagnon, C. M. Beavers, K. M. Kadish and A. Ghosh, *Chem. Eur. J.*, 2015, **21**, 16839.