Aromaticity of the planar hetero[8]circulenes and of their doubly charged ions: NICS and GIMIC characterization

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Electronic Supplementary Information

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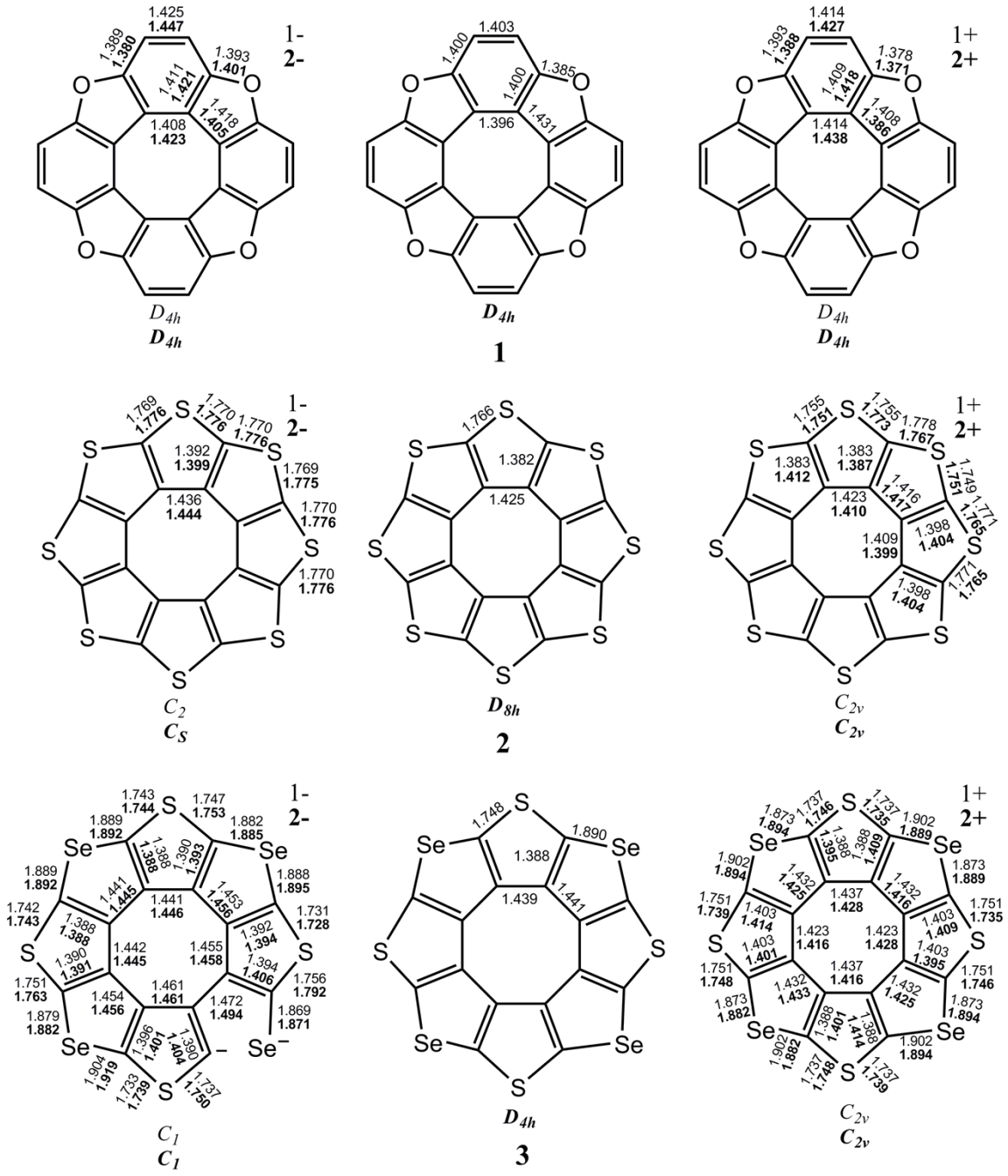


Figure S1. The bond lengths (Å) for the ground state of the molecules **1-3** and for their ions, calculated at the B3LYP/6-31+G(d) level of theory

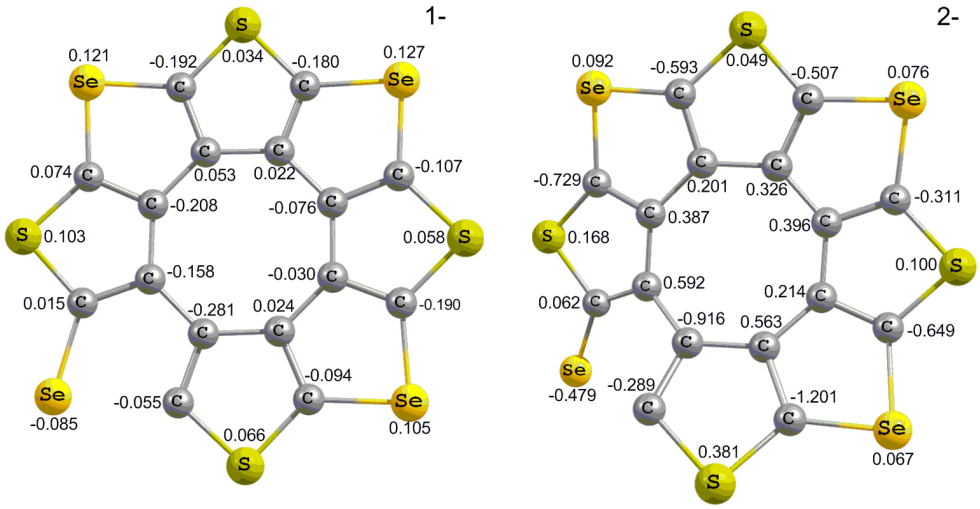


Figure S2. Mulliken charge distribution for the ground singlet state for the anionic forms of the compound **3** calculated at the B3LYP/6-31+G(d) level of theory

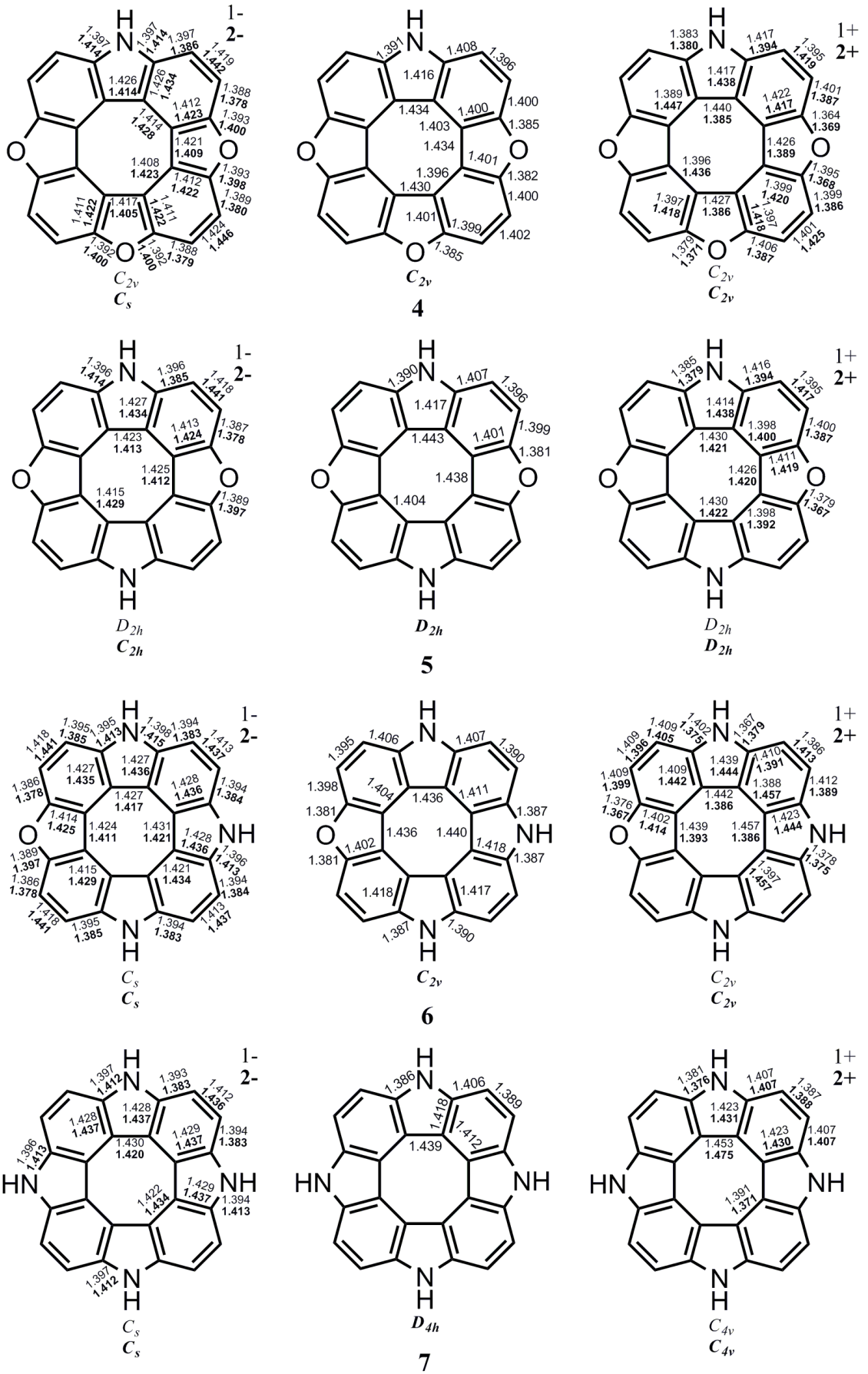
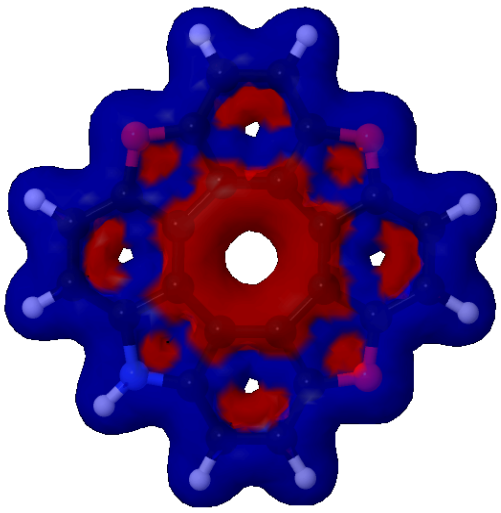
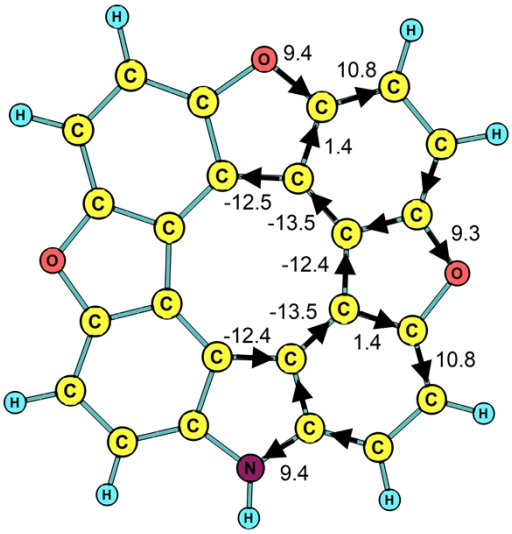


Figure S3. The bond lengths (Å) for the ground state of the molecules **4-7** and for their charged ions, calculated at the B3LYP/6-31+G(d) level of theory

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-13.5
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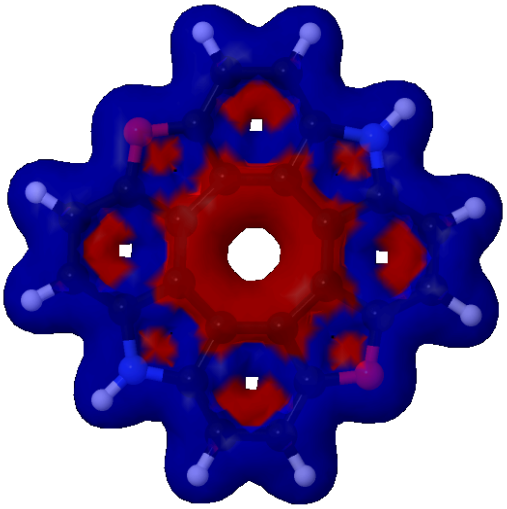
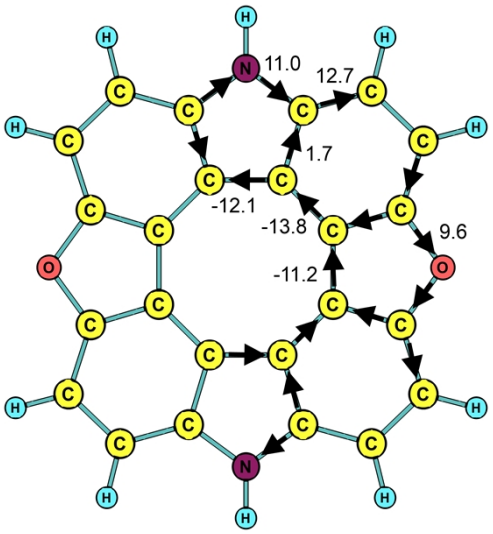
1.4
10.8
9.4

4

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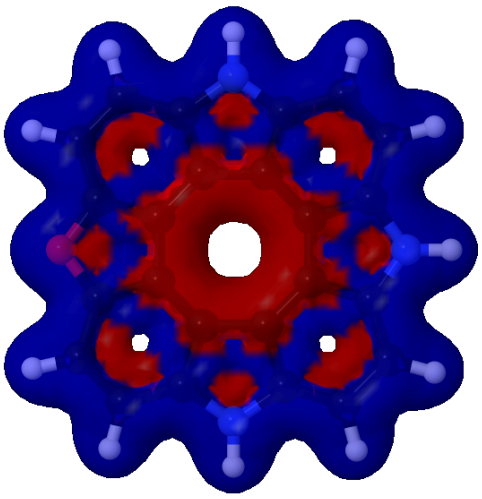
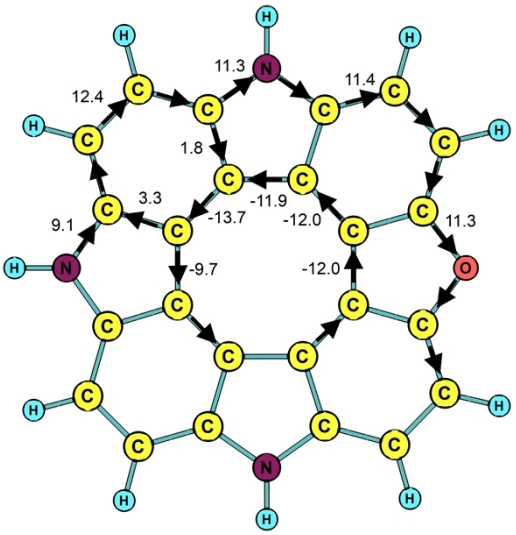
-11.2

5

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11.4
12.4
1.8
3.3
-11.9
9.1
-13.7
-12.0
11.3
-9.7
-12.0

6

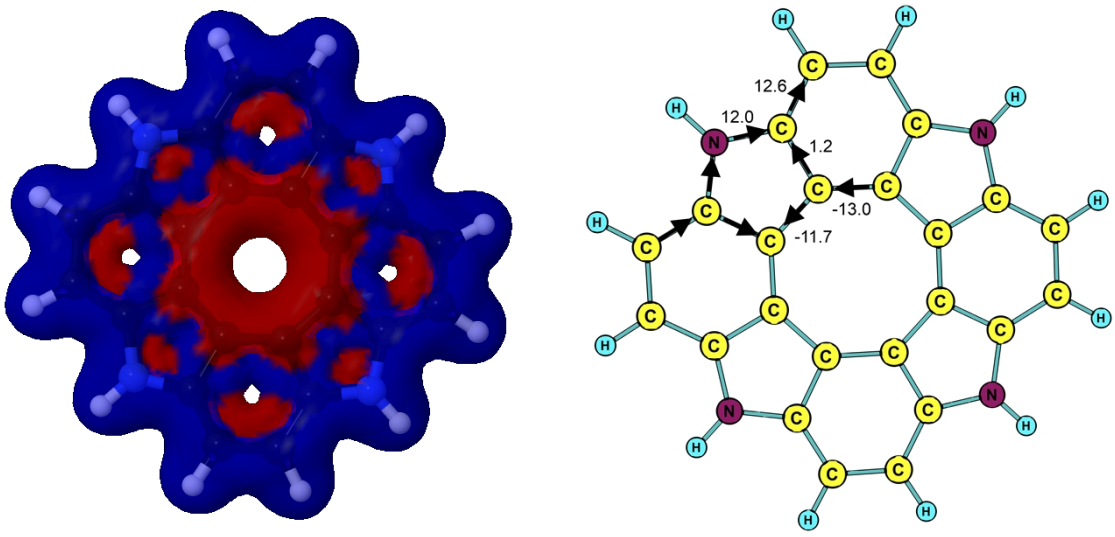

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Figure S4. The ring-current densities (right) and ring-current strengths (right, in $nA \cdot T^{-1}$) in hetero[8]circulenes **4–7** molecules (red and blue colours denote the paratropic and diatropic ring currents, respectively).

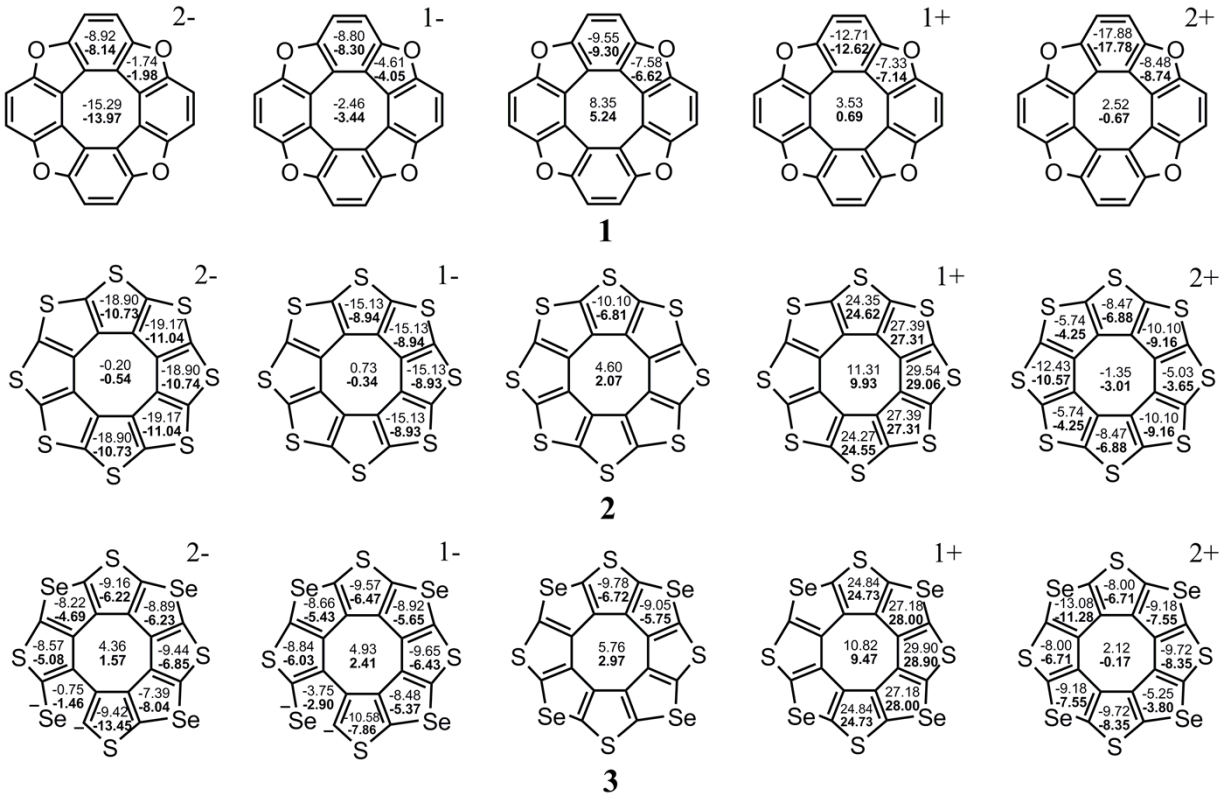

Figure S5. The NICS(0) (top number) and NICS (1) (bottom number in bold) indexes for the ground state of the molecules **1-3** and their ions calculated at the GIAO B3LYP/6-311++G(d,p) level of theory.

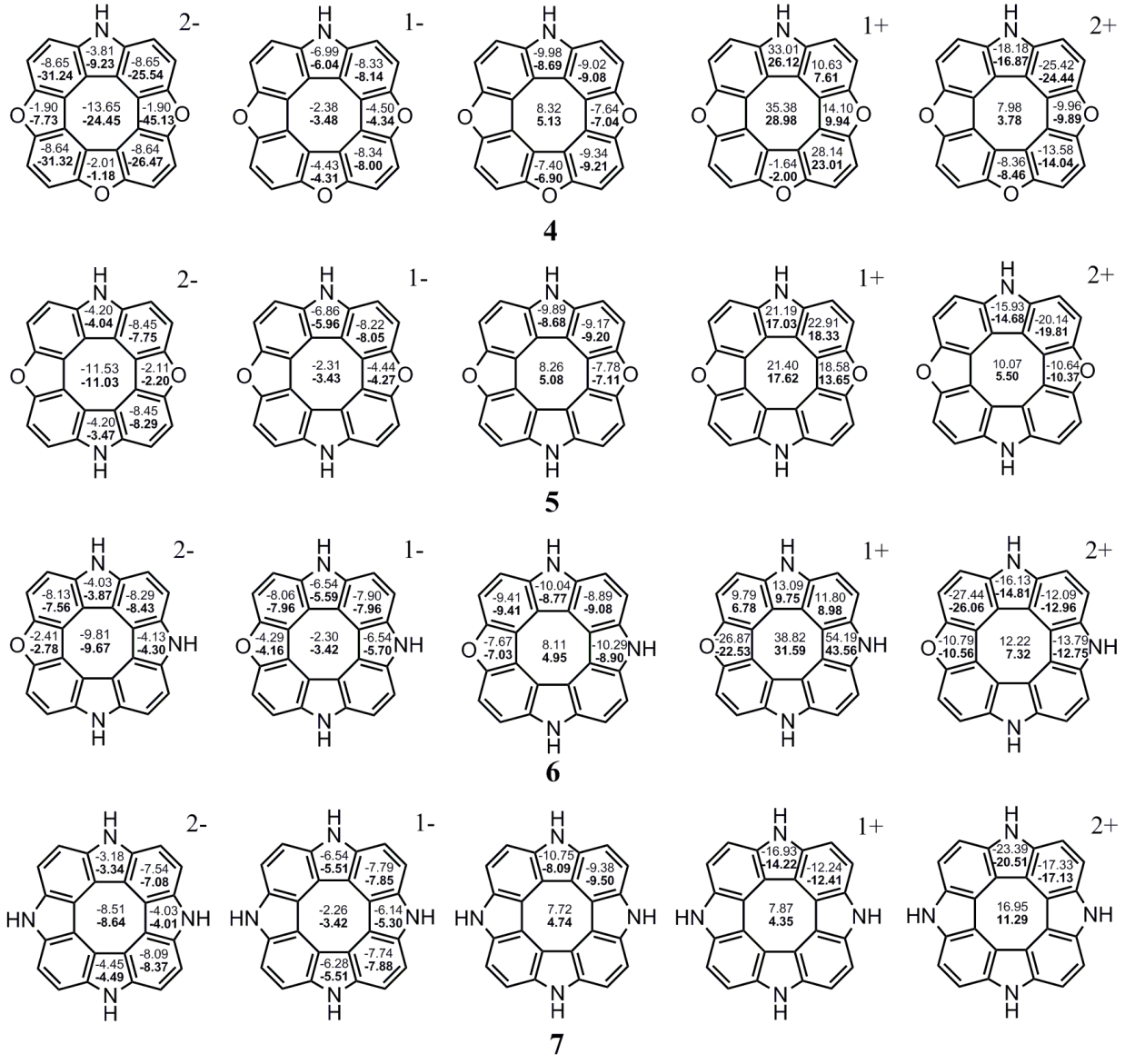

Figure S6. The NICS(0) (top number) and NICS (1) (bottom number in bold) indexes for the ground state of the molecules **4-7** and their ions calculated at the GIAO B3LYP/6-311++G(d,p) level of theory.

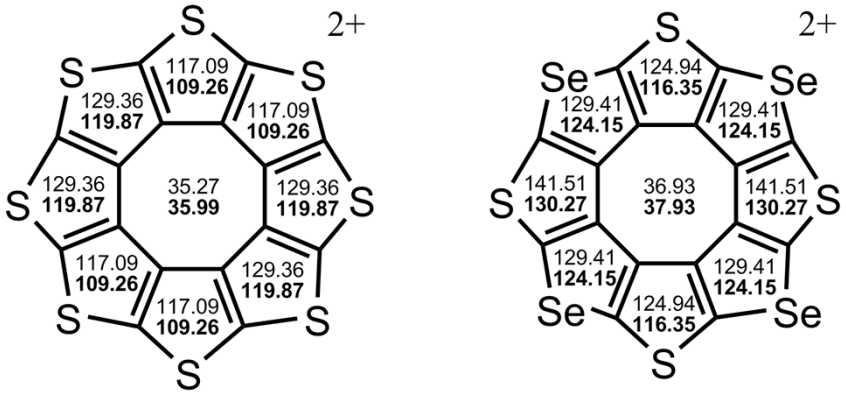

Figure S7. NICS(0) (top number) and NICS(1) (bottom number in bold) indexes, calculated for the singlet state dications of the compounds **2** and **3** at the GIAO B3LYP/6-311++G(d,p) level of theory.

Table S1. The optimized Cartesian coordinates of the compound **1** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.939892	4.119326	0.000000
2	6	-2.236788	3.584554	0.000000
3	6	-2.388164	2.192346	0.000000
4	6	-1.297308	1.314881	0.000000
5	6	-0.006540	1.847127	0.000000
6	6	0.148785	3.238452	0.000000
7	8	1.490579	3.582420	0.000000
8	6	2.192346	2.388164	0.000000
9	6	1.314881	1.297308	0.000000
10	6	3.584554	2.236788	0.000000
11	6	4.119326	0.939892	0.000000
12	1	-0.786271	5.192879	0.000000
13	1	-3.102454	4.237806	0.000000
14	1	4.237806	3.102454	0.000000
15	1	5.192879	0.786271	0.000000
16	6	1.847127	0.006540	0.000000
17	6	3.238452	-0.148785	0.000000
18	8	3.582420	-1.490579	0.000000
19	6	2.388164	-2.192346	0.000000
20	6	1.297308	-1.314881	0.000000
21	6	2.236788	-3.584554	0.000000
22	6	0.939892	-4.119326	0.000000
23	1	3.102454	-4.237806	0.000000
24	1	0.786271	-5.192879	0.000000
25	6	0.006540	-1.847127	0.000000
26	6	-0.148785	-3.238452	0.000000
27	8	-1.490579	-3.582420	0.000000
28	6	-2.192346	-2.388164	0.000000
29	6	-1.314881	-1.297308	0.000000
30	6	-3.584554	-2.236788	0.000000
31	6	-4.119326	-0.939892	0.000000
32	6	-3.238452	0.148785	0.000000
33	6	-1.847127	-0.006540	0.000000
34	1	-4.237806	-3.102454	0.000000
35	1	-5.192879	-0.786271	0.000000
36	8	-3.582420	1.490579	0.000000

Table S2. The optimized Cartesian coordinates for the anion of the compound **1** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.545213	4.195156	0.000000
2	6	-1.906819	3.776325	0.000000
3	6	-2.179256	2.414492	0.000000
4	6	-1.174616	1.424335	0.000000
5	6	0.171040	1.838260	0.000000
6	6	0.445508	3.221870	0.000000
7	8	1.821243	3.439427	0.000000
8	6	2.414492	2.179256	0.000000
9	6	1.424335	1.174616	0.000000
10	6	3.776325	1.906819	0.000000
11	6	4.195156	0.545213	0.000000
12	1	-0.291859	5.249862	0.000000
13	1	-2.709143	4.506304	0.000000
14	1	4.506304	2.709143	0.000000
15	1	5.249862	0.291859	0.000000
16	6	1.838260	-0.171040	0.000000
17	6	3.221870	-0.445508	0.000000
18	8	3.439427	-1.821243	0.000000
19	6	2.179256	-2.414492	0.000000
20	6	1.174616	-1.424335	0.000000
21	6	1.906819	-3.776325	0.000000

22	6	0.545213	-4.195156	0.000000
23	1	2.709143	-4.506304	0.000000
24	1	0.291859	-5.249862	0.000000
25	6	-0.171040	-1.838260	0.000000
26	6	-0.445508	-3.221870	0.000000
27	8	-1.821243	-3.439427	0.000000
28	6	-2.414492	-2.179256	0.000000
29	6	-1.424335	-1.174616	0.000000
30	6	-3.776325	-1.906819	0.000000
31	6	-4.195156	-0.545213	0.000000
32	6	-3.221870	0.445508	0.000000
33	6	-1.838260	0.171040	0.000000
34	1	-4.506304	-2.709143	0.000000
35	1	-5.249862	-0.291859	0.000000
36	8	-3.439427	1.821243	0.000000

Table S3. The optimized Cartesian coordinates for the dianion of the compound **1** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.135431	4.085830	0.000000
2	6	-0.304573	4.229709	0.000000
3	6	-1.074265	3.083790	0.000000
4	6	-0.538535	1.767503	0.000000
5	6	0.877602	1.626008	0.000000
6	6	1.663178	2.810275	0.000000
7	8	3.022959	2.473749	0.000000
8	6	3.083790	1.074265	0.000000
9	6	1.767503	0.538535	0.000000
10	6	4.229709	0.304573	0.000000
11	6	4.085830	-1.135431	0.000000
12	1	1.779306	4.961166	0.000000
13	1	-0.762527	5.215137	0.000000
14	1	5.215137	0.762527	0.000000
15	1	4.961166	-1.779306	0.000000
16	6	1.626008	-0.877602	0.000000
17	6	2.810275	-1.663178	0.000000
18	8	2.473749	-3.022959	0.000000
19	6	1.074265	-3.083790	0.000000
20	6	0.538535	-1.767503	0.000000
21	6	0.304573	-4.229709	0.000000
22	6	-1.135431	-4.085830	0.000000
23	1	0.762527	-5.215137	0.000000
24	1	-1.779306	-4.961166	0.000000
25	6	-0.877602	-1.626008	0.000000
26	6	-1.663178	-2.810275	0.000000
27	8	-3.022959	-2.473749	0.000000
28	6	-3.083790	-1.074265	0.000000
29	6	-1.767503	-0.538535	0.000000
30	6	-4.229709	-0.304573	0.000000
31	6	-4.085830	1.135431	0.000000
32	6	-2.810275	1.663178	0.000000
33	6	-1.626008	0.877602	0.000000
34	1	-5.215137	-0.762527	0.000000
35	1	-4.961166	1.779306	0.000000
36	8	-2.473749	3.022959	0.000000

Table S4. The optimized Cartesian coordinates for the cation of the compound **1** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.959032	3.006524	0.000000
2	6	1.799538	3.815326	0.000000
3	6	0.549136	3.201734	0.000000
4	6	0.394246	1.801199	0.000000
5	6	1.554198	0.992077	0.000000
6	6	2.815055	1.621146	0.000000
7	8	3.822028	0.680970	0.000000
8	6	3.201734	-0.549136	0.000000
9	6	1.801199	-0.394246	0.000000
10	6	3.815326	-1.799538	0.000000
11	6	3.006524	-2.959032	0.000000
12	1	3.941967	3.463228	0.000000
13	1	1.888657	4.895511	0.000000
14	1	4.895511	-1.888657	0.000000
15	1	3.463228	-3.941967	0.000000
16	6	0.992077	-1.554198	0.000000
17	6	1.621146	-2.815055	0.000000
18	8	0.680970	-3.822028	0.000000
19	6	-0.549136	-3.201734	0.000000
20	6	-0.394246	-1.801199	0.000000
21	6	-1.799538	-3.815326	0.000000
22	6	-2.959032	-3.006524	0.000000
23	1	-1.888657	-4.895511	0.000000
24	1	-3.941967	-3.463228	0.000000
25	6	-1.554198	-0.992077	0.000000
26	6	-2.815055	-1.621146	0.000000
27	8	-3.822028	-0.680970	0.000000
28	6	-3.201734	0.549136	0.000000
29	6	-1.801199	0.394246	0.000000
30	6	-3.815326	1.799538	0.000000
31	6	-3.006524	2.959032	0.000000
32	6	-1.621146	2.815055	0.000000
33	6	-0.992077	1.554198	0.000000
34	1	-4.895511	1.888657	0.000000
35	1	-3.463228	3.941967	0.000000
36	8	-0.680970	3.822028	0.000000

Table S5. The optimized Cartesian coordinates for the dication of the compound **1** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.950140	3.014012	0.000000
2	6	1.776573	3.825099	0.000000
3	6	0.529888	3.215537	0.000000
4	6	0.374579	1.806162	0.000000
5	6	1.557142	0.988858	0.000000
6	6	2.820625	1.632341	0.000000
7	8	3.824294	0.698475	0.000000
8	6	3.215537	-0.529888	0.000000
9	6	1.806162	-0.374579	0.000000
10	6	3.825099	-1.776573	0.000000
11	6	3.014012	-2.950140	0.000000
12	1	3.928720	3.482355	0.000000
13	1	1.868759	4.906055	0.000000
14	1	4.906055	-1.868759	0.000000
15	1	3.482355	-3.928720	0.000000
16	6	0.988858	-1.557142	0.000000
17	6	1.632341	-2.820625	0.000000
18	8	0.698475	-3.824294	0.000000
19	6	-0.529888	-3.215537	0.000000
20	6	-0.374579	-1.806162	0.000000
21	6	-1.776573	-3.825099	0.000000
22	6	-2.950140	-3.014012	0.000000

23	1	-1.868759	-4.906055	0.000000
24	1	-3.928720	-3.482355	0.000000
25	6	-1.557142	-0.988858	0.000000
26	6	-2.820625	-1.632341	0.000000
27	8	-3.824294	-0.698475	0.000000
28	6	-3.215537	0.529888	0.000000
29	6	-1.806162	0.374579	0.000000
30	6	-3.825099	1.776573	0.000000
31	6	-3.014012	2.950140	0.000000
32	6	-1.632341	2.820625	0.000000
33	6	-0.988858	1.557142	0.000000
34	1	-4.906055	1.868759	0.000000
35	1	-3.482355	3.928720	0.000000
36	8	-0.698475	3.824294	0.000000

Table S6. The optimized Cartesian coordinates of the compound **2** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	16	3.007081	-3.007081	0.000000
2	6	-0.712573	1.720303	0.000000
3	6	0.712573	1.720303	0.000000
4	6	-1.720303	-0.712573	0.000000
5	6	-1.720303	0.712573	0.000000
6	6	1.720303	0.712573	0.000000
7	6	1.720303	-0.712573	0.000000
8	6	-0.712573	-1.720303	0.000000
9	16	-3.007081	3.007081	0.000000
10	16	0.000000	4.252655	0.000000
11	16	3.007081	3.007081	0.000000
12	16	4.252655	0.000000	0.000000
13	16	-3.007081	-3.007081	0.000000
14	16	-4.252655	0.000000	0.000000
15	6	-2.996866	-1.241342	0.000000
16	6	-2.996866	1.241342	0.000000
17	6	-1.241342	2.996866	0.000000
18	6	1.241342	2.996866	0.000000
19	6	2.996866	1.241342	0.000000
20	6	2.996866	-1.241342	0.000000
21	6	-1.241342	-2.996866	0.000000
22	6	0.712573	-1.720303	0.000000
23	6	1.241342	-2.996866	0.000000
24	16	0.000000	-4.252655	0.000000

Table S7. The optimized Cartesian coordinates for the anion of the compound **2** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.320983	1.333060	-0.277357
2	6	2.290951	2.311936	-0.081585
3	6	-0.008442	1.876498	-0.277051
4	6	-0.014665	3.254412	-0.080590
5	6	-1.876310	-0.008576	-0.275631
6	6	-1.332743	1.320828	-0.277039
7	6	-3.253937	-0.014887	-0.077773
8	6	-2.311533	2.290638	-0.080846
9	16	-1.642584	3.914872	0.133252
10	16	1.606697	3.930017	0.132832
11	16	-3.929272	1.607052	0.134861
12	6	1.332743	-1.320828	-0.277039
13	6	1.876310	0.008576	-0.275631
14	6	3.253937	0.014887	-0.077773
15	6	2.311533	-2.290638	-0.080846

16	16	3.929272	-1.607052	0.134861
17	6	0.014665	-3.254412	-0.080590
18	6	0.008442	-1.876498	-0.277051
19	16	1.642584	-3.914872	0.133252
20	6	-1.320983	-1.333060	-0.277357
21	6	-2.290951	-2.311936	-0.081585
22	16	-1.606697	-3.930017	0.132832
23	16	-3.914789	-1.642360	0.134507
24	16	3.914789	1.642360	0.134507

Table S8. The optimized Cartesian coordinates for the dianion of the compound **2** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.348649	-1.743095	0.722012
2	6	0.119633	-3.017955	1.250074
3	6	0.348681	-0.722019	1.743185
4	6	0.120115	-1.250169	3.018131
5	6	0.348706	1.742983	0.721974
6	6	0.348643	0.721962	1.743171
7	6	0.119768	3.017870	1.250039
8	6	0.119999	1.250057	3.018115
9	16	-0.175690	0.000034	4.244001
10	16	-0.175144	-3.001439	3.000951
11	16	-0.175634	3.001497	3.000708
12	6	0.348681	-0.722019	-1.743185
13	6	0.348649	-1.743095	-0.722012
14	6	0.119633	-3.017955	-1.250074
15	6	0.120115	-1.250169	-3.018131
16	16	-0.175144	-3.001439	-3.000951
17	6	0.119999	1.250057	-3.018115
18	6	0.348643	0.721962	-1.743171
19	16	-0.175690	0.000034	-4.244001
20	6	0.348706	1.742983	-0.721974
21	6	0.119768	3.017870	-1.250039
22	16	-0.175634	3.001497	-3.000708
23	16	-0.176024	4.243990	0.000000
24	16	-0.176684	-4.243899	0.000000

Table S9. The optimized Cartesian coordinates for the cation of the compound **2** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.711385	1.706366
2	6	0.000000	-0.711385	1.706366
3	6	0.000000	-1.712594	0.704744
4	6	0.000000	-1.712581	-0.704644
5	6	0.000000	-0.711380	-1.706365
6	6	0.000000	0.711380	-1.706365
7	6	0.000000	1.712581	-0.704644
8	6	0.000000	1.712594	0.704744
9	6	0.000000	1.238929	2.985036
10	6	0.000000	-1.238929	2.985036
11	6	0.000000	-3.003378	1.241120
12	6	0.000000	-3.003620	-1.240895
13	6	0.000000	-1.239218	-2.984976
14	6	0.000000	1.239218	-2.984976
15	6	0.000000	3.003620	-1.240895
16	6	0.000000	3.003378	1.241120
17	16	0.000000	-4.267208	-0.000056
18	16	0.000000	-3.016898	-2.989799
19	16	0.000000	0.000000	-4.227568
20	16	0.000000	3.016898	-2.989799

21	16	0.000000	4.267208	-0.000056
22	16	0.000000	3.016656	2.989734
23	16	0.000000	0.000000	4.227519
24	16	0.000000	-3.016656	2.989734

Table S10. The optimized Cartesian coordinates for the singlet state dication of the compound **2** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.836672	0.000058
2	6	1.309854	1.293964	0.000047
3	6	-1.309854	1.293964	0.000047
4	6	0.000000	3.215795	0.000038
5	6	2.293816	2.286017	-0.000026
6	6	-2.293816	2.286017	-0.000026
7	16	-3.959247	1.605746	0.000003
8	16	-1.638791	3.887277	-0.000046
9	16	1.638791	3.887277	-0.000046
10	16	3.959247	1.605746	0.000003
11	6	-3.267153	0.000000	0.000080
12	6	-1.846330	0.000000	0.000013
13	6	1.309854	-1.293964	0.000047
14	6	0.000000	-1.836672	0.000058
15	6	-1.309854	-1.293964	0.000047
16	6	2.293816	-2.286017	-0.000026
17	6	0.000000	-3.215795	0.000038
18	6	-2.293816	-2.286017	-0.000026
19	16	3.959247	-1.605746	0.000003
20	16	1.638791	-3.887277	-0.000046
21	16	-1.638791	-3.887277	-0.000046
22	16	-3.959247	-1.605746	0.000003
23	6	1.846330	0.000000	0.000013
24	6	3.267153	0.000000	0.000080

Table S11. The optimized Cartesian coordinates for the triplet state dication of the compound **2** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.699457	1.703110
2	6	0.000000	-0.699457	1.703110
3	6	0.000000	-1.702966	0.702959
4	6	0.000000	-1.699918	-0.706635
5	6	0.000000	-0.709908	-1.699562
6	6	0.000000	0.709908	-1.699562
7	6	0.000000	1.699918	-0.706635
8	6	0.000000	1.702966	0.702959
9	6	0.000000	1.237247	3.000327
10	6	0.000000	-1.237247	3.000327
11	6	0.000000	-2.983874	1.233983
12	6	0.000000	-3.004121	-1.246655
13	6	0.000000	-1.242955	-2.987558
14	6	0.000000	1.242955	-2.987558
15	6	0.000000	3.004121	-1.246655
16	6	0.000000	2.983874	1.233983
17	16	0.000000	-4.245084	-0.011572
18	16	0.000000	-3.014664	-3.003132
19	16	0.000000	0.000000	-4.230879
20	16	0.000000	3.014664	-3.003132
21	16	0.000000	4.245084	-0.011572
22	16	0.000000	2.987974	3.000604
23	16	0.000000	0.000000	4.259103
24	16	0.000000	-2.987974	3.000604

Table S12. The optimized Cartesian coordinates of the compound **3** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	34	0.826039	4.328534	0.000000
2	34	-4.328534	0.826039	0.000000
3	16	-2.402075	3.535100	0.000000
4	16	3.535100	2.402075	0.000000
5	6	-1.572462	1.033751	0.000000
6	6	-0.382027	1.842643	0.000000
7	6	-1.842643	-0.382027	0.000000
8	6	1.816301	2.718288	0.000000
9	6	-0.687620	3.196125	0.000000
10	6	1.033751	1.572462	0.000000
11	6	-2.718288	1.816301	0.000000
12	6	-3.196125	-0.687620	0.000000
13	34	-0.826039	-4.328534	0.000000
14	34	4.328534	-0.826039	0.000000
15	16	2.402075	-3.535100	0.000000
16	16	-3.535100	-2.402075	0.000000
17	6	1.572462	-1.033751	0.000000
18	6	0.382027	-1.842643	0.000000
19	6	1.842643	0.382027	0.000000
20	6	-1.816301	-2.718288	0.000000
21	6	0.687620	-3.196125	0.000000
22	6	-1.033751	-1.572462	0.000000
23	6	2.718288	-1.816301	0.000000
24	6	3.196125	0.687620	0.000000

Table S13. The optimized Cartesian coordinates for the anion of the compound **3** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.572531	1.127193	0.000151
2	6	-0.339424	1.897298	-0.000155
3	6	-0.585380	3.271467	-0.000219
4	6	-2.729250	1.897900	0.000322
5	34	-2.427545	3.752738	0.000093
6	6	-3.278036	-0.486092	-0.000300
7	6	-1.906231	-0.275427	-0.000113
8	16	-4.219680	0.978927	-0.000078
9	6	-1.141916	-1.496979	0.000122
10	6	-1.929180	-2.639777	0.000231
11	34	-3.788457	-2.305037	-0.000169
12	6	1.094308	1.616657	0.000216
13	6	1.852792	2.781241	0.000318
14	6	1.867965	0.364451	0.000001
15	6	3.254419	0.513332	-0.000220
16	6	0.265102	-1.810290	-0.000073
17	6	1.498350	-1.042432	0.000268
18	6	0.452615	-3.187869	-0.000151
19	6	2.616769	-1.871916	0.000336
20	34	2.255980	-3.725197	0.000058
21	16	4.120348	-1.014246	0.000007
22	34	4.179856	2.137313	-0.000208
23	16	-1.020193	-4.126571	0.000148
24	16	0.869738	4.212745	0.000126

Table S14. The optimized Cartesian coordinates for the dianion of the compound **3** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.854759	-1.471335	-0.233164
2	6	-1.602949	-0.874266	-0.187137
3	6	-0.539441	-1.796884	0.137897
4	6	-0.982554	-3.094971	0.351146
5	34	-2.849987	-3.323319	0.155066
6	6	0.901348	-1.695270	0.168269
7	6	1.837062	-0.645866	-0.210435
8	6	1.469057	-2.947524	0.381005
9	6	3.106396	-1.168781	-0.491406
10	34	3.315100	-3.007009	0.017657
11	16	0.300311	-4.251686	0.584641
12	6	-1.671714	0.555770	-0.393007
13	6	-0.727625	1.650884	-0.218625
14	6	-1.390212	2.870475	-0.087471
15	6	-2.994565	0.951590	-0.574979
16	34	-3.253058	2.813663	-0.431378
17	6	0.718203	1.765979	-0.071114
18	6	1.080915	3.045612	0.383418
19	6	1.771776	0.788605	-0.479387
20	6	2.919503	1.320836	-1.088042
21	34	2.630404	3.830302	1.080073
22	16	-0.322930	4.158986	0.344682
23	16	4.130139	0.060477	-1.172940
24	16	-4.162912	-0.354827	-0.522009

Table S15. The optimized Cartesian coordinates for the cation of the compound **3** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.718332	1.723486	0.000000
2	6	-1.730776	0.711265	0.000000
3	6	-1.224655	3.016255	0.000000
4	16	0.000000	4.247616	0.000000
5	34	-3.124545	3.097251	0.000000
6	6	-3.036223	1.225947	0.000000
7	16	-4.286682	0.000000	0.000000
8	6	1.730776	0.711265	0.000000
9	6	0.718332	1.723486	0.000000
10	6	3.036223	1.225947	0.000000
11	34	3.124545	3.097251	0.000000
12	6	1.224655	3.016255	0.000000
13	6	-1.730776	-0.711265	0.000000
14	6	-0.718332	-1.723486	0.000000
15	6	-3.036223	-1.225947	0.000000
16	34	-3.124545	-3.097251	0.000000
17	6	-1.224655	-3.016255	0.000000
18	6	0.718332	-1.723486	0.000000
19	6	1.730776	-0.711265	0.000000
20	6	1.224655	-3.016255	0.000000
21	6	3.036223	-1.225947	0.000000
22	16	4.286682	0.000000	0.000000
23	34	3.124545	-3.097251	0.000000
24	16	0.000000	-4.247616	0.000000

Table S16. The optimized Cartesian coordinates for the dication singlet state of the compound **3** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.717425	1.712223	0.000000
2	6	-1.725595	0.704803	0.000000
3	6	-1.221850	3.006633	0.000000
4	16	0.000000	4.229200	0.000000
5	34	-3.137788	3.079804	0.000000
6	6	-3.044985	1.226363	0.000000
7	16	-4.302173	0.000000	0.000000
8	6	1.725595	0.704803	0.000000
9	6	0.717425	1.712223	0.000000
10	6	3.044985	1.226363	0.000000
11	34	3.137788	3.079804	0.000000
12	6	1.221850	3.006633	0.000000
13	6	-1.725595	-0.704803	0.000000
14	6	-0.717425	-1.712223	0.000000
15	6	-3.044985	-1.226363	0.000000
16	34	-3.137788	-3.079804	0.000000
17	6	-1.221850	-3.006633	0.000000
18	6	0.717425	-1.712223	0.000000
19	6	1.725595	-0.704803	0.000000
20	6	1.221850	-3.006633	0.000000
21	6	3.044985	-1.226363	0.000000
22	16	4.302173	0.000000	0.000000
23	34	3.137788	-3.079804	0.000000
24	16	0.000000	-4.229200	0.000000

Table S17. The optimized Cartesian coordinates for the triplet state dication of the compound **3** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.707963	1.718852
2	6	0.000000	-0.707963	1.718852
3	6	0.000000	-1.718749	0.710454
4	6	0.000000	-1.717184	-0.714554
5	6	0.000000	-0.716709	-1.717203
6	6	0.000000	0.716709	-1.717203
7	6	0.000000	1.717184	-0.714554
8	6	0.000000	1.718749	0.710454
9	6	0.000000	1.270687	3.010316
10	6	0.000000	-1.270687	3.010316
11	6	0.000000	-2.997455	1.267751
12	6	0.000000	-3.013326	-1.278914
13	6	0.000000	-1.275656	-3.001368
14	6	0.000000	1.275656	-3.001368
15	6	0.000000	3.013326	-1.278914
16	6	0.000000	2.997455	1.267751
17	34	0.000000	-4.396691	-0.008694
18	16	0.000000	-3.023882	-3.017619
19	34	0.000000	0.000000	-4.385603
20	16	0.000000	3.023882	-3.017619
21	34	0.000000	4.396691	-0.008694
22	16	0.000000	3.005745	3.013358
23	34	0.000000	0.000000	4.408647
24	16	0.000000	-3.005745	3.013358

Table S18. The optimized Cartesian coordinates of the compound **4** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.714964	1.706034
2	6	0.000000	1.106024	3.050997
3	6	0.000000	-1.106024	3.050997
4	6	0.000000	-0.714964	1.706034
5	6	0.000000	-1.699544	0.715783
6	6	0.000000	-1.702407	-0.718537
7	6	0.000000	-3.051446	-1.092868
8	6	0.000000	-3.042586	1.115631
9	6	0.000000	-0.717242	-1.717996
10	6	0.000000	1.699544	0.715783
11	6	0.000000	1.702407	-0.718537
12	6	0.000000	0.717242	-1.717996
13	8	0.000000	-3.880112	0.016753
14	8	0.000000	0.000000	3.884098
15	6	0.000000	3.042586	1.115631
16	6	0.000000	3.051446	-1.092868
17	8	0.000000	3.880112	0.016753
18	6	0.000000	-1.136853	-3.070317
19	6	0.000000	1.136853	-3.070317
20	6	0.000000	-3.437959	2.458280
21	6	0.000000	-2.447205	3.450118
22	6	0.000000	-2.498611	-3.428897
23	6	0.000000	-3.472295	-2.427950
24	6	0.000000	3.437959	2.458280
25	6	0.000000	2.447205	3.450118
26	6	0.000000	2.498611	-3.428897
27	6	0.000000	3.472295	-2.427950
28	1	0.000000	-4.488305	2.726228
29	1	0.000000	-2.715255	4.500363
30	1	0.000000	-2.798229	-4.472302
31	1	0.000000	-4.527291	-2.677023
32	1	0.000000	4.488305	2.726228
33	1	0.000000	2.715255	4.500363
34	1	0.000000	2.798229	-4.472302
35	1	0.000000	4.527291	-2.677023
36	7	0.000000	0.000000	-3.871513
37	1	0.000000	0.000000	-4.878113

Table S19. The optimized Cartesian coordinates for the anion of the compound **4** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.708535	1.707667
2	6	0.000000	1.113169	3.059693
3	6	0.000000	-1.113169	3.059693
4	6	0.000000	-0.708535	1.707667
5	6	0.000000	-1.701788	0.709215
6	6	0.000000	-1.704822	-0.712190
7	6	0.000000	-3.061709	-1.101032
8	6	0.000000	-3.051691	1.122211
9	6	0.000000	-0.712165	-1.719703
10	6	0.000000	1.701788	0.709215
11	6	0.000000	1.704822	-0.712190
12	6	0.000000	0.712165	-1.719703
13	8	0.000000	-3.892675	0.016602
14	8	0.000000	0.000000	3.895757
15	6	0.000000	3.051691	1.122211
16	6	0.000000	3.061709	-1.101032
17	8	0.000000	3.892675	0.016602
18	6	0.000000	-1.145175	-3.077852
19	6	0.000000	1.145175	-3.077852
20	6	0.000000	-3.448639	2.452950
21	6	0.000000	-2.442096	3.460181

22	6	0.000000	-2.494017	-3.440587
23	6	0.000000	-3.482827	-2.423357
24	6	0.000000	3.448639	2.452950
25	6	0.000000	2.442096	3.460181
26	6	0.000000	2.494017	-3.440587
27	6	0.000000	3.482827	-2.423357
28	1	0.000000	-4.499897	2.720449
29	1	0.000000	-2.709578	4.511409
30	1	0.000000	-2.791508	-4.485900
31	1	0.000000	-4.538861	-2.671969
32	1	0.000000	4.499897	2.720449
33	1	0.000000	2.709578	4.511409
34	1	0.000000	2.791508	-4.485900
35	1	0.000000	4.538861	-2.671969
36	7	0.000000	0.000000	-3.877572
37	1	0.000000	0.000000	-4.883015

Table S20. The optimized Cartesian coordinates for the dianion of the compound **4** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.022030	-1.712126	0.702318
2	6	0.011809	-3.070901	1.120881
3	6	0.011809	-3.070901	-1.120881
4	6	0.022030	-1.712126	-0.702318
5	6	0.015111	-0.703069	-1.705684
6	6	0.016813	0.705743	-1.708437
7	6	-0.014615	1.109493	-3.073134
8	6	-0.008659	-1.129696	-3.061989
9	6	0.025993	1.724385	-0.707189
10	6	0.015111	-0.703069	1.705684
11	6	0.016813	0.705743	1.708437
12	6	0.025993	1.724385	0.707189
13	8	-0.026486	-0.016138	-3.906277
14	8	0.011274	-3.910284	0.000000
15	6	-0.008659	-1.129696	3.061989
16	6	-0.014615	1.109493	3.073134
17	8	-0.026486	-0.016138	3.906277
18	6	0.020131	3.086987	-1.152795
19	6	0.020131	3.086987	1.152795
20	6	-0.016059	-2.450637	-3.462183
21	6	-0.004064	-3.474019	-2.440037
22	6	-0.013137	3.453943	-2.488969
23	6	-0.036287	2.421256	-3.495670
24	6	-0.016059	-2.450637	3.462183
25	6	-0.004064	-3.474019	2.440037
26	6	-0.013137	3.453943	2.488969
27	6	-0.036287	2.421256	3.495670
28	1	-0.034689	-2.718693	-4.515103
29	1	-0.014096	-4.526930	-2.708528
30	1	-0.010541	4.502038	-2.785282
31	1	-0.066129	2.671998	-4.552791
32	1	-0.034689	-2.718693	4.515103
33	1	-0.014096	-4.526930	2.708528
34	1	-0.010541	4.502038	2.785282
35	1	-0.066129	2.671998	4.552791
36	7	0.095168	3.902936	0.000000
37	1	-0.310457	4.826792	0.000000

Table S21. The optimized Cartesian coordinates for the cation of the compound **4** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.713411	1.703521
2	6	0.000000	1.102444	3.044997
3	6	0.000000	-1.102444	3.044997
4	6	0.000000	-0.713411	1.703521
5	6	0.000000	-1.700519	0.716573
6	6	0.000000	-1.696293	-0.709453
7	6	0.000000	-3.065164	-1.096337
8	6	0.000000	-3.042087	1.112333
9	6	0.000000	-0.720065	-1.697568
10	6	0.000000	1.700519	0.716573
11	6	0.000000	1.696293	-0.709453
12	6	0.000000	0.720065	-1.697568
13	8	0.000000	-3.880491	-0.002784
14	8	0.000000	0.000000	3.873871
15	6	0.000000	3.042087	1.112333
16	6	0.000000	3.065164	-1.096337
17	8	0.000000	3.880491	-0.002784
18	6	0.000000	-1.137255	-3.051312
19	6	0.000000	1.137255	-3.051312
20	6	0.000000	-3.444815	2.452445
21	6	0.000000	-2.451762	3.441315
22	6	0.000000	-2.503471	-3.427176
23	6	0.000000	-3.482803	-2.433695
24	6	0.000000	3.444815	2.452445
25	6	0.000000	2.451762	3.441315
26	6	0.000000	2.503471	-3.427176
27	6	0.000000	3.482803	-2.433695
28	1	0.000000	-4.494239	2.721462
29	1	0.000000	-2.721150	4.491244
30	1	0.000000	-2.793697	-4.472555
31	1	0.000000	-4.536120	-2.686778
32	1	0.000000	4.494239	2.721462
33	1	0.000000	2.721150	4.491244
34	1	0.000000	2.793697	-4.472555
35	1	0.000000	4.536120	-2.686778
36	7	0.000000	0.000000	-3.838559
37	1	0.000000	0.000000	-4.850988

Table S22. The optimized Cartesian coordinates for the dication of the compound **4** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.707166	-0.693690
2	6	0.000000	3.069702	-1.083332
3	6	0.000000	0.692389	-1.725177
4	6	0.000000	-1.707166	-0.693690
5	6	0.000000	-0.692389	-1.725177
6	6	0.000000	-3.069702	-1.083332
7	6	0.000000	1.127823	-3.095839
8	6	0.000000	-1.127823	-3.095839
9	6	0.000000	2.481288	-3.430019
10	6	0.000000	3.469499	-2.411714
11	6	0.000000	-2.481288	-3.430019
12	6	0.000000	-3.469499	-2.411714
13	1	0.000000	2.800861	-4.467107
14	1	0.000000	4.521553	-2.676122
15	1	0.000000	-2.800861	-4.467107
16	1	0.000000	-4.521553	-2.676122
17	6	0.000000	-0.692827	1.713863
18	6	0.000000	-1.098640	3.072626
19	6	0.000000	1.098640	3.072626
20	6	0.000000	0.692827	1.713863
21	6	0.000000	1.704495	0.694897

22	6	0.000000	3.062651	1.109765
23	6	0.000000	-1.704495	0.694897
24	8	0.000000	0.000000	3.891982
25	6	0.000000	-3.062651	1.109765
26	6	0.000000	3.439504	2.444013
27	6	0.000000	2.432557	3.452142
28	6	0.000000	-3.439504	2.444013
29	6	0.000000	-2.432557	3.452142
30	1	0.000000	4.486708	2.726809
31	1	0.000000	2.715827	4.499205
32	1	0.000000	-4.486708	2.726809
33	1	0.000000	-2.715827	4.499205
34	8	0.000000	3.885260	0.016523
35	8	0.000000	-3.885260	0.016523
36	7	0.000000	0.000000	-3.890579
37	1	0.000000	0.000000	-4.902188

Table S23. The optimized Cartesian coordinates of the compound **5** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.716606	1.721241
2	6	0.000000	1.136238	3.074292
3	6	0.000000	-1.136238	3.074292
4	6	0.000000	-0.716606	1.721241
5	6	0.000000	-1.699123	0.718780
6	6	0.000000	-1.699123	-0.718780
7	6	0.000000	-3.047009	-1.101869
8	6	0.000000	-3.047009	1.101869
9	6	0.000000	-0.716606	-1.721241
10	6	0.000000	1.699123	0.718780
11	6	0.000000	1.699123	-0.718780
12	6	0.000000	0.716606	-1.721241
13	8	0.000000	-3.880265	0.000000
14	7	0.000000	0.000000	3.875463
15	6	0.000000	3.047009	1.101869
16	6	0.000000	3.047009	-1.101869
17	8	0.000000	3.880265	0.000000
18	6	0.000000	-1.136238	-3.074292
19	7	0.000000	0.000000	-3.875463
20	6	0.000000	1.136238	-3.074292
21	6	0.000000	-3.468302	2.436140
22	6	0.000000	-2.495760	3.437175
23	6	0.000000	-2.495760	-3.437175
24	6	0.000000	-3.468302	-2.436140
25	6	0.000000	3.468302	2.436140
26	6	0.000000	2.495760	3.437175
27	6	0.000000	2.495760	-3.437175
28	6	0.000000	3.468302	-2.436140
29	1	0.000000	-4.523989	2.682642
30	1	0.000000	-2.793089	4.481287
31	1	0.000000	-2.793089	-4.481287
32	1	0.000000	-4.523989	-2.682642
33	1	0.000000	4.523989	2.682642
34	1	0.000000	2.793089	4.481287
35	1	0.000000	2.793089	-4.481287
36	1	0.000000	4.523989	-2.682642
37	1	0.000000	0.000000	-4.881893
38	1	0.000000	0.000000	4.881893

Table S24. The optimized Cartesian coordinates for the anion of the compound **5** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.711500	1.722601
2	6	0.000000	1.144767	3.081728
3	6	0.000000	-1.144767	3.081728
4	6	0.000000	-0.711500	1.722601
5	6	0.000000	-1.701901	0.712307
6	6	0.000000	-1.701901	-0.712307
7	6	0.000000	-3.057789	-1.109573
8	6	0.000000	-3.057789	1.109573
9	6	0.000000	-0.711500	-1.722601
10	6	0.000000	1.701901	0.712307
11	6	0.000000	1.701901	-0.712307
12	6	0.000000	0.711500	-1.722601
13	8	0.000000	-3.893594	0.000000
14	7	0.000000	0.000000	3.881286
15	6	0.000000	3.057789	1.109573
16	6	0.000000	3.057789	-1.109573
17	8	0.000000	3.893594	0.000000
18	6	0.000000	-1.144767	-3.081728
19	7	0.000000	0.000000	-3.881286
20	6	0.000000	1.144767	-3.081728
21	6	0.000000	-3.479325	2.431388
22	6	0.000000	-2.491257	3.448572
23	6	0.000000	-2.491257	-3.448572
24	6	0.000000	-3.479325	-2.431388
25	6	0.000000	3.479325	2.431388
26	6	0.000000	2.491257	3.448572
27	6	0.000000	2.491257	-3.448572
28	6	0.000000	3.479325	-2.431388
29	1	0.000000	-4.536000	2.677844
30	1	0.000000	-2.786551	4.494654
31	1	0.000000	-2.786551	-4.494654
32	1	0.000000	-4.536000	-2.677844
33	1	0.000000	4.536000	2.677844
34	1	0.000000	2.786551	4.494654
35	1	0.000000	2.786551	-4.494654
36	1	0.000000	4.536000	-2.677844
37	1	0.000000	0.000000	-4.886558
38	1	0.000000	0.000000	4.886558

Table S25. The optimized Cartesian coordinates for the dianion of the compound **5** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.005804	1.727816	0.706718
2	6	-0.009184	3.091229	1.152226
3	6	-0.009184	3.091229	-1.152226
4	6	-0.005804	1.727816	-0.706718
5	6	-0.002433	0.706065	-1.705302
6	6	0.002433	-0.706065	-1.705302
7	6	-0.005899	-1.117650	-3.068927
8	6	0.005899	1.117650	-3.068927
9	6	0.005804	-1.727816	-0.706718
10	6	-0.002433	0.706065	1.705302
11	6	0.002433	-0.706065	1.705302
12	6	0.005804	-1.727816	0.706718
13	8	0.000000	0.000000	-3.907111
14	7	-0.085773	3.907001	0.000000
15	6	0.005899	1.117650	3.068927
16	6	-0.005899	-1.117650	3.068927
17	8	0.000000	0.000000	3.907111
18	6	0.009184	-3.091229	-1.152226
19	7	0.085773	-3.907001	0.000000

20	6	0.009184	-3.091229	1.152226
21	6	0.021197	2.429239	-3.492502
22	6	0.010183	3.461853	-2.486884
23	6	-0.010183	-3.461853	-2.486884
24	6	-0.021197	-2.429239	-3.492502
25	6	0.021197	2.429239	3.492502
26	6	0.010183	3.461853	2.486884
27	6	-0.010183	-3.461853	2.486884
28	6	-0.021197	-2.429239	3.492502
29	1	0.033540	2.677061	-4.550759
30	1	-0.001818	4.510617	-2.780960
31	1	0.001818	-4.510617	-2.780960
32	1	-0.033540	-2.677061	-4.550759
33	1	0.033540	2.677061	4.550759
34	1	-0.001818	4.510617	2.780960
35	1	0.001818	-4.510617	2.780960
36	1	-0.033540	-2.677061	4.550759
37	1	-0.319650	-4.831016	0.000000
38	1	0.319650	4.831016	0.000000

Table S26. The optimized Cartesian coordinates for the cation of the compound **5** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.714981	1.708812
2	6	0.000000	1.132609	3.059875
3	6	0.000000	-1.132609	3.059875
4	6	0.000000	-0.714981	1.708812
5	6	0.000000	-1.696253	0.712964
6	6	0.000000	-1.696253	-0.712964
7	6	0.000000	-3.052581	-1.100608
8	6	0.000000	-3.052581	1.100608
9	6	0.000000	-0.714981	-1.708812
10	6	0.000000	1.696253	0.712964
11	6	0.000000	1.696253	-0.712964
12	6	0.000000	0.714981	-1.708812
13	8	0.000000	-3.883808	0.000000
14	7	0.000000	0.000000	3.856377
15	6	0.000000	3.052581	1.100608
16	6	0.000000	3.052581	-1.100608
17	8	0.000000	3.883808	0.000000
18	6	0.000000	-1.132609	-3.059875
19	7	0.000000	0.000000	-3.856377
20	6	0.000000	1.132609	-3.059875
21	6	0.000000	-3.476590	2.434344
22	6	0.000000	-2.499090	3.429803
23	6	0.000000	-2.499090	-3.429803
24	6	0.000000	-3.476590	-2.434344
25	6	0.000000	3.476590	2.434344
26	6	0.000000	2.499090	3.429803
27	6	0.000000	2.499090	-3.429803
28	6	0.000000	3.476590	-2.434344
29	1	0.000000	-4.530740	2.683530
30	1	0.000000	-2.793321	4.474197
31	1	0.000000	-2.793321	-4.474197
32	1	0.000000	-4.530740	-2.683530
33	1	0.000000	4.530740	2.683530
34	1	0.000000	2.793321	4.474197
35	1	0.000000	2.793321	-4.474197
36	1	0.000000	4.530740	-2.683530
37	1	0.000000	0.000000	-4.866676
38	1	0.000000	0.000000	4.866676

Table S27. The optimized Cartesian coordinates for the dication of the compound **5** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	0.692050	1.729955
2	6	0.000000	1.127381	3.100209
3	6	0.000000	-1.127381	3.100209
4	6	0.000000	-0.692050	1.729955
5	6	0.000000	-1.702653	0.695354
6	6	0.000000	-1.702653	-0.695354
7	6	0.000000	-3.064303	-1.093936
8	6	0.000000	-3.064303	1.093936
9	6	0.000000	-0.692050	-1.729955
10	6	0.000000	1.702653	0.695354
11	6	0.000000	1.702653	-0.695354
12	6	0.000000	0.692050	-1.729955
13	8	0.000000	-3.883396	0.000000
14	7	0.000000	0.000000	3.894821
15	6	0.000000	3.064303	1.093936
16	6	0.000000	3.064303	-1.093936
17	8	0.000000	3.883396	0.000000
18	6	0.000000	-1.127381	-3.100209
19	7	0.000000	0.000000	-3.894821
20	6	0.000000	1.127381	-3.100209
21	6	0.000000	-3.465655	2.420953
22	6	0.000000	-2.479326	3.438670
23	6	0.000000	-2.479326	-3.438670
24	6	0.000000	-3.465655	-2.420953
25	6	0.000000	3.465655	2.420953
26	6	0.000000	2.479326	3.438670
27	6	0.000000	2.479326	-3.438670
28	6	0.000000	3.465655	-2.420953
29	1	0.000000	-4.518353	2.681946
30	1	0.000000	-2.796251	4.476411
31	1	0.000000	-2.796251	-4.476411
32	1	0.000000	-4.518353	-2.681946
33	1	0.000000	4.518353	2.681946
34	1	0.000000	2.796251	4.476411
35	1	0.000000	2.796251	-4.476411
36	1	0.000000	4.518353	-2.681946
37	1	0.000000	0.000000	-4.906245
38	1	0.000000	0.000000	4.906245

Table S28. The optimized Cartesian coordinates of the compound **6** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.720932	-0.719199
2	6	0.000000	3.078920	-1.122154
3	6	0.000000	3.070096	1.145616
4	6	0.000000	1.718107	0.716777
5	6	0.000000	0.718104	1.702439
6	6	0.000000	-0.718104	1.702439
7	6	0.000000	-1.101155	3.050971
8	6	0.000000	1.101155	3.050971
9	6	0.000000	-1.718107	0.716777
10	6	0.000000	0.720099	-1.714492
11	6	0.000000	-0.720099	-1.714492
12	6	0.000000	-1.720932	-0.719199
13	8	0.000000	0.000000	3.884359
14	7	0.000000	3.875613	0.016609
15	6	0.000000	1.132250	-3.070764
16	6	0.000000	-1.132250	-3.070764
17	6	0.000000	-3.070096	1.145616
18	7	0.000000	-3.875613	0.016609
19	6	0.000000	-3.078920	-1.122154

20	6	0.000000	2.433213	3.476594
21	6	0.000000	3.433453	2.504347
22	6	0.000000	-3.433453	2.504347
23	6	0.000000	-2.433213	3.476594
24	6	0.000000	2.485229	-3.456227
25	6	0.000000	3.468337	-2.473768
26	6	0.000000	-3.468337	-2.473768
27	6	0.000000	-2.485229	-3.456227
28	1	0.000000	2.677095	4.532891
29	1	0.000000	4.478281	2.799619
30	1	0.000000	-4.478281	2.799619
31	1	0.000000	-2.677095	4.532891
32	1	0.000000	2.762154	-4.506228
33	1	0.000000	4.518341	-2.750334
34	1	0.000000	-4.518341	-2.750334
35	1	0.000000	-2.762154	-4.506228
36	1	0.000000	-4.881845	0.020128
37	1	0.000000	4.881845	0.020128
38	7	0.000000	0.000000	-3.871880
39	1	0.000000	0.000000	-4.878056

Table S29. The optimized Cartesian coordinates for the anion of the compound **6** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.008028	0.714631	1.722844
2	6	-0.018885	1.131576	3.087754
3	6	-0.024340	-1.153163	3.077463
4	6	-0.013886	-0.711938	1.719941
5	6	-0.006306	-1.704712	0.711817
6	6	-0.006306	-1.704712	-0.711817
7	6	0.005572	-3.061487	-1.108975
8	6	0.005572	-3.061487	1.108975
9	6	-0.013886	-0.711938	-1.719941
10	6	0.008381	1.716964	0.715541
11	6	0.008381	1.716964	-0.715541
12	6	-0.008028	0.714631	-1.722844
13	8	0.014545	-3.897174	0.000000
14	7	-0.065062	-0.016104	3.884457
15	6	0.035312	3.079419	1.140939
16	6	0.035312	3.079419	-1.140939
17	6	-0.024340	-1.153163	-3.077463
18	7	-0.065062	-0.016104	-3.884457
19	6	-0.018885	1.131576	-3.087754
20	6	0.006324	-3.486919	2.428510
21	6	-0.012738	-2.498910	3.444846
22	6	-0.012738	-2.498910	-3.444846
23	6	0.006324	-3.486919	-2.428510
24	6	0.030287	3.467671	2.480291
25	6	-0.003927	2.469174	3.479497
26	6	-0.003927	2.469174	-3.479497
27	6	0.030287	3.467671	-2.480291
28	1	0.016901	-4.543998	2.673127
29	1	-0.020244	-2.792488	4.491502
30	1	-0.020244	-2.792488	-4.491502
31	1	0.016901	-4.543998	-2.673127
32	1	0.053608	4.519135	2.756182
33	1	-0.015921	2.744890	4.531157
34	1	-0.015921	2.744890	-4.531157
35	1	0.053608	4.519135	-2.756182
36	1	0.101460	-0.020570	-4.876499
37	1	0.101460	-0.020570	4.876499
38	7	0.091149	3.881408	0.000000
39	1	-0.088330	4.871390	0.000000

Table S30. The optimized Cartesian coordinates for the dianion of the compound **6** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.026665	0.709695	1.727156
2	6	-0.050464	1.140082	3.097108
3	6	-0.061569	-1.159720	3.085998
4	6	-0.040215	-0.707044	1.724538
5	6	-0.017857	-1.708164	0.705514
6	6	-0.017857	-1.708164	-0.705514
7	6	0.020101	-3.072063	-1.117118
8	6	0.020101	-3.072063	1.117118
9	6	-0.040215	-0.707044	-1.724538
10	6	0.017609	1.720438	0.710625
11	6	0.017609	1.720438	-0.710625
12	6	-0.026665	0.709695	-1.727156
13	8	0.047680	-3.909634	0.000000
14	7	-0.157970	-0.014711	3.908215
15	6	0.083724	3.086733	1.148882
16	6	0.083724	3.086733	-1.148882
17	6	-0.061569	-1.159720	-3.085998
18	7	-0.157970	-0.014711	-3.908215
19	6	-0.050464	1.140082	-3.097108
20	6	0.025515	-3.498683	2.427009
21	6	-0.026571	-2.493461	3.457891
22	6	-0.026571	-2.493461	-3.457891
23	6	0.025515	-3.498683	-2.427009
24	6	0.073214	3.478489	2.476231
25	6	-0.010734	2.465268	3.491514
26	6	-0.010734	2.465268	-3.491514
27	6	0.073214	3.478489	-2.476231
28	1	0.057033	-4.556970	2.673248
29	1	-0.047039	-2.785281	4.507263
30	1	-0.047039	-2.785281	-4.507263
31	1	0.057033	-4.556970	-2.673248
32	1	0.135847	4.531055	2.751036
33	1	-0.040033	2.740536	4.545408
34	1	-0.040033	2.740536	-4.545408
35	1	0.135847	4.531055	-2.751036
36	1	0.268146	-0.020357	-4.823665
37	1	0.268146	-0.020357	4.823665
38	7	0.206454	3.900003	0.000000
39	1	-0.195968	4.826200	0.000000

Table S31. The optimized Cartesian coordinates for the cation of the compound **6** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.712294	-0.715701
2	6	0.000000	3.090079	-1.130252
3	6	0.000000	3.062383	1.144129
4	6	0.000000	1.716290	0.726228
5	6	0.000000	0.719260	1.704553
6	6	0.000000	-0.719260	1.704553
7	6	0.000000	-1.101422	3.053934
8	6	0.000000	1.101422	3.053934
9	6	0.000000	-1.716290	0.726228
10	6	0.000000	0.728359	-1.694436
11	6	0.000000	-0.728359	-1.694436
12	6	0.000000	-1.712294	-0.715701
13	8	0.000000	0.000000	3.879116
14	7	0.000000	3.866082	-0.004811
15	6	0.000000	1.137203	-3.057334

16	6	0.000000	-1.137203	-3.057334
17	6	0.000000	-3.062383	1.144129
18	7	0.000000	-3.866082	-0.004811
19	6	0.000000	-3.090079	-1.130252
20	6	0.000000	2.436408	3.472886
21	6	0.000000	3.435737	2.498288
22	6	0.000000	-3.435737	2.498288
23	6	0.000000	-2.436408	3.472886
24	6	0.000000	2.489921	-3.460906
25	6	0.000000	3.475861	-2.486895
26	6	0.000000	-3.475861	-2.486895
27	6	0.000000	-2.489921	-3.460906
28	1	0.000000	2.686138	4.527428
29	1	0.000000	4.479882	2.791868
30	1	0.000000	-4.479882	2.791868
31	1	0.000000	-2.686138	4.527428
32	1	0.000000	2.756611	-4.512345
33	1	0.000000	4.523560	-2.766743
34	1	0.000000	-4.523560	-2.766743
35	1	0.000000	-2.756611	-4.512345
36	1	0.000000	-4.875738	-0.001131
37	1	0.000000	4.875738	-0.001131
38	7	0.000000	0.000000	-3.835690
39	1	0.000000	0.000000	-4.847819

Table S32. The optimized Cartesian coordinates for the dication of the compound **6** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	1.727621	-0.691123
2	6	0.000000	3.100322	-1.110765
3	6	0.000000	3.096956	1.139540
4	6	0.000000	1.725572	0.695261
5	6	0.000000	0.696687	1.708439
6	6	0.000000	-0.696687	1.708439
7	6	0.000000	-1.093750	3.065291
8	6	0.000000	1.093750	3.065291
9	6	0.000000	-1.725572	0.695261
10	6	0.000000	0.693108	-1.716908
11	6	0.000000	-0.693108	-1.716908
12	6	0.000000	-1.727621	-0.691123
13	8	0.000000	0.000000	3.884870
14	7	0.000000	3.892850	0.018339
15	6	0.000000	1.123258	-3.095791
16	6	0.000000	-1.123258	-3.095791
17	6	0.000000	-3.096956	1.139540
18	7	0.000000	-3.892850	0.018339
19	6	0.000000	-3.100322	-1.110765
20	6	0.000000	2.422431	3.472386
21	6	0.000000	3.437928	2.491433
22	6	0.000000	-3.437928	2.491433
23	6	0.000000	-2.422431	3.472386
24	6	0.000000	2.465264	-3.455107
25	6	0.000000	3.462935	-2.454150
26	6	0.000000	-3.462935	-2.454150
27	6	0.000000	-2.465264	-3.455107
28	1	0.000000	2.678591	4.526200
29	1	0.000000	4.476424	2.805174
30	1	0.000000	-4.476424	2.805174
31	1	0.000000	-2.678591	4.526200
32	1	0.000000	2.763680	-4.498295
33	1	0.000000	4.506947	-2.750503
34	1	0.000000	-4.506947	-2.750503
35	1	0.000000	-2.763680	-4.498295
36	1	0.000000	-4.903889	0.020492
37	1	0.000000	4.903889	0.020492
38	7	0.000000	0.000000	-3.889104
39	1	0.000000	0.000000	-4.900185

Table S33. The optimized Cartesian coordinates of the compound **7** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.132494	1.478421	0.000000
2	6	2.104687	2.510951	0.000000
3	6	3.230304	0.547470	0.000000
4	6	1.848041	0.230247	0.000000
5	6	1.478421	-1.132494	0.000000
6	6	0.230247	-1.848041	0.000000
7	6	0.547470	-3.230304	0.000000
8	6	2.510951	-2.104687	0.000000
9	6	-1.132494	-1.478421	0.000000
10	6	-0.230247	1.848041	0.000000
11	6	-1.478421	1.132494	0.000000
12	6	-1.848041	-0.230247	0.000000
13	7	1.927629	-3.362482	0.000000
14	7	3.362482	1.927629	0.000000
15	6	-0.547470	3.230304	0.000000
16	6	-2.510951	2.104687	0.000000
17	6	-2.104687	-2.510951	0.000000
18	7	-3.362482	-1.927629	0.000000
19	6	-3.230304	-0.547470	0.000000
20	6	3.876808	-1.771183	0.000000
21	6	4.240450	-0.430485	0.000000
22	6	-1.771183	-3.876808	0.000000
23	6	-0.430485	-4.240450	0.000000
24	6	0.430485	4.240450	0.000000
25	6	1.771183	3.876808	0.000000
26	6	-4.240450	0.430485	0.000000
27	6	-3.876808	1.771183	0.000000
28	1	4.637442	-2.546226	0.000000
29	1	5.288461	-0.146006	0.000000
30	1	-2.546226	-4.637442	0.000000
31	1	-0.146006	-5.288461	0.000000
32	1	0.146006	5.288461	0.000000
33	1	2.546226	4.637442	0.000000
34	1	-5.288461	0.146006	0.000000
35	1	-4.637442	2.546226	0.000000
36	1	-4.235283	-2.427985	0.000000
37	1	4.235283	2.427985	0.000000
38	7	-1.927629	3.362482	0.000000
39	1	-2.427985	4.235283	0.000000
40	1	2.427985	-4.235283	0.000000

Table S34. The optimized Cartesian coordinates for the anion of the compound **7** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.025853	3.083078	1.140262
2	6	-0.005518	1.719891	0.714990
3	6	-0.019896	0.714984	1.720291
4	6	-0.019813	-0.715114	1.720377
5	6	-0.021229	-1.139992	3.083677
6	6	-0.028755	1.140090	3.083555
7	6	-0.006827	-1.719864	0.714859
8	7	-0.080989	-0.000035	3.888616
9	6	0.017567	-3.083516	1.140523
10	6	-0.012051	2.477048	3.475840
11	6	0.023782	3.475479	2.477396
12	6	0.032372	-3.475605	2.477859
13	6	0.009213	-2.476678	3.476139
14	1	-0.023744	2.750301	4.528268
15	1	0.051542	4.527586	2.750721
16	1	0.052663	-4.527837	2.751396
17	1	0.010006	-2.749656	4.528707

18	1	0.166879	0.001080	4.864277
19	6	-0.005518	1.719891	-0.714990
20	6	0.025853	3.083078	-1.140262
21	6	-0.019896	0.714984	-1.720291
22	6	-0.019813	-0.715114	-1.720377
23	6	-0.006827	-1.719864	-0.714859
24	6	-0.028755	1.140090	-3.083555
25	6	-0.021229	-1.139992	-3.083677
26	6	0.017567	-3.083516	-1.140523
27	6	-0.012051	2.477048	-3.475840
28	6	0.023782	3.475479	-2.477396
29	6	0.032372	-3.475605	-2.477859
30	6	0.009213	-2.476678	-3.476139
31	1	-0.023744	2.750301	-4.528268
32	1	0.051542	4.527586	-2.750721
33	1	0.052663	-4.527837	-2.751396
34	1	0.010006	-2.749656	-4.528707
35	7	-0.080989	-0.000035	-3.888616
36	1	0.166879	0.001080	-4.864277
37	7	0.087505	3.885536	0.000000
38	7	0.001446	-3.884955	0.000000
39	1	-0.111980	4.871862	0.000000
40	1	0.172107	-4.875987	0.000000

Table S35. The optimized Cartesian coordinates for the dianion of the compound **7** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.048341	3.091641	1.148244
2	6	-0.012317	1.724111	0.710178
3	6	-0.043145	0.710079	1.724335
4	6	-0.046252	-0.710411	1.724563
5	6	-0.037358	-1.147600	3.093585
6	6	-0.053267	1.148023	3.092948
7	6	-0.025458	-1.724519	0.710232
8	7	-0.138139	-0.000319	3.912132
9	6	0.025520	-3.092567	1.148353
10	6	-0.020908	2.473001	3.488319
11	6	0.045106	3.486971	2.473713
12	6	0.066484	-3.486257	2.473687
13	6	0.029260	-2.471218	3.488912
14	1	-0.040373	2.744997	4.543395
15	1	0.105295	4.540448	2.745881
16	1	0.099980	-4.540972	2.745732
17	1	0.036132	-2.742759	4.544283
18	1	0.317684	0.003963	4.813481
19	6	-0.012317	1.724111	-0.710178
20	6	0.048341	3.091641	-1.148244
21	6	-0.043145	0.710079	-1.724335
22	6	-0.046252	-0.710411	-1.724563
23	6	-0.025458	-1.724519	-0.710232
24	6	-0.053267	1.148023	-3.092948
25	6	-0.037358	-1.147600	-3.093585
26	6	0.025520	-3.092567	-1.148353
27	6	-0.020908	2.473001	-3.488319
28	6	0.045106	3.486971	-2.473713
29	6	0.066484	-3.486257	-2.473687
30	6	0.029260	-2.471218	-3.488912
31	1	-0.040373	2.744997	-4.543395
32	1	0.105295	4.540448	-2.745881
33	1	0.099980	-4.540972	-2.745732
34	1	0.036132	-2.742759	-4.544283
35	7	-0.138139	-0.000319	-3.912132
36	1	0.317684	0.003963	-4.813481
37	7	0.164896	3.905849	0.000000
38	7	-0.024345	-3.912302	0.000000
39	1	-0.247767	4.827590	0.000000
40	1	0.448347	-4.804355	0.000000

Table S36. The optimized Cartesian coordinates for the cation of the compound **7** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.381033	1.819128	0.000000
2	6	-0.519253	3.235252	0.000000
3	6	1.711701	2.794022	0.000000
4	6	1.044821	1.537128	0.000000
5	6	1.819128	0.381033	0.000000
6	6	1.537128	-1.044821	0.000000
7	6	2.794022	-1.711701	0.000000
8	6	3.235252	0.519253	0.000000
9	6	0.381033	-1.819128	0.000000
10	6	-1.537128	1.044821	0.000000
11	6	-1.819128	-0.381033	0.000000
12	6	-1.044821	-1.537128	0.000000
13	7	3.783286	-0.748244	0.000000
14	7	0.748244	3.783286	0.000000
15	6	-2.794022	1.711701	0.000000
16	6	-3.235252	-0.519253	0.000000
17	6	0.519253	-3.235252	0.000000
18	7	-0.748244	-3.783286	0.000000
19	6	-1.711701	-2.794022	0.000000
20	6	3.885097	1.767302	0.000000
21	6	3.113161	2.919857	0.000000
22	6	1.767302	-3.885097	0.000000
23	6	2.919857	-3.113161	0.000000
24	6	-2.919857	3.113161	0.000000
25	6	-1.767302	3.885097	0.000000
26	6	-3.113161	-2.919857	0.000000
27	6	-3.885097	-1.767302	0.000000
28	1	4.967755	1.831106	0.000000
29	1	3.584289	3.896718	0.000000
30	1	1.831106	-4.967755	0.000000
31	1	3.896718	-3.584289	0.000000
32	1	-3.896718	3.584289	0.000000
33	1	-1.831106	4.967755	0.000000
34	1	-3.584289	-3.896718	0.000000
35	1	-4.967755	-1.831106	0.000000
36	1	-0.944247	-4.774316	0.000000
37	1	0.944247	4.774316	0.000000
38	7	-3.783286	0.748244	0.000000
39	1	-4.774316	0.944247	0.000000
40	1	4.774316	-0.944247	0.000000

Table S37. The optimized Cartesian coordinates for the dication of the compound **7** calculated at the B3LYP/6–31+G(d) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.390335	1.817607	0.000000
2	6	-0.521044	3.242123	0.000000
3	6	1.721645	2.796209	0.000000
4	6	1.055948	1.530043	0.000000
5	6	1.817607	0.390335	0.000000
6	6	1.530043	-1.055948	0.000000
7	6	2.796209	-1.721645	0.000000
8	6	3.242123	0.521044	0.000000
9	6	0.390335	-1.817607	0.000000
10	6	-1.530043	1.055948	0.000000
11	6	-1.817607	-0.390335	0.000000
12	6	-1.055948	-1.530043	0.000000
13	7	3.769508	-0.749491	0.000000
14	7	0.749491	3.769508	0.000000
15	6	-2.796209	1.721645	0.000000
16	6	-3.242123	-0.521044	0.000000

17	6	0.521044	-3.242123	0.000000
18	7	-0.749491	-3.769508	0.000000
19	6	-1.721645	-2.796209	0.000000
20	6	3.894433	1.768162	0.000000
21	6	3.123441	2.921836	0.000000
22	6	1.768162	-3.894433	0.000000
23	6	2.921836	-3.123441	0.000000
24	6	-2.921836	3.123441	0.000000
25	6	-1.768162	3.894433	0.000000
26	6	-3.123441	-2.921836	0.000000
27	6	-3.894433	-1.768162	0.000000
28	1	4.976912	1.832389	0.000000
29	1	3.596870	3.897413	0.000000
30	1	1.832389	-4.976912	0.000000
31	1	3.897413	-3.596870	0.000000
32	1	-3.897413	3.596870	0.000000
33	1	-1.832389	4.976912	0.000000
34	1	-3.596870	-3.897413	0.000000
35	1	-4.976912	-1.832389	0.000000
36	1	-0.947392	-4.764835	0.000000
37	1	0.947392	4.764835	0.000000
38	7	-3.769508	0.749491	0.000000
39	1	-4.764835	0.947392	0.000000
40	1	4.764835	-0.947392	0.000000