Supporting Information

Conformation-selective coordination-driven self-assembly of a ditopic donor with Pd^{II} acceptors

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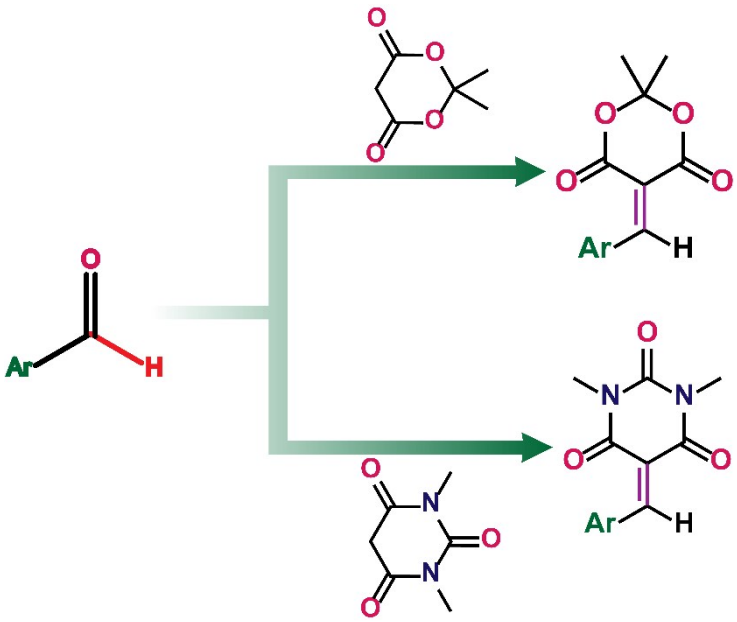

Table S1: Knoevenegal condensation products from different aromatic aldehydes and active methylene compounds.

Aldhydes	Active methylene compound	Product
Pyrene-1	Meldrum's acid (5eqv)	1a
Pyrene-1	Dimethyl Barbituric acid (2eqv)	1b
9-Anthracene	Dimethyl Barbituric acid	2b
1-naphthyl	Meldrum's acid	3a
1-naphthyl	Dimethyl Barbituric acid	3b
2-naphthyl	Meldrum's acid	4a
2-naphthyl	Dimethyl Barbituric acid	4b

Same reaction was studied in case of 9-anthracenealdehyde and dimethylbarbituric acid with equivalent amount of the ligand (**L-meta**) and also with **$Pd(NO_3)_2$** in water to confirm the catalytic activity of the cage (**$([CG\text{-}1](NO_3)_{12}$**). The results are assembled in Table S2.

Table S2: Knoevenegal condensation products from 9-anthracene aldehydes and dimethyl barbituric acid.

Aldehyde	Active Methylene Compound	Solvent	Time	Reagent	Yield
9-Anthracene	Dimethyl Barbituric acid	Water	55 hrs	**L-meta**	9%
9-Anthracene	Dimethyl Barbituric acid	Water	55 hrs	**$Pd(NO_3)_2$**	8%
9-Anthracene	Dimethyl Barbituric acid	Water	55 hrs	**MC-3**	12%

Characterization of the Knoevenegal products:

All the Knoevenegal products were isolated and purified by preparative TLC using chloroform. The products were characterized by ^{1}H-NMR spectroscopy.

2,2-dimethyl-5-(pyren-1-ylmethylene)-1,3-dioxane-4,6-dione (1a):

^{1}H NMR (400 MHz, $CDCl_3$): δ=9.61 (s, 1H), 8.52 (d, 1H), 8.37–8.07 (m, 8H), 1.92 ppm (s, 6H).

1,3-dimethyl-5-(pyren-1-ylmethylene)pyrimidine-2,4,6(1H,3H,5H)-trione (1b):

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.56 (s, 1H), 8.47 (d, 1H, H), 8.27-8.03 (m, 8H), 3.51 (s, 3H), 3.35 (s, 3H).

5-(anthracen-10-ylmethylene)-2,2-dimethyl-1,3-dioxane-4,6-dione (2a):

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.47(s, 1H), 8.55(s, 1H), 8.06 (d, 2H), 7.83(d, 2H), 7.52-7.49(m, 4H), 1.90(s, 6H).

5-(anthracen-10-ylmethylene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione(2b):

^{1}H NMR ($CDCl_3$, 400 MHz) δ= 9.45 (s, 1H), 8.54 (s, 1H), 8.05 (dd, 2H), 7.82 (dd, 2H), 7.49 (m, 4H), 3.54 (s, 3H, H), 3.17 (s, 3H).

2,2-dimethyl-5-(naphthalen-1-ylmethylene)-1,3-dioxane-4,6-dione (3a):

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.23 (s, 1H), 8.02 (d, 2H), 7.98 (d, 1H), 7.91 (d, 1H), 7.64–7.52 (m, 3H), 1.87 (s, 6H).

1,3-dimethyl-5-(naphthalen-1-ylmethylene)pyrimidine-2,4,6(1H,3H,5H)-trione(3b):

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.23 (s, 1H), 7.97 (t, 2H), 7.90 (d, 1H), 7.86 (d, 1H), 7.55 (m, 3H), 3.46 (s, 3H), 3.30 (s, 3H).

2,2-dimethyl-5-(naphthalen-2-ylmethylene)-1,3-dioxane-4,6-dione (4a):

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.59 (s, 1H), 8.55 (s, 1H), 8.12 (dd, 1H), 7.94 (d, 1H), 7.88 (d, 1H), 7.86 (d, 1H), 7.63 (td, 1H), 7.56 (td, 1H), 1.84 (s, 6H).

1,3-dimethyl-5-(naphthalen-2-ylmethylene)pyrimidine-2,4,6(1H,3H,5H)-trione (4b):

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.74 (s, 1H,), 8.51 (s, 1H), 8.14 (d, 1H), 7.94 (d, 1H), 7.87 (dd, 2H), 7.62 (t, 1H), 7.54 (t, 1H), 3.45 (s, 3H), 3.41 (s, 3H).

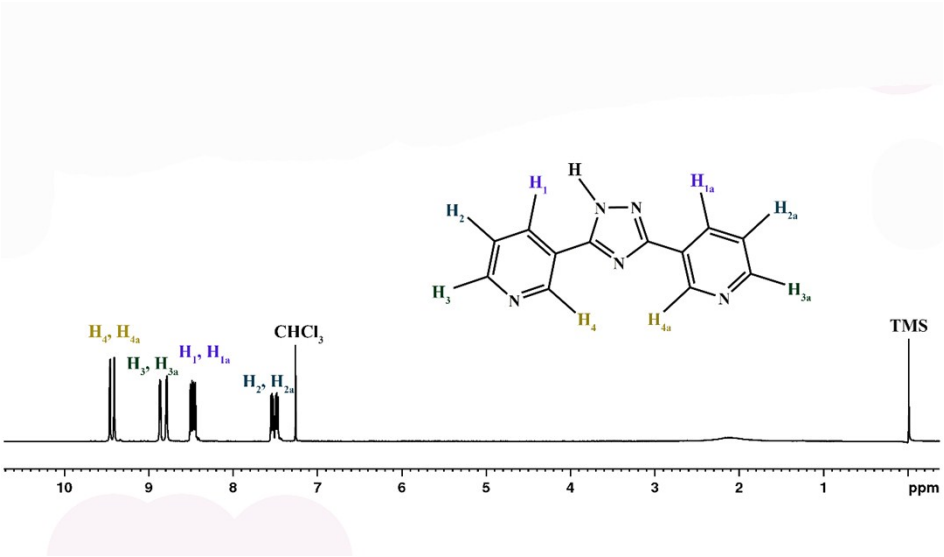

Figure S1. ^{1}H-NMR spectra of ligand **L** recorded in $CDCl_3$.

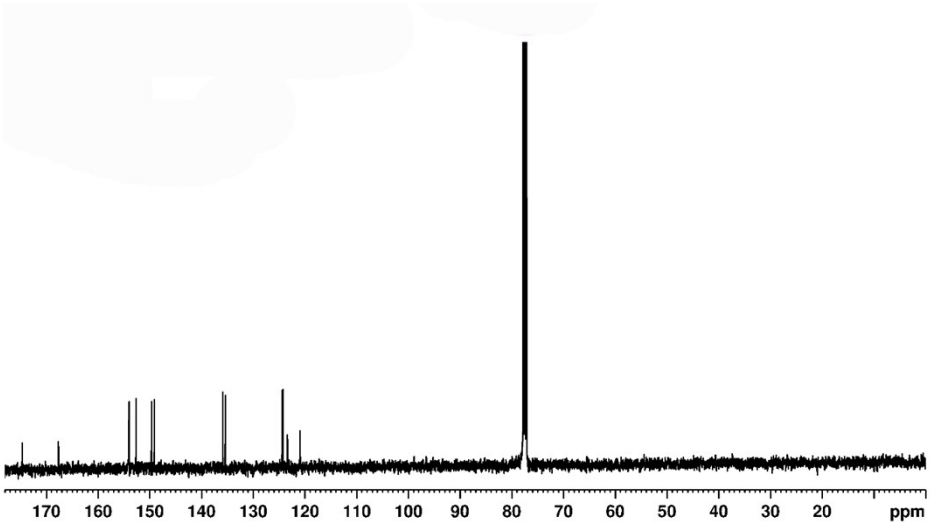

Figure S2. ^{13}C-NMR spectra of ligand **L** recorded in $CDCl_3$.

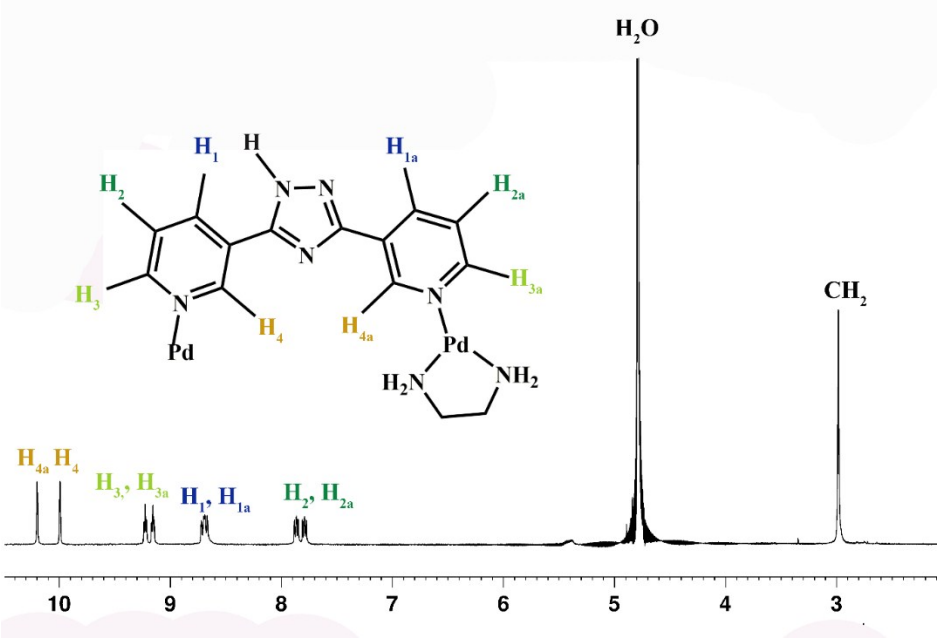

Figure S3. ^{1}H-NMR spectra of **[MC-1](NO$_3$)$_4$** recorded in D_2O.

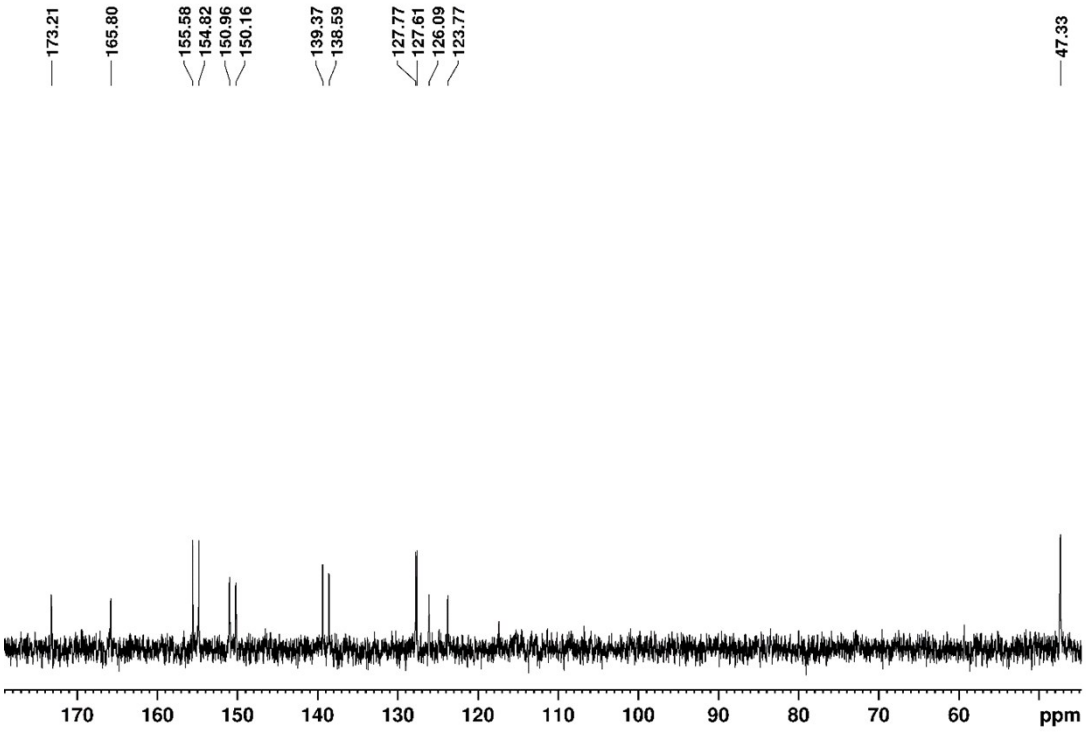

Figure S4. ^{13}C-NMR spectra of **[MC-1](NO$_3$)$_4$** recorded in D_2O.

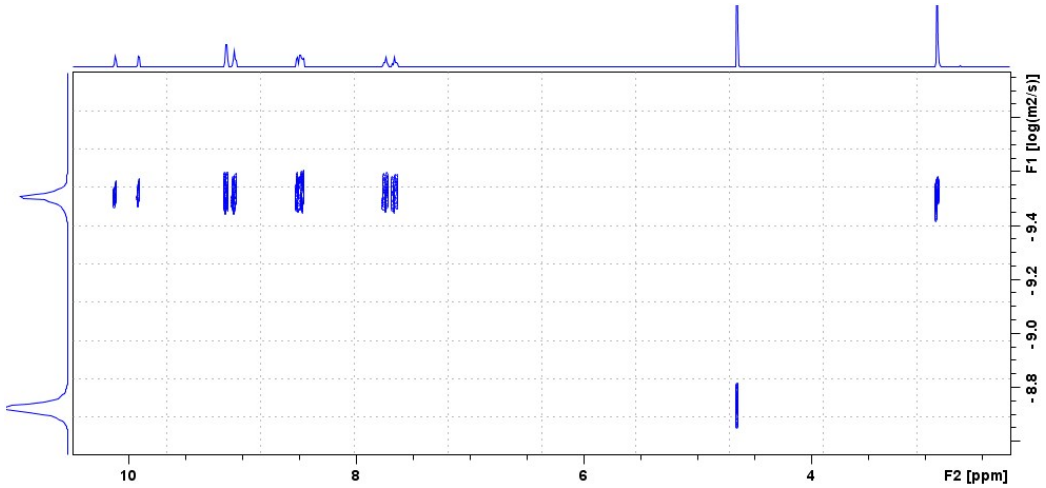

Figure S5. ^{1}H-DOSY spectra of **[MC-1](NO$_3$)$_4$** recorded in D_2O.

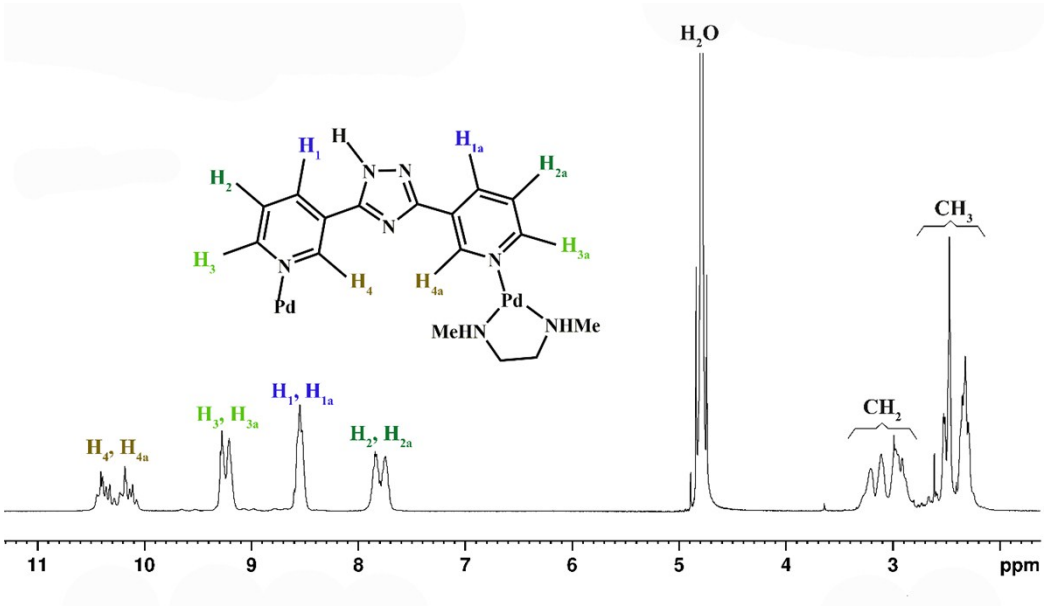

Figure S6. ^{1}H-NMR spectra of **[MC-2](NO$_3$)$_4$** recorded in D_2O.

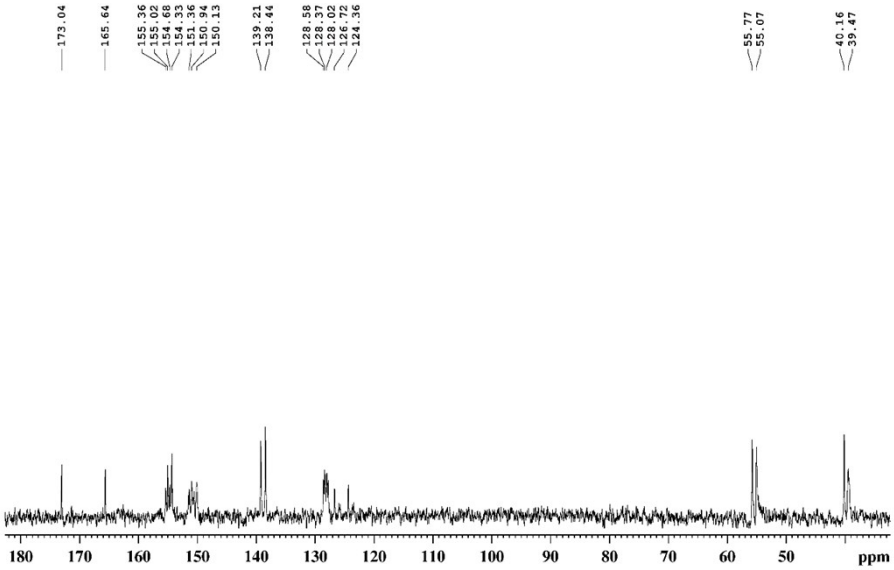

Figure S7. ^{13}C-NMR spectra of **[MC-2](NO$_3$)$_4$** recorded in D_2O.

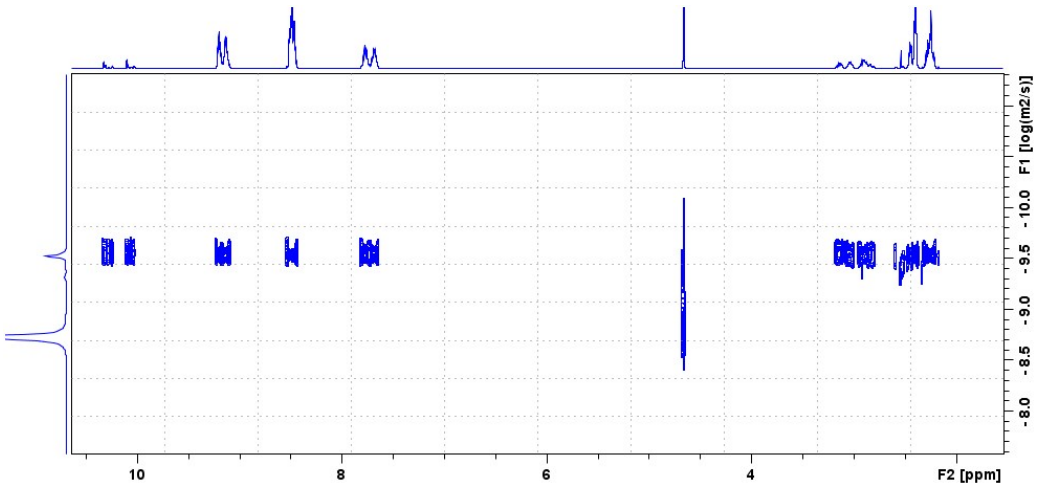

Figure S8. ^{1}H-DOSY spectra of **[MC-2](NO$_3$)$_4$** recorded in D_2O.

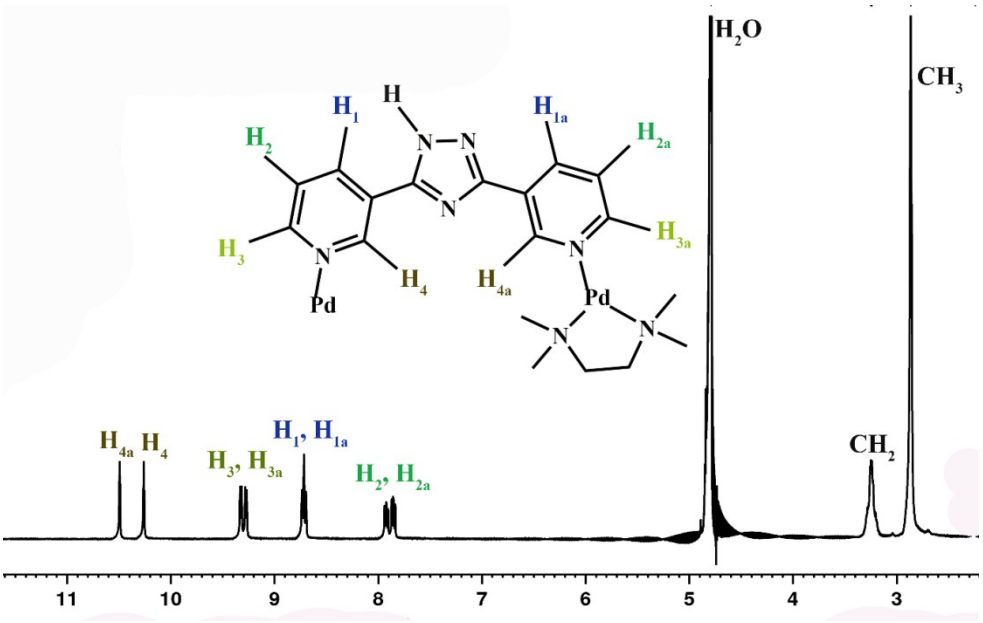

Figure S9. ^{1}H-NMR spectra of **[MC-3](NO$_3$)$_4$** recorded in D_2O.

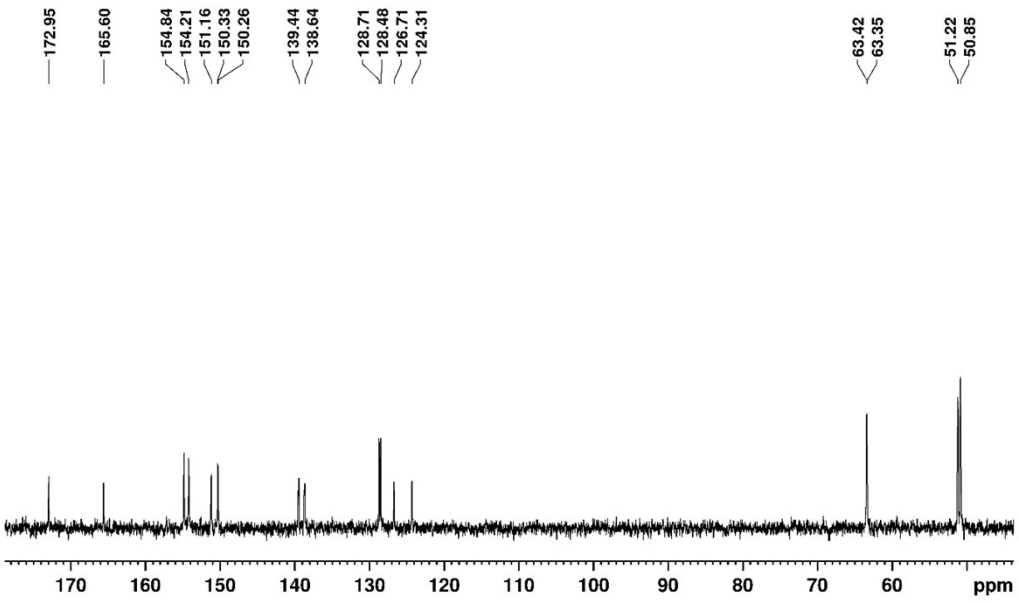

Figure S10. ^{13}C-NMR spectra of **[MC-3](NO$_3$)$_4$** recorded in D_2O.

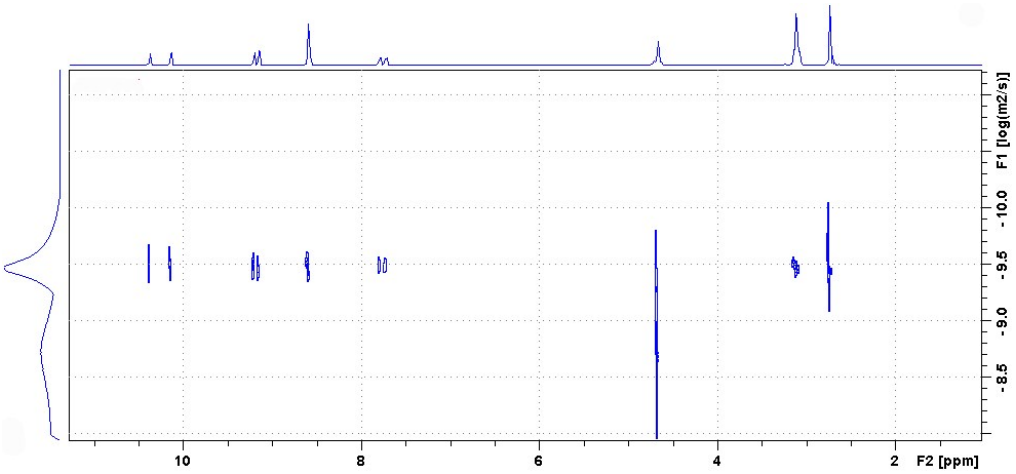

Figure S11. ^{1}H-DOSY spectra of **[MC-3](NO$_3$)$_4$** recorded in D_2O.

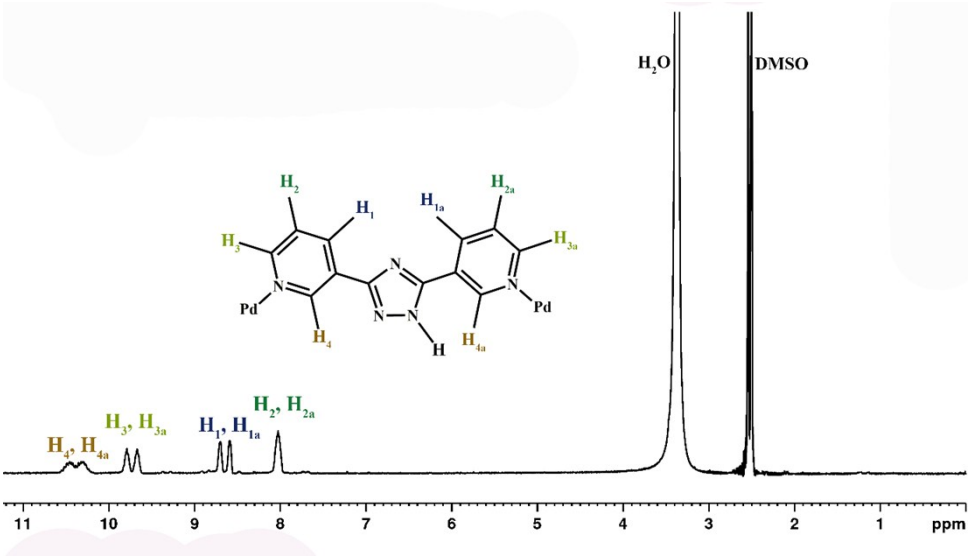

Figure S12. ^{1}H-NMR spectra of **[CG-1](NO$_3$)$_{12}$** recorded in DMSO-d_6.

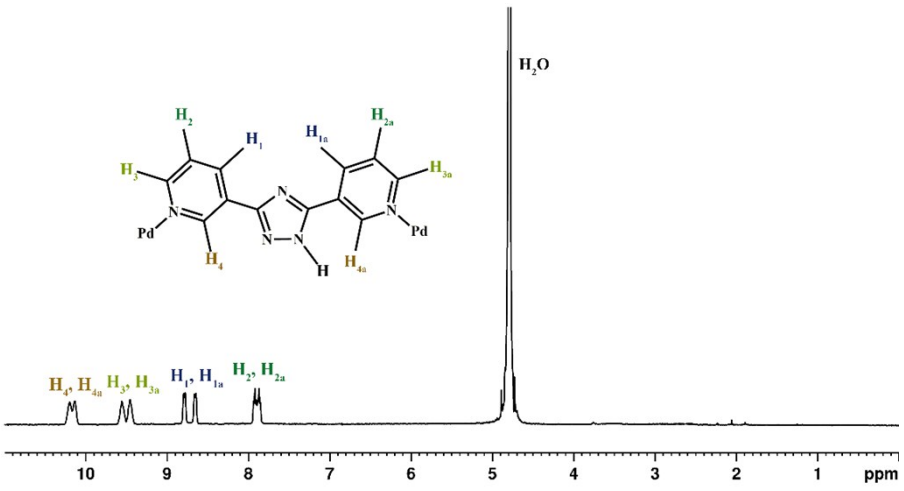

Figure S13. ^{1}H-NMR spectra of **[CG-1](NO$_3$)$_{12}$** recorded in D_2O.

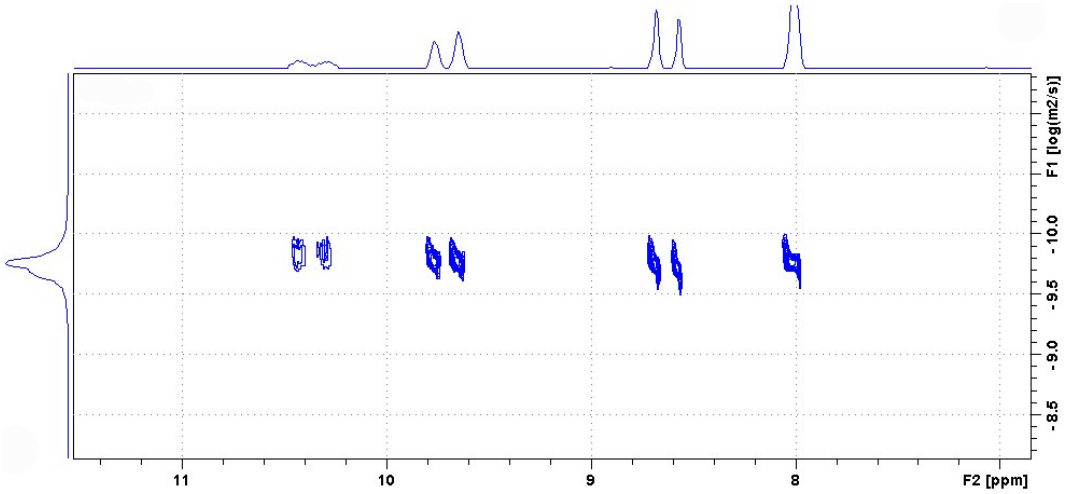

Figure S14. ^{1}H-DOSY spectra of **[CG-1](NO$_3$)$_{12}$** recorded in DMSO-d$_6$.

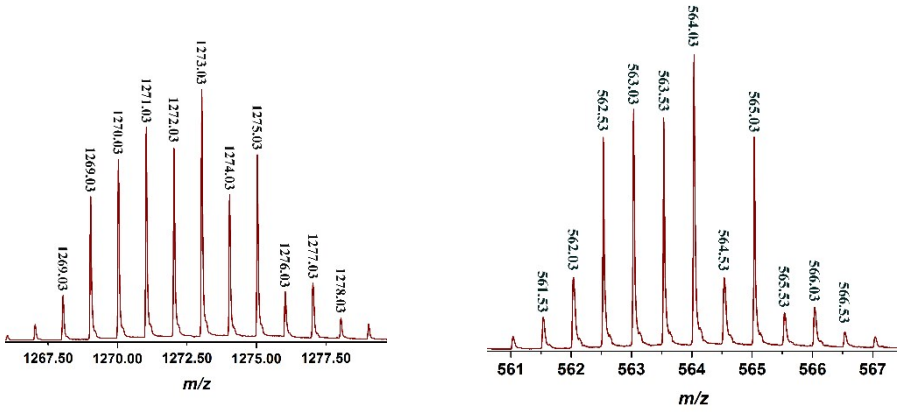

Figure S15. ESI-MS spectra of **[MC-2](PF$_6$)$_4$.** [**MC-2-PF$_6$**]$^+$ (left) and [**MC-2-2PF$_6$**]$^{2+}$.

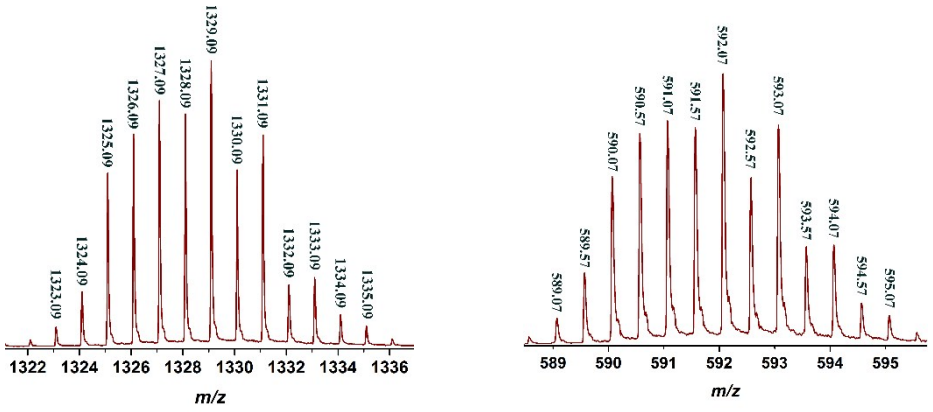

Figure S16. ESI-MS spectra of **[MC-3](PF$_6$)$_4$.** [**MC-3-PF$_6$**]$^+$ (left) and [**MC-3-2PF$_6$**]$^{2+}$.

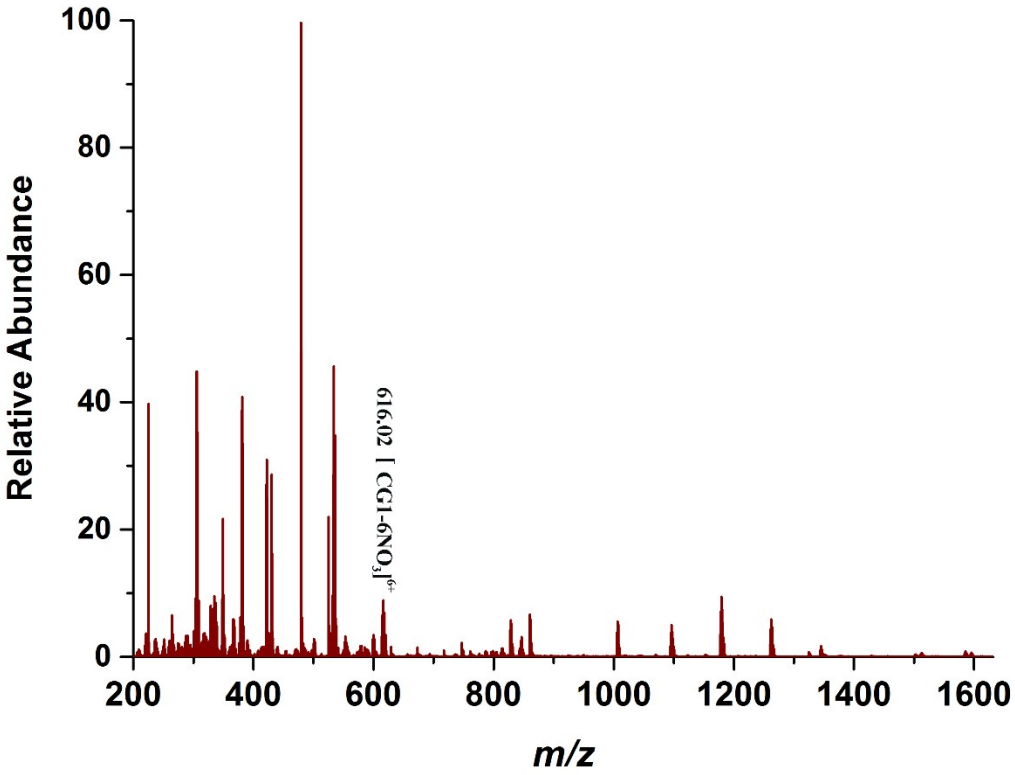

Figure S17. ESI-MS spectra of the cage **[CG-1](NO$_3$)$_{12}$ (** [**CG-1-6NO$_3$**]$^{6+}$).

Computed Geometry and Energy for [MC-1$_1$]$^{4+}$

Energy = - 2106.07183612 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-4.080825	-0.058429	1.228177
2	46	0	4.111777	0.020738	1.167537
3	6	0	-1.106918	3.171275	-1.688127
4	6	0	-2.412879	-2.798224	-1.579314
5	7	0	3.871251	1.488161	-0.232092
6	7	0	-3.939218	1.450390	-0.130440
7	7	0	4.263576	-1.407498	2.600458
8	1	0	4.815190	-2.172602	2.268285
9	7	0	3.845067	-1.382417	-0.280978
10	7	0	-0.075031	2.607397	-1.131157
11	7	0	0.005396	-2.655212	-1.201056
12	7	0	0.704160	-3.961443	-2.827507
13	7	0	4.526159	1.306578	2.678370
14	1	0	5.436229	1.701437	2.552434
15	7	0	-3.830697	-1.421524	-0.262674
16	7	0	-4.052343	-1.558631	2.627544
17	1	0	-4.566214	-2.355941	2.310947
18	7	0	0.601856	4.021987	-2.680512
19	7	0	-0.705373	-3.961790	-2.843631
20	7	0	-0.810822	4.045133	-2.629280
21	7	0	-4.436408	1.193086	2.790891
22	1	0	-5.371285	1.545781	2.750746
23	6	0	0.949616	3.178635	-1.728632
24	6	0	-2.510805	2.871233	-1.382357
25	6	0	-1.025538	-3.156061	-1.842989
26	6	0	2.620898	-1.825222	-0.578868
27	1	0	1.890749	-1.473436	-0.123372

28	6	0	2.372948	2.860821	-1.438524
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30	6	0	-3.518464	-3.304813	-2.240021
31	1	0	-3.416306	-3.957748	-2.894731
32	6	0	2.611598	1.850647	-0.568080
33	1	0	1.892959	1.392604	-0.194850
34	6	0	3.522477	-3.311741	-2.202261
35	1	0	3.412079	-3.962396	-2.856908
36	6	0	-2.728716	1.833775	-0.475752
37	1	0	-1.995773	1.398663	-0.101859
38	6	0	4.903495	-1.911413	-0.926051
39	1	0	5.755246	-1.612059	-0.703039
40	6	0	2.409966	-2.796596	-1.552524
41	6	0	3.425164	3.524388	-2.036355
42	1	0	3.273014	4.222771	-2.630273
43	6	0	-3.593879	3.497673	-1.932064
44	1	0	-3.471302	4.185713	-2.544851
45	6	0	4.712919	3.119911	-1.730825
46	1	0	5.445636	3.523950	-2.136119
47	6	0	4.784058	-2.869718	-1.891422
48	1	0	5.531291	-3.209819	-2.325233
49	6	0	-2.626258	-1.849004	-0.577913
50	1	0	-1.892828	-1.507321	-0.119272
51	6	0	-4.769718	-2.835648	-1.919682
52	1	0	-5.514122	-3.153794	-2.376297
53	6	0	4.880129	2.121469	-0.825649
54	1	0	5.748176	1.867435	-0.608742
55	6	0	-4.921479	-1.912392	-0.940755
56	1	0	-5.772562	-1.607935	-0.724793
57	6	0	-5.006263	2.088823	-0.709824
58	1	0	-5.866640	1.805233	-0.497635
59	6	0	-4.851848	3.111432	-1.580630
60	1	0	-5.594202	3.547113	-1.933297
61	6	0	4.473731	0.552523	3.941896
62	1	0	5.027385	0.999627	4.602686
63	1	0	3.561211	0.549653	4.272586
64	6	0	4.915524	-0.779691	3.794238
65	1	0	4.695263	-1.286714	4.590884
66	1	0	5.879211	-0.791540	3.684605
67	6	0	-4.682821	-0.960712	3.851529
68	1	0	-5.649263	-0.989474	3.771071
69	1	0	-4.428012	-1.470390	4.636748
70	6	0	-4.239526	0.422169	3.993368
71	1	0	-4.726892	0.838163	4.721035
72	1	0	-3.297591	0.430804	4.224914
73	1	0	1.313881	-4.465553	-3.439155
74	1	0	-1.438860	4.596019	-3.178909
75	1	0	3.853699	2.046572	2.692742
76	1	0	3.356282	-1.750840	2.843221
77	1	0	-3.807423	1.970128	2.766747
78	1	0	-3.116926	-1.858665	2.814558

Computed Geometry and Energy for $[MC\text{-}1_{II}]^{4+}$

Energy = - 2105.90879335 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	6.073261	0.007595	-0.409996
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4	7	0	0.647120	-1.813514	-1.242296
5	7	0	0.006100	-2.856772	0.716856
6	7	0	7.343983	1.387407	-1.192044
7	6	0	5.162900	-2.076517	1.610558
8	6	0	4.181452	-2.930959	2.285709
9	6	0	2.843270	-3.094544	1.706073

10	6	0	2.502806	-2.440379	0.429653
11	6	0	3.554639	-1.683381	-0.274135
12	6	0	1.108671	-2.454419	-0.062460
13	7	0	-0.742986	-1.774625	-1.297488
14	6	0	-1.111711	-2.433007	-0.054913
15	46	0	-6.080266	-0.008710	-0.399356
16	7	0	-7.354189	1.352388	-1.206319
17	7	0	4.832502	1.447940	0.354538
18	7	0	-4.847078	1.459763	0.323185
19	7	0	0.706417	1.714885	-1.247358
20	7	0	-0.661418	1.724949	-1.261793
21	7	0	-0.007954	2.879663	0.657352
22	6	0	5.164068	2.068549	1.600644
23	6	0	4.180478	2.923447	2.287583
24	6	0	2.836939	3.089151	1.708552
25	6	0	2.507597	2.433343	0.426187
26	6	0	3.568326	1.680055	-0.276589
27	6	0	1.122682	2.426406	-0.085602
28	6	0	-1.121079	2.428842	-0.111221
29	6	0	-2.518583	2.442769	0.377449
30	6	0	-2.859460	3.138713	1.636457
31	6	0	-4.207877	2.996924	2.209746
32	6	0	-5.187540	2.121848	1.544720
33	6	0	-3.580229	1.672427	-0.309184
34	6	0	8.256500	-0.700143	-2.116722
35	6	0	8.573636	0.718663	-1.605986
36	1	0	6.127375	-1.886912	2.069303
37	1	0	4.428969	-3.404616	3.229905
38	1	0	2.103969	-3.684667	2.238384
39	1	0	3.360053	-1.220393	-1.232625
40	1	0	-1.235542	1.243444	-1.994390
41	1	0	6.131215	1.875500	2.059207
42	1	0	4.430162	3.392247	3.237017
43	1	0	2.089904	3.672961	2.243045
44	1	0	3.364292	1.215791	-1.238448
45	1	0	-2.117091	3.739702	2.158093
46	1	0	-4.464527	3.500461	3.139306
47	1	0	-6.159720	1.948055	2.000237
48	1	0	-3.385477	1.184299	-1.258668
49	1	0	1.247071	-1.395368	-1.992699
50	1	0	6.792234	-2.124747	-1.673363
51	1	0	7.860042	-1.832028	-0.407751
52	1	0	9.196579	-1.289631	-2.227883
53	1	0	7.773150	-0.617455	-3.118465
54	1	0	9.259844	0.635978	-0.730657
55	1	0	9.087516	1.308866	-2.400495
56	1	0	6.867096	1.855253	-2.001671
57	1	0	7.529535	2.138256	-0.482435
58	1	0	-7.575331	2.092653	-0.495996
59	1	0	-6.864187	1.837747	-1.997727
60	7	0	-4.821376	-1.434088	0.399856
61	6	0	-2.488548	-2.420218	0.473469
62	6	0	-2.804643	-3.036108	1.777378
63	6	0	-3.552221	-1.688570	-0.241742
64	6	0	-5.138634	-2.026052	1.678048
65	6	0	-4.141447	-2.858942	2.370823
66	7	0	-7.348272	-1.440930	-1.145232
67	6	0	-8.183897	-0.748474	-2.146295
68	6	0	-8.553745	0.662122	-1.659269
69	1	0	-3.357662	-1.251623	-1.218316
70	1	0	-6.100211	-1.823664	2.144351
71	1	0	-4.375966	-3.305107	3.334957
72	1	0	-2.051706	-3.605068	2.319775
73	1	0	-7.957855	-1.820302	-0.358813
74	1	0	-6.796078	-2.227076	-1.604116
75	1	0	-9.109825	-1.337090	-2.344982
76	1	0	-7.615264	-0.658892	-3.101404
77	1	0	-9.272972	0.572288	-0.811540
78	1	0	-9.044626	1.235866	-2.480088

Computed Geometry and Energy for $[MC\text{-}1_{III}]^{4+}$

Energy = - 2105.89553418 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-5.855046	-0.021502	0.211170
2	7	0	-7.276091	1.363683	-0.314887
3	7	0	-4.507116	1.450951	0.721368
4	7	0	-1.049345	2.656970	-1.959576
5	7	0	0.341092	2.468531	-0.043072
6	7	0	-7.220123	-1.468203	-0.293223
7	6	0	-4.484663	1.924676	2.082555
8	6	0	-3.300194	2.615449	2.600997
9	6	0	-2.133666	2.799238	1.732078
10	6	0	-2.191678	2.379051	0.322654
11	6	0	-3.420045	1.741324	-0.181341
12	6	0	-1.006923	2.508062	-0.535872
13	7	0	0.264960	2.737362	-2.421676
14	6	0	1.099688	2.614075	-1.258115
15	7	0	-4.450321	-1.434467	0.736863
16	6	0	4.761792	-2.586737	-2.722003
17	7	0	-1.068544	-2.499815	-2.026210
18	7	0	0.245582	-2.582972	-2.488959
19	7	0	0.377343	-2.545492	-0.118927
20	6	0	-4.384849	-1.865699	2.110462
21	6	0	-3.186095	-2.544482	2.611773
22	6	0	-2.048853	-2.760532	1.711419
23	6	0	-2.141283	-2.360335	0.297177
24	6	0	-3.385756	-1.739572	-0.187622
25	6	0	-0.980537	-2.498724	-0.592309
26	6	0	1.115507	-2.598637	-1.349784
27	6	0	2.574583	-2.432631	-1.426998
28	6	0	3.302303	-1.769974	-0.330764
29	7	0	4.696907	-1.436115	-0.482609
30	6	0	5.440054	-1.866030	-1.640002
31	6	0	3.320247	-2.843408	-2.629039
32	6	0	-8.312168	0.610060	-1.041818
33	6	0	-8.511340	-0.768218	-0.399571
34	6	0	4.751426	2.708342	-2.598540
35	6	0	2.560930	2.473858	-1.322480
36	6	0	3.288457	1.763203	-0.256411
37	6	0	3.306869	2.945037	-2.501259
38	6	0	5.432131	1.945602	-1.547093
39	7	0	4.687991	1.453265	-0.415235
40	1	0	-5.309012	1.691742	2.747204
41	1	0	-3.267404	2.942760	3.634879
42	1	0	-1.237823	3.264123	2.131884
43	1	0	-3.458595	1.352173	-1.193142
44	1	0	0.525513	-2.517779	-3.512140
45	1	0	-5.191840	-1.616818	2.790653
46	1	0	-3.124194	-2.846491	3.652190
47	1	0	-1.148392	-3.230052	2.094660
48	1	0	-3.457615	-1.384730	-1.210481
49	1	0	2.768334	-1.414248	0.544584
50	1	0	6.487200	-1.600386	-1.736867
51	1	0	2.818871	-3.356161	-3.443551
52	1	0	-1.911631	2.736299	-2.575516
53	1	0	-6.854820	2.113722	-0.942008
54	1	0	-7.689308	1.799728	0.564161
55	1	0	-9.273018	1.175789	-1.034472
56	1	0	-7.995624	0.470993	-2.101704
57	1	0	-8.944783	-0.632993	0.618857
58	1	0	-9.224711	-1.371843	-1.007583
59	1	0	-6.955721	-1.897632	-1.230829
60	1	0	-7.266729	-2.216595	0.462462
61	1	0	2.797268	3.473399	-3.301028
62	1	0	6.481190	1.691436	-1.653168
63	1	0	2.751396	1.353139	0.592894
64	46	0	5.521903	-0.017217	0.763686
65	7	0	6.358939	1.372925	2.021132
66	6	0	7.330389	0.628032	2.840499
67	6	0	6.775405	-0.759600	3.185676
68	7	0	6.363965	-1.459617	1.956998
69	1	0	7.214306	-1.874244	1.468106
70	1	0	5.653874	-2.219785	2.183858
71	1	0	7.548576	-1.355563	3.724729

72	1	0	5.893112	-0.638898	3.857146
73	1	0	8.280335	0.504234	2.269313
74	1	0	7.554005	1.192087	3.775968
75	1	0	5.601885	1.794283	2.640271
76	1	0	6.852725	2.132936	1.462441
77	1	0	5.316088	-2.897108	-3.601642
78	1	0	5.304054	3.055937	-3.465028

Computed Geometry and Energy for [CG-1]$^{12+}$

Energy = - 9591.43852287 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	6.204579	6.180600	0.000000
2	46	0	0.000000	0.000000	8.635188
3	7	0	6.224590	6.161800	2.051246
4	7	0	1.453953	1.412200	8.657391
5	7	0	3.782102	3.555300	4.120240
6	7	0	3.057600	2.860300	5.124898
7	1	0	2.464974	2.247900	5.018620
8	7	0	4.360091	4.313800	6.105372
9	7	0	4.778769	7.571300	0.000000
10	7	0	0.705268	6.484500	0.000000
11	7	0	0.000000	8.561500	0.000000
12	7	0	7.612429	4.727600	0.000000
13	7	0	6.533667	0.719900	0.000000
14	7	0	8.655836	0.000000	0.000000
15	6	0	7.085917	6.939600	2.693653
16	1	0	7.617308	7.527100	2.207375
17	6	0	7.214752	6.892700	4.068692
18	1	0	7.850794	7.403000	4.514665
19	6	0	6.363042	6.059800	4.746454
20	1	0	6.408155	6.015600	5.673896
21	6	0	5.443662	5.290200	4.071874
22	6	0	5.416297	5.392300	2.701714
23	1	0	4.794820	4.890300	2.225194
24	6	0	4.525908	4.382800	4.806063
25	6	0	3.497067	3.354000	6.231025
26	6	0	2.951322	2.865800	7.511030
27	6	0	3.455277	3.279500	8.675140
28	1	0	4.128231	3.919400	8.681574
29	6	0	2.973808	2.755400	9.900343
30	1	0	3.328069	3.031300	10.715072
31	6	0	1.975586	1.839700	9.842431
32	1	0	1.639074	1.492200	10.636159
33	6	0	1.944968	1.900400	7.531960
34	1	0	1.605274	1.588700	6.725293
35	6	0	5.049167	8.867600	0.000000
36	1	0	5.941253	9.129600	0.000000
37	6	0	4.063884	9.877100	0.000000
38	1	0	4.276440	10.784600	0.000000
39	6	0	2.798304	9.433000	0.000000
40	1	0	2.118916	10.067400	0.000000
41	6	0	2.460166	8.180800	0.000000
42	6	0	3.445590	7.256800	0.000000
43	1	0	3.207295	6.357700	0.000000
44	6	0	1.040154	7.747800	0.000000
45	6	0	8.955225	5.064100	0.000000
46	1	0	9.229016	5.955000	0.000000
47	6	0	9.824683	4.095900	0.000000
48	1	0	10.719880	4.338600	0.000000
49	6	0	9.554285	2.794100	0.000000
50	1	0	10.224057	2.151400	0.000000
51	6	0	8.208237	2.463100	0.000000
52	6	0	7.261421	3.461500	0.000000
53	1	0	6.359860	3.235400	0.000000

54	6	0	7.808863	1.114300	0.000000
55	7	0	-4.778769	7.571300	0.000000
56	7	0	-0.705268	6.484500	0.000000
57	6	0	-5.049167	8.867600	0.000000
58	1	0	-5.941253	9.129600	0.000000
59	6	0	-4.063884	9.877100	0.000000
60	1	0	-4.276440	10.784600	0.000000
61	6	0	-2.798304	9.433000	0.000000
62	1	0	-2.118916	10.067400	0.000000
63	6	0	-2.460166	8.180800	0.000000
64	6	0	-3.445590	7.256800	0.000000
65	1	0	-3.207295	6.357700	0.000000
66	6	0	-1.040154	7.747800	0.000000
67	7	0	7.612429	-4.727600	0.000000
68	7	0	6.533667	-0.719900	0.000000
69	6	0	8.955225	-5.064100	0.000000
70	1	0	9.229016	-5.955000	0.000000
71	6	0	9.824683	-4.095900	0.000000
72	1	0	10.719880	-4.338600	0.000000
73	6	0	9.554285	-2.794100	0.000000
74	1	0	10.224057	-2.151400	0.000000
75	6	0	8.208237	-2.463100	0.000000
76	6	0	7.261421	-3.461500	0.000000
77	1	0	6.359860	-3.235400	0.000000
78	6	0	7.808863	-1.114300	0.000000
79	46	0	-6.204579	6.180600	0.000000
80	46	0	0.000000	0.000000	-8.635188
81	7	0	-6.224590	6.161800	-2.051246
82	7	0	-1.453953	1.412200	-8.657391
83	7	0	-3.782102	3.555300	-4.120240
84	7	0	-3.057600	2.860300	-5.124898
85	1	0	-2.464974	2.247900	-5.018620
86	7	0	-4.360091	4.313800	-6.105372
87	7	0	-7.612429	4.727600	0.000000
88	7	0	-6.533667	0.719900	0.000000
89	7	0	-8.655836	0.000000	0.000000
90	6	0	-7.085917	6.939600	-2.693653
91	1	0	-7.617308	7.527100	-2.207375
92	6	0	-7.214752	6.892700	-4.068692
93	1	0	-7.850794	7.403000	-4.514665
94	6	0	-6.363042	6.059800	-4.746454
95	1	0	-6.408155	6.015600	-5.673896
96	6	0	-5.443662	5.290200	-4.071874
97	6	0	-5.416297	5.392300	-2.701714
98	1	0	-4.794820	4.890300	-2.225194
99	6	0	-4.525908	4.382800	-4.806063
100	6	0	-3.497067	3.354000	-6.231025
101	6	0	-2.951322	2.865800	-7.511030
102	6	0	-3.455277	3.279500	-8.675140
103	1	0	-4.128231	3.919400	-8.681574
104	6	0	-2.973808	2.755400	-9.900343
105	1	0	-3.328069	3.031300	-10.715072
106	6	0	-1.975586	1.839700	-9.842431
107	1	0	-1.639074	1.492200	-10.636159
108	6	0	-1.944968	1.900400	-7.531960
109	1	0	-1.605274	1.588700	-6.725293
110	6	0	-8.955225	5.064100	0.000000
111	1	0	-9.229016	5.955000	0.000000
112	6	0	-9.824683	4.095900	0.000000
113	1	0	-10.719880	4.338600	0.000000
114	6	0	-9.554285	2.794100	0.000000
115	1	0	-10.224057	2.151400	0.000000
116	6	0	-8.208237	2.463100	0.000000
117	6	0	-7.261421	3.461500	0.000000
118	1	0	-6.359860	3.235400	0.000000
119	6	0	-7.808863	1.114300	0.000000
120	7	0	-7.612429	-4.727600	0.000000
121	7	0	-6.533667	-0.719900	0.000000
122	6	0	-8.955225	-5.064100	0.000000
123	1	0	-9.229016	-5.955000	0.000000
124	6	0	-9.824683	-4.095900	0.000000
125	1	0	-10.719880	-4.338600	0.000000
126	6	0	-9.554285	-2.794100	0.000000
127	1	0	-10.224057	-2.151400	0.000000
128	6	0	-8.208237	-2.463100	0.000000
129	6	0	-7.261421	-3.461500	0.000000
130	1	0	-6.359860	-3.235400	0.000000
131	6	0	-7.808863	-1.114300	0.000000
132	46	0	6.204579	-6.180600	0.000000

133	7	0	6.224590	-6.161800	-2.051246
134	7	0	1.453953	-1.412200	-8.657391
135	7	0	3.782102	-3.555300	-4.120240
136	7	0	3.057600	-2.860300	-5.124898
137	1	0	2.464974	-2.247900	-5.018620
138	7	0	4.360091	-4.313800	-6.105372
139	7	0	4.778769	-7.571300	0.000000
140	7	0	0.705268	-6.484500	0.000000
141	7	0	0.000000	-8.561500	0.000000
142	6	0	7.085917	-6.939600	-2.693653
143	1	0	7.617308	-7.527100	-2.207375
144	6	0	7.214752	-6.892700	-4.068692
145	1	0	7.850794	-7.403000	-4.514665
146	6	0	6.363042	-6.059800	-4.746454
147	1	0	6.408155	-6.015600	-5.673896
148	6	0	5.443662	-5.290200	-4.071874
149	6	0	5.416297	-5.392300	-2.701714
150	1	0	4.794820	-4.890300	-2.225194
151	6	0	4.525908	-4.382800	-4.806063
152	6	0	3.497067	-3.354000	-6.231025
153	6	0	2.951322	-2.865800	-7.511030
154	6	0	3.455277	-3.279500	-8.675140
155	1	0	4.128231	-3.919400	-8.681574
156	6	0	2.973808	-2.755400	-9.900343
157	1	0	3.328069	-3.031300	-10.715072
158	6	0	1.975586	-1.839700	-9.842431
159	1	0	1.639074	-1.492200	-10.636159
160	6	0	1.944968	-1.900400	-7.531960
161	1	0	1.605274	-1.588700	-6.725293
162	6	0	5.049167	-8.867600	0.000000
163	1	0	5.941253	-9.129600	0.000000
164	6	0	4.063884	-9.877100	0.000000
165	1	0	4.276440	-10.784600	0.000000
166	6	0	2.798304	-9.433000	0.000000
167	1	0	2.118916	-10.067400	0.000000
168	6	0	2.460166	-8.180800	0.000000
169	6	0	3.445590	-7.256800	0.000000
170	1	0	3.207295	-6.357700	0.000000
171	6	0	1.040154	-7.747800	0.000000
172	7	0	-4.778769	-7.571300	0.000000
173	7	0	-0.705268	-6.484500	0.000000
174	6	0	-5.049167	-8.867600	0.000000
175	1	0	-5.941253	-9.129600	0.000000
176	6	0	-4.063884	-9.877100	0.000000
177	1	0	-4.276440	-10.784600	0.000000
178	6	0	-2.798304	-9.433000	0.000000
179	1	0	-2.118916	-10.067400	0.000000
180	6	0	-2.460166	-8.180800	0.000000
181	6	0	-3.445590	-7.256800	0.000000
182	1	0	-3.207295	-6.357700	0.000000
183	6	0	-1.040154	-7.747800	0.000000
184	46	0	-6.204579	-6.180600	0.000000
185	7	0	-6.224590	-6.161800	2.051246
186	7	0	-1.453953	-1.412200	8.657391
187	7	0	-3.782102	-3.555300	4.120240
188	7	0	-3.057600	-2.860300	5.124898
189	1	0	-2.464974	-2.247900	5.018620
190	7	0	-4.360091	-4.313800	6.105372
191	6	0	-7.085917	-6.939600	2.693653
192	1	0	-7.617308	-7.527100	2.207375
193	6	0	-7.214752	-6.892700	4.068692
194	1	0	-7.850794	-7.403000	4.514665
195	6	0	-6.363042	-6.059800	4.746454
196	1	0	-6.408155	-6.015600	5.673896
197	6	0	-5.443662	-5.290200	4.071874
198	6	0	-5.416297	-5.392300	2.701714
199	1	0	-4.794820	-4.890300	2.225194
200	6	0	-4.525908	-4.382800	4.806063
201	6	0	-3.497067	-3.354000	6.231025
202	6	0	-2.951322	-2.865800	7.511030
203	6	0	-3.455277	-3.279500	8.675140
204	1	0	-4.128231	-3.919400	8.681574
205	6	0	-2.973808	-2.755400	9.900343
206	1	0	-3.328069	-3.031300	10.715072
207	6	0	-1.975586	-1.839700	9.842431
208	1	0	-1.639074	-1.492200	10.636159
209	6	0	-1.944968	-1.900400	7.531960
210	1	0	-1.605274	-1.588700	6.725293
211	7	0	-6.224590	-6.161800	-2.051246

212	7	0	-1.453953	-1.412200	-8.657391
213	7	0	-3.782102	-3.555300	-4.120240
214	7	0	-3.057600	-2.860300	-5.124898
215	1	0	-2.464974	-2.247900	-5.018620
216	7	0	-4.360091	-4.313800	-6.105372
217	6	0	-7.085917	-6.939600	-2.693653
218	1	0	-7.617308	-7.527100	-2.207375
219	6	0	-7.214752	-6.892700	-4.068692
220	1	0	-7.850794	-7.403000	-4.514665
221	6	0	-6.363042	-6.059800	-4.746454
222	1	0	-6.408155	-6.015600	-5.673896
223	6	0	-5.443662	-5.290200	-4.071874
224	6	0	-5.416297	-5.392300	-2.701714
225	1	0	-4.794820	-4.890300	-2.225194
226	6	0	-4.525908	-4.382800	-4.806063
227	6	0	-3.497067	-3.354000	-6.231025
228	6	0	-2.951322	-2.865800	-7.511030
229	6	0	-3.455277	-3.279500	-8.675140
230	1	0	-4.128231	-3.919400	-8.681574
231	6	0	-2.973808	-2.755400	-9.900343
232	1	0	-3.328069	-3.031300	-10.715072
233	6	0	-1.975586	-1.839700	-9.842431
234	1	0	-1.639074	-1.492200	-10.636159
235	6	0	-1.944968	-1.900400	-7.531960
236	1	0	-1.605274	-1.588700	-6.725293
237	7	0	6.224590	-6.161800	2.051246
238	7	0	1.453953	-1.412200	8.657391
239	7	0	3.782102	-3.555300	4.120240
240	7	0	3.057600	-2.860300	5.124898
241	1	0	2.464974	-2.247900	5.018620
242	7	0	4.360091	-4.313800	6.105372
243	6	0	7.085917	-6.939600	2.693653
244	1	0	7.617308	-7.527100	2.207375
245	6	0	7.214752	-6.892700	4.068692
246	1	0	7.850794	-7.403000	4.514665
247	6	0	6.363042	-6.059800	4.746454
248	1	0	6.408155	-6.015600	5.673896
249	6	0	5.443662	-5.290200	4.071874
250	6	0	5.416297	-5.392300	2.701714
251	1	0	4.794820	-4.890300	2.225194
252	6	0	4.525908	-4.382800	4.806063
253	6	0	3.497067	-3.354000	6.231025
254	6	0	2.951322	-2.865800	7.511030
255	6	0	3.455277	-3.279500	8.675140
256	1	0	4.128231	-3.919400	8.681574
257	6	0	2.973808	-2.755400	9.900343
258	1	0	3.328069	-3.031300	10.715072
259	6	0	1.975586	-1.839700	9.842431
260	1	0	1.639074	-1.492200	10.636159
261	6	0	1.944968	-1.900400	7.531960
262	1	0	1.605274	-1.588700	6.725293
263	7	0	-6.224590	6.161800	2.051246
264	7	0	-1.453953	1.412200	8.657391
265	7	0	-3.782102	3.555300	4.120240
266	7	0	-3.057600	2.860300	5.124898
267	1	0	-2.464974	2.247900	5.018620
268	7	0	-4.360091	4.313800	6.105372
269	6	0	-7.085917	6.939600	2.693653
270	1	0	-7.617308	7.527100	2.207375
271	6	0	-7.214752	6.892700	4.068692
272	1	0	-7.850794	7.403000	4.514665
273	6	0	-6.363042	6.059800	4.746454
274	1	0	-6.408155	6.015600	5.673896
275	6	0	-5.443662	5.290200	4.071874
276	6	0	-5.416297	5.392300	2.701714
277	1	0	-4.794820	4.890300	2.225194
278	6	0	-4.525908	4.382800	4.806063
279	6	0	-3.497067	3.354000	6.231025
280	6	0	-2.951322	2.865800	7.511030
281	6	0	-3.455277	3.279500	8.675140
282	1	0	-4.128231	3.919400	8.681574
283	6	0	-2.973808	2.755400	9.900343
284	1	0	-3.328069	3.031300	10.715072
285	6	0	-1.975586	1.839700	9.842431
286	1	0	-1.639074	1.492200	10.636159
287	6	0	-1.944968	1.900400	7.531960
288	1	0	-1.605274	1.588700	6.725293
289	7	0	6.224590	6.161800	-2.051246
290	7	0	1.453953	1.412200	-8.657391

291	7	0	3.782102	3.555300	-4.120240
292	7	0	3.057600	2.860300	-5.124898
293	1	0	2.464974	2.247900	-5.018620
294	7	0	4.360091	4.313800	-6.105372
295	6	0	7.085917	6.939600	-2.693653
296	1	0	7.617308	7.527100	-2.207375
297	6	0	7.214752	6.892700	-4.068692
298	1	0	7.850794	7.403000	-4.514665
299	6	0	6.363042	6.059800	-4.746454
300	1	0	6.408155	6.015600	-5.673896
301	6	0	5.443662	5.290200	-4.071874
302	6	0	5.416297	5.392300	-2.701714
303	1	0	4.794820	4.890300	-2.225194
304	6	0	4.525908	4.382800	-4.806063
305	6	0	3.497067	3.354000	-6.231025
306	6	0	2.951322	2.865800	-7.511030
307	6	0	3.455277	3.279500	-8.675140
308	1	0	4.128231	3.919400	-8.681574
309	6	0	2.973808	2.755400	-9.900343
310	1	0	3.328069	3.031300	-10.715072
311	6	0	1.975586	1.839700	-9.842431
312	1	0	1.639074	1.492200	-10.636159
313	6	0	1.944968	1.900400	-7.531960
314	1	0	1.605274	1.588700	-6.725293
315	1	0	5.728845	1.313417	0.000000
316	1	0	1.315089	5.691960	0.000000
317	1	0	-1.315089	-5.691960	0.000000
318	1	0	-5.728845	-1.313417	0.000000

Computed Geometry and Energy for [CG-2]$^{4+}$

Energy = - 3197.71968491 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	4.253359	0.324201	0.098450
2	46	0	-3.879047	-0.659381	-0.060303
3	6	0	1.565631	-3.136498	3.027550
4	6	0	2.971651	-2.443247	-2.879633
5	7	0	-3.510674	-2.127393	1.310604
6	7	0	4.236654	-1.149017	1.502650
7	7	0	-3.343362	-1.992760	-1.500203
8	7	0	0.488736	-2.658654	2.475351
9	7	0	0.523641	-2.349795	-2.779152
10	7	0	0.041137	-3.943756	-4.216627
11	7	0	4.202211	-1.080946	-1.373342
12	7	0	-0.036048	-4.373916	3.756843
13	7	0	1.443065	-3.801824	-4.177959
14	7	0	1.360864	-4.166612	3.823794
15	6	0	-0.472661	-3.407535	2.973432
16	6	0	2.931411	-2.654163	2.790025
17	6	0	1.630874	-2.833618	-3.294616
18	6	0	-2.161977	-2.087243	-1.982046
19	1	0	-1.495689	-1.579948	-1.578237
20	6	0	-1.913011	-3.256093	2.636535
21	6	0	-0.433522	-3.065950	-3.359812
22	6	0	4.155287	-2.936891	-3.400024
23	1	0	4.141563	-3.549105	-4.100315
24	6	0	-2.228592	-2.345920	1.684132
25	1	0	-1.547937	-1.861865	1.274322
26	6	0	-2.842624	-3.687627	-3.604846
27	1	0	-2.645270	-4.276138	-4.296804
28	6	0	3.065770	-1.655007	1.825985
29	1	0	2.304031	-1.334577	1.397731
30	6	0	-4.388024	-2.680630	-2.157593
31	1	0	-5.265519	-2.577057	-1.867589
32	6	0	-1.821954	-2.957032	-3.013510

33	6	0	-2.903626	-4.015207	3.225866
34	1	0	-2.699098	-4.638100	3.884500
35	6	0	4.057055	-3.123678	3.406576
36	1	0	3.991055	-3.795282	4.045735
37	6	0	-4.209303	-3.826920	2.807513
38	1	0	-4.899197	-4.340354	3.160807
39	6	0	-4.140091	-3.553420	-3.178045
40	1	0	-4.826053	-4.041997	-3.569154
41	6	0	3.050390	-1.496806	-1.856206
42	1	0	2.262753	-1.149590	-1.503944
43	6	0	5.352183	-2.513800	-2.873901
44	1	0	6.150011	-2.859510	-3.202239
45	6	0	-4.458112	-2.875189	1.871303
46	1	0	-5.339866	-2.738783	1.608635
47	6	0	5.372801	-1.594621	-1.879709
48	1	0	6.187427	-1.307673	-1.536605
49	6	0	5.349509	-1.650619	2.128602
50	1	0	6.185735	-1.323111	1.885372
51	6	0	5.274449	-2.606094	3.082180
52	1	0	6.043109	-2.904478	3.512772
53	1	0	-0.484670	-4.581098	-4.779941
54	1	0	2.036047	-4.681462	4.352053
55	6	0	-3.564142	1.552778	1.943668
56	6	0	-5.845925	0.806370	1.669594
57	6	0	-3.983339	2.486097	2.891514
58	1	0	-2.499626	1.478833	1.677898
59	6	0	-6.265220	1.740701	2.617027
60	1	0	-6.580309	0.144172	1.188296
61	6	0	-5.334015	2.580379	3.228048
62	1	0	-7.329779	1.814754	2.882280
63	1	0	-5.664369	3.316593	3.975041
64	6	0	-5.437579	1.099131	-1.927742
65	6	0	-3.093134	1.666960	-1.786587
66	6	0	-5.633673	2.135718	-2.840023
67	1	0	-6.284131	0.466553	-1.623617
68	1	0	-2.091522	1.482222	-1.371714
69	6	0	-4.559754	2.938717	-3.225198
70	1	0	-6.635025	2.321157	-3.254930
71	1	0	-4.714658	3.756207	-3.944126
72	6	0	5.658762	2.226199	1.946681
73	6	0	3.254380	2.466451	1.948418
74	6	0	5.761947	3.252478	2.885472
75	1	0	6.565577	1.726776	1.575791
76	6	0	3.155311	3.508219	2.918430
77	1	0	2.265782	2.156616	1.579431
78	6	0	4.611470	3.886573	3.355364
79	1	0	6.750192	3.562970	3.254533
80	1	0	4.693071	4.695984	4.095187
81	6	0	5.248002	2.407803	-1.819360
82	6	0	2.839134	2.241436	-1.727407
83	6	0	5.141556	3.423395	-2.769342
84	1	0	6.239257	2.072871	-1.480938
85	6	0	2.732848	3.256670	-2.678413
86	1	0	1.931378	1.775897	-1.316644
87	6	0	3.883926	3.847707	-3.199223
88	1	0	6.048866	3.889028	-3.180700
89	1	0	3.800229	4.648121	-3.948539
90	6	0	-2.955711	3.414105	3.565592
91	6	0	-0.776915	3.790287	3.533361
92	7	0	-2.666126	4.486500	4.509962
93	7	0	-1.366182	4.739612	4.505977
94	7	0	-1.860239	3.013825	2.991382
95	1	0	-3.344302	4.958063	5.073617
96	7	0	-4.418881	0.684323	1.390745
97	7	0	4.404568	1.832783	1.478239
98	6	0	-3.289653	2.704446	-2.698406
99	6	0	-2.124206	3.646081	-3.054294
100	6	0	0.025888	4.613853	-3.479909
101	7	0	-0.705817	3.782539	-2.799083
102	7	0	-2.345501	4.652549	-3.846790
103	7	0	-1.114099	5.063908	-3.913361
104	1	0	-0.833036	5.910736	-4.364899
105	7	0	-4.166844	0.864412	-1.401097
106	7	0	4.096438	1.816847	-1.297931
