Aromaticity of the doubly charged [8]circulenes

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Electronic Supplementary Information

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Table S1. Total energy of the ground singlet state of **1–13** circulenes and their doubly charged forms calculated at the B3LYP/6–311++G(d, p) level of theory

Compound	E_{tot}, *a.u.*		
	2+	**0**	**2–**
1	–1219.9211	–1220.5974	–1220.5641
2	–1372.3413	–1373.0657	–1373.1604
3	–2511.8312	–2512.4846	–2512.4550
4	–10525.1314	–10525.7640	–10525.7500
5	–1140.5524	–1141.1532	–1141.0785
6	–2286.8453	–2287.4722	–2287.4502
7	–9864.8275	–9865.4397	–9865.4242
8	–1073.8595	–1074.4246	–1074.4577
9	–1076.2922	–1076.9209	–1074.4577
10	–2079.3454	–2079.8421	–2079.9143
11	–9229.2906	–9229.7951	–9229.8892
12	–2081.8299	–2082.4416	–2082.3986
13	–9231.7554	–9232.3570	–9232.3412

Table S2. The optimized Cartesian coordinates of the dication **1** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.438346	2.430747	-0.004671
2	6	0	2.430710	3.438324	-0.005652
3	6	0	1.098173	3.063856	-0.006257
4	6	0	0.692219	1.706875	-0.011794
5	6	0	1.706965	0.692233	0.000922
6	6	0	3.063910	1.098182	-0.004397
7	8	0	3.881129	-0.000010	-0.005219
8	6	0	3.063898	-1.098190	-0.006125
9	6	0	1.706955	-0.692198	-0.011888
10	6	0	3.438347	-2.430741	-0.005970
11	6	0	2.430706	-3.438307	-0.005486
12	1	0	4.483476	2.716564	-0.006691
13	1	0	2.716438	4.483481	-0.003562
14	1	0	4.483495	-2.716504	-0.003770
15	1	0	2.716417	-4.483468	-0.007524
16	6	0	0.692185	-1.706838	-0.000224
17	6	0	1.098188	-3.063833	-0.005663
18	8	0	0.000027	-3.881053	-0.006030
19	6	0	-1.098173	-3.063856	-0.006257
20	6	0	-0.692219	-1.706875	-0.011794
21	6	0	-2.430710	-3.438324	-0.005652
22	6	0	-3.438346	-2.430747	-0.004671
23	1	0	-2.716438	-4.483481	-0.003562
24	1	0	-4.483476	-2.716564	-0.006691
25	6	0	-1.706965	-0.692233	0.000922
26	6	0	-3.063910	-1.098182	-0.004397
27	8	0	-3.881129	0.000010	-0.005219
28	6	0	-3.063898	1.098190	-0.006125
29	6	0	-1.706955	0.692198	-0.011888
30	6	0	-3.438347	2.430741	-0.005970
31	6	0	-2.430706	3.438307	-0.005486
32	6	0	-1.098188	3.063833	-0.005663
33	6	0	-0.692185	1.706838	-0.000224
34	1	0	-4.483495	2.716504	-0.003770
35	1	0	-2.716417	4.483468	-0.007524
36	8	0	-0.000027	3.881053	-0.006030

Table S3. The optimized Cartesian coordinates of the dianion **1** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.134904	4.082281	0.000000
2	6	0	-0.304758	4.226127	0.000000
3	6	0	-1.071987	3.080501	0.000000
4	6	0	-0.537538	1.766654	0.000000
5	6	0	0.876457	1.625373	0.000000
6	6	0	1.660294	2.807501	0.000000
7	8	0	3.017246	2.469073	0.000000
8	6	0	3.080501	1.071987	0.000000
9	6	0	1.766654	0.537538	0.000000
10	6	0	4.226127	0.304758	0.000000
11	6	0	4.082281	-1.134904	0.000000
12	1	0	1.777225	4.955868	0.000000
13	1	0	-0.761536	5.209532	0.000000
14	1	0	5.209532	0.761536	0.000000
15	1	0	4.955868	-1.777225	0.000000
16	6	0	1.625373	-0.876457	0.000000
17	6	0	2.807501	-1.660294	0.000000
18	8	0	2.469073	-3.017246	0.000000
19	6	0	1.071987	-3.080501	0.000000
20	6	0	0.537538	-1.766654	0.000000
21	6	0	0.304758	-4.226127	0.000000
22	6	0	-1.134904	-4.082281	0.000000
23	1	0	0.761536	-5.209532	0.000000

24	1	0	-1.777225	-4.955868	0.000000
25	6	0	-0.876457	-1.625373	0.000000
26	6	0	-1.660294	-2.807501	0.000000
27	8	0	-3.017246	-2.469073	0.000000
28	6	0	-3.080501	-1.071987	0.000000
29	6	0	-1.766654	-0.537538	0.000000
30	6	0	-4.226127	-0.304758	0.000000
31	6	0	-4.082281	1.134904	0.000000
32	6	0	-2.807501	1.660294	0.000000
33	6	0	-1.625373	0.876457	0.000000
34	1	0	-5.209532	-0.761536	0.000000
35	1	0	-4.955868	1.777225	0.000000
36	8	0	-2.469073	3.017246	0.000000

Table S4. The optimized Cartesian coordinates of the dication **2** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.363210	3.027528	0.004736
2	6	0	0.722089	1.742801	0.004281
3	6	0	-0.722091	1.742801	0.003362
4	6	0	-1.742801	0.722091	0.003362
5	6	0	-3.027531	1.363212	0.002363
6	6	0	-1.363212	3.027531	0.002363
7	6	0	-1.742801	-0.722089	0.004281
8	6	0	-2.842083	2.842083	0.001666
9	6	0	-3.027528	-1.363210	0.004736
10	6	0	-0.710400	4.230935	0.002819
11	6	0	0.710399	4.230933	0.004195
12	6	0	-4.230933	-0.710399	0.004195
13	6	0	-4.230935	0.710400	0.002819
14	1	0	-1.278445	5.155614	0.002127
15	1	0	1.278447	5.155611	0.004507
16	1	0	-5.155611	-1.278447	0.004507
17	1	0	-5.155614	1.278445	0.002127
18	6	0	1.742801	0.722089	0.004281
19	6	0	3.027528	1.363210	0.004736
20	6	0	1.742801	-0.722091	0.003362
21	6	0	0.722091	-1.742801	0.003362
22	6	0	-0.722089	-1.742801	0.004281
23	6	0	3.027531	-1.363212	0.002363
24	6	0	1.363212	-3.027531	0.002363
25	6	0	-1.363210	-3.027528	0.004736
26	6	0	4.230935	-0.710400	0.002819
27	6	0	4.230933	0.710399	0.004195
28	6	0	-0.710399	-4.230933	0.004195
29	6	0	0.710400	-4.230935	0.002819
30	1	0	5.155614	-1.278445	0.002127
31	1	0	5.155611	1.278447	0.004507
32	1	0	-1.278447	-5.155611	0.004507
33	1	0	1.278445	-5.155614	0.002127
34	6	0	2.842083	-2.842083	0.001666
35	6	0	2.842081	2.842081	0.005134
36	6	0	-2.842081	-2.842081	0.005134
37	8	0	-3.690905	-3.690905	0.006381
38	8	0	3.690908	-3.690908	0.000038
39	8	0	3.690905	3.690905	0.006381
40	8	0	-3.690908	3.690908	0.000038

Table S5. The optimized Cartesian coordinates of the dianion **2** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.385470	-2.293170	0.006406
2	6	0	1.289510	-1.367261	0.010170
3	6	0	0.000068	-1.879423	0.001921

4	6	0	-1.367246	-1.289491	0.010201
5	6	0	-2.293155	-2.385463	0.006506
6	6	0	-0.161959	-3.304976	0.005403
7	6	0	-1.879407	-0.000059	0.002116
8	6	0	-1.579375	-3.660644	0.005894
9	6	0	-3.304967	0.161974	0.005778
10	6	0	0.919768	-4.192393	0.005417
11	6	0	2.207414	-3.680959	0.006077
12	6	0	-4.192378	-0.919753	0.005912
13	6	0	-3.680940	-2.207403	0.006486
14	1	0	0.721315	-5.259348	0.005771
15	1	0	3.083838	-4.320999	0.005473
16	1	0	-5.259334	-0.721309	0.006527
17	1	0	-4.320982	-3.083828	0.005897
18	6	0	1.879445	0.000054	0.002118
19	6	0	3.305003	-0.161977	0.005779
20	6	0	1.367282	1.289487	0.010202
21	6	0	-0.000031	1.879419	0.001921
22	6	0	-1.289473	1.367257	0.010170
23	6	0	2.293192	2.385457	0.006507
24	6	0	0.161997	3.304972	0.005404
25	6	0	-2.385434	2.293165	0.006405
26	6	0	3.680977	2.207398	0.006486
27	6	0	4.192415	0.919749	0.005913
28	6	0	-2.207377	3.680954	0.006077
29	6	0	-0.919732	4.192388	0.005417
30	1	0	4.321016	3.083825	0.005897
31	1	0	5.259371	0.721303	0.006528
32	1	0	-3.083801	4.320994	0.005473
33	1	0	-0.721281	5.259343	0.005771
34	6	0	1.579412	3.660639	0.005895
35	6	0	3.660665	-1.579396	0.006112
36	6	0	-3.660628	1.579391	0.006110
37	8	0	-4.805590	2.073404	0.006145
38	8	0	2.073414	4.805613	0.005785
39	8	0	4.805627	-2.073407	0.006145
40	8	0	-2.073375	-4.805619	0.005785

Table S6. The optimized Cartesian coordinates of the dication **3** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.098560	3.087809	0.469401
2	6	0	-2.993122	1.335149	-0.469401
3	16	0	-4.197879	0.163326	-0.875520
4	1	0	4.562320	2.661370	-0.478141
5	1	0	3.007799	4.341751	0.478141
6	6	0	3.087809	1.098560	-0.469401
7	16	0	4.197879	-0.163326	-0.875520
8	6	0	2.993122	-1.335149	-0.469401
9	6	0	1.695680	-0.770942	-0.177005
10	6	0	1.750454	0.636864	-0.177005
11	6	0	3.533333	2.393859	-0.268605
12	6	0	2.661148	3.336659	0.268605
13	6	0	1.335149	2.993122	0.469401
14	6	0	0.770942	1.695680	0.177005
15	6	0	3.336659	-2.661148	-0.268605
16	6	0	2.393859	-3.533333	0.268605
17	6	0	1.098560	-3.087809	0.469401
18	6	0	0.636864	-1.750454	0.177005
19	1	0	2.661370	-4.562320	0.478141
20	1	0	4.341751	-3.007799	-0.478141
21	6	0	-0.636864	1.750454	0.177005
22	6	0	-1.695680	0.770942	-0.177005
23	6	0	-1.750454	-0.636864	-0.177005
24	6	0	-0.770942	-1.695680	0.177005
25	6	0	-1.335149	-2.993122	0.469401
26	6	0	-2.661148	-3.336659	0.268605
27	6	0	-3.533333	-2.393859	-0.268605
28	6	0	-3.087809	-1.098560	-0.469401
29	1	0	-4.562320	-2.661370	-0.478141

30	1	0	-3.007799	-4.341751	0.478141
31	16	0	-0.163326	-4.197879	0.875520
32	16	0	0.163326	4.197879	0.875520
33	6	0	-2.393859	3.533333	0.268605
34	6	0	-3.336659	2.661148	-0.268605
35	1	0	-2.661370	4.562320	0.478141
36	1	0	-4.341751	3.007799	-0.478141

Table S7. The optimized Cartesian coordinates of the dianion **3** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.294335	3.032163	0.434326
2	6	0	-3.068740	1.205054	-0.434326
3	16	0	-4.187871	-0.061286	-0.931352
4	1	0	4.466676	2.886694	-0.435374
5	1	0	2.754754	4.549234	0.435374
6	6	0	3.032163	1.294335	-0.434326
7	16	0	4.187871	0.061286	-0.931352
8	6	0	3.068740	-1.205054	-0.434326
9	6	0	1.742233	-0.694363	-0.159897
10	6	0	1.721169	0.745047	-0.159897
11	6	0	3.438481	2.594256	-0.249426
12	6	0	2.492528	3.512922	0.249426
13	6	0	1.205054	3.068740	0.434326
14	6	0	0.694363	1.742233	0.159897
15	6	0	3.512922	-2.492528	-0.249426
16	6	0	2.594256	-3.438481	0.249426
17	6	0	1.294335	-3.032163	0.434326
18	6	0	0.745047	-1.721169	0.159897
19	1	0	2.886694	-4.466676	0.435374
20	1	0	4.549234	-2.754754	-0.435374
21	6	0	-0.745047	1.721169	0.159897
22	6	0	-1.742233	0.694363	-0.159897
23	6	0	-1.721169	-0.745047	-0.159897
24	6	0	-0.694363	-1.742233	0.159897
25	6	0	-1.205054	-3.068740	0.434326
26	6	0	-2.492528	-3.512922	0.249426
27	6	0	-3.438481	-2.594256	-0.249426
28	6	0	-3.032163	-1.294335	-0.434326
29	1	0	-4.466676	-2.886694	-0.435374
30	1	0	-2.754754	-4.549234	0.435374
31	16	0	0.061286	-4.187871	0.931352
32	16	0	-0.061286	4.187871	0.931352
33	6	0	-2.594256	3.438481	0.249426
34	6	0	-3.512922	2.492528	-0.249426
35	1	0	-2.886694	4.466676	0.435374
36	1	0	-4.549234	2.754754	-0.435374

Table S8. The optimized Cartesian coordinates of the dication **4** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.609448	1.714015	0.276410
2	34	0	-4.123461	-0.229081	-1.427266
3	1	0	-2.657087	-4.477004	0.717392
4	1	0	-4.155130	-3.136650	-0.717392
5	34	0	0.229081	-4.123461	1.427266
6	6	0	1.422858	-2.858559	0.716401
7	6	0	-1.097461	-2.998577	0.716401
8	6	0	-2.352708	-3.485256	0.404358
9	6	0	-3.203200	-2.724289	-0.404358

10	6	0	-0.609448	-1.714015	0.276410
11	6	0	0.795558	-1.635959	0.276410
12	6	0	2.724289	-3.203200	0.404358
13	1	0	3.136650	-4.155130	0.717392
14	6	0	-2.858559	-1.422858	-0.716401
15	6	0	-1.635959	-0.795558	-0.276410
16	6	0	-1.714015	0.609448	-0.276410
17	6	0	-2.998577	1.097461	-0.716401
18	6	0	-3.485256	2.352708	-0.404358
19	6	0	-2.724289	3.203200	0.404358
20	6	0	-1.422858	2.858559	0.716401
21	6	0	-0.795558	1.635959	0.276410
22	1	0	-3.136650	4.155130	0.717392
23	1	0	-4.477004	2.657087	-0.717392
24	34	0	-0.229081	4.123461	1.427266
25	6	0	1.097461	2.998577	0.716401
26	6	0	2.352708	3.485256	0.404358
27	6	0	3.203200	2.724289	-0.404358
28	6	0	2.858559	1.422858	-0.716401
29	6	0	1.635959	0.795558	-0.276410
30	6	0	1.714015	-0.609448	-0.276410
31	6	0	2.998577	-1.097461	-0.716401
32	34	0	4.123461	0.229081	-1.427266
33	1	0	4.155130	3.136650	-0.717392
34	1	0	2.657087	4.477004	0.717392
35	6	0	3.485256	-2.352708	-0.404358
36	1	0	4.477004	-2.657087	-0.717392

Table S9. The optimized Cartesian coordinates of the dianion **4** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.370969	1.808118	0.238981
2	34	0	-4.041932	-0.808386	-1.443729
3	1	0	-1.954939	-4.888206	0.651628
4	1	0	-3.760291	-3.684639	-0.651628
5	34	0	0.808386	-4.041932	1.443729
6	6	0	1.847540	-2.654390	0.643258
7	6	0	-0.684502	-3.160798	0.643258
8	6	0	-1.840707	-3.847195	0.368919
9	6	0	-2.843293	-3.178804	-0.368919
10	6	0	-0.370969	-1.808118	0.238981
11	6	0	1.037863	-1.526352	0.238981
12	6	0	3.178804	-2.843293	0.368919
13	1	0	3.684639	-3.760291	0.651628
14	6	0	-2.654390	-1.847540	-0.643258
15	6	0	-1.526352	-1.037863	-0.238981
16	6	0	-1.808118	0.370969	-0.238981
17	6	0	-3.160798	0.684502	-0.643258
18	6	0	-3.847195	1.840707	-0.368919
19	6	0	-3.178804	2.843293	0.368919
20	6	0	-1.847540	2.654390	0.643258
21	6	0	-1.037863	1.526352	0.238981
22	1	0	-3.684639	3.760291	0.651628
23	1	0	-4.888206	1.954939	-0.651628
24	34	0	-0.808386	4.041932	1.443729
25	6	0	0.684502	3.160798	0.643258
26	6	0	1.840707	3.847195	0.368919
27	6	0	2.843293	3.178804	-0.368919
28	6	0	2.654390	1.847540	-0.643258
29	6	0	1.526352	1.037863	-0.238981
30	6	0	1.808118	-0.370969	-0.238981
31	6	0	3.160798	-0.684502	-0.643258
32	34	0	4.041932	0.808386	-1.443729
33	1	0	3.760291	3.684639	-0.651628
34	1	0	1.954939	4.888206	0.651628
35	6	0	3.847195	-1.840707	-0.368919
36	1	0	4.888206	-1.954939	-0.651628

Table S10. The optimized Cartesian coordinates of the dication **5** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.390195	1.815023	0.000000
2	6	0	-0.520823	3.237874	0.000000
3	6	0	1.719816	2.792368	0.000000
4	6	0	1.054830	1.527708	0.000000
5	6	0	1.815023	0.390195	0.000000
6	6	0	1.527708	-1.054830	0.000000
7	6	0	2.792368	-1.719816	0.000000
8	6	0	3.237874	0.520823	0.000000
9	6	0	0.390195	-1.815023	0.000000
10	6	0	-1.527708	1.054830	0.000000
11	6	0	-1.815023	-0.390195	0.000000
12	6	0	-1.054830	-1.527708	0.000000
13	7	0	3.765134	-0.748621	0.000000
14	7	0	0.748621	3.765134	0.000000
15	6	0	-2.792368	1.719816	0.000000
16	6	0	-3.237874	-0.520823	0.000000
17	6	0	0.520823	-3.237874	0.000000
18	7	0	-0.748621	-3.765134	0.000000
19	6	0	-1.719816	-2.792368	0.000000
20	6	0	3.888599	1.765822	0.000000
21	6	0	3.119046	2.917341	0.000000
22	6	0	1.765822	-3.888599	0.000000
23	6	0	2.917341	-3.119046	0.000000
24	6	0	-2.917341	3.119046	0.000000
25	6	0	-1.765822	3.888599	0.000000
26	6	0	-3.119046	-2.917341	0.000000
27	6	0	-3.888599	-1.765822	0.000000
28	1	0	4.969481	1.831090	0.000000
29	1	0	3.592828	3.891044	0.000000
30	1	0	1.831090	-4.969481	0.000000
31	1	0	3.891044	-3.592828	0.000000
32	1	0	-3.891044	3.592828	0.000000
33	1	0	-1.831090	4.969481	0.000000
34	1	0	-3.592828	-3.891044	0.000000
35	1	0	-4.969481	-1.831090	0.000000
36	1	0	-0.946420	-4.759948	0.000000
37	1	0	0.946420	4.759948	0.000000
38	7	0	-3.765134	0.748621	0.000000
39	1	0	-4.759948	0.946420	0.000000
40	1	0	4.759948	-0.946420	0.000000

Table S11. The optimized Cartesian coordinates of the dianion **5** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.069043	3.081376	1.139655
2	6	0	0.034991	1.720219	0.714905
3	6	0	-0.007571	0.715344	1.719315
4	6	0	0.007201	-0.714405	1.719317
5	6	0	-0.036483	-1.139621	3.080026
6	6	0	-0.060016	1.139570	3.080019
7	6	0	0.070505	-1.718192	0.714912
8	7	0	-0.153889	-0.001119	3.888039
9	6	0	0.132675	-3.078337	1.139660
10	6	0	-0.043569	2.474429	3.472962
11	6	0	0.034835	3.473990	2.474285
12	6	0	0.106569	-3.471576	2.474278
13	6	0	0.007510	-2.473857	3.472969
14	1	0	-0.106134	2.747538	4.522024
15	1	0	0.083758	4.523610	2.748035
16	1	0	0.177202	-4.519961	2.748018

17	1	0	-0.049414	-2.748203	4.522029
18	1	0	0.179811	0.002327	4.838966
19	6	0	0.034991	1.720219	-0.714905
20	6	0	0.069043	3.081376	-1.139655
21	6	0	-0.007571	0.715344	-1.719315
22	6	0	0.007201	-0.714405	-1.719317
23	6	0	0.070505	-1.718192	-0.714912
24	6	0	-0.060016	1.139570	-3.080019
25	6	0	-0.036483	-1.139621	-3.080026
26	6	0	0.132675	-3.078337	-1.139660
27	6	0	-0.043569	2.474429	-3.472962
28	6	0	0.034835	3.473990	-2.474285
29	6	0	0.106569	-3.471576	-2.474278
30	6	0	0.007510	-2.473857	-3.472969
31	1	0	-0.106134	2.747538	-4.522024
32	1	0	0.083758	4.523610	-2.748035
33	1	0	0.177202	-4.519961	-2.748018
34	1	0	-0.049414	-2.748203	-4.522029
35	7	0	-0.153889	-0.001119	-3.888039
36	1	0	0.179811	0.002327	-4.838966
37	7	0	0.166145	3.890306	0.000000
38	7	0	0.246638	-3.885172	0.000000
39	1	0	-0.175810	4.838283	0.000000
40	1	0	-0.076717	-4.839669	0.000000

Table S12. The optimized Cartesian coordinates of the dication **6** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.247866	2.923454	0.735116
2	15	0	0.000000	3.935747	1.595181
3	6	0	-0.709102	1.666324	0.281688
4	6	0	0.709102	1.666324	0.281688
5	6	0	1.247866	2.923454	0.735116
6	6	0	-1.666324	0.709102	-0.281688
7	6	0	-1.666324	-0.709102	-0.281688
8	6	0	-0.709102	-1.666324	0.281688
9	6	0	0.709102	-1.666324	0.281688
10	6	0	1.666324	-0.709102	-0.281688
11	6	0	1.666324	0.709102	-0.281688
12	6	0	2.923454	1.247866	-0.735116
13	6	0	2.923454	-1.247866	-0.735116
14	15	0	3.935747	0.000000	-1.595181
15	6	0	3.324798	2.527417	-0.424550
16	6	0	2.527417	3.324798	0.424550
17	1	0	2.908252	4.280064	0.768229
18	1	0	4.280064	2.908252	-0.768229
19	6	0	3.324798	-2.527417	-0.424550
20	6	0	2.527417	-3.324798	0.424550
21	6	0	1.247866	-2.923454	0.735116
22	15	0	0.000000	-3.935747	1.595181
23	6	0	-1.247866	-2.923454	0.735116
24	6	0	-2.527417	-3.324798	0.424550
25	6	0	-3.324798	-2.527417	-0.424550
26	6	0	-2.923454	-1.247866	-0.735116
27	15	0	-3.935747	0.000000	-1.595181
28	6	0	-2.923454	1.247866	-0.735116
29	6	0	-3.324798	2.527417	-0.424550
30	6	0	-2.527417	3.324798	0.424550
31	1	0	-4.280064	2.908252	-0.768229
32	1	0	-2.908252	4.280064	0.768229
33	1	0	-4.280064	-2.908252	-0.768229
34	1	0	-2.908252	-4.280064	0.768229
35	1	0	2.908252	-4.280064	0.768229
36	1	0	4.280064	-2.908252	-0.768229
37	1	0	0.000000	5.067131	0.736553
38	1	0	0.000000	-5.067131	0.736553
39	1	0	-5.067131	0.000000	-0.736553
40	1	0	5.067131	0.000000	-0.736553

Table S13. The optimized Cartesian coordinates of the dianion **6** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.272652	2.983540	0.622733
2	15	0	0.000000	4.019569	1.415692
3	6	0	-0.721937	1.703843	0.226437
4	6	0	0.721937	1.703843	0.226437
5	6	0	1.272652	2.983540	0.622733
6	6	0	-1.703843	0.721937	-0.226437
7	6	0	-1.703843	-0.721937	-0.226437
8	6	0	-0.721937	-1.703843	0.226437
9	6	0	0.721937	-1.703843	0.226437
10	6	0	1.703843	-0.721937	-0.226437
11	6	0	1.703843	0.721937	-0.226437
12	6	0	2.983540	1.272652	-0.622733
13	6	0	2.983540	-1.272652	-0.622733
14	15	0	4.019569	0.000000	-1.415692
15	6	0	3.408512	2.553718	-0.369754
16	6	0	2.553718	3.408512	0.369754
17	1	0	2.884963	4.397486	0.676515
18	1	0	4.397486	2.884963	-0.676515
19	6	0	3.408512	-2.553718	-0.369754
20	6	0	2.553718	-3.408512	0.369754
21	6	0	1.272652	-2.983540	0.622733
22	15	0	0.000000	-4.019569	1.415692
23	6	0	-1.272652	-2.983540	0.622733
24	6	0	-2.553718	-3.408512	0.369754
25	6	0	-3.408512	-2.553718	-0.369754
26	6	0	-2.983540	-1.272652	-0.622733
27	15	0	-4.019569	0.000000	-1.415692
28	6	0	-2.983540	1.272652	-0.622733
29	6	0	-3.408512	2.553718	-0.369754
30	6	0	-2.553718	3.408512	0.369754
31	1	0	-4.397486	2.884963	-0.676515
32	1	0	-2.884963	4.397486	0.676515
33	1	0	-4.397486	-2.884963	-0.676515
34	1	0	-2.884963	-4.397486	0.676515
35	1	0	2.884963	-4.397486	0.676515
36	1	0	4.397486	-2.884963	-0.676515
37	1	0	0.000000	5.124115	0.505355
38	1	0	0.000000	-5.124115	0.505355
39	1	0	-5.124115	0.000000	-0.505355
40	1	0	5.124115	0.000000	-0.505355

Table S14. The optimized Cartesian coordinates of the dication **7** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.538269	3.270408	0.483551
2	6	0	-3.270408	2.538269	-0.483551
3	6	0	-2.851217	1.281702	-0.845721
4	6	0	-1.636089	0.710526	-0.331176
5	6	0	-0.710526	1.636089	0.331176
6	6	0	-1.281702	2.851217	0.845721
7	33	0	-3.897934	0.000000	-1.894563
8	6	0	-2.851217	-1.281702	-0.845721
9	6	0	-1.636089	-0.710526	-0.331176
10	6	0	-3.270408	-2.538269	-0.483551
11	6	0	-2.538269	-3.270408	0.483551
12	6	0	-1.281702	-2.851217	0.845721
13	6	0	-0.710526	-1.636089	0.331176
14	1	0	-2.952136	-4.194293	0.871907
15	1	0	-4.194293	-2.952136	-0.871907
16	1	0	-4.194293	2.952136	-0.871907
17	1	0	-2.952136	4.194293	0.871907
18	33	0	0.000000	3.897934	1.894563
19	6	0	1.281702	2.851217	0.845721
20	6	0	0.710526	1.636089	0.331176
21	6	0	1.636089	0.710526	-0.331176

22	6	0	2.851217	1.281702	-0.845721
23	6	0	3.270408	2.538269	-0.483551
24	6	0	2.538269	3.270408	0.483551
25	6	0	1.636089	-0.710526	-0.331176
26	6	0	2.851217	-1.281702	-0.845721
27	33	0	3.897934	0.000000	-1.894563
28	6	0	0.710526	-1.636089	0.331176
29	6	0	1.281702	-2.851217	0.845721
30	6	0	2.538269	-3.270408	0.483551
31	6	0	3.270408	-2.538269	-0.483551
32	1	0	2.952136	-4.194293	0.871907
33	33	0	0.000000	-3.897934	1.894563
34	1	0	4.194293	-2.952136	-0.871907
35	1	0	4.194293	2.952136	-0.871907
36	1	0	2.952136	4.194293	0.871907
37	1	0	-5.105192	0.000000	-0.965521
38	1	0	0.000000	5.105192	0.965521
39	1	0	0.000000	-5.105192	0.965521
40	1	0	5.105192	0.000000	-0.965521

Table S15. The optimized Cartesian coordinates of the dianion **7** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.567474	3.365869	0.430376
2	6	0	-3.365869	2.567474	-0.430376
3	6	0	-2.923687	1.304905	-0.731290
4	6	0	-1.683565	0.721338	-0.269434
5	6	0	-0.721338	1.683565	0.269434
6	6	0	-1.304905	2.923687	0.731290
7	33	0	-3.981842	0.000000	-1.715959
8	6	0	-2.923687	-1.304905	-0.731290
9	6	0	-1.683565	-0.721338	-0.269434
10	6	0	-3.365869	-2.567474	-0.430376
11	6	0	-2.567474	-3.365869	0.430376
12	6	0	-1.304905	-2.923687	0.731290
13	6	0	-0.721338	-1.683565	0.269434
14	1	0	-2.926061	-4.328477	0.785350
15	1	0	-4.328477	-2.926061	-0.785350
16	1	0	-4.328477	2.926061	-0.785350
17	1	0	-2.926061	4.328477	0.785350
18	33	0	0.000000	3.981842	1.715959
19	6	0	1.304905	2.923687	0.731290
20	6	0	0.721338	1.683565	0.269434
21	6	0	1.683565	0.721338	-0.269434
22	6	0	2.923687	1.304905	-0.731290
23	6	0	3.365869	2.567474	-0.430376
24	6	0	2.567474	3.365869	0.430376
25	6	0	1.683565	-0.721338	-0.269434
26	6	0	2.923687	-1.304905	-0.731290
27	33	0	3.981842	0.000000	-1.715959
28	6	0	0.721338	-1.683565	0.269434
29	6	0	1.304905	-2.923687	0.731290
30	6	0	2.567474	-3.365869	0.430376
31	6	0	3.365869	-2.567474	-0.430376
32	1	0	2.926061	-4.328477	0.785350
33	33	0	0.000000	-3.981842	1.715959
34	1	0	4.328477	-2.926061	-0.785350
35	1	0	4.328477	2.926061	-0.785350
36	1	0	2.926061	4.328477	0.785350
37	1	0	-5.211679	0.000000	-0.792530
38	1	0	0.000000	5.211679	0.792530
39	1	0	0.000000	-5.211679	0.792530
40	1	0	5.211679	0.000000	-0.792530

Table S16. The optimized Cartesian coordinates of the dication **8** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.778658	3.210971	-0.004818
2	6	0	-0.459633	3.882939	-0.005489
3	6	0	0.534447	1.776269	-0.001060
4	6	0	-0.934404	1.602365	-0.009196
5	6	0	-1.506809	2.940447	-0.005438
6	6	0	1.602380	0.934401	-0.009085
7	6	0	1.776217	-0.534428	-0.000859
8	6	0	0.934404	-1.602365	-0.009196
9	6	0	-0.534447	-1.776269	-0.001060
10	6	0	-1.602380	-0.934401	-0.009085
11	6	0	-1.776217	0.534428	-0.000859
12	6	0	-3.210982	0.778651	-0.004400
13	6	0	-2.940436	-1.506808	-0.005319
14	6	0	-3.882939	-0.459627	-0.004702
15	6	0	-3.754763	2.078892	-0.004277
16	6	0	-2.898071	3.165646	-0.005296
17	1	0	-3.286375	4.177203	-0.004977
18	1	0	-4.829026	2.220282	-0.004483
19	6	0	-3.165644	-2.898079	-0.005530
20	6	0	-2.078914	-3.754779	-0.004653
21	6	0	-0.778658	-3.210971	-0.004818
22	6	0	0.459633	-3.882939	-0.005489
23	6	0	1.506809	-2.940447	-0.005438
24	6	0	2.898071	-3.165646	-0.005296
25	6	0	3.754763	-2.078892	-0.004277
26	6	0	3.210982	-0.778651	-0.004400
27	6	0	3.882939	0.459627	-0.004702
28	6	0	2.940436	1.506808	-0.005319
29	6	0	3.165644	2.898079	-0.005530
30	6	0	2.078914	3.754779	-0.004653
31	1	0	4.177221	3.286338	-0.005095
32	1	0	2.220304	4.829038	-0.005161
33	1	0	4.829026	-2.220282	-0.004483
34	1	0	3.286375	-4.177203	-0.004977
35	1	0	-2.220304	-4.829038	-0.005161
36	1	0	-4.177221	-3.286338	-0.005095
37	1	0	-0.586921	4.958335	-0.005635
38	1	0	0.586921	-4.958335	-0.005635
39	1	0	4.958333	0.586949	-0.004529
40	1	0	-4.958333	-0.586949	-0.004529

Table S17. The optimized Cartesian coordinates of the dianion **8** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394788	3.024797
2	6	0	0.000000	2.781336	2.782479
3	6	0	0.000000	0.693436	1.747918
4	6	0	0.000000	1.747592	0.694143
5	6	0	0.000000	3.024138	1.396265
6	6	0	0.000000	-0.694341	1.747431
7	6	0	0.000000	-1.747669	0.693421
8	6	0	0.000000	-1.747592	-0.694143
9	6	0	0.000000	-0.693436	-1.747918
10	6	0	0.000000	0.694341	-1.747431
11	6	0	0.000000	1.747669	-0.693421
12	6	0	0.000000	3.024790	-1.395090
13	6	0	0.000000	1.396190	-3.024287
14	6	0	0.000000	2.782433	-2.781329
15	6	0	0.000000	4.253210	-0.687959
16	6	0	0.000000	4.253019	0.689601
17	1	0	0.000000	5.188524	1.246389

18	1	0	0.000000	5.189038	-1.244268
19	6	0	0.000000	0.689661	-4.253016
20	6	0	0.000000	-0.688121	-4.253263
21	6	0	0.000000	-1.394788	-3.024797
22	6	0	0.000000	-2.781336	-2.782479
23	6	0	0.000000	-3.024138	-1.396265
24	6	0	0.000000	-4.253019	-0.689601
25	6	0	0.000000	-4.253210	0.687959
26	6	0	0.000000	-3.024790	1.395090
27	6	0	0.000000	-2.782433	2.781329
28	6	0	0.000000	-1.396190	3.024287
29	6	0	0.000000	-0.689661	4.253016
30	6	0	0.000000	0.688121	4.253263
31	1	0	0.000000	-1.246397	5.188559
32	1	0	0.000000	1.244379	5.188970
33	1	0	0.000000	-5.189038	1.244268
34	1	0	0.000000	-5.188524	-1.246389
35	1	0	0.000000	-1.244379	-5.188970
36	1	0	0.000000	1.246397	-5.188559
37	1	0	0.000000	3.548909	3.550710
38	1	0	0.000000	-3.548909	-3.550710
39	1	0	0.000000	-3.550794	3.548780
40	1	0	0.000000	3.550794	-3.548780

Table S18. The optimized Cartesian coordinates of the dication **9** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.382062	3.023501	0.000015
2	6	0	2.863940	2.863940	0.000000
3	6	0	0.731180	1.743976	0.000007
4	6	0	1.743976	0.731180	-0.000007
5	6	0	3.023501	1.382062	-0.000015
6	6	0	-0.731180	1.743976	0.000007
7	6	0	-1.743976	0.731180	-0.000007
8	6	0	-1.743976	-0.731180	-0.000007
9	6	0	-0.731180	-1.743976	0.000007
10	6	0	0.731180	-1.743976	0.000007
11	6	0	1.743976	-0.731180	-0.000007
12	6	0	3.023501	-1.382062	-0.000015
13	6	0	1.382062	-3.023501	0.000015
14	6	0	2.863940	-2.863940	0.000000
15	6	0	4.217412	-0.704538	-0.000032
16	6	0	4.217412	0.704538	-0.000032
17	1	0	5.155448	1.248097	-0.000042
18	1	0	5.155448	-1.248097	-0.000042
19	6	0	0.704538	-4.217412	0.000032
20	6	0	-0.704538	-4.217412	0.000032
21	6	0	-1.382062	-3.023501	0.000015
22	6	0	-2.863940	-2.863940	0.000000
23	6	0	-3.023501	-1.382062	-0.000015
24	6	0	-4.217412	-0.704538	-0.000032
25	6	0	-4.217412	0.704538	-0.000032
26	6	0	-3.023501	1.382062	-0.000015
27	6	0	-2.863940	2.863940	0.000000
28	6	0	-1.382062	3.023501	0.000015
29	6	0	-0.704538	4.217412	0.000032
30	6	0	0.704538	4.217412	0.000032
31	1	0	-1.248097	5.155448	0.000042
32	1	0	1.248097	5.155448	0.000042
33	1	0	-5.155448	1.248097	-0.000042
34	1	0	-5.155448	-1.248097	-0.000042
35	1	0	-1.248097	-5.155448	0.000042
36	1	0	1.248097	-5.155448	0.000042
37	1	0	3.326159	3.326139	0.879745
38	1	0	-3.326159	-3.326139	0.879745
39	1	0	-3.326159	3.326139	0.879745
40	1	0	3.326159	-3.326139	0.879745
41	1	0	3.326139	3.326159	-0.879745
42	1	0	3.326139	-3.326159	-0.879745
43	1	0	-3.326139	-3.326159	-0.879745
44	1	0	-3.326139	3.326159	-0.879745

Table S19. The optimized Cartesian coordinates of the dianion **9** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394788	3.024797
2	6	0	0.000000	2.781336	2.782479
3	6	0	0.000000	0.693436	1.747918
4	6	0	0.000000	1.747592	0.694143
5	6	0	0.000000	3.024138	1.396265
6	6	0	0.000000	-0.694341	1.747431
7	6	0	0.000000	-1.747669	0.693421
8	6	0	0.000000	-1.747592	-0.694143
9	6	0	0.000000	-0.693436	-1.747918
10	6	0	0.000000	0.694341	-1.747431
11	6	0	0.000000	1.747669	-0.693421
12	6	0	0.000000	3.024790	-1.395090
13	6	0	0.000000	1.396190	-3.024287
14	6	0	0.000000	2.782433	-2.781329
15	6	0	0.000000	4.253210	-0.687959
16	6	0	0.000000	4.253019	0.689601
17	1	0	0.000000	5.188524	1.246389
18	1	0	0.000000	5.189038	-1.244268
19	6	0	0.000000	0.689661	-4.253016
20	6	0	0.000000	-0.688121	-4.253263
21	6	0	0.000000	-1.394788	-3.024797
22	6	0	0.000000	-2.781336	-2.782479
23	6	0	0.000000	-3.024138	-1.396265
24	6	0	0.000000	-4.253019	-0.689601
25	6	0	0.000000	-4.253210	0.687959
26	6	0	0.000000	-3.024790	1.395090
27	6	0	0.000000	-2.782433	2.781329
28	6	0	0.000000	-1.396190	3.024287
29	6	0	0.000000	-0.689661	4.253016
30	6	0	0.000000	0.688121	4.253263
31	1	0	0.000000	-1.246397	5.188559
32	1	0	0.000000	1.244379	5.188970
33	1	0	0.000000	-5.189038	1.244268
34	1	0	0.000000	-5.188524	-1.246389
35	1	0	0.000000	-1.244379	-5.188970
36	1	0	0.000000	1.246397	-5.188559
37	1	0	0.000000	3.548909	3.550710
38	1	0	0.000000	-3.548909	-3.550710
39	1	0	0.000000	-3.550794	3.548780
40	1	0	0.000000	3.550794	-3.548780

Table S20. The optimized Cartesian coordinates of the dication **10** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.060777	2.984088	0.810040
2	6	0	-0.683455	1.666604	0.323957
3	6	0	0.683455	1.666604	-0.323957
4	6	0	1.666604	0.683455	-0.323957
5	6	0	2.984088	1.060777	-0.810040
6	6	0	-1.666604	0.683455	0.323957
7	6	0	-1.666604	-0.683455	-0.323957
8	6	0	-0.683455	-1.666604	-0.323957
9	6	0	0.683455	-1.666604	0.323957
10	6	0	1.666604	-0.683455	0.323957
11	6	0	2.984088	-1.060777	0.810040
12	14	0	4.178236	0.000000	0.000000
13	6	0	3.230987	-2.255444	1.498299
14	6	0	2.255444	-3.230987	1.498299
15	6	0	1.060777	-2.984088	0.810040
16	14	0	0.000000	-4.178236	0.000000
17	6	0	-1.060777	-2.984088	-0.810040
18	6	0	-2.984088	-1.060777	-0.810040
19	6	0	-3.230987	-2.255444	-1.498299

20	6	0	-2.255444	-3.230987	-1.498299
21	1	0	-2.454532	-4.206649	-1.926331
22	1	0	-4.206649	-2.454532	-1.926331
23	1	0	0.000000	-5.646629	0.000000
24	1	0	2.454532	-4.206649	1.926331
25	1	0	4.206649	-2.454532	1.926331
26	1	0	5.646629	0.000000	0.000000
27	6	0	3.230987	2.255444	-1.498299
28	6	0	2.255444	3.230987	-1.498299
29	6	0	1.060777	2.984088	-0.810040
30	14	0	0.000000	4.178236	0.000000
31	6	0	-2.255444	3.230987	1.498299
32	6	0	-3.230987	2.255444	1.498299
33	6	0	-2.984088	1.060777	0.810040
34	14	0	-4.178236	0.000000	0.000000
35	1	0	-5.646629	0.000000	0.000000
36	1	0	-4.206649	2.454532	1.926331
37	1	0	-2.454532	4.206649	1.926331
38	1	0	0.000000	5.646629	0.000000
39	1	0	2.454532	4.206649	-1.926331
40	1	0	4.206649	2.454532	-1.926331

Table S21. The optimized Cartesian coordinates of the dianion **10** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.096381	-2.953617	-0.789400
2	6	0	0.533297	-1.730014	-0.269824
3	6	0	1.588860	-0.868752	0.395744
4	6	0	1.730472	0.532292	0.397191
5	6	0	2.987290	1.079781	0.840371
6	6	0	-0.869626	-1.588216	-0.268325
7	6	0	-1.730472	-0.532292	0.397191
8	6	0	-1.588860	0.868752	0.395744
9	6	0	-0.533297	1.730014	-0.269824
10	6	0	0.869626	1.588216	-0.268325
11	6	0	1.667212	2.674832	-0.785552
12	14	0	3.255672	2.789463	0.173679
13	6	0	1.070652	3.712516	-1.513057
14	6	0	-0.302592	3.850883	-1.515203
15	6	0	-1.096381	2.953617	-0.789400
16	14	0	-2.631909	3.384847	0.166031
17	6	0	-2.710976	1.657524	0.836690
18	6	0	-2.987290	-1.079781	0.840371
19	6	0	-3.946558	-0.294438	1.481973
20	6	0	-3.807813	1.081412	1.479858
21	1	0	-4.604840	1.717307	1.860575
22	1	0	-4.854351	-0.757226	1.864464
23	1	0	-3.865034	3.613300	-0.682628
24	1	0	-0.759290	4.734948	-1.956594
25	1	0	1.695922	4.487585	-1.952685
26	1	0	4.511615	2.769619	-0.672045
27	6	0	3.946558	0.294438	1.481973
28	6	0	3.807813	-1.081412	1.479858
29	6	0	2.710976	-1.657524	0.836690
30	14	0	2.631909	-3.384847	0.166031
31	6	0	0.302592	-3.850883	-1.515203
32	6	0	-1.070652	-3.712516	-1.513057
33	6	0	-1.667212	-2.674832	-0.785552
34	14	0	-3.255672	-2.789463	0.173679
35	1	0	-4.511615	-2.769619	-0.672045
36	1	0	-1.695922	-4.487585	-1.952685
37	1	0	0.759290	-4.734948	-1.956594
38	1	0	3.865034	-3.613300	-0.682628
39	1	0	4.604840	-1.717307	1.860575
40	1	0	4.854351	0.757226	1.864464

Table S22. The optimized Cartesian coordinates of the compound **10** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.225573	0.158726	0.695838
2	6	0	-1.819452	0.001232	0.312157
3	6	0	-1.286458	1.244650	-0.333493
4	6	0	0.000810	1.795665	-0.251150
5	6	0	0.160060	3.164887	-0.674767
6	6	0	-1.247505	-1.260989	0.427462
7	6	0	-0.000810	-1.795665	-0.251150
8	6	0	1.286458	-1.244650	-0.333493
9	6	0	1.819452	-0.001232	0.312157
10	6	0	1.247505	1.260989	0.427462
11	6	0	2.061113	2.309749	1.032217
12	14	0	1.562751	3.807813	0.253271
13	6	0	3.272478	2.019027	1.712075
14	6	0	3.852565	0.796624	1.532824
15	6	0	3.225573	-0.158726	0.695838
16	14	0	3.998612	-1.355438	-0.423758
17	6	0	2.344467	-2.068121	-0.861575
18	6	0	-0.160060	-3.164887	-0.674767
19	6	0	0.844413	-3.874287	-1.335749
20	6	0	2.098849	-3.302844	-1.459605
21	1	0	2.910708	-3.862864	-1.911703
22	1	0	0.665174	-4.889272	-1.675623
23	1	0	4.987401	-2.338752	0.103605
24	1	0	4.840104	0.592428	1.933392
25	1	0	3.775422	2.797626	2.276265
26	1	0	2.086234	5.182971	0.343236
27	6	0	-0.844413	3.874287	-1.335749
28	6	0	-2.098849	3.302844	-1.459605
29	6	0	-2.344467	2.068121	-0.861575
30	14	0	-3.998612	1.355438	-0.423758
31	6	0	-3.852565	-0.796624	1.532824
32	6	0	-3.272478	-2.019027	1.712075
33	6	0	-2.061113	-2.309749	1.032217
34	14	0	-1.562751	-3.807813	0.253271
35	1	0	-2.086234	-5.182971	0.343236
36	1	0	-3.775422	-2.797626	2.276265
37	1	0	-4.840104	-0.592428	1.933392
38	1	0	-4.987401	2.338752	0.103605
39	1	0	-2.910708	3.862864	-1.911703
40	1	0	-0.665174	4.889272	-1.675623

Table S23. The optimized Cartesian coordinates of the dication **11** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.037186	2.953551	0.877517
2	6	0	-0.671658	1.657065	0.348391
3	6	0	0.671658	1.657065	-0.348391
4	6	0	1.657065	0.671658	-0.348391
5	6	0	2.953551	1.037186	-0.877517
6	6	0	-1.657065	0.671658	0.348391
7	6	0	-1.657065	-0.671658	-0.348391
8	6	0	-0.671658	-1.657065	-0.348391
9	6	0	0.671658	-1.657065	0.348391
10	6	0	1.657065	-0.671658	0.348391
11	6	0	2.953551	-1.037186	0.877517
12	32	0	4.242734	0.000000	0.000000
13	6	0	3.182525	-2.205628	1.609886
14	6	0	2.205628	-3.182525	1.609886
15	6	0	1.037186	-2.953551	0.877517
16	32	0	0.000000	-4.242734	0.000000
17	6	0	-1.037186	-2.953551	-0.877517

18	6	0	-2.953551	-1.037186	-0.877517
19	6	0	-3.182525	-2.205628	-1.609886
20	6	0	-2.205628	-3.182525	-1.609886
21	1	0	-2.392967	-4.146259	-2.068670
22	1	0	-4.146259	-2.392967	-2.068670
23	1	0	0.000000	-5.755927	0.000000
24	1	0	2.392967	-4.146259	2.068670
25	1	0	4.146259	-2.392967	2.068670
26	1	0	5.755927	0.000000	0.000000
27	6	0	3.182525	2.205628	-1.609886
28	6	0	2.205628	3.182525	-1.609886
29	6	0	1.037186	2.953551	-0.877517
30	32	0	0.000000	4.242734	0.000000
31	6	0	-2.205628	3.182525	1.609886
32	6	0	-3.182525	2.205628	1.609886
33	6	0	-2.953551	1.037186	0.877517
34	32	0	-4.242734	0.000000	0.000000
35	1	0	-5.755927	0.000000	0.000000
36	1	0	-4.146259	2.392967	2.068670
37	1	0	-2.392967	4.146259	2.068670
38	1	0	0.000000	5.755927	0.000000
39	1	0	2.392967	4.146259	-2.068670
40	1	0	4.146259	2.392967	-2.068670

Table S24. The optimized Cartesian coordinates of the dianion **11** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.630107	1.652810	0.903813
2	6	0	-1.572091	0.863057	0.338762
3	6	0	-0.540412	1.708436	-0.380546
4	6	0	0.861587	1.571007	-0.381113
5	6	0	1.639721	2.668132	-0.881567
6	6	0	-1.709819	-0.541589	0.338201
7	6	0	-0.861587	-1.571007	-0.381113
8	6	0	0.540412	-1.708436	-0.380546
9	6	0	1.572091	-0.863057	0.338762
10	6	0	1.709819	0.541589	0.338201
11	6	0	2.901354	1.111124	0.902374
12	32	0	3.439408	2.703268	-0.112857
13	6	0	3.785390	0.325585	1.643390
14	6	0	3.649981	-1.053308	1.644193
15	6	0	2.630107	-1.652810	0.903813
16	32	0	2.849040	-3.320317	-0.109759
17	6	0	1.090954	-2.936105	-0.880010
18	6	0	-1.639721	-2.668132	-0.881567
19	6	0	-1.060993	-3.720202	-1.585423
20	6	0	0.319507	-3.855705	-1.584533
21	1	0	0.786697	-4.742936	-2.007671
22	1	0	-1.691255	-4.499651	-2.009327
23	1	0	2.591367	-4.598223	0.786454
24	1	0	4.418472	-1.673226	2.102401
25	1	0	4.659863	0.784719	2.100898
26	1	0	3.437795	4.007961	0.781670
27	6	0	1.060993	3.720202	-1.585423
28	6	0	-0.319507	3.855705	-1.584533
29	6	0	-1.090954	2.936105	-0.880010
30	32	0	-2.849040	3.320317	-0.109759
31	6	0	-3.649981	1.053308	1.644193
32	6	0	-3.785390	-0.325585	1.643390
33	6	0	-2.901354	-1.111124	0.902374
34	32	0	-3.439408	-2.703268	-0.112857
35	1	0	-3.437795	-4.007961	0.781670
36	1	0	-4.659863	-0.784719	2.100898
37	1	0	-4.418472	1.673226	2.102401
38	1	0	-2.591367	4.598223	0.786454
39	1	0	-0.786697	4.742936	-2.007671
40	1	0	1.691255	4.499651	-2.009327

Table S25. The optimized Cartesian coordinates of the compound **11** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.740845	1.640294	0.722089
2	6	0	-1.597212	0.854279	0.309401
3	6	0	-0.564249	1.693834	-0.379970
4	6	0	0.828466	1.581449	-0.278978
5	6	0	1.607367	2.706250	-0.728816
6	6	0	-1.657535	-0.536857	0.450511
7	6	0	-0.828466	-1.581449	-0.278978
8	6	0	0.564249	-1.693834	-0.379970
9	6	0	1.597212	-0.854279	0.309401
10	6	0	1.657535	0.536857	0.450511
11	6	0	2.808668	1.075623	1.126020
12	32	0	3.141141	2.725038	0.335326
13	6	0	3.752308	0.267379	1.783012
14	6	0	3.718104	-1.092470	1.565408
15	6	0	2.740845	-1.640294	0.722089
16	32	0	3.014364	-3.144099	-0.503332
17	6	0	1.115283	-2.897234	-0.940910
18	6	0	-1.607367	-2.706250	-0.728816
19	6	0	-1.057201	-3.777215	-1.442309
20	6	0	0.315169	-3.841114	-1.587202
21	1	0	0.770359	-4.692941	-2.081665
22	1	0	-1.692262	-4.580968	-1.800430
23	1	0	3.028174	-4.493135	0.290701
24	1	0	4.516785	-1.722030	1.944371
25	1	0	4.554038	0.719467	2.358028
26	1	0	4.285638	3.718582	0.468095
27	6	0	1.057201	3.777215	-1.442309
28	6	0	-0.315169	3.841114	-1.587202
29	6	0	-1.115283	2.897234	-0.940910
30	32	0	-3.014364	3.144099	-0.503332
31	6	0	-3.718104	1.092470	1.565408
32	6	0	-3.752308	-0.267379	1.783012
33	6	0	-2.808668	-1.075623	1.126020
34	32	0	-3.141141	-2.725038	0.335326
35	1	0	-4.285638	-3.718582	0.468095
36	1	0	-4.554038	-0.719467	2.358028
37	1	0	-4.516785	1.722030	1.944371
38	1	0	-3.028174	4.493135	0.290701
39	1	0	-0.770359	4.692941	-2.081665
40	1	0	1.692262	4.580968	-1.800430

Table S26. The optimized Cartesian coordinates of the dication **12** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.039540	0.807517	-0.508021
2	6	0	4.115383	-0.184868	0.507810
3	6	0	2.982685	-0.849099	0.908843
4	6	0	1.693489	-0.508059	0.356189
5	6	0	1.596591	0.759282	-0.356275
6	6	0	2.819114	1.292035	-0.908969
7	14	0	2.457937	2.864365	-1.888185
8	6	0	0.849102	2.982685	-0.908822
9	6	0	0.508062	1.693490	-0.356167
10	6	0	-0.759280	1.596593	0.356296
11	6	0	-1.292034	2.819117	0.908987
12	6	0	-0.807515	4.039542	0.508039
13	6	0	0.184871	4.115384	-0.507792
14	6	0	-1.693489	0.508064	0.356188
15	6	0	-2.982684	0.849105	0.908841
16	14	0	-2.864365	2.457941	1.888202
17	6	0	-1.596591	-0.759279	-0.356273

18	6	0	-2.819113	-1.292034	-0.908964
19	6	0	-4.039539	-0.807515	-0.508018
20	6	0	-4.115382	0.184873	0.507811
21	6	0	-0.508061	-1.693487	-0.356162
22	6	0	-0.849101	-2.982684	-0.908814
23	14	0	-2.457937	-2.864366	-1.888177
24	6	0	-0.184870	-4.115381	-0.507782
25	6	0	0.807517	-4.039537	0.508048
26	6	0	1.292035	-2.819110	0.908994
27	6	0	0.759281	-1.596589	0.356300
28	14	0	2.864366	-2.457932	1.888208
29	1	0	-0.453138	-5.086553	-0.909358
30	1	0	1.220157	-4.958651	0.909738
31	1	0	3.967635	-3.404792	1.640971
32	1	0	5.086554	-0.453135	0.909388
33	1	0	4.958654	1.220157	-0.909711
34	1	0	3.404796	3.967634	-1.640948
35	1	0	0.453139	5.086554	-0.909370
36	1	0	-1.220156	4.958657	0.909727
37	1	0	-5.086553	0.453142	0.909388
38	1	0	-4.958654	-1.220156	-0.909706
39	1	0	-3.404796	-3.967635	-1.640937
40	1	0	2.227650	2.596013	-3.323252
41	1	0	-2.596015	2.227656	3.323270
42	1	0	-2.227651	-2.596018	-3.323245
43	1	0	2.596015	-2.227643	3.323275
44	1	0	-3.967634	3.404800	1.640962

Table S27. The optimized Cartesian coordinates of the dianion **12** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.690264	3.849159	1.508911
2	6	0	-0.690172	3.848385	1.511274
3	6	0	-1.381989	2.841078	0.816933
4	6	0	-0.704370	1.659959	0.330476
5	6	0	0.702787	1.660557	0.328439
6	6	0	1.380883	2.842338	0.812662
7	14	0	3.018025	3.018821	-0.002350
8	6	0	2.842048	1.381083	-0.816207
9	6	0	1.660976	0.702609	-0.330962
10	6	0	1.661476	-0.704557	-0.331493
11	6	0	2.843338	-1.381800	-0.816852
12	6	0	3.850200	-0.689913	-1.511755
13	6	0	3.849415	0.690518	-1.511735
14	6	0	0.703511	-1.663913	0.326079
15	6	0	1.381936	-2.845945	0.809161
16	14	0	3.019750	-3.020452	-0.004874
17	6	0	-0.703651	-1.664504	0.326452
18	6	0	-1.380920	-2.847225	0.809539
19	6	0	-0.689115	-3.855369	1.502712
20	6	0	0.691312	-3.854573	1.502765
21	6	0	-1.662968	-0.705301	-0.329462
22	6	0	-2.844835	-1.382849	-0.814030
23	14	0	-3.019413	-3.022178	-0.003076
24	6	0	-3.853386	-0.690958	-1.506521
25	6	0	-3.854165	0.689475	-1.503916
26	6	0	-2.846120	1.380024	-0.809384
27	6	0	-1.663470	0.701857	-0.327277
28	14	0	-3.021171	3.017140	0.005982
29	1	0	-4.689115	-1.237371	-1.940706
30	1	0	-4.690728	1.236554	-1.935596
31	1	0	-4.228409	3.166396	0.909210
32	1	0	-1.236629	4.683396	1.946788
33	1	0	1.237273	4.684964	1.942137
34	1	0	3.167226	4.227737	-0.903338
35	1	0	4.684413	1.237756	-1.946285
36	1	0	4.686070	-1.236151	-1.945854
37	1	0	1.238530	-4.690373	1.935807
38	1	0	-1.235404	-4.692010	1.935254
39	1	0	-3.170110	-4.229264	-0.906275

40	1	0	4.227194	3.169287	0.898061
41	1	0	3.170357	-4.227928	-0.907548
42	1	0	-4.227080	-3.174502	0.899033
43	1	0	-3.173302	4.226308	-0.894168
44	1	0	4.228535	-3.171401	0.896018

Table S28. The optimized Cartesian coordinates of the compound **12** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.227436	3.209884	-1.496326
2	6	0	3.209884	2.227436	-1.496326
3	6	0	2.968812	1.029694	-0.837669
4	6	0	1.678822	0.679917	-0.332546
5	6	0	0.679917	1.678822	-0.332546
6	6	0	1.029694	2.968812	-0.837669
7	14	0	0.000000	4.276507	0.000000
8	6	0	-1.029694	2.968812	0.837669
9	6	0	-0.679917	1.678822	0.332546
10	6	0	-1.678822	0.679917	0.332546
11	6	0	-2.968812	1.029694	0.837669
12	6	0	-3.209884	2.227436	1.496326
13	6	0	-2.227436	3.209884	1.496326
14	6	0	-1.678822	-0.679917	-0.332546
15	6	0	-2.968812	-1.029694	-0.837669
16	14	0	-4.276507	0.000000	0.000000
17	6	0	-0.679917	-1.678822	-0.332546
18	6	0	-1.029694	-2.968812	-0.837669
19	6	0	-2.227436	-3.209884	-1.496326
20	6	0	-3.209884	-2.227436	-1.496326
21	6	0	0.679917	-1.678822	0.332546
22	6	0	1.029694	-2.968812	0.837669
23	14	0	0.000000	-4.276507	0.000000
24	6	0	2.227436	-3.209884	1.496326
25	6	0	3.209884	-2.227436	1.496326
26	6	0	2.968812	-1.029694	0.837669
27	6	0	1.678822	-0.679917	0.332546
28	14	0	4.276507	0.000000	0.000000
29	1	0	2.441444	-4.192324	1.905750
30	1	0	4.192324	-2.441444	1.905750
31	1	0	5.152528	-0.844436	-0.855789
32	1	0	4.192324	2.441444	-1.905750
33	1	0	2.441444	4.192324	-1.905750
34	1	0	0.844436	5.152528	0.855789
35	1	0	-2.441444	4.192324	1.905750
36	1	0	-4.192324	2.441444	1.905750
37	1	0	-4.192324	-2.441444	-1.905750
38	1	0	-2.441444	-4.192324	-1.905750
39	1	0	-0.844436	-5.152528	0.855789
40	1	0	-0.844436	5.152528	-0.855789
41	1	0	-5.152528	-0.844436	0.855789
42	1	0	0.844436	-5.152528	-0.855789
43	1	0	5.152528	0.844436	0.855789
44	1	0	-5.152528	0.844436	-0.855789

Table S29. The optimized Cartesian coordinates of the dication **13** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.089152	2.871230	-0.956214
2	32	0	0.306091	3.746530	-2.031964
3	6	0	1.541036	2.656071	-0.956751
4	6	0	2.801318	2.995029	-0.533677

5	6	0	3.410568	2.277305	0.533248
6	6	0	2.871140	1.089042	0.956613
7	6	0	1.652599	0.584094	0.379001
8	6	0	0.844833	1.535786	-0.379015
9	6	0	-0.584138	1.652635	-0.378777
10	6	0	-1.535743	0.844797	0.379272
11	6	0	-2.655961	1.540945	0.957203
12	6	0	-2.994968	2.801267	0.534287
13	6	0	-2.277367	3.410618	-0.532662
14	6	0	-1.652591	-0.584174	0.378913
15	6	0	-2.871120	-1.089243	0.956443
16	32	0	-3.746296	0.305898	2.032425
17	6	0	-0.844840	-1.535708	-0.379319
18	6	0	-1.541055	-2.655872	-0.957275
19	6	0	-2.801328	-2.994919	-0.534246
20	6	0	-3.410556	-2.277419	0.532841
21	6	0	0.584131	-1.652555	-0.379136
22	6	0	1.089134	-2.871029	-0.956842
23	32	0	-0.306132	-3.746101	-2.032746
24	6	0	1.535751	-0.844876	0.379063
25	6	0	2.655981	-1.541146	0.956824
26	6	0	2.994980	-2.801379	0.533636
27	6	0	2.277357	-3.410505	-0.533428
28	32	0	3.746336	-0.306325	2.032286
29	1	0	5.246387	-0.429033	1.798960
30	1	0	3.323853	-0.271661	3.497947
31	1	0	3.849024	-3.319246	0.956087
32	1	0	2.649495	-4.337455	-0.955695
33	1	0	-0.428861	-5.246179	-1.799605
34	1	0	-0.271331	-3.323451	-3.498356
35	1	0	-3.319154	-3.848914	-0.956845
36	1	0	-4.337546	-2.649605	0.954977
37	1	0	-5.246351	0.428655	1.799151
38	1	0	-3.323789	0.270928	3.498072
39	1	0	-3.849003	3.319044	0.956865
40	1	0	-2.649513	4.337657	-0.954725
41	1	0	0.428827	5.246558	-1.798506
42	1	0	0.271257	3.324190	-3.497662
43	1	0	3.319136	3.849112	-0.956107
44	1	0	4.337567	2.649403	0.955442

Table S30. The optimized Cartesian coordinates of the dianion **13** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.350936	2.851235	0.850125
2	32	0	0.012348	3.821705	1.854989
3	6	0	-1.333391	2.858480	0.852816
4	6	0	-2.574764	3.322984	0.489031
5	6	0	-3.308054	2.594688	-0.485629
6	6	0	-2.851163	1.350832	-0.850534
7	6	0	-1.656740	0.728463	-0.311636
8	6	0	-0.718443	1.660849	0.312494
9	6	0	0.728501	1.656767	0.311405
10	6	0	1.660810	0.718416	-0.312760
11	6	0	2.858375	1.333319	-0.853282
12	6	0	3.322925	2.574722	-0.489658
13	6	0	2.594748	3.308094	0.485029
14	6	0	1.656728	-0.728528	-0.311548
15	6	0	2.851130	-1.351009	-0.850361
16	32	0	3.821476	-0.012506	-1.855458
17	6	0	0.718455	-1.660783	0.312812
18	6	0	1.333424	-2.858302	0.853361
19	6	0	2.574782	-3.322883	0.489624
20	6	0	3.308034	-2.594789	-0.485216
21	6	0	-0.728490	-1.656701	0.311778
22	6	0	-1.350904	-2.851058	0.850770
23	32	0	-0.012277	-3.821318	1.855784
24	6	0	-1.660822	-0.718481	-0.312547
25	6	0	-2.858407	-1.333496	-0.852895
26	6	0	-3.322942	-2.574824	-0.488997

27	6	0	-2.594729	-3.307994	0.485816
28	32	0	-3.821547	0.012120	-1.855315
29	1	0	-5.367781	0.015869	-1.689267
30	1	0	-3.568014	0.013224	-3.392550
31	1	0	-4.252339	-2.967574	-0.894677
32	1	0	-2.993071	-4.235452	0.890477
33	1	0	-0.016012	-5.367573	1.689926
34	1	0	-0.013511	-3.567597	3.392988
35	1	0	2.967498	-4.252230	0.895453
36	1	0	4.235527	-2.993182	-0.889749
37	1	0	5.367717	-0.016219	-1.689470
38	1	0	3.567883	-0.013928	-3.392683
39	1	0	4.252307	2.967387	-0.895455
40	1	0	2.993106	4.235638	0.889481
41	1	0	0.016076	5.367925	1.688812
42	1	0	0.013640	3.568300	3.392245
43	1	0	-2.967463	4.252417	0.894680
44	1	0	-4.235563	2.992995	-0.890208

Table S31. The optimized Cartesian coordinates of the compound **13** in the ground singlet state calculated at the B3LYP/6–311++G(d, p) level of theory

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.784875	1.368383	-0.910224
2	32	0	-3.064761	3.065697	-0.002151
3	6	0	-1.368726	2.785401	0.908489
4	6	0	-0.695983	3.773380	1.611313
5	6	0	0.694737	3.772942	1.612453
6	6	0	1.368407	2.784745	0.910589
7	6	0	0.707546	1.649070	0.359673
8	6	0	-0.707337	1.649311	0.358964
9	6	0	-1.649120	0.707536	-0.359455
10	6	0	-1.649362	-0.707347	-0.358708
11	6	0	-2.785532	-1.368750	-0.908052
12	6	0	-3.773612	-0.696025	-1.610752
13	6	0	-3.773173	0.694695	-1.611929
14	6	0	-0.707483	-1.649112	0.359599
15	6	0	-1.368250	-2.784853	0.910493
16	32	0	-3.065698	-3.064759	0.002676
17	6	0	0.707400	-1.649353	0.358651
18	6	0	1.368882	-2.785507	0.907930
19	6	0	0.696258	-3.773569	1.610751
20	6	0	-0.694462	-3.773132	1.612127
21	6	0	1.649060	-0.707492	-0.359817
22	6	0	2.784720	-1.368275	-0.910859
23	32	0	3.064758	-3.065699	-0.003039
24	6	0	1.649302	0.707390	-0.358905
25	6	0	2.785378	1.368857	-0.908365
26	6	0	3.773338	0.696215	-1.611312
27	6	0	3.772900	-0.694505	-1.612652
28	32	0	3.065698	3.064760	0.002513
29	1	0	3.033002	4.362096	-0.823059
30	1	0	4.361415	3.029977	0.830411
31	1	0	4.603055	1.239069	-2.052735
32	1	0	4.602345	-1.236900	-2.055136
33	1	0	4.362118	-3.033128	0.822499
34	1	0	3.029944	-4.361294	-0.831126
35	1	0	1.239124	-4.603348	2.052042
36	1	0	-1.236845	-4.602642	2.054504
37	1	0	-3.033147	-4.361997	-0.823056
38	1	0	-4.361271	-3.030069	0.830803
39	1	0	-4.603403	-1.238827	-2.052098
40	1	0	-4.602695	1.237141	-2.054207
41	1	0	-4.361975	3.033019	0.823612
42	1	0	-3.030100	4.361394	-0.830084
43	1	0	-1.238774	4.603107	2.052794
44	1	0	1.237195	4.602400	2.054836