

Alkali and alkaline-earth metal complexes with tetraoxa[8]circulene sheet: A computational study by DFT and QTAIM methods

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Electronic Supplementary Information

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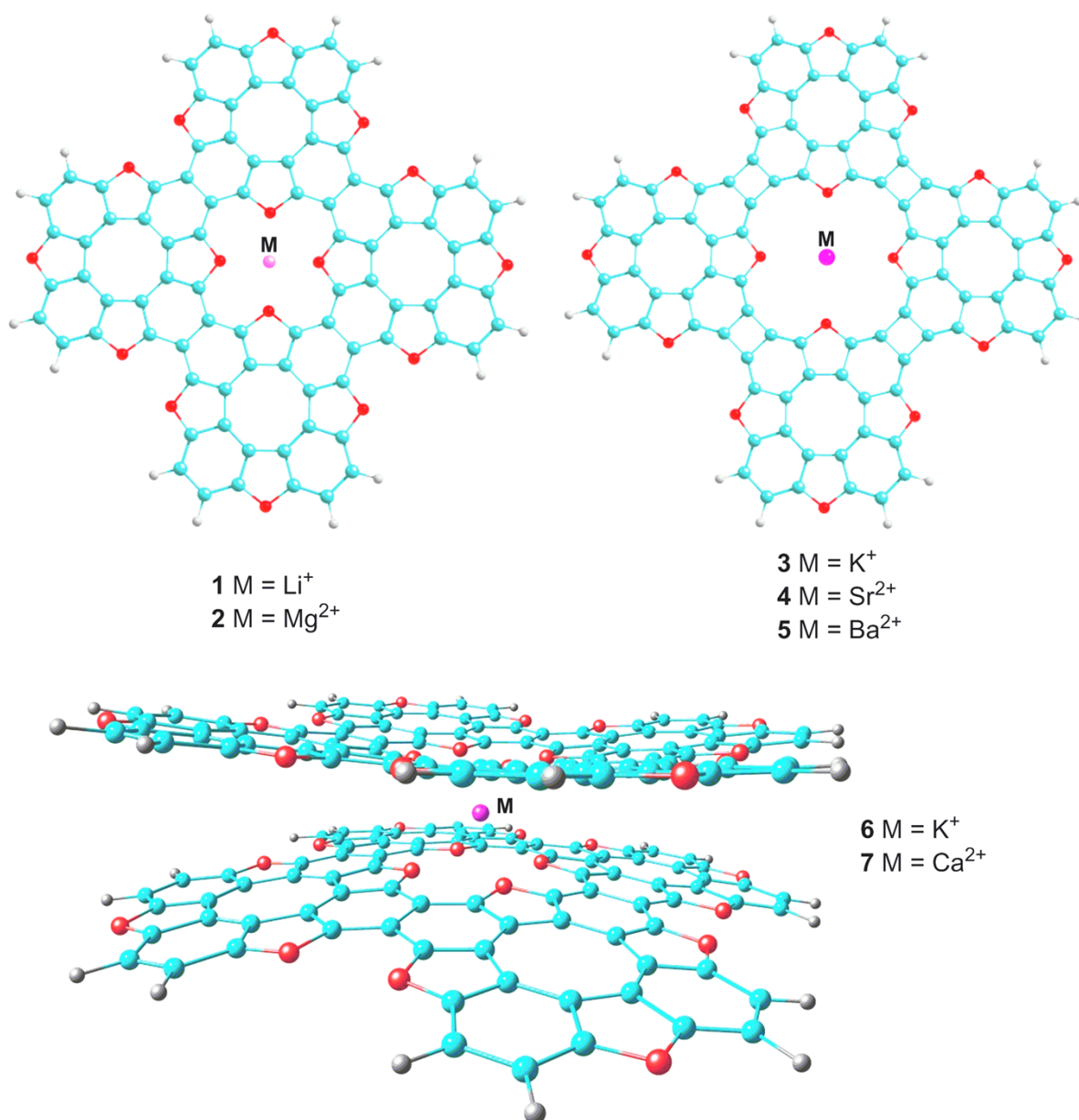


Figure S1. The optimized structures of the studied complexes 1–7 based on tetraoxa[8]circulene sheet (Carbon atoms in blue, Oxygen – red, Hydrogen – grey, metal atoms (M) – pink).

Table S1. The optimized Cartesian coordinates of the complex **1** in the ground singlet state calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.495557	5.282644	0.000000
2	6	-0.172264	5.722552	0.000000
3	6	-1.414443	7.544349	0.000000
4	6	-2.302690	6.461952	0.000000
5	6	-3.674420	6.727196	0.000000
6	6	-4.857466	5.929718	0.000000
7	6	-5.933808	6.825764	0.000000
8	6	-4.101244	8.061074	0.000000
9	6	-5.126186	4.558665	0.000000
10	6	-1.761032	3.896447	0.000000
11	6	-2.951244	3.094139	0.000000
12	6	-4.335795	3.368071	0.000000
13	8	-5.481219	8.131299	0.000000
14	6	-0.689919	3.019254	0.000000
15	6	-2.539933	1.772180	0.000000
16	6	-6.462751	4.141341	0.000000
17	8	-6.535297	2.757608	0.000000
18	6	-3.211004	9.142876	0.000000
19	6	-1.835251	8.879129	0.000000
20	6	-7.542186	5.032148	0.000000
21	6	-7.270568	6.406369	0.000000
22	1	-3.577646	10.163275	0.000000
23	1	-1.115181	9.689582	0.000000
24	1	-8.563577	4.668701	0.000000
25	1	-8.078903	7.129027	0.000000
26	8	-1.140407	1.691775	0.000000
27	6	0.943751	4.847712	0.000000
28	6	0.664703	3.414342	0.000000
29	6	3.896447	1.761032	0.000000
30	6	3.019254	0.689919	0.000000
31	6	1.772180	2.539933	0.000000
32	6	3.094139	2.951244	0.000000
33	6	3.368071	4.335795	0.000000
34	6	4.558665	5.126186	0.000000
35	6	4.141341	6.462751	0.000000
36	6	2.306450	5.239997	0.000000
37	6	5.929718	4.857466	0.000000
38	6	5.282644	1.495557	0.000000
39	6	6.461952	2.302690	0.000000
40	6	6.727196	3.674420	0.000000
41	8	2.757608	6.535297	0.000000
42	8	1.691775	1.140407	0.000000
43	6	5.722552	0.172264	0.000000
44	6	7.544349	1.414443	0.000000
45	6	6.825764	5.933808	0.000000
46	8	8.131299	5.481219	0.000000
47	6	8.061074	4.101244	0.000000
48	6	6.406369	7.270568	0.000000
49	6	5.032148	7.542186	0.000000
50	6	9.142876	3.211004	0.000000
51	6	8.879129	1.835251	0.000000
52	1	7.129027	8.078903	0.000000
53	1	4.668701	8.563577	0.000000
54	1	10.163275	3.577646	0.000000
55	1	9.689582	1.115181	0.000000
56	8	7.092502	0.104552	0.000000
57	6	-3.094139	-2.951244	0.000000
58	6	-1.772180	-2.539933	0.000000
59	6	-3.019254	-0.689919	0.000000
60	6	-3.896447	-1.761032	0.000000
61	6	-5.282644	-1.495557	0.000000
62	6	-6.461952	-2.302690	0.000000
63	6	-7.544349	-1.414443	0.000000
64	6	-5.722552	-0.172264	0.000000
65	6	-6.727196	-3.674420	0.000000
66	6	-3.368071	-4.335795	0.000000
67	6	-4.558665	-5.126186	0.000000
68	6	-5.929718	-4.857466	0.000000
69	8	-7.092502	-0.104552	0.000000
70	8	-1.691775	-1.140407	0.000000

71	6	-2.306450	-5.239997	0.000000
72	6	-4.141341	-6.462751	0.000000
73	6	-8.061074	-4.101244	0.000000
74	8	-8.131299	-5.481219	0.000000
75	6	-6.825764	-5.933808	0.000000
76	6	-4.847712	0.943751	0.000000
77	6	-3.414342	0.664703	0.000000
78	6	-9.142876	-3.211004	0.000000
79	6	-8.879129	-1.835251	0.000000
80	6	-6.406369	-7.270568	0.000000
81	6	-5.032148	-7.542186	0.000000
82	1	-10.163275	-3.577646	0.000000
83	1	-9.689582	-1.115181	0.000000
84	1	-7.129027	-8.078903	0.000000
85	1	-4.668701	-8.563577	0.000000
86	8	-2.757608	-6.535297	0.000000
87	6	-0.664703	-3.414342	0.000000
88	6	-0.943751	-4.847712	0.000000
89	6	2.302690	-6.461952	0.000000
90	6	1.414443	-7.544349	0.000000
91	6	0.172264	-5.722552	0.000000
92	6	1.495557	-5.282644	0.000000
93	6	1.761032	-3.896447	0.000000
94	6	2.951244	-3.094139	0.000000
95	6	2.539933	-1.772180	0.000000
96	6	0.689919	-3.019254	0.000000
97	6	4.335795	-3.368071	0.000000
98	6	3.674420	-6.727196	0.000000
99	6	4.857466	-5.929718	0.000000
100	6	5.126186	-4.558665	0.000000
101	8	1.140407	-1.691775	0.000000
102	8	0.104552	-7.092502	0.000000
103	6	4.101244	-8.061074	0.000000
104	6	5.933808	-6.825764	0.000000
105	6	5.239997	-2.306450	0.000000
106	8	6.535297	-2.757608	0.000000
107	6	6.462751	-4.141341	0.000000
108	6	4.847712	-0.943751	0.000000
109	6	3.414342	-0.664703	0.000000
110	6	3.211004	-9.142876	0.000000
111	6	1.835251	-8.879129	0.000000
112	6	7.542186	-5.032148	0.000000
113	6	7.270568	-6.406369	0.000000
114	1	3.577646	-10.163275	0.000000
115	1	1.115181	-9.689582	0.000000
116	1	8.563577	-4.668701	0.000000
117	1	8.078903	-7.129027	0.000000
118	8	5.481219	-8.131299	0.000000
119	6	-5.239997	2.306450	0.000000
120	8	-0.104552	7.092502	0.000000
121	3	0.000000	0.000000	0.000000

Table S2. The optimized Cartesian coordinates of the complex **2** in the ground singlet state calculated at the B3LYP/6-31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	1.714867	5.226122	0.000000
2	6	3.063127	4.852767	0.000000
3	6	3.043514	7.056365	0.000000
4	6	1.702751	6.653587	0.000000
5	6	0.712378	7.639123	0.000000
6	6	-0.712378	7.639123	0.000000
7	6	-1.103717	8.983456	0.000000
8	6	1.103717	8.983456	0.000000
9	6	-1.702751	6.653587	0.000000
10	6	0.720632	4.222747	0.000000
11	6	-0.720632	4.222747	0.000000
12	6	-1.714867	5.226122	0.000000
13	8	0.000000	9.810165	0.000000
14	6	1.134652	2.906451	0.000000
15	6	-1.134652	2.906451	0.000000
16	6	-3.043514	7.056365	0.000000
17	8	-3.877942	5.947465	0.000000

18	6	2.447487	9.383657	0.000000
19	6	3.441706	8.398272	0.000000
20	6	-3.441706	8.398272	0.000000
21	6	-2.447487	9.383657	0.000000
22	1	2.713091	10.434843	0.000000
23	1	4.491271	8.669159	0.000000
24	1	-4.491271	8.669159	0.000000
25	1	-2.713091	10.434843	0.000000
26	8	0.000000	2.035665	0.000000
27	6	3.506009	3.506009	0.000000
28	6	2.471939	2.471939	0.000000
29	6	4.222747	-0.720632	0.000000
30	6	2.906451	-1.134652	0.000000
31	6	2.906451	1.134652	0.000000
32	6	4.222747	0.720632	0.000000
33	6	5.226122	1.714867	0.000000
34	6	6.653587	1.702751	0.000000
35	6	7.056365	3.043514	0.000000
36	6	4.852767	3.063127	0.000000
37	6	7.639123	0.712378	0.000000
38	6	5.226122	-1.714867	0.000000
39	6	6.653587	-1.702751	0.000000
40	6	7.639123	-0.712378	0.000000
41	8	5.947465	3.877942	0.000000
42	8	2.035665	0.000000	0.000000
43	6	4.852767	-3.063127	0.000000
44	6	7.056365	-3.043514	0.000000
45	6	8.983456	1.103717	0.000000
46	8	9.810165	0.000000	0.000000
47	6	8.983456	-1.103717	0.000000
48	6	9.383657	2.447487	0.000000
49	6	8.398272	3.441706	0.000000
50	6	9.383657	-2.447487	0.000000
51	6	8.398272	-3.441706	0.000000
52	1	10.434843	2.713091	0.000000
53	1	8.669159	4.491271	0.000000
54	1	10.434843	-2.713091	0.000000
55	1	8.669159	-4.491271	0.000000
56	8	5.947465	-3.877942	0.000000
57	6	-4.222747	-0.720632	0.000000
58	6	-2.906451	-1.134652	0.000000
59	6	-2.906451	1.134652	0.000000
60	6	-4.222747	0.720632	0.000000
61	6	-5.226122	1.714867	0.000000
62	6	-6.653587	1.702751	0.000000
63	6	-7.056365	3.043514	0.000000
64	6	-4.852767	3.063127	0.000000
65	6	-7.639123	0.712378	0.000000
66	6	-5.226122	-1.714867	0.000000
67	6	-6.653587	-1.702751	0.000000
68	6	-7.639123	-0.712378	0.000000
69	8	-5.947465	3.877942	0.000000
70	8	-2.035665	0.000000	0.000000
71	6	-4.852767	-3.063127	0.000000
72	6	-7.056365	-3.043514	0.000000
73	6	-8.983456	1.103717	0.000000
74	8	-9.810165	0.000000	0.000000
75	6	-8.983456	-1.103717	0.000000
76	6	-3.506009	3.506009	0.000000
77	6	-2.471939	2.471939	0.000000
78	6	-9.383657	2.447487	0.000000
79	6	-8.398272	3.441706	0.000000
80	6	-9.383657	-2.447487	0.000000
81	6	-8.398272	-3.441706	0.000000
82	1	-10.434843	2.713091	0.000000
83	1	-8.669159	4.491271	0.000000
84	1	-10.434843	-2.713091	0.000000
85	1	-8.669159	-4.491271	0.000000
86	8	-5.947465	-3.877942	0.000000
87	6	-2.471939	-2.471939	0.000000
88	6	-3.506009	-3.506009	0.000000
89	6	-1.702751	-6.653587	0.000000
90	6	-3.043514	-7.056365	0.000000
91	6	-3.063127	-4.852767	0.000000
92	6	-1.714867	-5.226122	0.000000
93	6	-0.720632	-4.222747	0.000000
94	6	0.720632	-4.222747	0.000000
95	6	1.134652	-2.906451	0.000000
96	6	-1.134652	-2.906451	0.000000

97	6	1.714867	-5.226122	0.000000
98	6	-0.712378	-7.639123	0.000000
99	6	0.712378	-7.639123	0.000000
100	6	1.702751	-6.653587	0.000000
101	8	0.000000	-2.035665	0.000000
102	8	-3.877942	-5.947465	0.000000
103	6	-1.103717	-8.983456	0.000000
104	6	1.103717	-8.983456	0.000000
105	6	3.063127	-4.852767	0.000000
106	8	3.877942	-5.947465	0.000000
107	6	3.043514	-7.056365	0.000000
108	6	3.506009	-3.506009	0.000000
109	6	2.471939	-2.471939	0.000000
110	6	-2.447487	-9.383657	0.000000
111	6	-3.441706	-8.398272	0.000000
112	6	3.441706	-8.398272	0.000000
113	6	2.447487	-9.383657	0.000000
114	1	-2.713091	-10.434843	0.000000
115	1	-4.491271	-8.669159	0.000000
116	1	4.491271	-8.669159	0.000000
117	1	2.713091	-10.434843	0.000000
118	8	0.000000	-9.810165	0.000000
119	6	-3.063127	4.852767	0.000000
120	8	3.877942	5.947465	0.000000
121	12	0.000000	0.000000	0.000000

Table S3. The optimized Cartesian coordinates of the complex **3** in the ground singlet state calculated the B3LYP/6-31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	19	0.000000	0.000000	0.000000
2	6	3.042296	8.034287	0.000000
3	6	1.703722	7.623279	0.000000
4	6	0.714931	8.610400	0.000000
5	6	-0.714931	8.610400	0.000000
6	6	-1.102961	9.956380	0.000000
7	6	1.102961	9.956380	0.000000
8	6	-1.703722	7.623279	0.000000
9	8	0.000000	10.786097	0.000000
10	6	-3.042296	8.034287	0.000000
11	6	2.443501	10.362941	0.000000
12	6	3.436540	9.377286	0.000000
13	6	-3.436540	9.377286	0.000000
14	6	-2.443501	10.362941	0.000000
15	1	2.705313	11.415325	0.000000
16	1	4.486984	9.645691	0.000000
17	1	-4.486984	9.645691	0.000000
18	1	-2.705313	11.415325	0.000000
19	6	1.710559	6.186981	0.000000
20	6	3.095710	5.832180	0.000000
21	6	0.721457	5.198211	0.000000
22	6	-0.721457	5.198211	0.000000
23	6	-1.710559	6.186981	0.000000
24	6	1.110088	3.827837	0.000000
25	6	-1.110088	3.827837	0.000000
26	6	-3.095710	5.832180	0.000000
27	6	2.435153	3.491441	0.000000
28	6	3.447890	4.504576	0.000000
29	6	-3.447890	4.504576	0.000000
30	6	-2.435153	3.491441	0.000000
31	8	0.000000	2.982693	0.000000
32	8	3.897962	6.945099	0.000000
33	8	-3.897962	6.945099	0.000000
34	6	9.956380	1.102961	0.000000
35	6	8.610400	0.714931	0.000000
36	6	7.623279	1.703722	0.000000
37	6	6.186981	1.710559	0.000000
38	6	5.832180	3.095710	0.000000
39	6	8.034287	3.042296	0.000000
40	6	5.198211	0.721457	0.000000
41	8	6.945099	3.897962	0.000000

42	6	3.827837	1.110088	0.000000
43	6	9.377286	3.436540	0.000000
44	6	10.362941	2.443501	0.000000
45	6	3.491441	2.435153	0.000000
46	6	4.504576	3.447890	0.000000
47	1	9.645691	4.486984	0.000000
48	1	11.415325	2.705313	0.000000
49	6	8.610400	-0.714931	0.000000
50	6	9.956380	-1.102961	0.000000
51	6	7.623279	-1.703722	0.000000
52	6	6.186981	-1.710559	0.000000
53	6	5.198211	-0.721457	0.000000
54	6	8.034287	-3.042296	0.000000
55	6	5.832180	-3.095710	0.000000
56	6	3.827837	-1.110088	0.000000
57	6	9.377286	-3.436540	0.000000
58	6	10.362941	-2.443501	0.000000
59	6	3.491441	-2.435153	0.000000
60	6	4.504576	-3.447890	0.000000
61	1	9.645691	-4.486984	0.000000
62	1	11.415325	-2.705313	0.000000
63	8	6.945099	-3.897962	0.000000
64	8	10.786097	0.000000	0.000000
65	8	2.982693	0.000000	0.000000
66	6	-3.827837	1.110088	0.000000
67	6	-5.198211	0.721457	0.000000
68	6	-6.186981	1.710559	0.000000
69	6	-7.623279	1.703722	0.000000
70	6	-8.034287	3.042296	0.000000
71	6	-5.832180	3.095710	0.000000
72	6	-8.610400	0.714931	0.000000
73	8	-6.945099	3.897962	0.000000
74	6	-9.956380	1.102961	0.000000
75	6	-4.504576	3.447890	0.000000
76	6	-3.491441	2.435153	0.000000
77	6	-10.362941	2.443501	0.000000
78	6	-9.377286	3.436540	0.000000
79	1	-11.415325	2.705313	0.000000
80	1	-9.645691	4.486984	0.000000
81	6	-5.198211	-0.721457	0.000000
82	6	-3.827837	-1.110088	0.000000
83	6	-6.186981	-1.710559	0.000000
84	6	-7.623279	-1.703722	0.000000
85	6	-8.610400	-0.714931	0.000000
86	6	-5.832180	-3.095710	0.000000
87	6	-8.034287	-3.042296	0.000000
88	6	-9.956380	-1.102961	0.000000
89	6	-4.504576	-3.447890	0.000000
90	6	-3.491441	-2.435153	0.000000
91	6	-10.362941	-2.443501	0.000000
92	6	-9.377286	-3.436540	0.000000
93	1	-11.415325	-2.705313	0.000000
94	1	-9.645691	-4.486984	0.000000
95	8	-6.945099	-3.897962	0.000000
96	8	-2.982693	0.000000	0.000000
97	8	-10.786097	0.000000	0.000000
98	6	3.095710	-5.832180	0.000000
99	6	1.710559	-6.186981	0.000000
100	6	0.721457	-5.198211	0.000000
101	6	-0.721457	-5.198211	0.000000
102	6	-1.110088	-3.827837	0.000000
103	6	1.110088	-3.827837	0.000000
104	6	-1.710559	-6.186981	0.000000
105	8	0.000000	-2.982693	0.000000
106	6	-3.095710	-5.832180	0.000000
107	6	2.435153	-3.491441	0.000000
108	6	3.447890	-4.504576	0.000000
109	6	-3.447890	-4.504576	0.000000
110	6	-2.435153	-3.491441	0.000000
111	6	1.703722	-7.623279	0.000000
112	6	3.042296	-8.034287	0.000000
113	6	0.714931	-8.610400	0.000000
114	6	-0.714931	-8.610400	0.000000
115	6	-1.703722	-7.623279	0.000000
116	6	1.102961	-9.956380	0.000000
117	6	-1.102961	-9.956380	0.000000
118	6	-3.042296	-8.034287	0.000000
119	6	2.443501	-10.362941	0.000000
120	6	3.436540	-9.377286	0.000000

121	6	-3.436540	-9.377286	0.000000
122	6	-2.443501	-10.362941	0.000000
123	1	2.705313	-11.415325	0.000000
124	1	4.486984	-9.645691	0.000000
125	1	-4.486984	-9.645691	0.000000
126	1	-2.705313	-11.415325	0.000000
127	8	0.000000	-10.786097	0.000000
128	8	3.897962	-6.945099	0.000000
129	8	-3.897962	-6.945099	0.000000

Table S4. The optimized Cartesian coordinates of the complex **4** in the ground singlet state calculated at the B3LYP/LanL2Dz level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	38	0.000000	0.000000	0.000000
2	6	-3.568048	7.891314	0.000000
3	6	-4.217291	6.635958	0.000000
4	6	-5.620234	6.637954	0.000000
5	6	-6.637746	5.620412	0.000000
6	6	-7.880779	6.291799	0.000000
7	6	-6.291551	7.880929	0.000000
8	6	-6.635872	4.217250	0.000000
9	8	-7.686339	7.686617	0.000000
10	6	-7.891472	3.568132	0.000000
11	6	-5.637764	9.126049	0.000000
12	6	-4.229209	9.130779	0.000000
13	6	-9.130947	4.229403	0.000000
14	6	-9.126082	5.638035	0.000000
15	1	-6.202455	10.051827	0.000000
16	1	-3.669525	10.059327	0.000000
17	1	-10.059579	3.669818	0.000000
18	1	-10.051837	6.202878	0.000000
19	6	-3.187911	5.617080	0.000000
20	6	-1.940655	6.348881	0.000000
21	6	-3.181817	4.208837	0.000000
22	6	-4.209021	3.181577	0.000000
23	6	-5.617178	3.187667	0.000000
24	6	-1.919448	3.525227	0.000000
25	6	-3.525425	1.919219	0.000000
26	6	-6.349069	1.940567	0.000000
27	6	-0.747224	4.220823	0.000000
28	6	-0.749916	5.665982	0.000000
29	6	-5.666219	0.749823	0.000000
30	6	-4.221078	0.747046	0.000000
31	8	-2.089377	2.089187	0.000000
32	8	-2.160552	7.725449	0.000000
33	8	-7.725629	2.160563	0.000000
34	6	6.291539	7.881410	0.000000
35	6	5.620350	6.638262	0.000000
36	6	4.217251	6.635998	0.000000
37	6	3.187758	5.617103	0.000000
38	6	1.940655	6.348821	0.000000
39	6	3.567909	7.891272	0.000000
40	6	3.181644	4.208903	0.000000
41	8	2.160567	7.725268	0.000000
42	6	1.919247	3.525148	0.000000
43	6	4.228702	9.130804	0.000000
44	6	5.637322	9.126598	0.000000
45	6	0.746964	4.220760	0.000000
46	6	0.749916	5.665985	0.000000
47	1	3.668906	10.059248	0.000000
48	1	6.201933	10.052549	0.000000
49	6	6.637819	5.620772	0.000000
50	6	7.881042	6.292068	0.000000
51	6	6.635814	4.217453	0.000000
52	6	5.617105	3.187880	0.000000
53	6	4.208842	3.181675	0.000000
54	6	7.891337	3.568257	0.000000
55	6	6.349041	1.940771	0.000000
56	6	3.525276	1.919275	0.000000
57	6	9.130854	4.229456	0.000000

58	6	9.126286	5.638099	0.000000
59	6	4.221000	0.747122	0.000000
60	6	5.666184	0.749996	0.000000
61	1	10.059434	3.669747	0.000000
62	1	10.052137	6.202834	0.000000
63	8	7.725544	2.160807	0.000000
64	8	7.686547	7.687045	0.000000
65	8	2.089233	2.089107	0.000000
66	6	-3.525276	-1.919275	0.000000
67	6	-4.208842	-3.181675	0.000000
68	6	-5.617105	-3.187880	0.000000
69	6	-6.635814	-4.217453	0.000000
70	6	-7.891337	-3.568257	0.000000
71	6	-6.349041	-1.940771	0.000000
72	6	-6.637819	-5.620772	0.000000
73	8	-7.725544	-2.160807	0.000000
74	6	-7.881042	-6.292068	0.000000
75	6	-5.666184	-0.749996	0.000000
76	6	-4.221000	-0.747122	0.000000
77	6	-9.126286	-5.638099	0.000000
78	6	-9.130854	-4.229456	0.000000
79	1	-10.052137	-6.202834	0.000000
80	1	-10.059434	-3.669747	0.000000
81	6	-3.181644	-4.208903	0.000000
82	6	-1.919247	-3.525148	0.000000
83	6	-3.187758	-5.617103	0.000000
84	6	-4.217251	-6.635998	0.000000
85	6	-5.620350	-6.638262	0.000000
86	6	-1.940655	-6.348821	0.000000
87	6	-3.567909	-7.891272	0.000000
88	6	-6.291539	-7.881410	0.000000
89	6	-0.749916	-5.665985	0.000000
90	6	-0.746964	-4.220760	0.000000
91	6	-5.637322	-9.126598	0.000000
92	6	-4.228702	-9.130804	0.000000
93	1	-6.201933	-10.052549	0.000000
94	1	-3.668906	-10.059248	0.000000
95	8	-2.160567	-7.725268	0.000000
96	8	-2.089233	-2.089107	0.000000
97	8	-7.686547	-7.687045	0.000000
98	6	6.349069	-1.940567	0.000000
99	6	5.617178	-3.187667	0.000000
100	6	4.209021	-3.181577	0.000000
101	6	3.181817	-4.208837	0.000000
102	6	1.919448	-3.525227	0.000000
103	6	3.525425	-1.919219	0.000000
104	6	3.187911	-5.617080	0.000000
105	8	2.089377	-2.089187	0.000000
106	6	1.940655	-6.348881	0.000000
107	6	4.221078	-0.747046	0.000000
108	6	5.666219	-0.749823	0.000000
109	6	0.749916	-5.665982	0.000000
110	6	0.747224	-4.220823	0.000000
111	6	6.635872	-4.217250	0.000000
112	6	7.891472	-3.568132	0.000000
113	6	6.637746	-5.620412	0.000000
114	6	5.620234	-6.637954	0.000000
115	6	4.217291	-6.635958	0.000000
116	6	7.880779	-6.291799	0.000000
117	6	6.291551	-7.880929	0.000000
118	6	3.568048	-7.891314	0.000000
119	6	9.126082	-5.638035	0.000000
120	6	9.130947	-4.229403	0.000000
121	6	4.229209	-9.130779	0.000000
122	6	5.637764	-9.126049	0.000000
123	1	10.051837	-6.202878	0.000000
124	1	10.059579	-3.669818	0.000000
125	1	3.669525	-10.059327	0.000000
126	1	6.202455	-10.051827	0.000000
127	8	7.686339	-7.686617	0.000000
128	8	7.725629	-2.160563	0.000000
129	8	2.160552	-7.725449	0.000000

Table S5. 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	56	0.000000	0.000000	0.000000
2	6	3.058802	8.110919	0.000000
3	6	1.712279	7.682853	0.000000
4	6	0.719924	8.674784	0.000000
5	6	-0.719924	8.674784	0.000000
6	6	-1.123911	10.028474	0.000000
7	6	1.123911	10.028474	0.000000
8	6	-1.712279	7.682853	0.000000
9	8	0.000000	10.877312	0.000000
10	6	-3.058802	8.110919	0.000000
11	6	2.466819	10.446945	0.000000
12	6	3.467043	9.454911	0.000000
13	6	-3.467043	9.454911	0.000000
14	6	-2.466819	10.446945	0.000000
15	1	2.721655	11.501070	0.000000
16	1	4.519038	9.716947	0.000000
17	1	-4.519038	9.716947	0.000000
18	1	-2.721655	11.501070	0.000000
19	6	1.720227	6.235015	0.000000
20	6	3.119460	5.868079	0.000000
21	6	0.727270	5.237925	0.000000
22	6	-0.727270	5.237925	0.000000
23	6	-1.720227	6.235015	0.000000
24	6	1.136695	3.862581	0.000000
25	6	-1.136695	3.862581	0.000000
26	6	-3.119460	5.868079	0.000000
27	6	2.458664	3.518931	0.000000
28	6	3.479905	4.542155	0.000000
29	6	-3.479905	4.542155	0.000000
30	6	-2.458664	3.518931	0.000000
31	8	0.000000	2.975614	0.000000
32	8	3.936682	6.998143	0.000000
33	8	-3.936682	6.998143	0.000000
34	6	10.028474	1.123911	0.000000
35	6	8.674784	0.719924	0.000000
36	6	7.682853	1.712279	0.000000
37	6	6.235015	1.720227	0.000000
38	6	5.868079	3.119460	0.000000
39	6	8.110919	3.058802	0.000000
40	6	5.237925	0.727270	0.000000
41	8	6.998143	3.936682	0.000000
42	6	3.862581	1.136695	0.000000
43	6	9.454911	3.467043	0.000000
44	6	10.446945	2.466819	0.000000
45	6	3.518931	2.458664	0.000000
46	6	4.542155	3.479905	0.000000
47	1	9.716947	4.519038	0.000000
48	1	11.501070	2.721655	0.000000
49	6	8.674784	-0.719924	0.000000
50	6	10.028474	-1.123911	0.000000
51	6	7.682853	-1.712279	0.000000
52	6	6.235015	-1.720227	0.000000
53	6	5.237925	-0.727270	0.000000
54	6	8.110919	-3.058802	0.000000
55	6	5.868079	-3.119460	0.000000
56	6	3.862581	-1.136695	0.000000
57	6	9.454911	-3.467043	0.000000
58	6	10.446945	-2.466819	0.000000
59	6	3.518931	-2.458664	0.000000
60	6	4.542155	-3.479905	0.000000
61	1	9.716947	-4.519038	0.000000
62	1	11.501070	-2.721655	0.000000
63	8	6.998143	-3.936682	0.000000
64	8	10.877312	0.000000	0.000000
65	8	2.975614	0.000000	0.000000
66	6	-3.862581	1.136695	0.000000
67	6	-5.237925	0.727270	0.000000
68	6	-6.235015	1.720227	0.000000
69	6	-7.682853	1.712279	0.000000
70	6	-8.110919	3.058802	0.000000

71	6	-5.868079	3.119460	0.000000
72	6	-8.674784	0.719924	0.000000
73	8	-6.998143	3.936682	0.000000
74	6	-10.028474	1.123911	0.000000
75	6	-4.542155	3.479905	0.000000
76	6	-3.518931	2.458664	0.000000
77	6	-10.446945	2.466819	0.000000
78	6	-9.454911	3.467043	0.000000
79	1	-11.501070	2.721655	0.000000
80	1	-9.716947	4.519038	0.000000
81	6	-5.237925	-0.727270	0.000000
82	6	-3.862581	-1.136695	0.000000
83	6	-6.235015	-1.720227	0.000000
84	6	-7.682853	-1.712279	0.000000
85	6	-8.674784	-0.719924	0.000000
86	6	-5.868079	-3.119460	0.000000
87	6	-8.110919	-3.058802	0.000000
88	6	-10.028474	-1.123911	0.000000
89	6	-4.542155	-3.479905	0.000000
90	6	-3.518931	-2.458664	0.000000
91	6	-10.446945	-2.466819	0.000000
92	6	-9.454911	-3.467043	0.000000
93	1	-11.501070	-2.721655	0.000000
94	1	-9.716947	-4.519038	0.000000
95	8	-6.998143	-3.936682	0.000000
96	8	-2.975614	0.000000	0.000000
97	8	-10.877312	0.000000	0.000000
98	6	3.119460	-5.868079	0.000000
99	6	1.720227	-6.235015	0.000000
100	6	0.727270	-5.237925	0.000000
101	6	-0.727270	-5.237925	0.000000
102	6	-1.136695	-3.862581	0.000000
103	6	1.136695	-3.862581	0.000000
104	6	-1.720227	-6.235015	0.000000
105	8	0.000000	-2.975614	0.000000
106	6	-3.119460	-5.868079	0.000000
107	6	2.458664	-3.518931	0.000000
108	6	3.479905	-4.542155	0.000000
109	6	-3.479905	-4.542155	0.000000
110	6	-2.458664	-3.518931	0.000000
111	6	1.712279	-7.682853	0.000000
112	6	3.058802	-8.110919	0.000000
113	6	0.719924	-8.674784	0.000000
114	6	-0.719924	-8.674784	0.000000
115	6	-1.712279	-7.682853	0.000000
116	6	1.123911	-10.028474	0.000000
117	6	-1.123911	-10.028474	0.000000
118	6	-3.058802	-8.110919	0.000000
119	6	2.466819	-10.446945	0.000000
120	6	3.467043	-9.454911	0.000000
121	6	-3.467043	-9.454911	0.000000
122	6	-2.466819	-10.446945	0.000000
123	1	2.721655	-11.501070	0.000000
124	1	4.519038	-9.716947	0.000000
125	1	-4.519038	-9.716947	0.000000
126	1	-2.721655	-11.501070	0.000000
127	8	0.000000	-10.877312	0.000000
128	8	3.936682	-6.998143	0.000000
129	8	-3.936682	-6.998143	0.000000

Table S6. The optimized Cartesian coordinates of the complex **6** in the ground singlet state calculated at the B3LYP/6-31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	19	0.000000	0.000000	0.000000
2	6	-1.713014	5.215802	2.242701
3	6	-3.054109	4.837694	2.245043
4	6	-3.045090	7.034428	2.446981
5	6	-1.703391	6.639100	2.376006
6	6	-0.713927	7.622172	2.462840
7	6	0.713927	7.622172	2.462840
8	6	1.105729	8.958648	2.613016

9	6	-1.105729	8.958648	2.613016
10	6	1.703391	6.639100	2.376006
11	6	-0.717321	4.221231	2.144076
12	6	0.717321	4.221231	2.144076
13	6	1.713014	5.215802	2.242701
14	8	0.000000	9.784762	2.700005
15	6	-1.109077	2.892605	2.050052
16	6	1.109077	2.892605	2.050052
17	6	3.045090	7.034428	2.446981
18	8	3.877536	5.931261	2.364644
19	6	-2.448160	9.353632	2.676880
20	6	-3.441409	8.368615	2.591846
21	6	3.441409	8.368615	2.591846
22	6	2.448160	9.353632	2.676880
23	1	-2.714017	10.398109	2.796844
24	1	-4.491276	8.634258	2.644258
25	1	4.491276	8.634258	2.644258
26	1	2.714017	10.398109	2.796844
27	8	0.000000	2.061100	1.972396
28	6	-3.488537	3.488537	2.174825
29	6	-2.458215	2.458215	2.070959
30	6	-4.221231	-0.717321	2.144076
31	6	-2.892605	-1.109077	2.050052
32	6	-2.892605	1.109077	2.050052
33	6	-4.221231	0.717321	2.144076
34	6	-5.215802	1.713014	2.242701
35	6	-6.639100	1.703391	2.376006
36	6	-7.034428	3.045090	2.446981
37	6	-4.837694	3.054109	2.245043
38	6	-7.622172	0.713927	2.462840
39	6	-5.215802	-1.713014	2.242701
40	6	-6.639100	-1.703391	2.376006
41	6	-7.622172	-0.713927	2.462840
42	8	-5.931261	3.877536	2.364644
43	8	-2.061100	0.000000	1.972396
44	6	-4.837694	-3.054109	2.245043
45	6	-7.034428	-3.045090	2.446981
46	6	-8.958648	1.105729	2.613016
47	8	-9.784762	0.000000	2.700005
48	6	-8.958648	-1.105729	2.613016
49	6	-9.353632	2.448160	2.676880
50	6	-8.368615	3.441409	2.591846
51	6	-9.353632	-2.448160	2.676880
52	6	-8.368615	-3.441409	2.591846
53	1	-10.398109	2.714017	2.796844
54	1	-8.634258	4.491276	2.644258
55	1	-10.398109	-2.714017	2.796844
56	1	-8.634258	-4.491276	2.644258
57	8	-5.931261	-3.877536	2.364644
58	6	4.221231	-0.717321	2.144076
59	6	2.892605	-1.109077	2.050052
60	6	2.892605	1.109077	2.050052
61	6	4.221231	0.717321	2.144076
62	6	5.215802	1.713014	2.242701
63	6	6.639100	1.703391	2.376006
64	6	7.034428	3.045090	2.446981
65	6	4.837694	3.054109	2.245043
66	6	7.622172	0.713927	2.462840
67	6	5.215802	-1.713014	2.242701
68	6	6.639100	-1.703391	2.376006
69	6	7.622172	-0.713927	2.462840
70	8	5.931261	3.877536	2.364644
71	8	2.061100	0.000000	1.972396
72	6	4.837694	-3.054109	2.245043
73	6	7.034428	-3.045090	2.446981
74	6	8.958648	1.105729	2.613016
75	8	9.784762	0.000000	2.700005
76	6	8.958648	-1.105729	2.613016
77	6	3.488537	3.488537	2.174825
78	6	2.458215	2.458215	2.070959
79	6	9.353632	2.448160	2.676880
80	6	8.368615	3.441409	2.591846
81	6	9.353632	-2.448160	2.676880
82	6	8.368615	-3.441409	2.591846
83	1	10.398109	2.714017	2.796844
84	1	8.634258	4.491276	2.644258
85	1	10.398109	-2.714017	2.796844
86	1	8.634258	-4.491276	2.644258
87	8	5.931261	-3.877536	2.364644

88	6	2.458215	-2.458215	2.070959
89	6	3.488537	-3.488537	2.174825
90	6	1.703391	-6.639100	2.376006
91	6	3.045090	-7.034428	2.446981
92	6	3.054109	-4.837694	2.245043
93	6	1.713014	-5.215802	2.242701
94	6	0.717321	-4.221231	2.144076
95	6	-0.717321	-4.221231	2.144076
96	6	-1.109077	-2.892605	2.050052
97	6	1.109077	-2.892605	2.050052
98	6	-1.713014	-5.215802	2.242701
99	6	0.713927	-7.622172	2.462840
100	6	-0.713927	-7.622172	2.462840
101	6	-1.703391	-6.639100	2.376006
102	8	0.000000	-2.061100	1.972396
103	8	3.877536	-5.931261	2.364644
104	6	1.105729	-8.958648	2.613016
105	6	-1.105729	-8.958648	2.613016
106	6	-3.054109	-4.837694	2.245043
107	8	-3.877536	-5.931261	2.364644
108	6	-3.045090	-7.034428	2.446981
109	6	-3.488537	-3.488537	2.174825
110	6	-2.458215	-2.458215	2.070959
111	6	2.448160	-9.353632	2.676880
112	6	3.441409	-8.368615	2.591846
113	6	-3.441409	-8.368615	2.591846
114	6	-2.448160	-9.353632	2.676880
115	1	2.714017	-10.398109	2.796844
116	1	4.491276	-8.634258	2.644258
117	1	-4.491276	-8.634258	2.644258
118	1	-2.714017	-10.398109	2.796844
119	8	0.000000	-9.784762	2.700005
120	6	3.054109	4.837694	2.245043
121	8	-3.877536	5.931261	2.364644
122	6	-1.713014	5.215802	-2.242701
123	6	-3.054109	4.837694	-2.245043
124	6	-3.045090	7.034428	-2.446981
125	6	-1.703391	6.639100	-2.376006
126	6	-0.713927	7.622172	-2.462840
127	6	0.713927	7.622172	-2.462840
128	6	1.105729	8.958648	-2.613016
129	6	-1.105729	8.958648	-2.613016
130	6	1.703391	6.639100	-2.376006
131	6	-0.717321	4.221231	-2.144076
132	6	0.717321	4.221231	-2.144076
133	6	1.713014	5.215802	-2.242701
134	8	0.000000	9.784762	-2.700005
135	6	-1.109077	2.892605	-2.050052
136	6	1.109077	2.892605	-2.050052
137	6	3.045090	7.034428	-2.446981
138	8	3.877536	5.931261	-2.364644
139	6	-2.448160	9.353632	-2.676880
140	6	-3.441409	8.368615	-2.591846
141	6	3.441409	8.368615	-2.591846
142	6	2.448160	9.353632	-2.676880
143	1	-2.714017	10.398109	-2.796844
144	1	-4.491276	8.634258	-2.644258
145	1	4.491276	8.634258	-2.644258
146	1	2.714017	10.398109	-2.796844
147	8	0.000000	2.061100	-1.972396
148	6	-3.488537	3.488537	-2.174825
149	6	-2.458215	2.458215	-2.070959
150	6	-4.221231	-0.717321	-2.144076
151	6	-2.892605	-1.109077	-2.050052
152	6	-2.892605	1.109077	-2.050052
153	6	-4.221231	0.717321	-2.144076
154	6	-5.215802	1.713014	-2.242701
155	6	-6.639100	1.703391	-2.376006
156	6	-7.034428	3.045090	-2.446981
157	6	-4.837694	3.054109	-2.245043
158	6	-7.622172	0.713927	-2.462840
159	6	-5.215802	-1.713014	-2.242701
160	6	-6.639100	-1.703391	-2.376006
161	6	-7.622172	-0.713927	-2.462840
162	8	-5.931261	3.877536	-2.364644
163	8	-2.061100	0.000000	-1.972396
164	6	-4.837694	-3.054109	-2.245043
165	6	-7.034428	-3.045090	-2.446981
166	6	-8.958648	1.105729	-2.613016

167	8	-9.784762	0.000000	-2.700005
168	6	-8.958648	-1.105729	-2.613016
169	6	-9.353632	2.448160	-2.676880
170	6	-8.368615	3.441409	-2.591846
171	6	-9.353632	-2.448160	-2.676880
172	6	-8.368615	-3.441409	-2.591846
173	1	-10.398109	2.714017	-2.796844
174	1	-8.634258	4.491276	-2.644258
175	1	-10.398109	-2.714017	-2.796844
176	1	-8.634258	-4.491276	-2.644258
177	8	-5.931261	-3.877536	-2.364644
178	6	4.221231	-0.717321	-2.144076
179	6	2.892605	-1.109077	-2.050052
180	6	2.892605	1.109077	-2.050052
181	6	4.221231	0.717321	-2.144076
182	6	5.215802	1.713014	-2.242701
183	6	6.639100	1.703391	-2.376006
184	6	7.034428	3.045090	-2.446981
185	6	4.837694	3.054109	-2.245043
186	6	7.622172	0.713927	-2.462840
187	6	5.215802	-1.713014	-2.242701
188	6	6.639100	-1.703391	-2.376006
189	6	7.622172	-0.713927	-2.462840
190	8	5.931261	3.877536	-2.364644
191	8	2.061100	0.000000	-1.972396
192	6	4.837694	-3.054109	-2.245043
193	6	7.034428	-3.045090	-2.446981
194	6	8.958648	1.105729	-2.613016
195	8	9.784762	0.000000	-2.700005
196	6	8.958648	-1.105729	-2.613016
197	6	3.488537	3.488537	-2.174825
198	6	2.458215	2.458215	-2.070959
199	6	9.353632	2.448160	-2.676880
200	6	8.368615	3.441409	-2.591846
201	6	9.353632	-2.448160	-2.676880
202	6	8.368615	-3.441409	-2.591846
203	1	10.398109	2.714017	-2.796844
204	1	8.634258	4.491276	-2.644258
205	1	10.398109	-2.714017	-2.796844
206	1	8.634258	-4.491276	-2.644258
207	8	5.931261	-3.877536	-2.364644
208	6	2.458215	-2.458215	-2.070959
209	6	3.488537	-3.488537	-2.174825
210	6	1.703391	-6.639100	-2.376006
211	6	3.045090	-7.034428	-2.446981
212	6	3.054109	-4.837694	-2.245043
213	6	1.713014	-5.215802	-2.242701
214	6	0.717321	-4.221231	-2.144076
215	6	-0.717321	-4.221231	-2.144076
216	6	-1.109077	-2.892605	-2.050052
217	6	1.109077	-2.892605	-2.050052
218	6	-1.713014	-5.215802	-2.242701
219	6	0.713927	-7.622172	-2.462840
220	6	-0.713927	-7.622172	-2.462840
221	6	-1.703391	-6.639100	-2.376006
222	8	0.000000	-2.061100	-1.972396
223	8	3.877536	-5.931261	-2.364644
224	6	1.105729	-8.958648	-2.613016
225	6	-1.105729	-8.958648	-2.613016
226	6	-3.054109	-4.837694	-2.245043
227	8	-3.877536	-5.931261	-2.364644
228	6	-3.045090	-7.034428	-2.446981
229	6	-3.488537	-3.488537	-2.174825
230	6	-2.458215	-2.458215	-2.070959
231	6	2.448160	-9.353632	-2.676880
232	6	3.441409	-8.368615	-2.591846
233	6	-3.441409	-8.368615	-2.591846
234	6	-2.448160	-9.353632	-2.676880
235	1	2.714017	-10.398109	-2.796844
236	1	4.491276	-8.634258	-2.644258
237	1	-4.491276	-8.634258	-2.644258
238	1	-2.714017	-10.398109	-2.796844
239	8	0.000000	-9.784762	-2.700005
240	6	3.054109	4.837694	-2.245043
241	8	-3.877536	5.931261	-2.364644

Table S7. The optimized Cartesian coordinates of the complex **7** in the ground singlet state calculated at the B3LYP/6–31G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	20	0.000000	0.000000	0.000000
2	6	-1.709360	5.210025	2.065277
3	6	-3.051517	4.832652	2.072651
4	6	-3.040732	7.021939	2.325166
5	6	-1.700203	6.628821	2.236061
6	6	-0.713013	7.611794	2.339403
7	6	0.713013	7.611794	2.339403
8	6	1.105086	8.944407	2.518809
9	6	-1.105086	8.944407	2.518809
10	6	1.700203	6.628821	2.236061
11	6	-0.718123	4.215779	1.916556
12	6	0.718123	4.215779	1.916556
13	6	1.709360	5.210025	2.065277
14	8	0.000000	9.767016	2.620392
15	6	-1.117911	2.898197	1.766891
16	6	1.117911	2.898197	1.766891
17	6	3.040732	7.021939	2.325166
18	8	3.872599	5.918474	2.224916
19	6	-2.448315	9.336473	2.597147
20	6	-3.439945	8.352012	2.499622
21	6	3.439945	8.352012	2.499622
22	6	2.448315	9.336473	2.597147
23	1	-2.715785	10.377404	2.741469
24	1	-4.489870	8.613412	2.567045
25	1	4.489870	8.613412	2.567045
26	1	2.715785	10.377404	2.741469
27	8	0.000000	2.056156	1.626898
28	6	-3.487846	3.487846	1.974188
29	6	-2.461108	2.461108	1.807448
30	6	-4.215779	-0.718123	1.916556
31	6	-2.898197	-1.117911	1.766891
32	6	-2.898197	1.117911	1.766891
33	6	-4.215779	0.718123	1.916556
34	6	-5.210025	1.709360	2.065277
35	6	-6.628821	1.700203	2.236061
36	6	-7.021939	3.040732	2.325166
37	6	-4.832652	3.051517	2.072651
38	6	-7.611794	0.713013	2.339403
39	6	-5.210025	-1.709360	2.065277
40	6	-6.628821	-1.700203	2.236061
41	6	-7.611794	-0.713013	2.339403
42	8	-5.918474	3.872599	2.224916
43	8	-2.056156	0.000000	1.626898
44	6	-4.832652	-3.051517	2.072651
45	6	-7.021939	-3.040732	2.325166
46	6	-8.944407	1.105086	2.518809
47	8	-9.767016	0.000000	2.620392
48	6	-8.944407	-1.105086	2.518809
49	6	-9.336473	2.448315	2.597147
50	6	-8.352012	3.439945	2.499622
51	6	-9.336473	-2.448315	2.597147
52	6	-8.352012	-3.439945	2.499622
53	1	-10.377404	2.715785	2.741469
54	1	-8.613412	4.489870	2.567045
55	1	-10.377404	-2.715785	2.741469
56	1	-8.613412	-4.489870	2.567045
57	8	-5.918474	-3.872599	2.224916
58	6	4.215779	-0.718123	1.916556
59	6	2.898197	-1.117911	1.766891
60	6	2.898197	1.117911	1.766891
61	6	4.215779	0.718123	1.916556
62	6	5.210025	1.709360	2.065277
63	6	6.628821	1.700203	2.236061
64	6	7.021939	3.040732	2.325166
65	6	4.832652	3.051517	2.072651
66	6	7.611794	0.713013	2.339403
67	6	5.210025	-1.709360	2.065277
68	6	6.628821	-1.700203	2.236061
69	6	7.611794	-0.713013	2.339403
70	8	5.918474	3.872599	2.224916

71	8	2.056156	0.000000	1.626898
72	6	4.832652	-3.051517	2.072651
73	6	7.021939	-3.040732	2.325166
74	6	8.944407	1.105086	2.518809
75	8	9.767016	0.000000	2.620392
76	6	8.944407	-1.105086	2.518809
77	6	3.487846	3.487846	1.974188
78	6	2.461108	2.461108	1.807448
79	6	9.336473	2.448315	2.597147
80	6	8.352012	3.439945	2.499622
81	6	9.336473	-2.448315	2.597147
82	6	8.352012	-3.439945	2.499622
83	1	10.377404	2.715785	2.741469
84	1	8.613412	4.489870	2.567045
85	1	10.377404	-2.715785	2.741469
86	1	8.613412	-4.489870	2.567045
87	8	5.918474	-3.872599	2.224916
88	6	2.461108	-2.461108	1.807448
89	6	3.487846	-3.487846	1.974188
90	6	1.700203	-6.628821	2.236061
91	6	3.040732	-7.021939	2.325166
92	6	3.051517	-4.832652	2.072651
93	6	1.709360	-5.210025	2.065277
94	6	0.718123	-4.215779	1.916556
95	6	-0.718123	-4.215779	1.916556
96	6	-1.117911	-2.898197	1.766891
97	6	1.117911	-2.898197	1.766891
98	6	-1.709360	-5.210025	2.065277
99	6	0.713013	-7.611794	2.339403
100	6	-0.713013	-7.611794	2.339403
101	6	-1.700203	-6.628821	2.236061
102	8	0.000000	-2.056156	1.626898
103	8	3.872599	-5.918474	2.224916
104	6	1.105086	-8.944407	2.518809
105	6	-1.105086	-8.944407	2.518809
106	6	-3.051517	-4.832652	2.072651
107	8	-3.872599	-5.918474	2.224916
108	6	-3.040732	-7.021939	2.325166
109	6	-3.487846	-3.487846	1.974188
110	6	-2.461108	-2.461108	1.807448
111	6	2.448315	-9.336473	2.597147
112	6	3.439945	-8.352012	2.499622
113	6	-3.439945	-8.352012	2.499622
114	6	-2.448315	-9.336473	2.597147
115	1	2.715785	-10.377404	2.741469
116	1	4.489870	-8.613412	2.567045
117	1	-4.489870	-8.613412	2.567045
118	1	-2.715785	-10.377404	2.741469
119	8	0.000000	-9.767016	2.620392
120	6	3.051517	4.832652	2.072651
121	8	-3.872599	5.918474	2.224916
122	6	-1.709360	5.210025	-2.065277
123	6	-3.051517	4.832652	-2.072651
124	6	-3.040732	7.021939	-2.325166
125	6	-1.700203	6.628821	-2.236061
126	6	-0.713013	7.611794	-2.339403
127	6	0.713013	7.611794	-2.339403
128	6	1.105086	8.944407	-2.518809
129	6	-1.105086	8.944407	-2.518809
130	6	1.700203	6.628821	-2.236061
131	6	-0.718123	4.215779	-1.916556
132	6	0.718123	4.215779	-1.916556
133	6	1.709360	5.210025	-2.065277
134	8	0.000000	9.767016	-2.620392
135	6	-1.117911	2.898197	-1.766891
136	6	1.117911	2.898197	-1.766891
137	6	3.040732	7.021939	-2.325166
138	8	3.872599	5.918474	-2.224916
139	6	-2.448315	9.336473	-2.597147
140	6	-3.439945	8.352012	-2.499622
141	6	3.439945	8.352012	-2.499622
142	6	2.448315	9.336473	-2.597147
143	1	-2.715785	10.377404	-2.741469
144	1	-4.489870	8.613412	-2.567045
145	1	4.489870	8.613412	-2.567045
146	1	2.715785	10.377404	-2.741469
147	8	0.000000	2.056156	-1.626898
148	6	-3.487846	3.487846	-1.974188
149	6	-2.461108	2.461108	-1.807448

150	6	-4.215779	-0.718123	-1.916556
151	6	-2.898197	-1.117911	-1.766891
152	6	-2.898197	1.117911	-1.766891
153	6	-4.215779	0.718123	-1.916556
154	6	-5.210025	1.709360	-2.065277
155	6	-6.628821	1.700203	-2.236061
156	6	-7.021939	3.040732	-2.325166
157	6	-4.832652	3.051517	-2.072651
158	6	-7.611794	0.713013	-2.339403
159	6	-5.210025	-1.709360	-2.065277
160	6	-6.628821	-1.700203	-2.236061
161	6	-7.611794	-0.713013	-2.339403
162	8	-5.918474	3.872599	-2.224916
163	8	-2.056156	0.000000	-1.626898
164	6	-4.832652	-3.051517	-2.072651
165	6	-7.021939	-3.040732	-2.325166
166	6	-8.944407	1.105086	-2.518809
167	8	-9.767016	0.000000	-2.620392
168	6	-8.944407	-1.105086	-2.518809
169	6	-9.336473	2.448315	-2.597147
170	6	-8.352012	3.439945	-2.499622
171	6	-9.336473	-2.448315	-2.597147
172	6	-8.352012	-3.439945	-2.499622
173	1	-10.377404	2.715785	-2.741469
174	1	-8.613412	4.489870	-2.567045
175	1	-10.377404	-2.715785	-2.741469
176	1	-8.613412	-4.489870	-2.567045
177	8	-5.918474	-3.872599	-2.224916
178	6	4.215779	-0.718123	-1.916556
179	6	2.898197	-1.117911	-1.766891
180	6	2.898197	1.117911	-1.766891
181	6	4.215779	0.718123	-1.916556
182	6	5.210025	1.709360	-2.065277
183	6	6.628821	1.700203	-2.236061
184	6	7.021939	3.040732	-2.325166
185	6	4.832652	3.051517	-2.072651
186	6	7.611794	0.713013	-2.339403
187	6	5.210025	-1.709360	-2.065277
188	6	6.628821	-1.700203	-2.236061
189	6	7.611794	-0.713013	-2.339403
190	8	5.918474	3.872599	-2.224916
191	8	2.056156	0.000000	-1.626898
192	6	4.832652	-3.051517	-2.072651
193	6	7.021939	-3.040732	-2.325166
194	6	8.944407	1.105086	-2.518809
195	8	9.767016	0.000000	-2.620392
196	6	8.944407	-1.105086	-2.518809
197	6	3.487846	3.487846	-1.974188
198	6	2.461108	2.461108	-1.807448
199	6	9.336473	2.448315	-2.597147
200	6	8.352012	3.439945	-2.499622
201	6	9.336473	-2.448315	-2.597147
202	6	8.352012	-3.439945	-2.499622
203	1	10.377404	2.715785	-2.741469
204	1	8.613412	4.489870	-2.567045
205	1	10.377404	-2.715785	-2.741469
206	1	8.613412	-4.489870	-2.567045
207	8	5.918474	-3.872599	-2.224916
208	6	2.461108	-2.461108	-1.807448
209	6	3.487846	-3.487846	-1.974188
210	6	1.700203	-6.628821	-2.236061
211	6	3.040732	-7.021939	-2.325166
212	6	3.051517	-4.832652	-2.072651
213	6	1.709360	-5.210025	-2.065277
214	6	0.718123	-4.215779	-1.916556
215	6	-0.718123	-4.215779	-1.916556
216	6	-1.117911	-2.898197	-1.766891
217	6	1.117911	-2.898197	-1.766891
218	6	-1.709360	-5.210025	-2.065277
219	6	0.713013	-7.611794	-2.339403
220	6	-0.713013	-7.611794	-2.339403
221	6	-1.700203	-6.628821	-2.236061
222	8	0.000000	-2.056156	-1.626898
223	8	3.872599	-5.918474	-2.224916
224	6	1.105086	-8.944407	-2.518809
225	6	-1.105086	-8.944407	-2.518809
226	6	-3.051517	-4.832652	-2.072651
227	8	-3.872599	-5.918474	-2.224916
228	6	-3.040732	-7.021939	-2.325166

229	6	-3.487846	-3.487846	-1.974188
230	6	-2.461108	-2.461108	-1.807448
231	6	2.448315	-9.336473	-2.597147
232	6	3.439945	-8.352012	-2.499622
233	6	-3.439945	-8.352012	-2.499622
234	6	-2.448315	-9.336473	-2.597147
235	1	2.715785	-10.377404	-2.741469
236	1	4.489870	-8.613412	-2.567045
237	1	-4.489870	-8.613412	-2.567045
238	1	-2.715785	-10.377404	-2.741469
239	8	0.000000	-9.767016	-2.620392
240	6	3.051517	4.832652	-2.072651
241	8	-3.872599	5.918474	-2.224916
