DFT and QTAIM study of the novel d-block metal complexes with tetraoxa[8]circulene-based ligand

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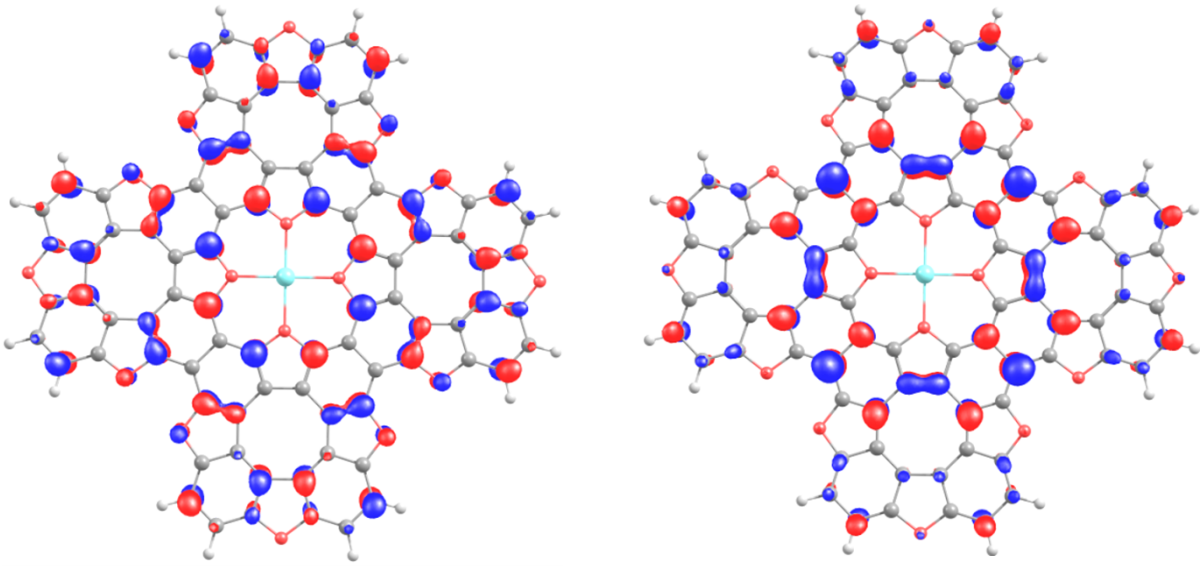
Electronic Supplementary Information

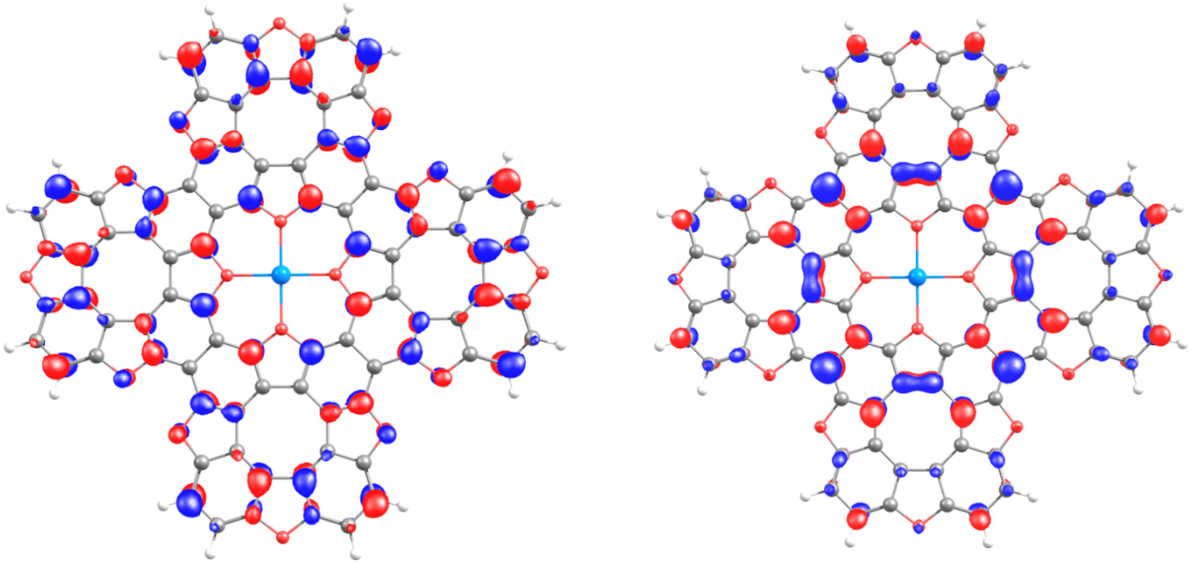
List of Content

Molecular HOMO-LUMO orbitals for the studied complexes **1–6** (Fig. **S1**–**S8**)	**2**
Table S1. Total energies of the studied complexes **1–6** with tetraoxa[8]circulene-based ligand	**6**
Optimized Cartesian coordinates of the complexes **1–6** (Tables **S2–S8**)	**7**

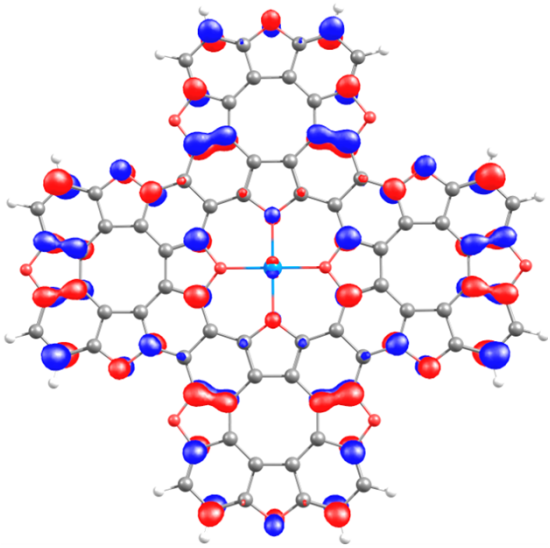


HOMO LUMO

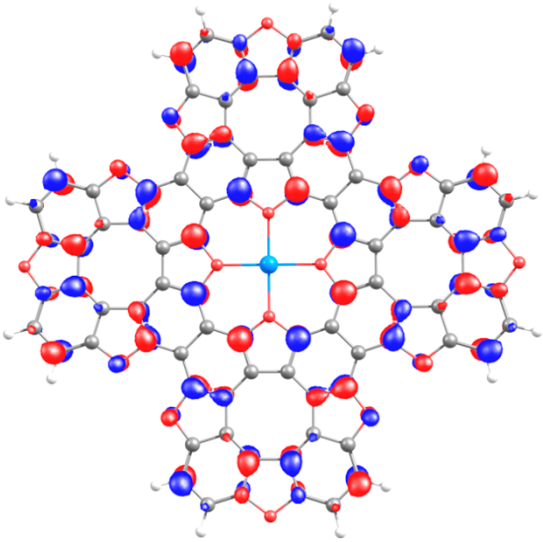
Fig. S1. Molecular HOMO-LUMO orbitals for complex **1** calculated at the B3LYP/LanL2Dz level of theory



HOMO-α (350) LUMO-α (351)

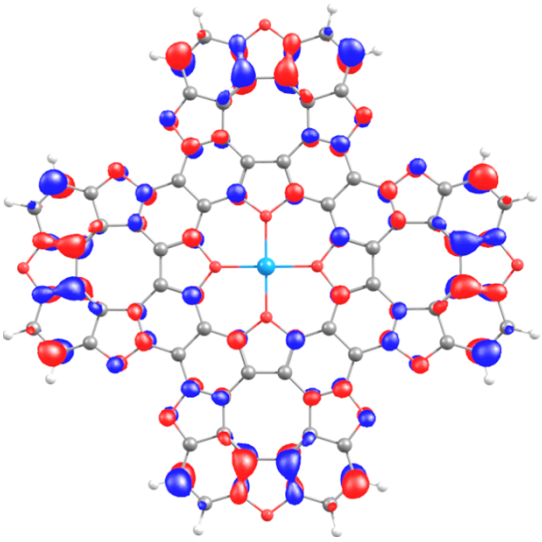


HOMO-β (349)

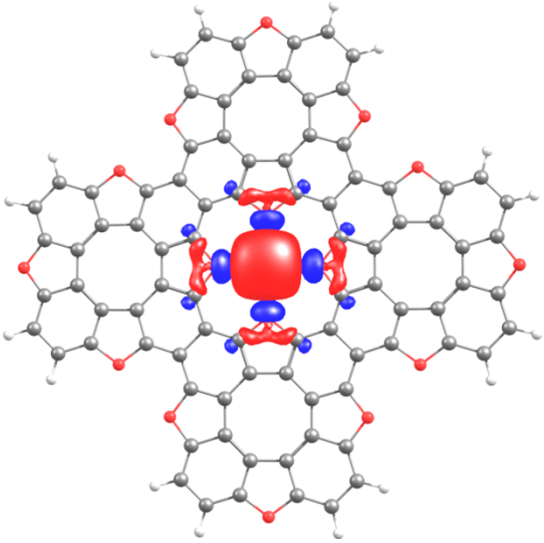


LUMO-β (350)

Fig. S2. Molecular HOMO-LUMO orbitals for complex **2** calculated at the B3LYP/LanL2Dz level of theory

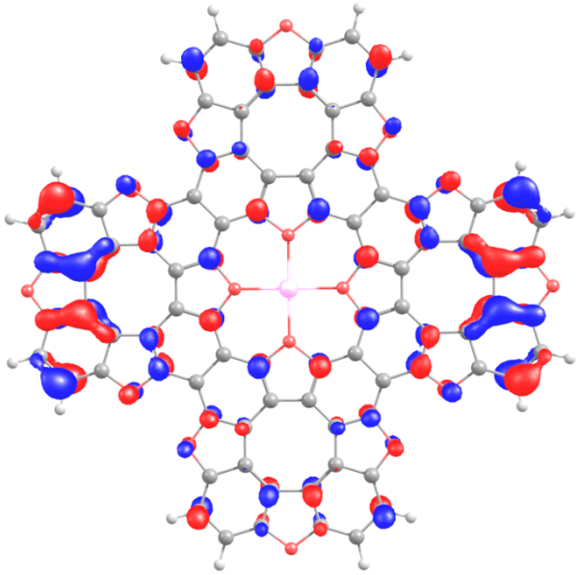


HOMO

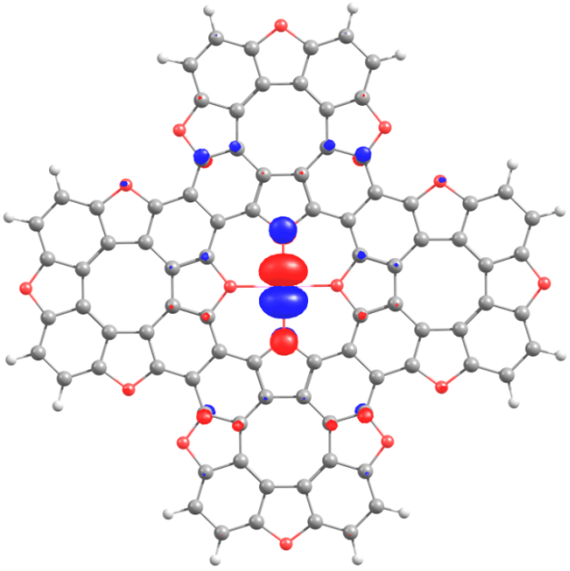


LUMO

Fig. S3. Molecular HOMO-LUMO orbitals for complex **3** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory

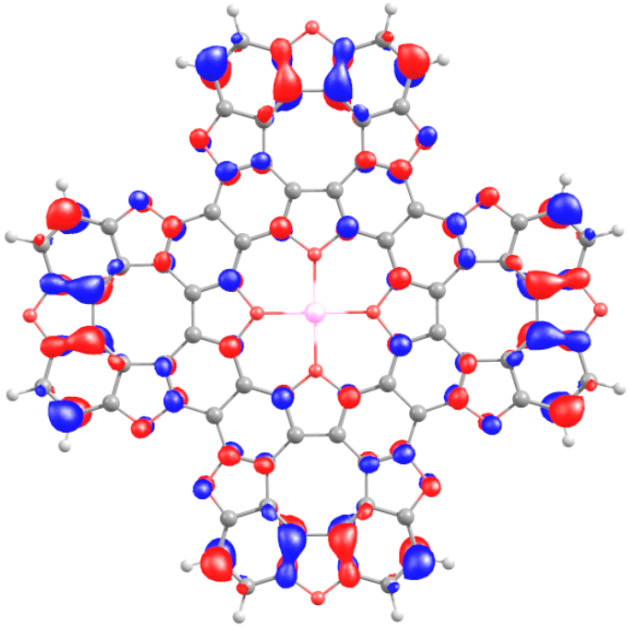


HOMO-348

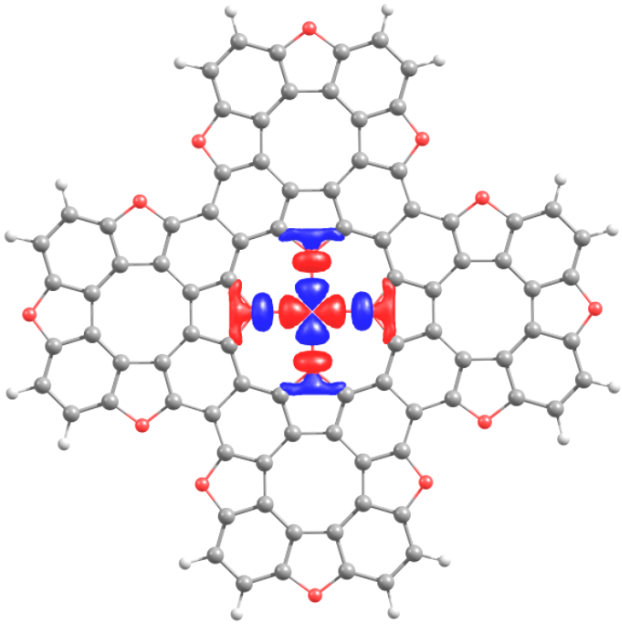


LUMO-349

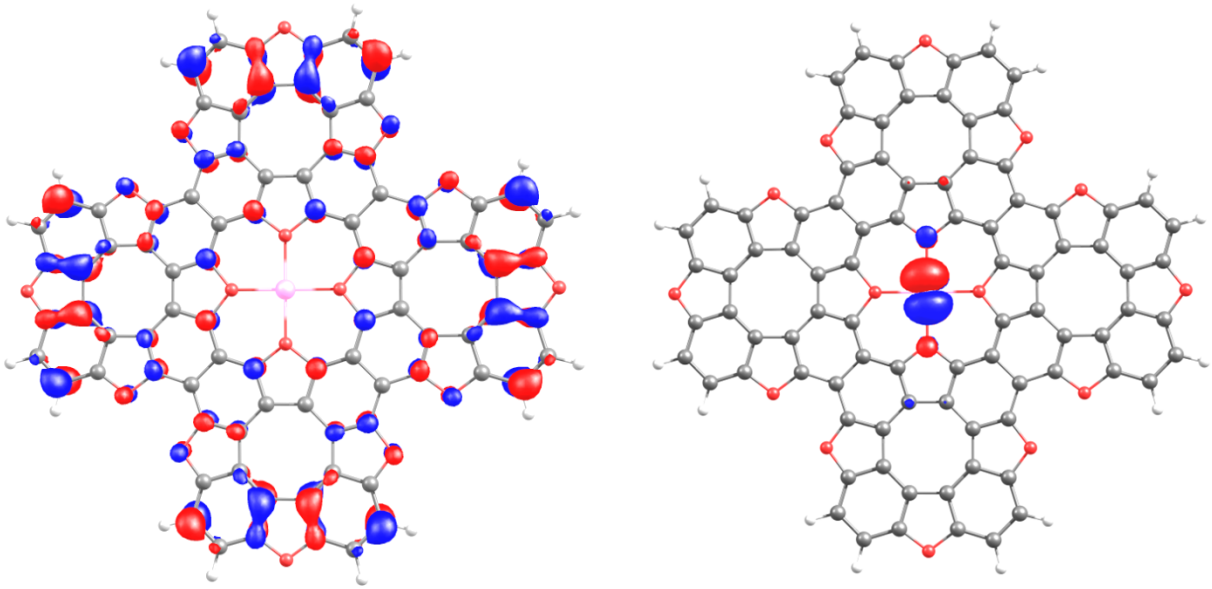
Fig. S4. Molecular HOMO-LUMO orbitals for complex **4** in the exited singlet state calculated at the B3LYP/LanL2Dz level of theory



HOMO-α (349)

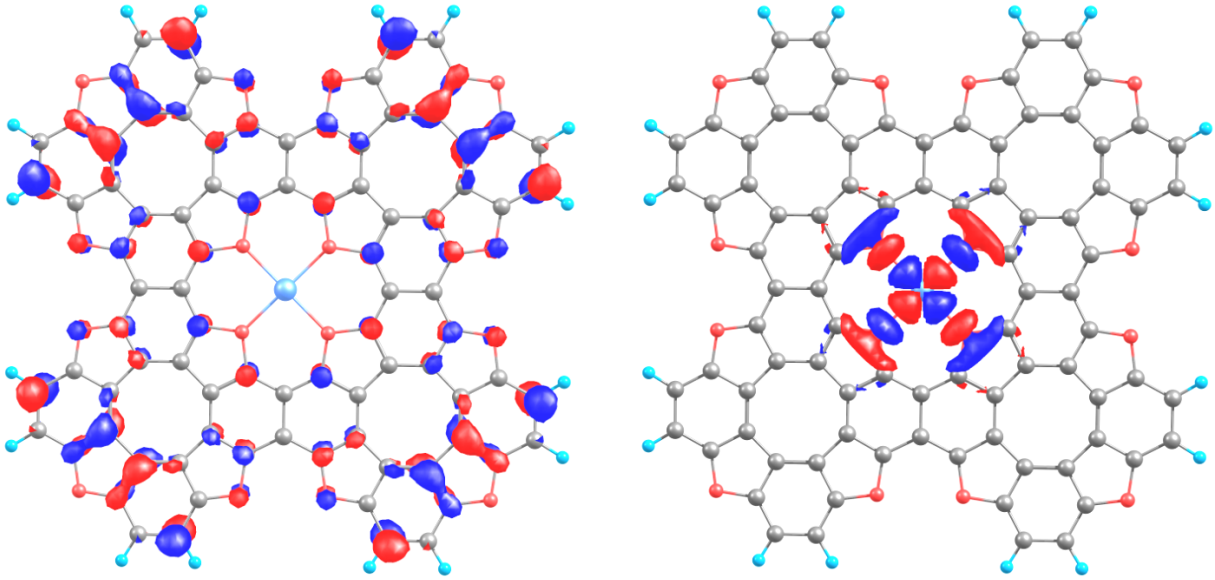


LUMO-α (350)



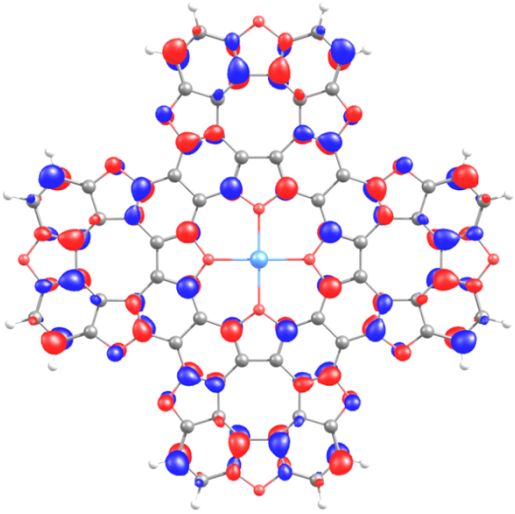
HOMO-β (347) LUMO-β (348)

Fig. S5. Molecular HOMO-LUMO orbitals for complex **4** in the ground triplet state calculated at the B3LYP/LanL2Dz level of theory

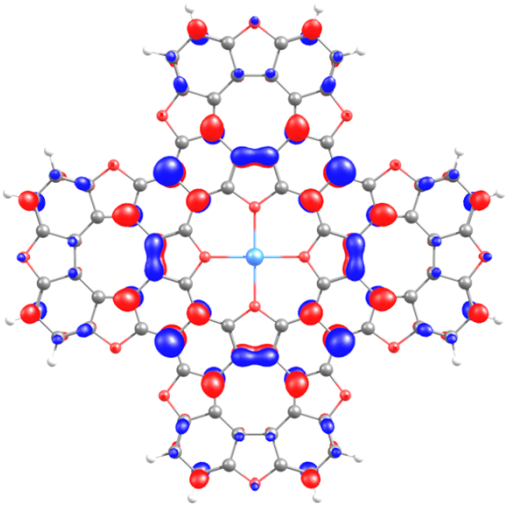


HOMO LUMO

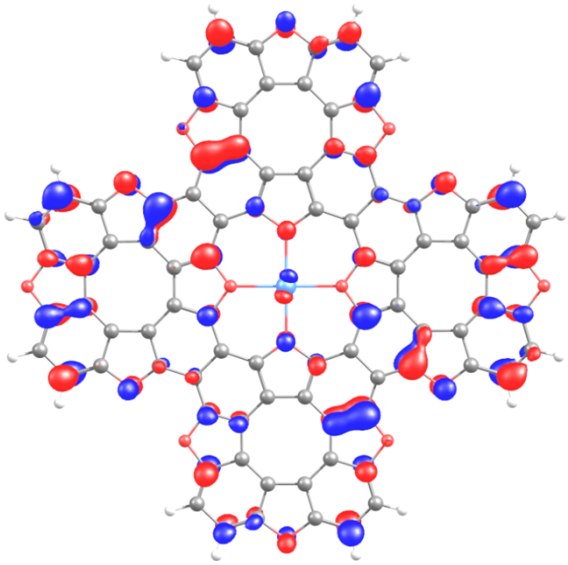
Fig. S6. Molecular HOMO-LUMO orbitals for complex **5** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory



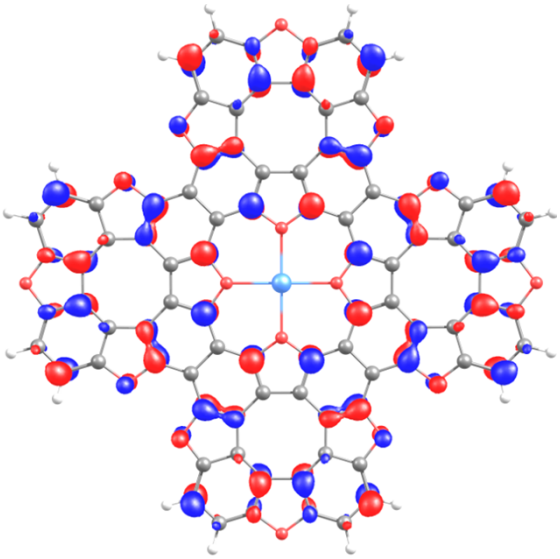
HOMO-α (375)



LUMO-α (376)

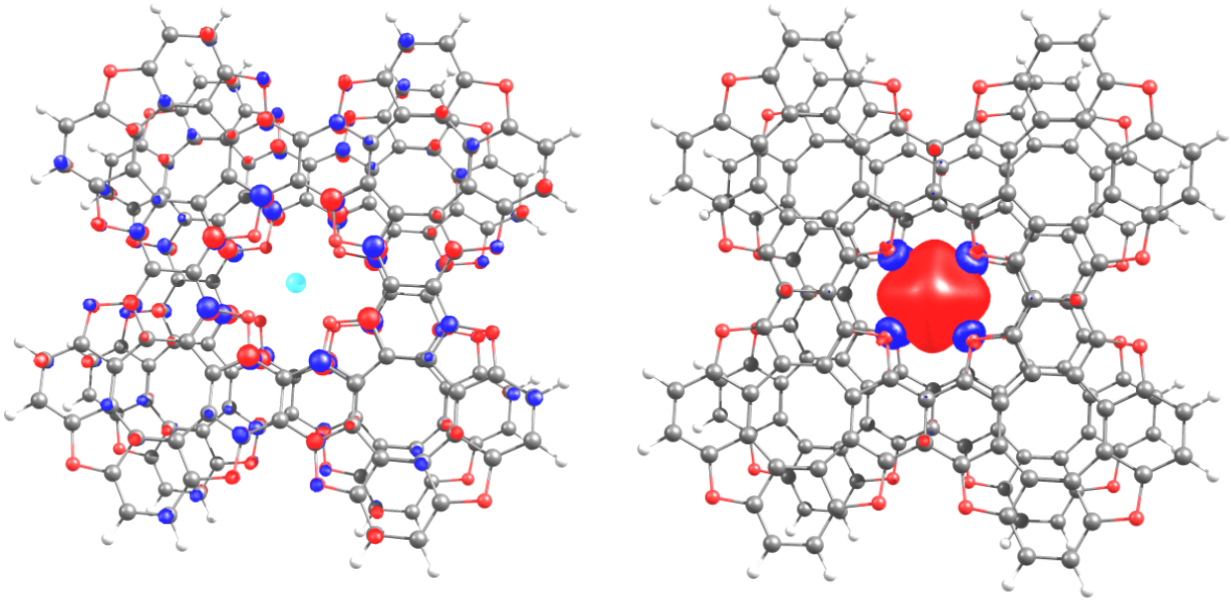


HOMO-β (373)



LUMO-β (374)

Fig. S7. Molecular HOMO-LUMO orbitals for complex **5** in the exited triplet state calculated at the B3LYP/LanL2Dz level of theory



HOMO LUMO

Fig. S8. Molecular HOMO-LUMO orbitals for complex **6** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory

Table S1. Total energies of the studied transition metal complexes **1–7** with tetraoxa[8]circulene-based ligand calculated at the B3LYP/LanL2Dz level of theory

Complex	Metal-ion	S	E_{tot}, *a.u.*
1	Cu^{1+}	0	–4762.0582
2	Cu^{2+}	1/2	–4761.7383
3	Zn^{2+}	0	–4631.1830
4	Fe^{2+}	0	–4688.9629
4	Fe^{2+}	1	–4689.0163
5	Pt^{2+}	0	–4684.6503
5	Pt^{2+}	1	–4684.6436
6	Cd^{2+}	0	–9179.7668

Table S2. The optimized Cartesian coordinates of the complex **1** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.502814	-4.949726	0.000000
2	6	1.268800	-5.626955	0.000000
3	6	2.869774	-7.207721	0.000000
4	6	3.530106	-5.959280	0.000000
5	6	4.933952	-5.954583	0.000000
6	6	5.952755	-4.936106	0.000000
7	6	7.197045	-5.605224	0.000000
8	6	5.602628	-7.199004	0.000000
9	6	5.957986	-3.532128	0.000000
10	6	2.504332	-3.531420	0.000000
11	6	3.530562	-2.505463	0.000000
12	6	4.948795	-2.504462	0.000000
13	8	7.001650	-7.004126	0.000000
14	6	1.268032	-2.882290	0.000000
15	6	2.881878	-1.268981	0.000000
16	6	7.206682	-2.872243	0.000000
17	8	7.014154	-1.469641	0.000000
18	6	4.942887	-8.440909	0.000000
19	6	3.531816	-8.446640	0.000000
20	6	8.445393	-3.534751	0.000000
21	6	8.439162	-4.945860	0.000000
22	1	5.504843	-9.368343	0.000000
23	1	2.975404	-9.377178	0.000000
24	1	9.376131	-2.978582	0.000000
25	1	9.366435	-5.508155	0.000000
26	8	1.471857	-1.472262	0.000000
27	6	-0.000622	-4.983514	0.000000
28	6	-0.000416	-3.519547	0.000000
29	6	-3.531348	-2.504189	0.000000
30	6	-2.882175	-1.267776	0.000000
31	6	-1.268800	-2.881702	0.000000
32	6	-2.505428	-3.530456	0.000000
33	6	-2.504126	-4.949138	0.000000
34	6	-3.531815	-5.958274	0.000000
35	6	-2.871925	-7.207075	0.000000
36	6	-1.270218	-5.626791	0.000000
37	6	-4.936142	-5.952992	0.000000
38	6	-4.949949	-2.502471	0.000000
39	6	-5.959433	-3.529857	0.000000
40	6	-5.954602	-4.934223	0.000000
41	8	-1.469451	-7.014342	0.000000
42	8	-1.472231	-1.471630	0.000000
43	6	-5.627207	-1.268385	0.000000
44	6	-7.208101	-2.869571	0.000000
45	6	-5.605173	-7.197271	0.000000
46	8	-7.004086	-7.001850	0.000000
47	6	-7.199077	-5.602887	0.000000
48	6	-4.945646	-8.439328	0.000000
49	6	-3.534615	-8.445617	0.000000
50	6	-8.440934	-4.942976	0.000000
51	6	-8.446859	-3.531933	0.000000
52	1	-5.507889	-9.366613	0.000000
53	1	-2.978687	-9.376424	0.000000
54	1	-9.368400	-5.504964	0.000000
55	1	-9.377500	-2.975625	0.000000

56	8	-7.014919	-1.467066	0.000000
57	6	2.505428	3.530456	0.000000
58	6	1.268800	2.881702	0.000000
59	6	2.882175	1.267776	0.000000
60	6	3.531348	2.504189	0.000000
61	6	4.949949	2.502471	0.000000
62	6	5.959433	3.529857	0.000000
63	6	7.208101	2.869571	0.000000
64	6	5.627207	1.268385	0.000000
65	6	5.954602	4.934223	0.000000
66	6	2.504126	4.949138	0.000000
67	6	3.531815	5.958274	0.000000
68	6	4.936142	5.952992	0.000000
69	8	7.014919	1.467066	0.000000
70	8	1.472231	1.471630	0.000000
71	6	1.270218	5.626791	0.000000
72	6	2.871925	7.207075	0.000000
73	6	7.199077	5.602887	0.000000
74	8	7.004086	7.001850	0.000000
75	6	5.605173	7.197271	0.000000
76	6	4.983502	-0.001027	0.000000
77	6	3.519513	-0.000786	0.000000
78	6	8.440934	4.942976	0.000000
79	6	8.446859	3.531933	0.000000
80	6	4.945646	8.439328	0.000000
81	6	3.534615	8.445617	0.000000
82	1	9.368400	5.504964	0.000000
83	1	9.377500	2.975625	0.000000
84	1	5.507889	9.366613	0.000000
85	1	2.978687	9.376424	0.000000
86	8	1.469451	7.014342	0.000000
87	6	0.000416	3.519547	0.000000
88	6	0.000622	4.983514	0.000000
89	6	-3.530106	5.959280	0.000000
90	6	-2.869774	7.207721	0.000000
91	6	-1.268800	5.626955	0.000000
92	6	-2.502814	4.949726	0.000000
93	6	-2.504332	3.531420	0.000000
94	6	-3.530562	2.505463	0.000000
95	6	-2.881878	1.268981	0.000000
96	6	-1.268032	2.882290	0.000000
97	6	-4.948795	2.504462	0.000000
98	6	-4.933952	5.954583	0.000000
99	6	-5.952755	4.936106	0.000000
100	6	-5.957986	3.532128	0.000000
101	8	-1.471857	1.472262	0.000000
102	8	-1.467311	7.014615	0.000000
103	6	-5.602628	7.199004	0.000000
104	6	-7.197045	5.605224	0.000000
105	6	-5.626491	1.270715	0.000000
106	8	-7.014154	1.469641	0.000000
107	6	-7.206682	2.872243	0.000000
108	6	-4.983502	0.001027	0.000000
109	6	-3.519513	0.000786	0.000000
110	6	-4.942887	8.440909	0.000000
111	6	-3.531816	8.446640	0.000000
112	6	-8.445393	3.534751	0.000000
113	6	-8.439162	4.945860	0.000000
114	1	-5.504843	9.368343	0.000000
115	1	-2.975404	9.377178	0.000000
116	1	-9.376131	2.978582	0.000000
117	1	-9.366435	5.508155	0.000000
118	8	-7.001650	7.004126	0.000000

119	6	5.626491	-1.270715	0.000000
120	8	1.467311	-7.014615	0.000000
121	29	0.000000	0.000000	0.000000

Table S3. The optimized Cartesian coordinates of the complex **2** in the ground doublet state calculated at the B3LYP/Lanl2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.726812	5.270858	-0.000560
2	6	3.083441	4.877197	-0.000463
3	6	3.064288	7.125508	-0.000335
4	6	1.715258	6.707594	-0.000439
5	6	0.716906	7.698846	-0.000316
6	6	-0.716906	7.698846	-0.000316
7	6	-1.125799	9.056402	-0.000127
8	6	1.125799	9.056402	-0.000127
9	6	-1.715258	6.707594	-0.000439
10	6	0.725018	4.268525	-0.000573
11	6	-0.725018	4.268525	-0.000573
12	6	-1.726812	5.270858	-0.000560
13	8	0.000000	9.904513	-0.000038
14	6	1.141381	2.934911	-0.000495
15	6	-1.141381	2.934911	-0.000495
16	6	-3.064288	7.125508	-0.000335
17	8	-3.918903	5.995207	-0.000352
18	6	2.468089	9.465787	-0.000048
19	6	3.471549	8.468625	-0.000133
20	6	-3.471549	8.468625	-0.000133
21	6	-2.468089	9.465787	-0.000048
22	1	2.729321	10.518221	0.000122
23	1	4.522514	8.735513	-0.000041
24	1	-4.522514	8.735513	-0.000041
25	1	-2.729321	10.518221	0.000122
26	8	0.000000	2.080926	-0.000575
27	6	3.524508	3.524312	-0.000422
28	6	2.489382	2.489051	-0.000416
29	6	4.268993	-0.725032	-0.000458
30	6	2.935313	-1.141293	-0.000439
31	6	2.935313	1.141293	-0.000439
32	6	4.268993	0.725032	-0.000458
33	6	5.271138	1.726748	-0.000416
34	6	6.707887	1.715236	-0.000252
35	6	7.125797	3.064218	-0.000132
36	6	4.877466	3.083321	-0.000385
37	6	7.698970	0.716969	-0.000091
38	6	5.271138	-1.726748	-0.000416
39	6	6.707887	-1.715236	-0.000252
40	6	7.698970	-0.716969	-0.000091
41	8	5.995458	3.918860	-0.000258
42	8	2.081535	0.000000	-0.000225
43	6	4.877466	-3.083321	-0.000385
44	6	7.125797	-3.064218	-0.000132
45	6	9.056478	1.125774	0.000201
46	8	9.904572	0.000000	0.000377
47	6	9.056478	-1.125774	0.000201
48	6	9.466013	2.468008	0.000324
49	6	8.468973	3.471497	0.000146
50	6	9.466013	-2.468008	0.000324

51	6	8.468973	-3.471497	0.000146
52	1	10.518464	2.729133	0.000565
53	1	8.735836	4.522467	0.000245
54	1	10.518464	-2.729133	0.000565
55	1	8.735836	-4.522467	0.000245
56	8	5.995458	-3.918860	-0.000258
57	6	-4.268993	-0.725032	-0.000458
58	6	-2.935313	-1.141293	-0.000439
59	6	-2.935313	1.141293	-0.000439
60	6	-4.268993	0.725032	-0.000458
61	6	-5.271138	1.726748	-0.000416
62	6	-6.707887	1.715236	-0.000252
63	6	-7.125797	3.064218	-0.000132
64	6	-4.877466	3.083321	-0.000385
65	6	-7.698970	0.716969	-0.000091
66	6	-5.271138	-1.726748	-0.000416
67	6	-6.707887	-1.715236	-0.000252
68	6	-7.698970	-0.716969	-0.000091
69	8	-5.995458	3.918860	-0.000258
70	8	-2.081535	0.000000	-0.000225
71	6	-4.877466	-3.083321	-0.000385
72	6	-7.125797	-3.064218	-0.000132
73	6	-9.056478	1.125774	0.000201
74	8	-9.904572	0.000000	0.000377
75	6	-9.056478	-1.125774	0.000201
76	6	-3.524508	3.524312	-0.000422
77	6	-2.489382	2.489051	-0.000416
78	6	-9.466013	2.468008	0.000324
79	6	-8.468973	3.471497	0.000146
80	6	-9.466013	-2.468008	0.000324
81	6	-8.468973	-3.471497	0.000146
82	1	-10.518464	2.729133	0.000565
83	1	-8.735836	4.522467	0.000245
84	1	-10.518464	-2.729133	0.000565
85	1	-8.735836	-4.522467	0.000245
86	8	-5.995458	-3.918860	-0.000258
87	6	-2.489382	-2.489051	-0.000416
88	6	-3.524508	-3.524312	-0.000422
89	6	-1.715258	-6.707594	-0.000439
90	6	-3.064288	-7.125508	-0.000335
91	6	-3.083441	-4.877197	-0.000463
92	6	-1.726812	-5.270858	-0.000560
93	6	-0.725018	-4.268525	-0.000573
94	6	0.725018	-4.268525	-0.000573
95	6	1.141381	-2.934911	-0.000495
96	6	-1.141381	-2.934911	-0.000495
97	6	1.726812	-5.270858	-0.000560
98	6	-0.716906	-7.698846	-0.000316
99	6	0.716906	-7.698846	-0.000316
100	6	1.715258	-6.707594	-0.000439
101	8	0.000000	-2.080926	-0.000575
102	8	-3.918903	-5.995207	-0.000352
103	6	-1.125799	-9.056402	-0.000127
104	6	1.125799	-9.056402	-0.000127
105	6	3.083441	-4.877197	-0.000463
106	8	3.918903	-5.995207	-0.000352
107	6	3.064288	-7.125508	-0.000335
108	6	3.524508	-3.524312	-0.000422
109	6	2.489382	-2.489051	-0.000416
110	6	-2.468089	-9.465787	-0.000048
111	6	-3.471549	-8.468625	-0.000133
112	6	3.471549	-8.468625	-0.000133
113	6	2.468089	-9.465787	-0.000048

114	1	-2.729321	-10.518221	0.000122
115	1	-4.522514	-8.735513	-0.000041
116	1	4.522514	-8.735513	-0.000041
117	1	2.729321	-10.518221	0.000122
118	8	0.000000	-9.904513	-0.000038
119	6	-3.083441	4.877197	-0.000463
120	8	3.918903	5.995207	-0.000352
121	29	0.000000	0.000000	0.005629

Table S4. The optimized Cartesian coordinates of the complex **3** in the ground singlet state calculated the B3LYP/Lanl2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	5.264726	1.725523	0.000000
2	6	4.875713	3.081888	0.000000
3	6	7.122563	3.062203	0.000000
4	6	6.704962	1.712625	0.000000
5	6	7.696273	0.718712	0.000000
6	6	7.696272	-0.718705	0.000000
7	6	9.048925	-1.126032	0.000000
8	6	9.048925	1.126032	0.000000
9	6	6.704961	-1.712627	0.000000
10	6	4.255430	0.726269	0.000000
11	6	4.255433	-0.726259	0.000000
12	6	5.264727	-1.725524	0.000000
13	8	9.897214	0.000001	0.000000
14	6	2.931395	1.152827	0.000000
15	6	2.931396	-1.152826	0.000000
16	6	7.122563	-3.062204	0.000000
17	8	5.991552	-3.916886	0.000000
18	6	9.459603	2.471784	0.000000
19	6	8.465942	3.472572	0.000000
20	6	8.465943	-3.472570	0.000000
21	6	9.459601	-2.471784	0.000000
22	1	10.512505	2.731322	0.000000
23	1	8.730081	4.523976	0.000000
24	1	8.730083	-4.523974	0.000000
25	1	10.512503	-2.731319	0.000000
26	8	2.042328	0.000001	0.000000
27	6	3.527142	3.527142	0.000000
28	6	2.492454	2.492453	0.000000
29	6	-0.726269	4.255422	0.000000
30	6	-1.152828	2.931390	0.000000
31	6	1.152826	2.931391	0.000000
32	6	0.726258	4.255424	0.000000
33	6	1.725516	5.264719	0.000000
34	6	1.712623	6.704948	0.000000
35	6	3.062200	7.122555	0.000000
36	6	3.081884	4.875709	0.000000
37	6	0.718705	7.696254	0.000000
38	6	-1.725515	5.264717	0.000000
39	6	-1.712622	6.704950	0.000000
40	6	-0.718712	7.696255	0.000000
41	8	3.916885	5.991544	0.000000
42	8	-0.000001	2.042317	0.000000
43	6	-3.081880	4.875710	0.000000
44	6	-3.062199	7.122555	0.000000

45	6	1.126034	9.048905	0.000000
46	8	-0.000001	9.897195	0.000000
47	6	-1.126034	9.048905	0.000000
48	6	2.471785	9.459591	0.000000
49	6	3.472573	8.465936	0.000000
50	6	-2.471784	9.459593	0.000000
51	6	-3.472574	8.465935	0.000000
52	1	2.731322	10.512495	0.000000
53	1	4.523978	8.730075	0.000000
54	1	-2.731324	10.512497	0.000000
55	1	-4.523980	8.730073	0.000000
56	8	-3.916886	5.991542	0.000000
57	6	-0.726258	-4.255424	0.000000
58	6	-1.152826	-2.931391	0.000000
59	6	1.152828	-2.931390	0.000000
60	6	0.726269	-4.255422	0.000000
61	6	1.725515	-5.264717	0.000000
62	6	1.712622	-6.704950	0.000000
63	6	3.062199	-7.122555	0.000000
64	6	3.081880	-4.875710	0.000000
65	6	0.718712	-7.696255	0.000000
66	6	-1.725516	-5.264719	0.000000
67	6	-1.712623	-6.704948	0.000000
68	6	-0.718705	-7.696254	0.000000
69	8	3.916886	-5.991542	0.000000
70	8	0.000001	-2.042317	0.000000
71	6	-3.081884	-4.875709	0.000000
72	6	-3.062200	-7.122555	0.000000
73	6	1.126034	-9.048905	0.000000
74	8	0.000001	-9.897195	0.000000
75	6	-1.126034	-9.048905	0.000000
76	6	3.527140	-3.527145	0.000000
77	6	2.492454	-2.492453	0.000000
78	6	2.471784	-9.459593	0.000000
79	6	3.472574	-8.465935	0.000000
80	6	-2.471785	-9.459591	0.000000
81	6	-3.472573	-8.465936	0.000000
82	1	2.731324	-10.512497	0.000000
83	1	4.523980	-8.730073	0.000000
84	1	-2.731322	-10.512495	0.000000
85	1	-4.523978	-8.730075	0.000000
86	8	-3.916885	-5.991544	0.000000
87	6	-2.492454	-2.492453	0.000000
88	6	-3.527142	-3.527142	0.000000
89	6	-6.704962	-1.712625	0.000000
90	6	-7.122563	-3.062203	0.000000
91	6	-4.875713	-3.081888	0.000000
92	6	-5.264726	-1.725523	0.000000
93	6	-4.255430	-0.726269	0.000000
94	6	-4.255433	0.726259	0.000000
95	6	-2.931396	1.152826	0.000000
96	6	-2.931395	-1.152827	0.000000
97	6	-5.264727	1.725524	0.000000
98	6	-7.696273	-0.718712	0.000000
99	6	-7.696272	0.718705	0.000000
100	6	-6.704961	1.712627	0.000000
101	8	-2.042328	-0.000001	0.000000
102	8	-5.991550	-3.916887	0.000000
103	6	-9.048925	-1.126032	0.000000
104	6	-9.048925	1.126032	0.000000
105	6	-4.875711	3.081891	0.000000
106	8	-5.991552	3.916886	0.000000
107	6	-7.122563	3.062204	0.000000

108	6	-3.527140	3.527145	0.000000
109	6	-2.492454	2.492453	0.000000
110	6	-9.459603	-2.471784	0.000000
111	6	-8.465942	-3.472572	0.000000
112	6	-8.465943	3.472570	0.000000
113	6	-9.459601	2.471784	0.000000
114	1	-10.512505	-2.731322	0.000000
115	1	-8.730081	-4.523976	0.000000
116	1	-8.730083	4.523974	0.000000
117	1	-10.512503	2.731319	0.000000
118	8	-9.897214	-0.000001	0.000000
119	6	4.875711	-3.081891	0.000000
120	8	5.991550	3.916887	0.000000
121	30	0.000000	0.000000	0.000000

Table S5. The optimized Cartesian coordinates of the complex **4** in the ground triplet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	5.244694	1.719063
2	6	0.000000	4.857437	3.078781
3	6	0.000000	7.102915	3.058184
4	6	0.000000	6.685532	1.708816
5	6	0.000000	7.678655	0.718272
6	6	0.000000	7.678655	-0.718272
7	6	0.000000	9.030627	-1.125522
8	6	0.000000	9.030627	1.125522
9	6	0.000000	6.685532	-1.708816
10	6	0.000000	4.233820	0.725025
11	6	0.000000	4.233820	-0.725025
12	6	0.000000	5.244694	-1.719063
13	8	0.000000	9.879109	0.000000
14	6	0.000000	2.906029	1.147503
15	6	0.000000	2.906029	-1.147503
16	6	0.000000	7.102915	-3.058184
17	8	0.000000	5.971719	-3.913476
18	6	0.000000	9.440660	2.471965
19	6	0.000000	8.445277	3.471095
20	6	0.000000	8.445277	-3.471095
21	6	0.000000	9.440660	-2.471965
22	1	0.000000	10.493254	2.732826
23	1	0.000000	8.707282	4.522999
24	1	0.000000	8.707282	-4.522999
25	1	0.000000	10.493254	-2.732826
26	8	0.000000	2.011907	0.000000
27	6	0.000000	3.513122	3.522382
28	6	0.000000	2.477487	2.488236
29	6	0.000000	-0.722423	4.251736
30	6	0.000000	-1.141000	2.920096
31	6	0.000000	1.141000	2.920096
32	6	0.000000	0.722423	4.251736
33	6	0.000000	1.719871	5.262250
34	6	0.000000	1.709355	6.702820
35	6	0.000000	3.059162	7.118768
36	6	0.000000	3.073696	4.873086
37	6	0.000000	0.718260	7.695527
38	6	0.000000	-1.719871	5.262250
39	6	0.000000	-1.709355	6.702820

40	6	0.000000	-0.718260	7.695527
41	8	0.000000	3.911845	5.985984
42	8	0.000000	0.000000	2.038485
43	6	0.000000	-3.073696	4.873086
44	6	0.000000	-3.059162	7.118768
45	6	0.000000	1.126138	9.047939
46	8	0.000000	0.000000	9.896666
47	6	0.000000	-1.126138	9.047939
48	6	0.000000	2.472276	9.457141
49	6	0.000000	3.471593	8.461606
50	6	0.000000	-2.472276	9.457141
51	6	0.000000	-3.471593	8.461606
52	1	0.000000	2.733576	10.509604
53	1	0.000000	4.523354	8.724413
54	1	0.000000	-2.733576	10.509604
55	1	0.000000	-4.523354	8.724413
56	8	0.000000	-3.911845	5.985984
57	6	0.000000	-0.722423	-4.251736
58	6	0.000000	-1.141000	-2.920096
59	6	0.000000	1.141000	-2.920096
60	6	0.000000	0.722423	-4.251736
61	6	0.000000	1.719871	-5.262250
62	6	0.000000	1.709355	-6.702820
63	6	0.000000	3.059162	-7.118768
64	6	0.000000	3.073696	-4.873086
65	6	0.000000	0.718260	-7.695527
66	6	0.000000	-1.719871	-5.262250
67	6	0.000000	-1.709355	-6.702820
68	6	0.000000	-0.718260	-7.695527
69	8	0.000000	3.911845	-5.985984
70	8	0.000000	0.000000	-2.038485
71	6	0.000000	-3.073696	-4.873086
72	6	0.000000	-3.059162	-7.118768
73	6	0.000000	1.126138	-9.047939
74	8	0.000000	0.000000	-9.896666
75	6	0.000000	-1.126138	-9.047939
76	6	0.000000	3.513122	-3.522382
77	6	0.000000	2.477487	-2.488236
78	6	0.000000	2.472276	-9.457141
79	6	0.000000	3.471593	-8.461606
80	6	0.000000	-2.472276	-9.457141
81	6	0.000000	-3.471593	-8.461606
82	1	0.000000	2.733576	-10.509604
83	1	0.000000	4.523354	-8.724413
84	1	0.000000	-2.733576	-10.509604
85	1	0.000000	-4.523354	-8.724413
86	8	0.000000	-3.911845	-5.985984
87	6	0.000000	-2.477487	-2.488236
88	6	0.000000	-3.513122	-3.522382
89	6	0.000000	-6.685532	-1.708816
90	6	0.000000	-7.102915	-3.058184
91	6	0.000000	-4.857437	-3.078781
92	6	0.000000	-5.244694	-1.719063
93	6	0.000000	-4.233820	-0.725025
94	6	0.000000	-4.233820	0.725025
95	6	0.000000	-2.906029	1.147503
96	6	0.000000	-2.906029	-1.147503
97	6	0.000000	-5.244694	1.719063
98	6	0.000000	-7.678655	-0.718272
99	6	0.000000	-7.678655	0.718272
100	6	0.000000	-6.685532	1.708816
101	8	0.000000	-2.011907	0.000000
102	8	0.000000	-5.971719	-3.913476

103	6	0.000000	-9.030627	-1.125522
104	6	0.000000	-9.030627	1.125522
105	6	0.000000	-4.857437	3.078781
106	8	0.000000	-5.971719	3.913476
107	6	0.000000	-7.102915	3.058184
108	6	0.000000	-3.513122	3.522382
109	6	0.000000	-2.477487	2.488236
110	6	0.000000	-9.440660	-2.471965
111	6	0.000000	-8.445277	-3.471095
112	6	0.000000	-8.445277	3.471095
113	6	0.000000	-9.440660	2.471965
114	1	0.000000	-10.493254	-2.732826
115	1	0.000000	-8.707282	-4.522999
116	1	0.000000	-8.707282	4.522999
117	1	0.000000	-10.493254	2.732826
118	8	0.000000	-9.879109	0.000000
119	6	0.000000	4.857437	-3.078781
120	8	0.000000	5.971719	3.913476
121	26	0.000000	0.000000	0.000000

Table S6. The optimized Cartesian coordinates of the complex **4** in the exited singlet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.095022	5.369624	0.000000
2	6	-2.476440	5.157991	0.000000
3	6	-2.205785	7.342260	0.000000
4	6	-0.920391	6.787812	0.000000
5	6	0.172478	7.656201	0.000000
6	6	1.585927	7.492000	0.000000
7	6	2.130885	8.781635	0.000000
8	6	-0.062397	9.036493	0.000000
9	6	2.450479	6.396184	0.000000
10	6	-0.229554	4.252907	0.000000
11	6	1.196923	4.087142	0.000000
12	6	2.295316	4.975748	0.000000
13	8	1.129751	9.730839	0.000000
14	6	-0.789766	2.992179	0.000000
15	6	1.453517	2.731532	0.000000
16	6	3.828755	6.641196	0.000000
17	8	4.528456	5.443291	0.000000
18	6	-1.351731	9.587888	0.000000
19	6	-2.450479	8.720325	0.000000
20	6	4.382932	7.926459	0.000000
21	6	3.512285	9.022903	0.000000
22	1	-1.496523	10.662655	0.000000
23	1	-3.463091	9.107301	0.000000
24	1	5.457238	8.070797	0.000000
25	1	3.899649	10.035787	0.000000
26	8	0.229554	1.983175	0.000000
27	6	-3.068084	3.873814	0.000000
28	6	-2.161848	2.729728	0.000000
29	6	-4.252634	-0.229765	0.000000
30	6	-2.991402	-0.789994	0.000000
31	6	-2.730946	1.453667	0.000000
32	6	-4.087054	1.197351	0.000000
33	6	-4.975942	2.295991	0.000000

34	6	-6.396695	2.450697	0.000000
35	6	-6.642178	3.829253	0.000000
36	6	-4.453704	3.592469	0.000000
37	6	-7.492726	1.585748	0.000000
38	6	-5.369343	-1.095663	0.000000
39	6	-6.787827	-0.920926	0.000000
40	6	-7.656681	0.172232	0.000000
41	8	-5.444158	4.529353	0.000000
42	8	-1.982660	0.229435	0.000000
43	6	-5.157546	-2.477208	0.000000
44	6	-7.342122	-2.206846	0.000000
45	6	-8.782444	2.130450	0.000000
46	8	-9.731414	1.129222	0.000000
47	6	-9.037036	-0.062882	0.000000
48	6	-9.023502	3.511455	0.000000
49	6	-7.927874	4.382283	0.000000
50	6	-9.587738	-1.352472	0.000000
51	6	-8.720291	-2.451089	0.000000
52	1	-10.036381	3.898241	0.000000
53	1	-8.072682	5.456454	0.000000
54	1	-10.662335	-1.497083	0.000000
55	1	-9.107227	-3.463495	0.000000
56	8	-6.335995	-3.162320	0.000000
57	6	4.087054	-1.197351	0.000000
58	6	2.730946	-1.453667	0.000000
59	6	2.991402	0.789994	0.000000
60	6	4.252634	0.229765	0.000000
61	6	5.369343	1.095663	0.000000
62	6	6.787827	0.920926	0.000000
63	6	7.342122	2.206846	0.000000
64	6	5.157546	2.477208	0.000000
65	6	7.656681	-0.172232	0.000000
66	6	4.975942	-2.295991	0.000000
67	6	6.396695	-2.450697	0.000000
68	6	7.492726	-1.585748	0.000000
69	8	6.335995	3.162320	0.000000
70	8	1.982660	-0.229435	0.000000
71	6	4.453704	-3.592469	0.000000
72	6	6.642178	-3.829253	0.000000
73	6	9.037036	0.062882	0.000000
74	8	9.731414	-1.129222	0.000000
75	6	8.782444	-2.130450	0.000000
76	6	3.873118	3.067991	0.000000
77	6	2.729343	2.162245	0.000000
78	6	9.587738	1.352472	0.000000
79	6	8.720291	2.451089	0.000000
80	6	9.023502	-3.511455	0.000000
81	6	7.927874	-4.382283	0.000000
82	1	10.662335	1.497083	0.000000
83	1	9.107227	3.463495	0.000000
84	1	10.036381	-3.898241	0.000000
85	1	8.072682	-5.456454	0.000000
86	8	5.444158	-4.529353	0.000000
87	6	2.161848	-2.729728	0.000000
88	6	3.068084	-3.873814	0.000000
89	6	0.920391	-6.787812	0.000000
90	6	2.205785	-7.342260	0.000000
91	6	2.476440	-5.157991	0.000000
92	6	1.095022	-5.369624	0.000000
93	6	0.229554	-4.252907	0.000000
94	6	-1.196923	-4.087142	0.000000
95	6	-1.453517	-2.731532	0.000000
96	6	0.789766	-2.992179	0.000000

97	6	-2.295316	-4.975748	0.000000
98	6	-0.172478	-7.656201	0.000000
99	6	-1.585927	-7.492000	0.000000
100	6	-2.450479	-6.396184	0.000000
101	8	-0.229554	-1.983175	0.000000
102	8	3.161641	-6.336778	0.000000
103	6	0.062397	-9.036493	0.000000
104	6	-2.130885	-8.781635	0.000000
105	6	-3.591427	-4.453243	0.000000
106	8	-4.528456	-5.443291	0.000000
107	6	-3.828755	-6.641196	0.000000
108	6	-3.873118	-3.067991	0.000000
109	6	-2.729343	-2.162245	0.000000
110	6	1.351731	-9.587888	0.000000
111	6	2.450479	-8.720325	0.000000
112	6	-4.382932	-7.926459	0.000000
113	6	-3.512285	-9.022903	0.000000
114	1	1.496523	-10.662655	0.000000
115	1	3.463091	-9.107301	0.000000
116	1	-5.457238	-8.070797	0.000000
117	1	-3.899649	-10.035787	0.000000
118	8	-1.129751	-9.730839	0.000000
119	6	3.591427	4.453243	0.000000
120	8	-3.161641	6.336778	0.000000
121	26	0.000000	0.000000	0.000000

Table S7. The optimized Cartesian coordinates of the complex **5** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.726848	5.266406	0.000000
2	6	-3.083454	4.877683	0.000000
3	6	-3.062455	7.124214	0.000000
4	6	-1.713104	6.706256	0.000000
5	6	-0.718695	7.696739	0.000000
6	6	0.718577	7.696711	0.000000
7	6	1.125869	9.049319	0.000000
8	6	-1.125957	9.049327	0.000000
9	6	1.713152	6.706224	0.000000
10	6	-0.726464	4.258690	0.000000
11	6	0.726413	4.258726	0.000000
12	6	1.726920	5.266477	0.000000
13	8	0.000001	9.897948	0.000000
14	6	-1.158141	2.936477	0.000000
15	6	1.158139	2.936488	0.000000
16	6	3.062539	7.124248	0.000000
17	8	3.917829	5.993752	0.000000
18	6	-2.471954	9.460761	0.000000
19	6	-3.472940	8.467448	0.000000
20	6	3.472793	8.467697	0.000000
21	6	2.471681	9.460821	0.000000
22	1	-2.730806	10.514060	0.000000
23	1	-4.524286	8.732017	0.000000
24	1	4.524159	8.732322	0.000000
25	1	2.730495	10.514061	0.000000
26	8	0.000010	2.062903	0.000000
27	6	-3.529468	3.529496	0.000000
28	6	-2.494562	2.494569	0.000000

29	6	-4.258744	-0.726487	0.000000
30	6	-2.936521	-1.158181	0.000000
31	6	-2.936531	1.158178	0.000000
32	6	-4.258780	0.726434	0.000000
33	6	-5.266519	1.726822	0.000000
34	6	-6.706297	1.713122	0.000000
35	6	-7.124237	3.062497	0.000000
36	6	-4.877717	3.083495	0.000000
37	6	-7.696592	0.718648	0.000000
38	6	-5.266447	-1.726751	0.000000
39	6	-6.706330	-1.713073	0.000000
40	6	-7.696620	-0.718764	0.000000
41	8	-5.993692	3.917777	0.000000
42	8	-2.062895	0.000010	0.000000
43	6	-4.877666	-3.083355	0.000000
44	6	-7.124204	-3.062412	0.000000
45	6	-9.049207	1.125823	0.000000
46	8	-9.897838	0.000002	0.000000
47	6	-9.049216	-1.125907	0.000000
48	6	-9.460804	2.471581	0.000000
49	6	-8.467680	3.472788	0.000000
50	6	-9.460746	-2.471851	0.000000
51	6	-8.467433	-3.472933	0.000000
52	1	-10.514049	2.730306	0.000000
53	1	-8.732237	4.524154	0.000000
54	1	-10.514050	-2.730613	0.000000
55	1	-8.731937	-4.524280	0.000000
56	8	-5.993658	-3.917601	0.000000
57	6	4.258780	-0.726434	0.000000
58	6	2.936531	-1.158178	0.000000
59	6	2.936521	1.158181	0.000000
60	6	4.258744	0.726487	0.000000
61	6	5.266447	1.726751	0.000000
62	6	6.706330	1.713073	0.000000
63	6	7.124204	3.062412	0.000000
64	6	4.877666	3.083355	0.000000
65	6	7.696620	0.718764	0.000000
66	6	5.266519	-1.726822	0.000000
67	6	6.706297	-1.713122	0.000000
68	6	7.696592	-0.718648	0.000000
69	8	5.993658	3.917601	0.000000
70	8	2.062895	-0.000010	0.000000
71	6	4.877717	-3.083495	0.000000
72	6	7.124237	-3.062497	0.000000
73	6	9.049216	1.125907	0.000000
74	8	9.897838	-0.000002	0.000000
75	6	9.049207	-1.125823	0.000000
76	6	3.529521	3.529445	0.000000
77	6	2.494562	2.494570	0.000000
78	6	9.460746	2.471851	0.000000
79	6	8.467433	3.472933	0.000000
80	6	9.460804	-2.471581	0.000000
81	6	8.467680	-3.472788	0.000000
82	1	10.514050	2.730613	0.000000
83	1	8.731937	4.524280	0.000000
84	1	10.514049	-2.730306	0.000000
85	1	8.732237	-4.524154	0.000000
86	8	5.993692	-3.917777	0.000000
87	6	2.494562	-2.494569	0.000000
88	6	3.529468	-3.529496	0.000000
89	6	1.713104	-6.706256	0.000000
90	6	3.062455	-7.124214	0.000000
91	6	3.083454	-4.877683	0.000000

92	6	1.726848	-5.266406	0.000000
93	6	0.726464	-4.258690	0.000000
94	6	-0.726413	-4.258726	0.000000
95	6	-1.158139	-2.936488	0.000000
96	6	1.158141	-2.936477	0.000000
97	6	-1.726920	-5.266477	0.000000
98	6	0.718695	-7.696739	0.000000
99	6	-0.718577	-7.696711	0.000000
100	6	-1.713152	-6.706224	0.000000
101	8	-0.000010	-2.062903	0.000000
102	8	3.917652	-5.993716	0.000000
103	6	1.125957	-9.049327	0.000000
104	6	-1.125869	-9.049319	0.000000
105	6	-3.083596	-4.877735	0.000000
106	8	-3.917829	-5.993752	0.000000
107	6	-3.062539	-7.124248	0.000000
108	6	-3.529521	-3.529445	0.000000
109	6	-2.494562	-2.494570	0.000000
110	6	2.471954	-9.460761	0.000000
111	6	3.472940	-8.467448	0.000000
112	6	-3.472793	-8.467697	0.000000
113	6	-2.471681	-9.460821	0.000000
114	1	2.730806	-10.514060	0.000000
115	1	4.524286	-8.732017	0.000000
116	1	-4.524159	-8.732322	0.000000
117	1	-2.730495	-10.514061	0.000000
118	8	-0.000001	-9.897948	0.000000
119	6	3.083596	4.877735	0.000000
120	8	-3.917652	5.993716	0.000000
121	78	0.000000	0.000000	0.000000

Table S8. The optimized Cartesian coordinates of the complex **5** in the exited triplet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.735499	5.291282	0.000000
2	6	3.093202	4.893183	0.000000
3	6	3.070348	7.144559	0.000000
4	6	1.721668	6.726027	0.000000
5	6	0.717722	7.713515	0.000000
6	6	-0.717790	7.713547	0.000000
7	6	-1.125677	9.071567	0.000000
8	6	1.125717	9.071597	0.000000
9	6	-1.721614	6.726133	0.000000
10	6	0.727903	4.296411	0.000000
11	6	-0.728072	4.296435	0.000000
12	6	-1.735533	5.291366	0.000000
13	8	-0.000001	9.919611	0.000000
14	6	1.151443	2.965601	0.000000
15	6	-1.151472	2.965611	0.000000
16	6	-3.070253	7.144621	0.000000
17	8	-3.926278	6.014617	0.000000
18	6	2.467849	9.482989	0.000000
19	6	3.474443	8.488826	0.000000
20	6	-3.474286	8.488848	0.000000
21	6	-2.467711	9.482969	0.000000
22	1	2.726341	10.536215	0.000000
23	1	4.524579	8.759086	0.000000

24	1	-4.524374	8.759162	0.000000
25	1	-2.726188	10.536166	0.000000
26	8	0.000004	2.138121	0.000000
27	6	3.538343	3.537784	0.000000
28	6	2.501091	2.500643	0.000000
29	6	4.297190	-0.727892	0.000000
30	6	2.965959	-1.151485	0.000000
31	6	2.965983	1.151502	0.000000
32	6	4.297184	0.727983	0.000000
33	6	5.292004	1.735354	0.000000
34	6	6.727236	1.721621	0.000000
35	6	7.145322	3.070277	0.000000
36	6	4.894027	3.092725	0.000000
37	6	7.714510	0.718107	0.000000
38	6	5.292034	-1.735400	0.000000
39	6	6.727229	-1.721598	0.000000
40	6	7.714514	-0.717966	0.000000
41	8	6.014932	3.926160	0.000000
42	8	2.138687	0.000047	0.000000
43	6	4.894057	-3.092853	0.000000
44	6	7.145358	-3.070267	0.000000
45	6	9.072288	1.125840	0.000000
46	8	9.920308	0.000052	0.000000
47	6	9.072288	-1.125777	0.000000
48	6	9.483453	2.468122	0.000000
49	6	8.489546	3.474455	0.000000
50	6	9.483468	-2.468079	0.000000
51	6	8.489549	-3.474413	0.000000
52	1	10.536563	2.726616	0.000000
53	1	8.759677	4.524543	0.000000
54	1	10.536582	-2.726564	0.000000
55	1	8.759758	-4.524469	0.000000
56	8	6.015011	-3.926113	0.000000
57	6	-4.297184	-0.727983	0.000000
58	6	-2.965983	-1.151502	0.000000
59	6	-2.965959	1.151485	0.000000
60	6	-4.297190	0.727892	0.000000
61	6	-5.292034	1.735400	0.000000
62	6	-6.727229	1.721598	0.000000
63	6	-7.145358	3.070267	0.000000
64	6	-4.894057	3.092853	0.000000
65	6	-7.714514	0.717966	0.000000
66	6	-5.292004	-1.735354	0.000000
67	6	-6.727236	-1.721621	0.000000
68	6	-7.714510	-0.718107	0.000000
69	8	-6.015011	3.926113	0.000000
70	8	-2.138687	-0.000047	0.000000
71	6	-4.894027	-3.092725	0.000000
72	6	-7.145322	-3.070277	0.000000
73	6	-9.072288	1.125777	0.000000
74	8	-9.920308	-0.000052	0.000000
75	6	-9.072288	-1.125840	0.000000
76	6	-3.538317	3.537881	0.000000
77	6	-2.501090	2.500677	0.000000
78	6	-9.483468	2.468079	0.000000
79	6	-8.489549	3.474413	0.000000
80	6	-9.483453	-2.468122	0.000000
81	6	-8.489546	-3.474455	0.000000
82	1	-10.536582	2.726564	0.000000
83	1	-8.759758	4.524469	0.000000
84	1	-10.536563	-2.726616	0.000000
85	1	-8.759677	-4.524543	0.000000
86	8	-6.014932	-3.926160	0.000000

87	6	-2.501091	-2.500643	0.000000
88	6	-3.538343	-3.537784	0.000000
89	6	-1.721668	-6.726027	0.000000
90	6	-3.070348	-7.144559	0.000000
91	6	-3.093202	-4.893183	0.000000
92	6	-1.735499	-5.291282	0.000000
93	6	-0.727903	-4.296411	0.000000
94	6	0.728072	-4.296435	0.000000
95	6	1.151472	-2.965611	0.000000
96	6	-1.151443	-2.965601	0.000000
97	6	1.735533	-5.291366	0.000000
98	6	-0.717722	-7.713515	0.000000
99	6	0.717790	-7.713547	0.000000
100	6	1.721614	-6.726133	0.000000
101	8	-0.000004	-2.138121	0.000000
102	8	-3.926362	-6.014498	0.000000
103	6	-1.125717	-9.071597	0.000000
104	6	1.125677	-9.071567	0.000000
105	6	3.093219	-4.893318	0.000000
106	8	3.926278	-6.014617	0.000000
107	6	3.070253	-7.144621	0.000000
108	6	3.538317	-3.537881	0.000000
109	6	2.501090	-2.500677	0.000000
110	6	-2.467849	-9.482989	0.000000
111	6	-3.474443	-8.488826	0.000000
112	6	3.474286	-8.488848	0.000000
113	6	2.467711	-9.482969	0.000000
114	1	-2.726341	-10.536215	0.000000
115	1	-4.524579	-8.759086	0.000000
116	1	4.524374	-8.759162	0.000000
117	1	2.726188	-10.536166	0.000000
118	8	0.000001	-9.919611	0.000000
119	6	-3.093219	4.893318	0.000000
120	8	3.926362	6.014498	0.000000
121	78	0.000000	0.000000	0.000000

Table S9. The optimized Cartesian coordinates of the complex **6** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	48	0.000000	0.000000	0.000000
2	6	-1.717942	5.245171	1.982498
3	6	-3.068357	4.853036	1.989326
4	6	-3.057434	7.083778	2.251531
5	6	-1.708196	6.676445	2.158946
6	6	-0.718738	7.665157	2.266123
7	6	0.718738	7.665157	2.266123
8	6	1.126764	9.004678	2.452178
9	6	-1.126764	9.004678	2.452178
10	6	1.708196	6.676445	2.158946
11	6	-0.723555	4.243798	1.830323
12	6	0.723555	4.243798	1.830323
13	6	1.717942	5.245171	1.982498
14	8	0.000000	9.847935	2.560596
15	6	-1.136999	2.919712	1.669359
16	6	1.136999	2.919712	1.669359
17	6	3.057434	7.083778	2.251531

18	8	3.909643	5.959067	2.147675
19	6	-2.471825	9.406632	2.534890
20	6	-3.469387	8.414358	2.432846
21	6	3.469387	8.414358	2.432846
22	6	2.471825	9.406632	2.534890
23	1	-2.732941	10.448519	2.684180
24	1	-4.521256	8.668121	2.501399
25	1	4.521256	8.668121	2.501399
26	1	2.732941	10.448519	2.684180
27	8	0.000000	2.057771	1.512104
28	6	-3.507121	3.507121	1.888706
29	6	-2.480104	2.480104	1.716719
30	6	-4.243798	-0.723555	1.830323
31	6	-2.919712	-1.136999	1.669359
32	6	-2.919712	1.136999	1.669359
33	6	-4.243798	0.723555	1.830323
34	6	-5.245171	1.717942	1.982498
35	6	-6.676445	1.708196	2.158946
36	6	-7.083778	3.057434	2.251531
37	6	-4.853036	3.068357	1.989326
38	6	-7.665157	0.718738	2.266123
39	6	-5.245171	-1.717942	1.982498
40	6	-6.676445	-1.708196	2.158946
41	6	-7.665157	-0.718738	2.266123
42	8	-5.959067	3.909643	2.147675
43	8	-2.057771	0.000000	1.512104
44	6	-4.853036	-3.068357	1.989326
45	6	-7.083778	-3.057434	2.251531
46	6	-9.004678	1.126764	2.452178
47	8	-9.847935	0.000000	2.560596
48	6	-9.004678	-1.126764	2.452178
49	6	-9.406632	2.471825	2.534890
50	6	-8.414358	3.469387	2.432846
51	6	-9.406632	-2.471825	2.534890
52	6	-8.414358	-3.469387	2.432846
53	1	-10.448519	2.732941	2.684180
54	1	-8.668121	4.521256	2.501399
55	1	-10.448519	-2.732941	2.684180
56	1	-8.668121	-4.521256	2.501399
57	8	-5.959067	-3.909643	2.147675
58	6	4.243798	-0.723555	1.830323
59	6	2.919712	-1.136999	1.669359
60	6	2.919712	1.136999	1.669359
61	6	4.243798	0.723555	1.830323
62	6	5.245171	1.717942	1.982498
63	6	6.676445	1.708196	2.158946
64	6	7.083778	3.057434	2.251531
65	6	4.853036	3.068357	1.989326
66	6	7.665157	0.718738	2.266123
67	6	5.245171	-1.717942	1.982498
68	6	6.676445	-1.708196	2.158946
69	6	7.665157	-0.718738	2.266123
70	8	5.959067	3.909643	2.147675
71	8	2.057771	0.000000	1.512104
72	6	4.853036	-3.068357	1.989326
73	6	7.083778	-3.057434	2.251531
74	6	9.004678	1.126764	2.452178
75	8	9.847935	0.000000	2.560596
76	6	9.004678	-1.126764	2.452178
77	6	3.507121	3.507121	1.888706
78	6	2.480104	2.480104	1.716719
79	6	9.406632	2.471825	2.534890
80	6	8.414358	3.469387	2.432846

81	6	9.406632	-2.471825	2.534890
82	6	8.414358	-3.469387	2.432846
83	1	10.448519	2.732941	2.684180
84	1	8.668121	4.521256	2.501399
85	1	10.448519	-2.732941	2.684180
86	1	8.668121	-4.521256	2.501399
87	8	5.959067	-3.909643	2.147675
88	6	2.480104	-2.480104	1.716719
89	6	3.507121	-3.507121	1.888706
90	6	1.708196	-6.676445	2.158946
91	6	3.057434	-7.083778	2.251531
92	6	3.068357	-4.853036	1.989326
93	6	1.717942	-5.245171	1.982498
94	6	0.723555	-4.243798	1.830323
95	6	-0.723555	-4.243798	1.830323
96	6	-1.136999	-2.919712	1.669359
97	6	1.136999	-2.919712	1.669359
98	6	-1.717942	-5.245171	1.982498
99	6	0.718738	-7.665157	2.266123
100	6	-0.718738	-7.665157	2.266123
101	6	-1.708196	-6.676445	2.158946
102	8	0.000000	-2.057771	1.512104
103	8	3.909643	-5.959067	2.147675
104	6	1.126764	-9.004678	2.452178
105	6	-1.126764	-9.004678	2.452178
106	6	-3.068357	-4.853036	1.989326
107	8	-3.909643	-5.959067	2.147675
108	6	-3.057434	-7.083778	2.251531
109	6	-3.507121	-3.507121	1.888706
110	6	-2.480104	-2.480104	1.716719
111	6	2.471825	-9.406632	2.534890
112	6	3.469387	-8.414358	2.432846
113	6	-3.469387	-8.414358	2.432846
114	6	-2.471825	-9.406632	2.534890
115	1	2.732941	-10.448519	2.684180
116	1	4.521256	-8.668121	2.501399
117	1	-4.521256	-8.668121	2.501399
118	1	-2.732941	-10.448519	2.684180
119	8	0.000000	-9.847935	2.560596
120	6	3.068357	4.853036	1.989326
121	8	-3.909643	5.959067	2.147675
122	6	-1.717942	5.245171	-1.982498
123	6	-3.068357	4.853036	-1.989326
124	6	-3.057434	7.083778	-2.251531
125	6	-1.708196	6.676445	-2.158946
126	6	-0.718738	7.665157	-2.266123
127	6	0.718738	7.665157	-2.266123
128	6	1.126764	9.004678	-2.452178
129	6	-1.126764	9.004678	-2.452178
130	6	1.708196	6.676445	-2.158946
131	6	-0.723555	4.243798	-1.830323
132	6	0.723555	4.243798	-1.830323
133	6	1.717942	5.245171	-1.982498
134	8	0.000000	9.847935	-2.560596
135	6	-1.136999	2.919712	-1.669359
136	6	1.136999	2.919712	-1.669359
137	6	3.057434	7.083778	-2.251531
138	8	3.909643	5.959067	-2.147675
139	6	-2.471825	9.406632	-2.534890
140	6	-3.469387	8.414358	-2.432846
141	6	3.469387	8.414358	-2.432846
142	6	2.471825	9.406632	-2.534890
143	1	-2.732941	10.448519	-2.684180

144	1	-4.521256	8.668121	-2.501399
145	1	4.521256	8.668121	-2.501399
146	1	2.732941	10.448519	-2.684180
147	8	0.000000	2.057771	-1.512104
148	6	-3.507121	3.507121	-1.888706
149	6	-2.480104	2.480104	-1.716719
150	6	-4.243798	-0.723555	-1.830323
151	6	-2.919712	-1.136999	-1.669359
152	6	-2.919712	1.136999	-1.669359
153	6	-4.243798	0.723555	-1.830323
154	6	-5.245171	1.717942	-1.982498
155	6	-6.676445	1.708196	-2.158946
156	6	-7.083778	3.057434	-2.251531
157	6	-4.853036	3.068357	-1.989326
158	6	-7.665157	0.718738	-2.266123
159	6	-5.245171	-1.717942	-1.982498
160	6	-6.676445	-1.708196	-2.158946
161	6	-7.665157	-0.718738	-2.266123
162	8	-5.959067	3.909643	-2.147675
163	8	-2.057771	0.000000	-1.512104
164	6	-4.853036	-3.068357	-1.989326
165	6	-7.083778	-3.057434	-2.251531
166	6	-9.004678	1.126764	-2.452178
167	8	-9.847935	0.000000	-2.560596
168	6	-9.004678	-1.126764	-2.452178
169	6	-9.406632	2.471825	-2.534890
170	6	-8.414358	3.469387	-2.432846
171	6	-9.406632	-2.471825	-2.534890
172	6	-8.414358	-3.469387	-2.432846
173	1	-10.448519	2.732941	-2.684180
174	1	-8.668121	4.521256	-2.501399
175	1	-10.448519	-2.732941	-2.684180
176	1	-8.668121	-4.521256	-2.501399
177	8	-5.959067	-3.909643	-2.147675
178	6	4.243798	-0.723555	-1.830323
179	6	2.919712	-1.136999	-1.669359
180	6	2.919712	1.136999	-1.669359
181	6	4.243798	0.723555	-1.830323
182	6	5.245171	1.717942	-1.982498
183	6	6.676445	1.708196	-2.158946
184	6	7.083778	3.057434	-2.251531
185	6	4.853036	3.068357	-1.989326
186	6	7.665157	0.718738	-2.266123
187	6	5.245171	-1.717942	-1.982498
188	6	6.676445	-1.708196	-2.158946
189	6	7.665157	-0.718738	-2.266123
190	8	5.959067	3.909643	-2.147675
191	8	2.057771	0.000000	-1.512104
192	6	4.853036	-3.068357	-1.989326
193	6	7.083778	-3.057434	-2.251531
194	6	9.004678	1.126764	-2.452178
195	8	9.847935	0.000000	-2.560596
196	6	9.004678	-1.126764	-2.452178
197	6	3.507121	3.507121	-1.888706
198	6	2.480104	2.480104	-1.716719
199	6	9.406632	2.471825	-2.534890
200	6	8.414358	3.469387	-2.432846
201	6	9.406632	-2.471825	-2.534890
202	6	8.414358	-3.469387	-2.432846
203	1	10.448519	2.732941	-2.684180
204	1	8.668121	4.521256	-2.501399
205	1	10.448519	-2.732941	-2.684180
206	1	8.668121	-4.521256	-2.501399

207	8	5.959067	-3.909643	-2.147675
208	6	2.480104	-2.480104	-1.716719
209	6	3.507121	-3.507121	-1.888706
210	6	1.708196	-6.676445	-2.158946
211	6	3.057434	-7.083778	-2.251531
212	6	3.068357	-4.853036	-1.989326
213	6	1.717942	-5.245171	-1.982498
214	6	0.723555	-4.243798	-1.830323
215	6	-0.723555	-4.243798	-1.830323
216	6	-1.136999	-2.919712	-1.669359
217	6	1.136999	-2.919712	-1.669359
218	6	-1.717942	-5.245171	-1.982498
219	6	0.718738	-7.665157	-2.266123
220	6	-0.718738	-7.665157	-2.266123
221	6	-1.708196	-6.676445	-2.158946
222	8	0.000000	-2.057771	-1.512104
223	8	3.909643	-5.959067	-2.147675
224	6	1.126764	-9.004678	-2.452178
225	6	-1.126764	-9.004678	-2.452178
226	6	-3.068357	-4.853036	-1.989326
227	8	-3.909643	-5.959067	-2.147675
228	6	-3.057434	-7.083778	-2.251531
229	6	-3.507121	-3.507121	-1.888706
230	6	-2.480104	-2.480104	-1.716719
231	6	2.471825	-9.406632	-2.534890
232	6	3.469387	-8.414358	-2.432846
233	6	-3.469387	-8.414358	-2.432846
234	6	-2.471825	-9.406632	-2.534890
235	1	2.732941	-10.448519	-2.684180
236	1	4.521256	-8.668121	-2.501399
237	1	-4.521256	-8.668121	-2.501399
238	1	-2.732941	-10.448519	-2.684180
239	8	0.000000	-9.847935	-2.560596
240	6	3.068357	4.853036	-1.989326
241	8	-3.909643	5.959067	-2.147675