Heteroatom impact (S, Se, Te) on the heterocirculenes aromaticity

Nataliya N. Karaush-Karmazin[a,*], Gleb V. Baryshnikov[a,b], Lenara I. Valiulina[c], Rashid Valiev[c,d], Hans Ågren[b] and Boris F. Minaev[a]

[a]*Department of Chemistry and Nanomaterials Science, Bohdan Khmelnytsky National University, 18031, Cherkasy, Ukraine*

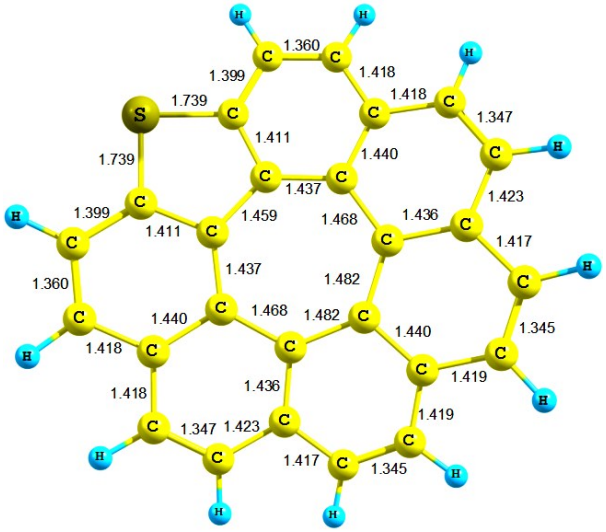
[b] *Division of Theoretical Chemistry and Biology, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH Royal Institute of Technology, 10691 Stockholm, Sweden*

[c] *Tomsk State University, 36, Lenin Avenue, 634050 Tomsk, Russia*

[d] *Tomsk Polytechnic University, 36, Lenin Avenue, 634050 Tomsk, Russia*

Electronic Supplementary Information

List of Content



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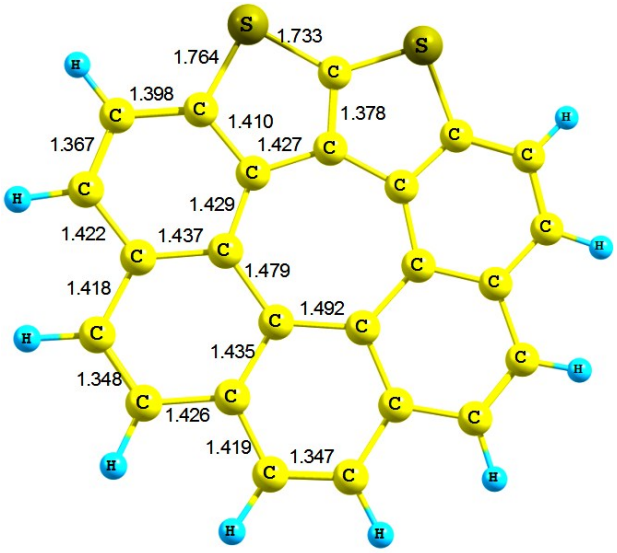

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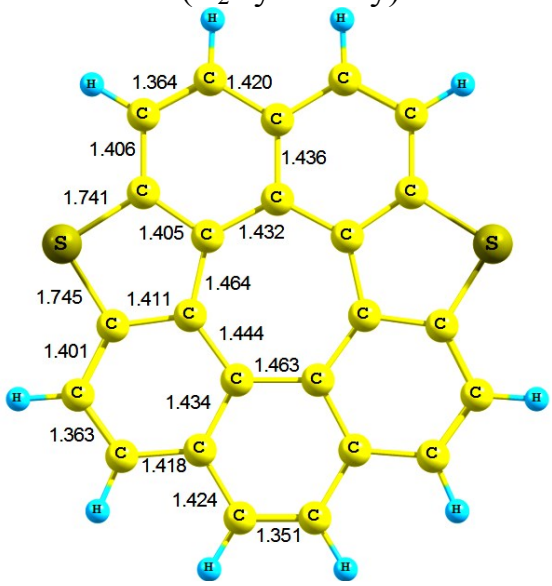

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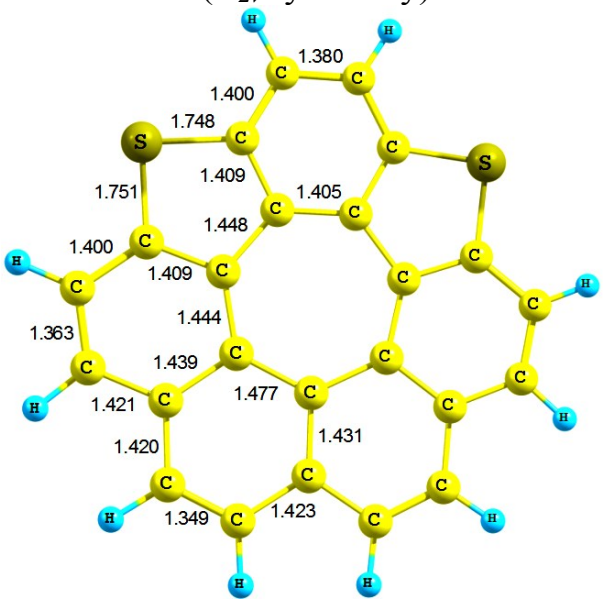

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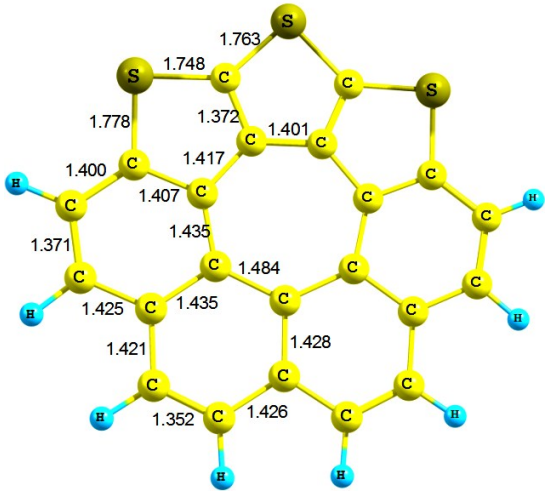

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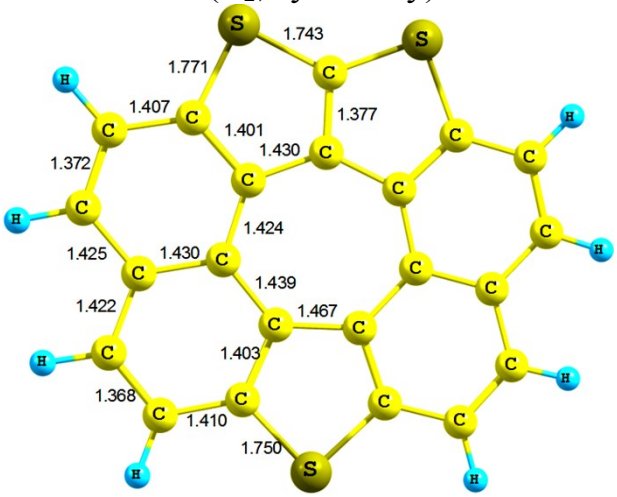

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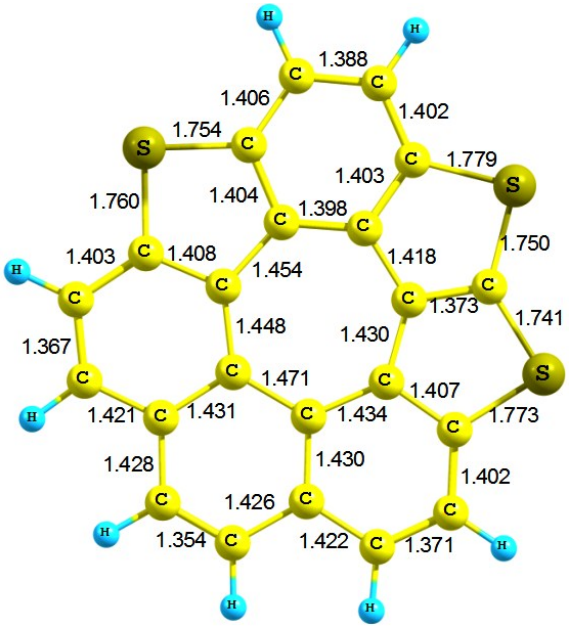

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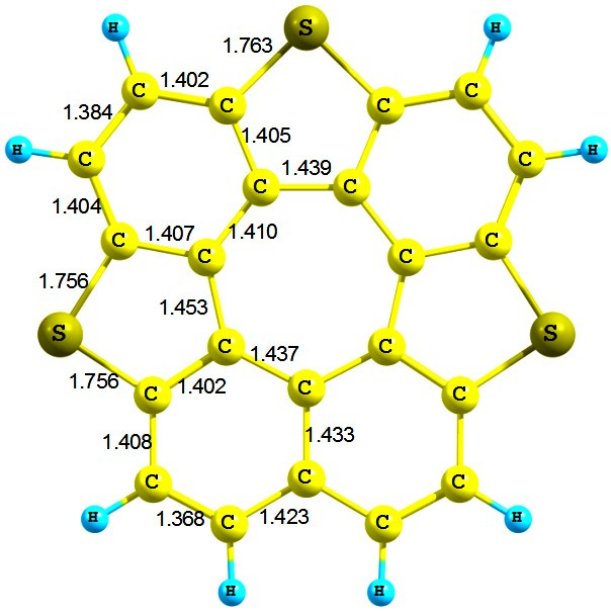

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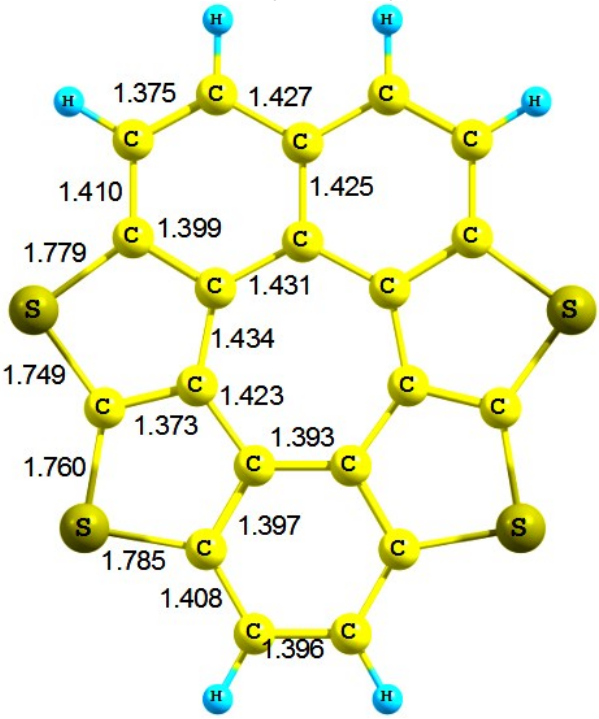

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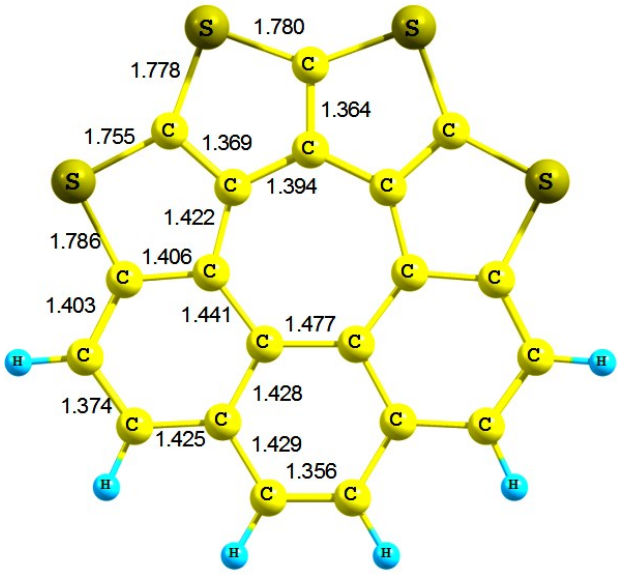

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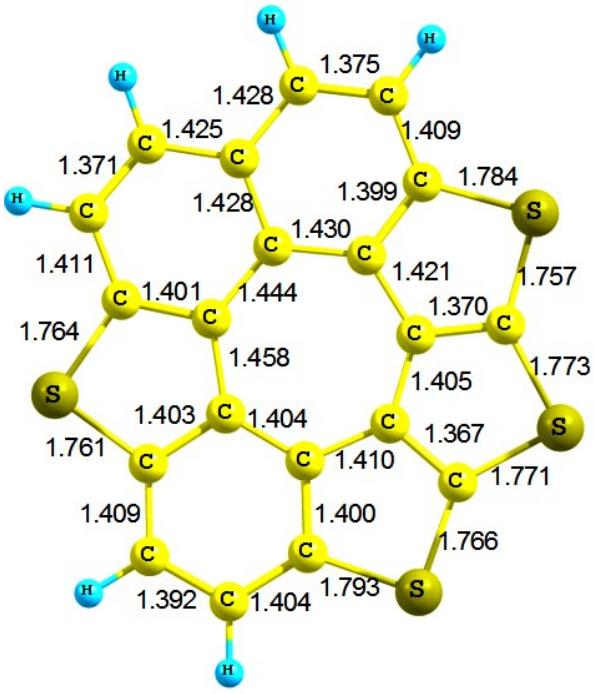

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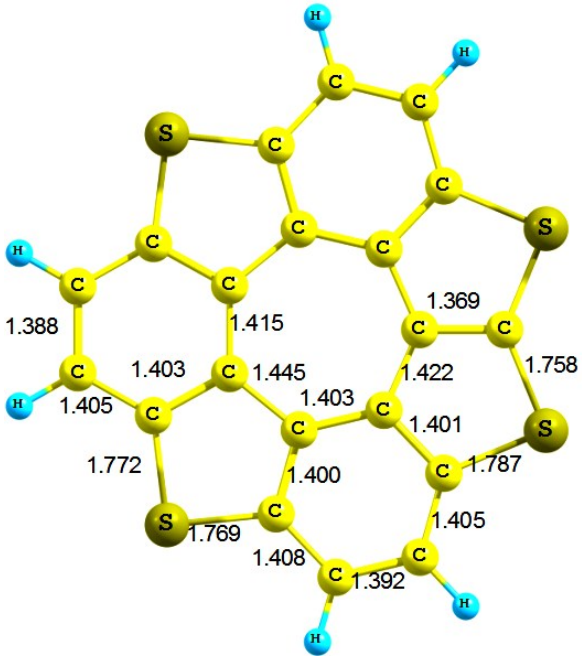

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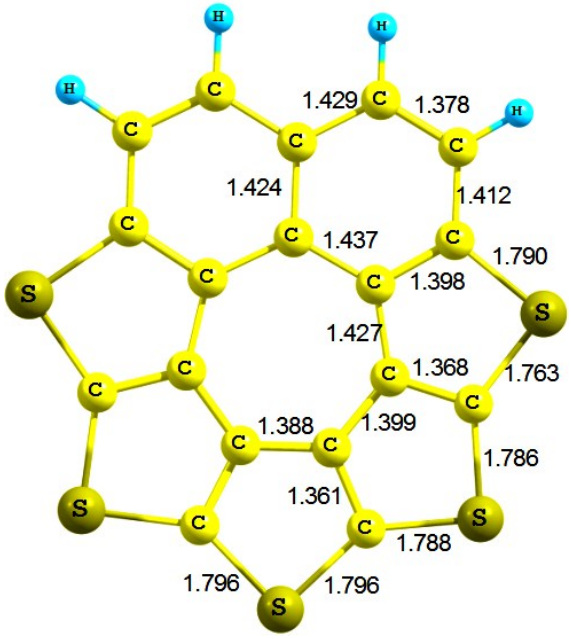

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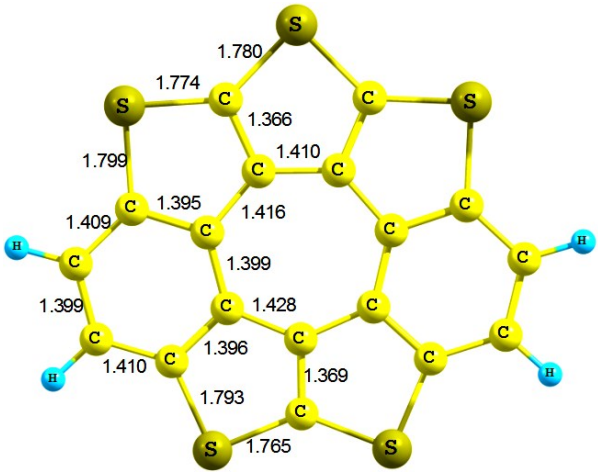

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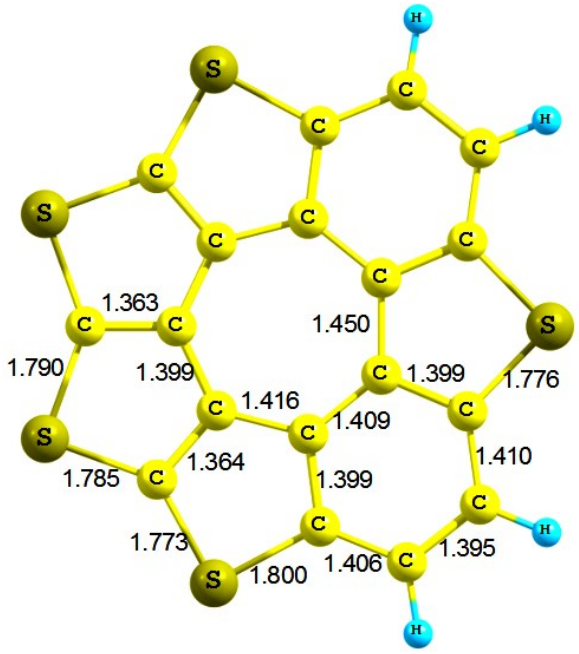

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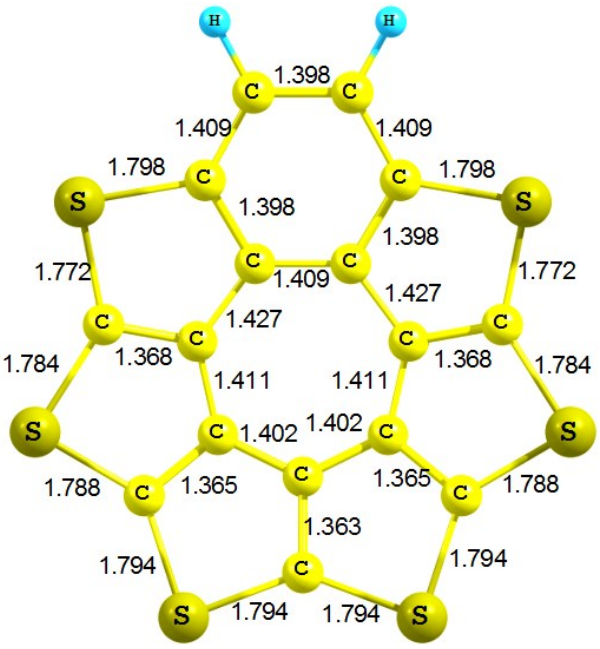

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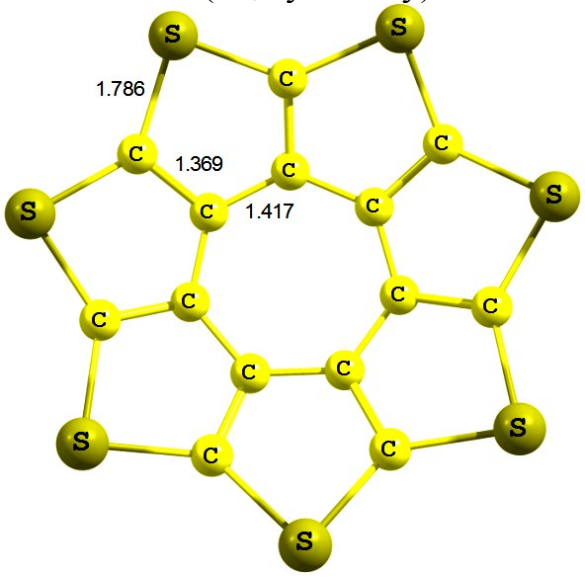


17 (C_{7v} symmetry)

Fig. S1. Bond lengths in thia[7]circulene molecules **1–17** calculated at the B3LYP/6-311++(d,p) level of theory

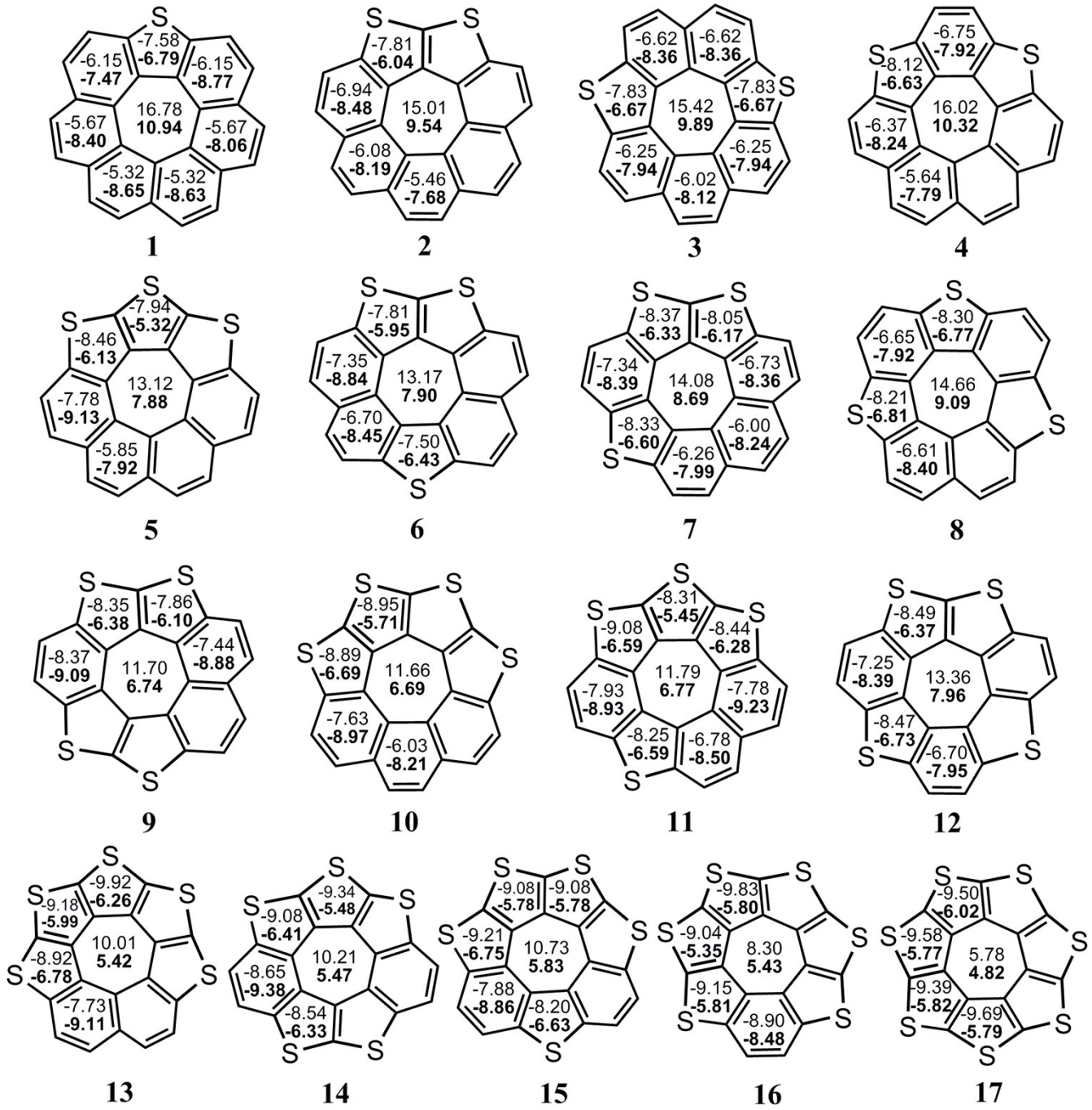
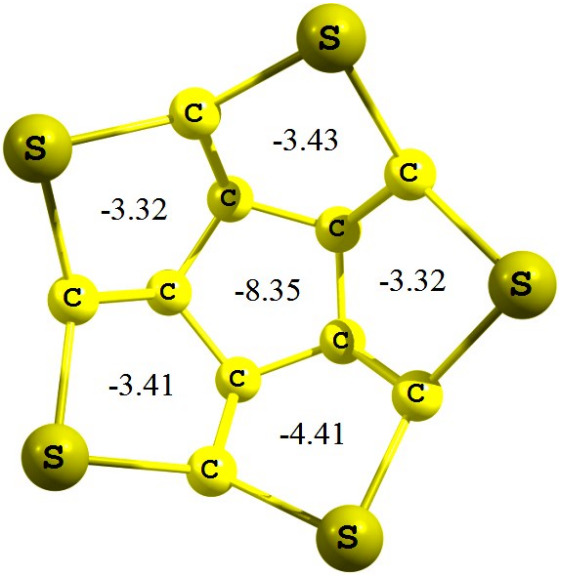
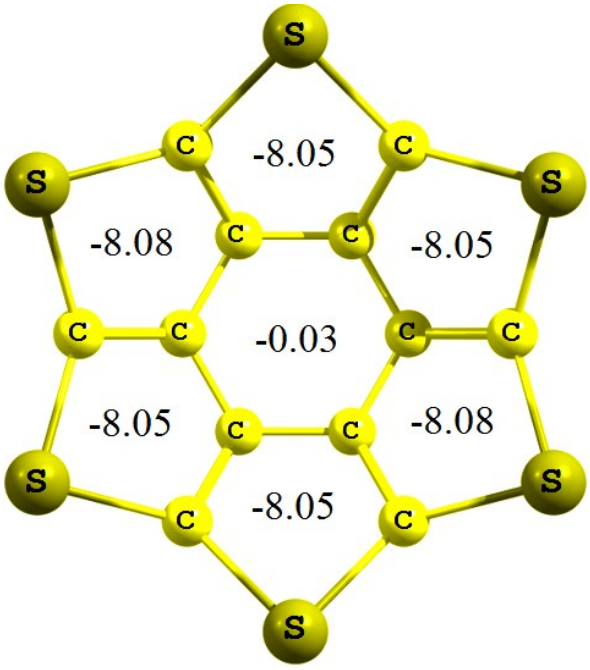


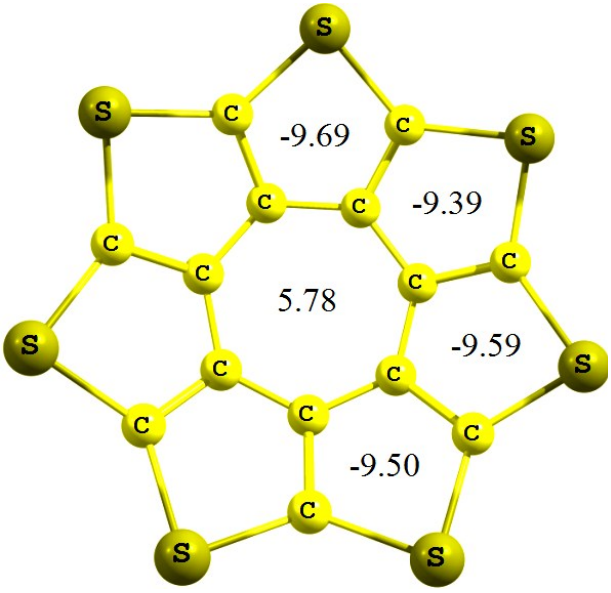
Fig. S2. The values of NICS(0) (top) and NICS(1) (bottom) indexes in the thia[7]circulene molecules **1**–**17**.


-3.43
-3.32
-8.35
-3.32
-3.41
-4.41

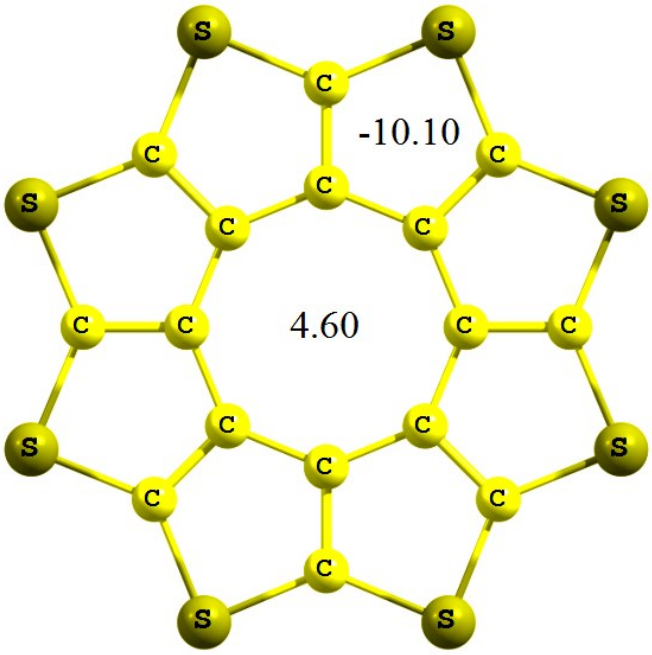
n = 5


-8.05
-8.08
-8.05
-0.03
-8.05
-8.08
-8.05

n = 6


-9.69
-9.39
5.78
-9.59
-9.50

n = 7


-10.10
4.60

n = 8

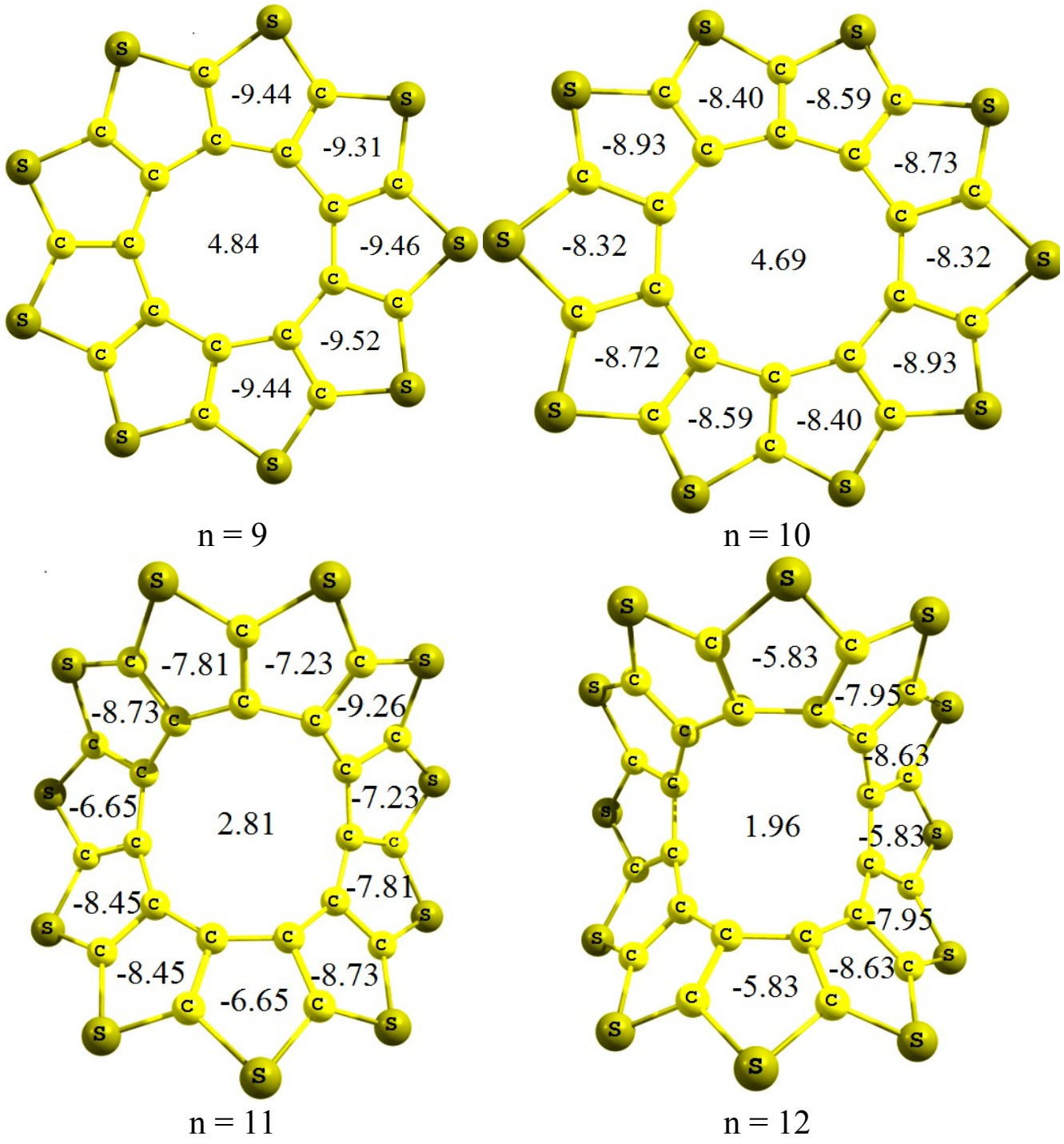


Fig. S3. The values of NICS(0) indexes in the thia[n]circulene molecules with n = 5–12.

Table S1. Total energies of the studied thia[7]circulene molecules **1**–**17** calculated at the B3LYP/6-311++(d,p) level of theory

Thiacirculene	E_{tot}, *a.u.*	Thiacirculene	E_{tot}, *a.u.*
1	–1396.49182	**10**	–2358.78675
2	–1717.26868	**11**	–2358.81337
3	–1717.29514	**12**	–2358.83428
4	–1717.28877	**13**	–2679.53706
5	–2038.03096	**14**	–2679.56457
6	–2038.06394	**15**	–2679.55790
7	–2038.05803	**16**	–3000.27943
8	–2038.07788	**17**	–3320.99972
9	–2358.82018		

Table S2. HOMO-LUMO gap for thia[n]circulenes (n = 5–12) calculated at the B3LYP/6-311++(d,p) level of theory

Circulene	HOMO-LUMO gap
n=5	1.96
n=6	2.51
n=7	3.45
n=8	4.45
n=9	4.27
n=10	4.30
n=11	3.62
n=12	3.26

Table S3. Relative energy (kcal·mol^{-1}) of the excited triplet state of the dicationic compounds **20**$^{2+}$–**22**$^{2+}$

Dication	CASSCF(10,10)/6-31G(d,p)
20^{2+}	+0.83
21^{2+}	+0.81
22^{2+}	+0.16

The total energy of the ground singlet state (S_0) is taken as zero.

Table S4. Total energies of the studied hetero[8]circulene molecules **18**–**23** calculated by the DFT/B3LYP method using the 6-311++G(d,p) basis set for the light atoms and the effective core potential Lanl2DZ basis set for the heavy Te atoms

Hetero[8]circulene	E_{tot}, *a.u.*
18	–3795.498419
19	–11808.83100
20	–2234.79915
21	–19822.14721
22	–10248.09111
23	–674.01613

Table S5. The optimized Cartesian coordinates of the thia[7]circulene **1** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.649098	0.234012	0.283399
2	6	1.338488	0.035578	-1.137554
3	6	-0.000000	-0.000000	-1.771763
4	6	-1.338488	-0.035578	-1.137554
5	6	-1.649098	-0.234012	0.283399
6	6	-0.712318	-0.156429	1.369903
7	6	0.712318	0.156429	1.369903
8	6	2.481937	-0.065594	-1.999652
9	6	3.014537	0.480382	0.670128
10	6	3.401513	0.731509	2.011365
11	6	2.505085	0.644615	3.030731
12	6	1.189119	0.314121	2.688972
13	16	0.000000	0.000000	3.917881
14	6	-1.189119	-0.314121	2.688972
15	6	-3.014537	-0.480382	0.670128
16	6	-2.481937	0.065594	-1.999652
17	6	-0.000000	-0.000000	-3.211710
18	1	4.444498	0.950329	2.208795
19	1	2.792244	0.790799	4.064969
20	6	4.080220	0.415060	-0.263253
21	6	3.821145	0.092154	-1.545061
22	6	2.378290	-0.248279	-3.401321
23	6	1.171845	-0.175464	-3.992426
24	6	-1.171845	0.175464	-3.992426
25	6	-2.378290	0.248279	-3.401321
26	6	-3.821145	-0.092154	-1.545061
27	6	-4.080220	-0.415060	-0.263253
28	6	-3.401513	-0.731509	2.011365
29	6	-2.505085	-0.644615	3.030731
30	1	5.091752	0.591350	0.083943
31	1	4.619645	-0.004183	-2.271429
32	1	3.286364	-0.375260	-3.978834
33	1	1.066554	-0.236031	-5.069328
34	1	-1.066554	0.236031	-5.069328
35	1	-3.286364	0.375260	-3.978834
36	1	-4.619645	0.004183	-2.271429
37	1	-5.091752	-0.591350	0.083943
38	1	-4.444498	-0.950329	2.208795
39	1	-2.792244	-0.790799	4.064969

Table S6. The optimized Cartesian coordinates of the thia[7]circulene **2** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	-1.680234	0.533510
2	6	0.000000	-0.745786	1.679871
3	6	0.000000	0.745786	1.679871
4	6	-0.000000	1.680234	0.533510
5	6	-0.000000	1.310384	-0.846823
6	6	-0.000000	-0.000000	-1.411749
7	6	-0.000000	-1.310384	-0.846823
8	6	0.000000	-1.390248	2.962081
9	6	0.000000	-2.806820	3.126326
10	6	0.000000	-3.640242	2.066440
11	6	0.000000	-3.100225	0.754860
12	6	0.000000	-4.039956	-0.312111
13	6	-0.000000	-3.654480	-1.623286
14	6	-0.000000	-2.278350	-1.871422
15	16	-0.000000	-1.584135	-3.493326
16	6	-0.000000	-0.000000	-2.789660
17	6	-0.000000	2.278350	-1.871422
18	6	-0.000000	3.100225	0.754860
19	6	-0.000000	3.640242	2.066440
20	6	0.000000	2.806820	3.126326
21	6	0.000000	1.390248	2.962081
22	1	0.000000	-3.195347	4.138166
23	1	0.000000	-4.716820	2.192971
24	1	0.000000	-5.092959	-0.054984
25	1	-0.000000	-4.376416	-2.430780
26	1	-0.000000	4.716820	2.192971
27	1	0.000000	3.195347	4.138166
28	6	0.000000	-0.673582	4.186332
29	6	0.000000	0.673582	4.186332
30	1	0.000000	-1.235294	5.113157
31	1	0.000000	1.235294	5.113157
32	6	-0.000000	4.039956	-0.312111
33	6	-0.000000	3.654480	-1.623286
34	16	-0.000000	1.584135	-3.493326
35	1	-0.000000	5.092959	-0.054984
36	1	-0.000000	4.376416	-2.430780

Table S7. The optimized Cartesian coordinates of the thia[7]circulene **3** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.000000	-0.731447	1.590922
2	6	-0.000000	0.731447	1.590922
3	6	-0.000000	1.578171	0.421394
4	6	-0.000000	1.264308	-1.008161
5	6	-0.000000	-0.000000	-1.680185

6	6	0.000000	-1.264308	-1.008161
7	6	0.000000	-1.578171	0.421394
8	6	-0.000000	1.401182	2.859317
9	6	-0.000000	0.675272	4.084712
10	6	0.000000	-0.675272	4.084712
11	6	0.000000	-1.401182	2.859317
12	6	0.000000	-2.815461	2.967872
13	6	0.000000	-3.609739	1.860489
14	6	0.000000	-2.976563	0.610339
15	16	0.000000	-3.897837	-0.871149
16	6	0.000000	-2.424837	-1.800105
17	6	0.000000	-0.000000	-3.116446
18	6	-0.000000	2.424837	-1.800105
19	6	-0.000000	2.976563	0.610339
20	1	-0.000000	1.234386	5.013593
21	1	0.000000	-1.234386	5.013593
22	1	0.000000	-3.253600	3.959390
23	1	0.000000	-4.690620	1.933931
24	6	-0.000000	2.815461	2.967872
25	6	-0.000000	3.609739	1.860489
26	1	-0.000000	3.253600	3.959390
27	1	-0.000000	4.690620	1.933931
28	6	-0.000000	2.423065	-3.206135
29	6	-0.000000	1.218412	-3.846583
30	1	-0.000000	3.356376	-3.756264
31	1	-0.000000	1.171736	-4.929782
32	6	0.000000	-1.218412	-3.846583
33	6	0.000000	-2.423065	-3.206135
34	1	0.000000	-1.171736	-4.929782
35	1	0.000000	-3.356376	-3.756264
36	16	-0.000000	3.897837	-0.871149

Table S8. The optimized Cartesian coordinates of the thia[7]circulene **4** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	-1.326981	1.171844
2	6	0.000000	-0.000000	1.820963
3	6	0.000000	1.326981	1.171844
4	6	0.000000	1.607708	-0.244479
5	6	0.000000	0.702738	-1.375227
6	6	-0.000000	-0.702738	-1.375227
7	6	-0.000000	-1.607708	-0.244479
8	6	0.000000	-0.000000	3.251940
9	6	-0.000000	-1.196196	4.022694
10	6	-0.000000	-2.405126	3.424775
11	6	-0.000000	-2.498372	2.007942
12	6	-0.000000	-3.817890	1.481411
13	6	-0.000000	-4.057870	0.140169
14	6	-0.000000	-2.940328	-0.702944
15	16	-0.000000	-3.101211	-2.446197
16	6	-0.000000	-1.362278	-2.620756
17	6	0.000000	1.362278	-2.620756

18	6	0.000000	0.689984	-3.849269
19	6	-0.000000	-0.689984	-3.849269
20	6	0.000000	2.940328	-0.702944
21	16	0.000000	3.101211	-2.446197
22	6	0.000000	4.057870	0.140169
23	6	0.000000	3.817890	1.481411
24	6	0.000000	2.498372	2.007942
25	1	-0.000000	-1.107227	5.102922
26	1	-0.000000	-3.320313	4.005811
27	1	-0.000000	-4.642576	2.184935
28	1	-0.000000	-5.063743	-0.261681
29	1	0.000000	1.242695	-4.780886
30	1	-0.000000	-1.242695	-4.780886
31	1	0.000000	5.063743	-0.261681
32	1	0.000000	4.642576	2.184935
33	6	0.000000	1.196196	4.022694
34	6	0.000000	2.405126	3.424775
35	1	0.000000	1.107227	5.102922
36	1	0.000000	3.320313	4.005811

Table S9. The optimized Cartesian coordinates of the thia[7]circulene **5** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	1.339721	1.247102
2	6	0.000000	-0.000000	1.884680
3	6	0.000000	-1.339721	1.247102
4	6	0.000000	-1.626664	-0.159415
5	6	0.000000	-0.700676	-1.231569
6	6	0.000000	0.700676	-1.231569
7	6	-0.000000	1.626664	-0.159415
8	6	0.000000	-0.000000	3.313131
9	6	-0.000000	2.517236	2.066448
10	6	-0.000000	3.827532	1.506954
11	6	-0.000000	4.060672	0.156417
12	6	-0.000000	2.934780	-0.676440
13	16	-0.000000	2.984860	-2.453453
14	6	0.000000	1.237378	-2.493864
15	6	0.000000	-1.237378	-2.493864
16	6	0.000000	-2.934780	-0.676440
17	6	0.000000	-2.517236	2.066448
18	1	-0.000000	4.664839	2.195688
19	1	-0.000000	5.067148	-0.243686
20	6	-0.000000	2.418660	3.484036
21	6	-0.000000	1.203848	4.077767
22	6	0.000000	-1.203848	4.077767
23	6	0.000000	-2.418660	3.484036
24	6	0.000000	-3.827532	1.506954
25	6	0.000000	-4.060672	0.156417
26	1	-0.000000	3.329408	4.072292
27	1	-0.000000	1.117034	5.158411
28	1	0.000000	-1.117034	5.158411
29	1	0.000000	-3.329408	4.072292

30	1	0.000000	-4.664839	2.195688
31	1	0.000000	-5.067148	-0.243686
32	16	0.000000	0.000000	-3.749601
33	16	0.000000	-2.984860	-2.453453

Table S10. The optimized Cartesian coordinates of the thia[7]circulene **6** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	-1.684043	-0.441313
2	6	-0.000000	-0.733286	-1.520909
3	6	-0.000000	0.733286	-1.520909
4	6	-0.000000	1.684043	-0.441313
5	6	-0.000000	1.317034	0.934228
6	6	0.000000	-0.000000	1.492570
7	6	0.000000	-1.317034	0.934228
8	6	-0.000000	-1.244693	-2.827674
9	6	0.000000	-3.082841	-0.739780
10	6	0.000000	-4.040709	0.315391
11	6	0.000000	-3.670741	1.636857
12	6	0.000000	-2.296154	1.936013
13	16	0.000000	-1.598757	3.563650
14	6	0.000000	-0.000000	2.869198
15	6	0.000000	2.296154	1.936013
16	6	-0.000000	3.082841	-0.739780
17	6	-0.000000	1.244693	-2.827674
18	1	0.000000	-5.092444	0.051486
19	1	0.000000	-4.414500	2.424449
20	6	-0.000000	-3.519831	-2.093064
21	6	-0.000000	-2.622471	-3.125580
22	6	-0.000000	2.622471	-3.125580
23	6	-0.000000	3.519831	-2.093064
24	1	-0.000000	-4.584847	-2.296762
25	1	-0.000000	-2.957740	-4.155868
26	1	-0.000000	2.957740	-4.155868
27	1	-0.000000	4.584847	-2.296762
28	16	0.000000	1.598757	3.563650
29	6	-0.000000	4.040709	0.315391
30	6	-0.000000	3.670741	1.636857
31	1	-0.000000	5.092444	0.051486
32	1	-0.000000	4.414500	2.424449
33	16	-0.000000	0.000000	-4.057251

Table S11. The optimized Cartesian coordinates of the thia[7]circulene **7** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.697124	-0.005329	-0.000000

2	6	-1.210152	1.358469	-0.000000
3	6	0.193128	1.798532	0.000000
4	6	1.340576	0.937815	0.000000
5	6	1.398513	-0.491453	0.000000
6	6	0.393876	-1.492047	0.000000
7	6	-0.987184	-1.273789	-0.000000
8	6	-2.216018	2.376782	-0.000000
9	6	-3.601064	2.060004	-0.000000
10	6	-4.046881	0.767895	-0.000000
11	6	-3.083338	-0.251342	-0.000000
12	6	-1.813953	-2.408171	-0.000000
13	6	0.919267	-2.793232	0.000000
14	6	2.667460	-1.016732	0.000000
15	6	2.646462	1.462543	0.000000
16	16	3.902272	0.210646	0.000000
17	6	2.903220	2.840348	0.000000
18	6	1.820690	3.681257	0.000000
19	6	0.482647	3.198445	0.000000
20	1	-4.311055	2.879414	-0.000000
21	1	-5.104916	0.535430	-0.000000
22	1	3.915611	3.225752	0.000000
23	1	1.972202	4.754798	0.000000
24	6	-1.865799	3.761017	-0.000000
25	6	-0.571740	4.158309	-0.000000
26	1	-2.668141	4.490472	-0.000000
27	1	-0.313506	5.211422	-0.000000
28	16	2.697747	-2.766906	0.000000
29	6	0.077738	-3.914260	0.000000
30	6	-1.296394	-3.715089	-0.000000
31	16	-3.509255	-1.958658	-0.000000
32	1	0.480864	-4.919601	0.000000
33	1	-1.964313	-4.567852	-0.000000

Table S12. The optimized Cartesian coordinates of the thia[7]circulene **8** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	0.000000	-1.753449
2	6	-0.000000	-1.275294	-1.090755
3	6	-0.000000	-1.587772	0.327812
4	6	-0.000000	-0.719346	1.438629
5	6	0.000000	0.719346	1.438629
6	6	0.000000	1.587772	0.327812
7	6	0.000000	1.275294	-1.090755
8	6	-0.000000	-2.446048	-1.861652
9	6	-0.000000	-2.436812	-3.269371
10	6	-0.000000	-1.226822	-3.907946
11	6	0.000000	0.000000	-3.186381
12	6	0.000000	1.226822	-3.907946
13	6	0.000000	2.436812	-3.269371
14	6	0.000000	2.446048	-1.861652
15	16	0.000000	3.914110	-0.897567
16	6	0.000000	2.971445	0.584230
17	6	0.000000	1.257310	2.736472

18	6	0.000000	2.640238	2.968909
19	6	0.000000	3.500540	1.884208
20	6	-0.000000	-1.257310	2.736472
21	16	-0.000000	-0.000000	3.972982
22	6	-0.000000	-2.640238	2.968909
23	6	-0.000000	-3.500540	1.884208
24	6	-0.000000	-2.971445	0.584230
25	16	-0.000000	-3.914110	-0.897567
26	1	-0.000000	-3.364921	-3.828066
27	1	-0.000000	-1.185535	-4.991546
28	1	0.000000	1.185535	-4.991546
29	1	0.000000	3.364921	-3.828066
30	1	0.000000	3.034184	3.977895
31	1	0.000000	4.572523	2.040581
32	1	-0.000000	-3.034184	3.977895
33	1	-0.000000	-4.572523	2.040581

Table S13. The optimized Cartesian coordinates of the thia[7]circulene **9** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	1.261015	-1.117790
2	6	-0.000000	-0.000000	-1.793845
3	6	0.000000	-1.261015	-1.117790
4	6	0.000000	-1.528599	0.291234
5	6	0.000000	-0.696271	1.445608
6	6	-0.000000	0.696271	1.445608
7	6	-0.000000	1.528599	0.291234
8	6	-0.000000	-0.000000	-3.218967
9	6	-0.000000	1.244004	-3.917756
10	6	-0.000000	2.452106	-3.260824
11	6	-0.000000	2.452790	-1.850472
12	6	-0.000000	2.862860	0.613464
13	16	-0.000000	3.155752	2.348721
14	6	-0.000000	1.396984	2.654630
15	6	0.000000	-1.396984	2.654630
16	6	0.000000	-2.862860	0.613464
17	6	0.000000	-2.452790	-1.850472
18	1	-0.000000	1.226613	-5.002050
19	1	-0.000000	3.381652	-3.817286
20	6	0.000000	-1.244004	-3.917756
21	6	0.000000	-2.452106	-3.260824
22	1	0.000000	-1.226613	-5.002050
23	1	0.000000	-3.381652	-3.817286
24	6	0.000000	-0.698161	3.876439
25	6	-0.000000	0.698161	3.876439
26	1	0.000000	-1.227883	4.821190
27	1	-0.000000	1.227883	4.821190
28	16	0.000000	-3.889929	-0.802695
29	16	-0.000000	3.889929	-0.802695
30	16	0.000000	-3.155752	2.348721

Table S14. The optimized Cartesian coordinates of the thia[7]circulene **10** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	-0.738676	1.720076
2	6	-0.000000	0.738676	1.720076
3	6	-0.000000	1.605190	0.569254
4	6	-0.000000	1.254228	-0.808831
5	6	-0.000000	-0.000000	-1.416956
6	6	0.000000	-1.254228	-0.808831
7	6	-0.000000	-1.605190	0.569254
8	6	-0.000000	1.418431	2.975454
9	6	-0.000000	-1.418431	2.975454
10	6	-0.000000	-2.841526	3.044457
11	6	-0.000000	-3.643309	1.928412
12	6	-0.000000	-3.006540	0.678325
13	16	0.000000	-3.830537	-0.905857
14	6	-0.000000	-2.275436	-1.720102
15	6	-0.000000	-0.000000	-2.780780
16	6	-0.000000	2.275436	-1.720102
17	6	-0.000000	3.006540	0.678325
18	1	-0.000000	-3.298376	4.027880
19	1	-0.000000	-4.722933	2.016328
20	6	-0.000000	-0.678151	4.197806
21	6	-0.000000	0.678151	4.197806
22	6	-0.000000	2.841526	3.044457
23	6	-0.000000	3.643309	1.928412
24	1	-0.000000	-1.228311	5.132388
25	1	-0.000000	1.228311	5.132388
26	1	-0.000000	3.298376	4.027880
27	1	-0.000000	4.722933	2.016328
28	16	0.000000	-1.672168	-3.392361
29	16	-0.000000	1.672168	-3.392361
30	16	-0.000000	3.830537	-0.905857

Table S15. The optimized Cartesian coordinates of the thia[7]circulene **11** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.074460	1.019880	0.000000
2	6	0.211024	1.598512	-0.000000
3	6	1.424988	0.892535	-0.000000
4	6	1.655631	-0.546637	-0.000000
5	6	0.730072	-1.654476	-0.000000
6	6	-0.694940	-1.530099	0.000000
7	6	-1.459226	-0.331688	0.000000
8	6	0.158085	2.997675	-0.000000
9	6	-2.116117	1.904841	0.000000
10	6	-2.819997	-0.493364	0.000000

11	16	-3.261850	-2.193974	0.000000
12	6	-1.536838	-2.646975	0.000000
13	6	1.251117	-2.983967	-0.000000
14	6	3.029307	-0.820139	-0.000000
15	6	2.598687	1.660344	-0.000000
16	6	1.346434	3.745119	-0.000000
17	6	2.563146	3.068496	-0.000000
18	1	1.333784	4.828130	-0.000000
19	1	3.485917	3.635977	-0.000000
20	6	0.357621	-4.097935	-0.000000
21	6	-1.010082	-3.953666	0.000000
22	1	0.786444	-5.094050	-0.000000
23	1	-1.657931	-4.821781	0.000000
24	16	4.029238	0.633074	-0.000000
25	16	-3.673209	1.060483	0.000000
26	6	3.540574	-2.135096	-0.000000
27	6	2.661052	-3.187188	-0.000000
28	16	-1.539484	3.573949	0.000000
29	1	4.610027	-2.308427	-0.000000
30	1	3.038249	-4.203961	-0.000000

Table S16. The optimized Cartesian coordinates of the thia[7]circulene **12** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	0.707251	1.522947
2	6	0.000000	-0.707251	1.522947
3	6	0.000000	-1.617767	0.401291
4	6	0.000000	-1.299676	-0.965518
5	6	0.000000	0.000000	-1.543453
6	6	-0.000000	1.299676	-0.965518
7	6	-0.000000	1.617767	0.401291
8	6	0.000000	-1.386847	2.750877
9	6	-0.000000	-0.694135	3.973213
10	6	-0.000000	0.694135	3.973213
11	6	-0.000000	1.386847	2.750877
12	6	-0.000000	2.967435	0.773326
13	6	-0.000000	2.313976	-1.932401
14	6	0.000000	0.000000	-2.912833
15	6	0.000000	-2.313976	-1.932401
16	16	0.000000	-1.625490	-3.581412
17	6	0.000000	-3.665426	-1.548726
18	6	0.000000	-3.989227	-0.194749
19	6	0.000000	-2.967435	0.773326
20	1	-0.000000	-1.232016	4.913486
21	1	-0.000000	1.232016	4.913486
22	1	0.000000	-4.456823	-2.288370
23	1	0.000000	-5.030393	0.103870
24	16	-0.000000	1.625490	-3.581412
25	6	-0.000000	3.665426	-1.548726
26	6	-0.000000	3.989227	-0.194749
27	16	-0.000000	3.145123	2.533370
28	1	-0.000000	4.456823	-2.288370
29	1	-0.000000	5.030393	0.103870

30	16	0.000000	-3.145123	2.533370

Table S17. The optimized Cartesian coordinates of the thia[7]circulene **13** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	0.000000	-1.856570
2	6	-0.000000	-1.274082	-1.191703
3	6	-0.000000	-1.549876	0.208247
4	6	-0.000000	-0.694057	1.315372
5	6	0.000000	0.694057	1.315372
6	6	0.000000	1.549876	0.208247
7	6	0.000000	1.274082	-1.191703
8	6	-0.000000	-2.471350	-1.913062
9	6	-0.000000	0.000000	-3.280293
10	6	0.000000	1.248502	-3.976003
11	6	0.000000	2.462492	-3.324915
12	6	0.000000	2.471350	-1.913062
13	16	0.000000	3.906871	-0.844121
14	6	0.000000	2.866965	0.579359
15	6	0.000000	1.273271	2.546871
16	6	-0.000000	-1.273271	2.546871
17	6	-0.000000	-2.866965	0.579359
18	1	0.000000	1.231585	-5.060436
19	1	0.000000	3.386577	-3.890284
20	6	-0.000000	-1.248502	-3.976003
21	6	-0.000000	-2.462492	-3.324915
22	1	-0.000000	-1.231585	-5.060436
23	1	-0.000000	-3.386577	-3.890284
24	16	0.000000	3.051446	2.355814
25	16	-0.000000	-0.000000	3.813622
26	16	-0.000000	-3.051446	2.355814
27	16	-0.000000	-3.906871	-0.844121

Table S18. The optimized Cartesian coordinates of the thia[7]circulene **14** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	1.309503	1.042527
2	6	0.000000	-0.000000	1.610999
3	6	0.000000	-1.309503	1.042527
4	6	0.000000	-1.634464	-0.318004
5	6	0.000000	-0.704754	-1.386036
6	6	0.000000	0.704754	-1.386036
7	6	-0.000000	1.634464	-0.318004
8	6	-0.000000	-0.000000	2.980233
9	6	-0.000000	2.330752	1.994783
10	6	-0.000000	3.677446	1.576634

11	6	-0.000000	3.994235	0.213821
12	6	-0.000000	2.962188	-0.745951
13	16	-0.000000	3.031973	-2.543834
14	6	0.000000	1.259951	-2.634142
15	6	0.000000	-1.259951	-2.634142
16	6	0.000000	-2.962188	-0.745951
17	6	0.000000	-2.330752	1.994783
18	1	-0.000000	4.482783	2.301268
19	1	-0.000000	5.035877	-0.083412
20	16	0.000000	0.000000	-3.891482
21	16	0.000000	-3.031973	-2.543834
22	16	0.000000	-1.634475	3.646997
23	6	0.000000	-3.677446	1.576634
24	6	0.000000	-3.994235	0.213821
25	16	-0.000000	1.634475	3.646997
26	1	0.000000	-4.482783	2.301268
27	1	0.000000	-5.035877	-0.083412

Table S19. The optimized Cartesian coordinates of the thia[7]circulene **15** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.000000	-0.724969	-1.572213
2	6	-0.000000	-1.612132	-0.477117
3	6	0.000000	-1.262973	0.894724
4	6	0.000000	0.000000	1.495852
5	6	0.000000	1.262973	0.894724
6	6	-0.000000	1.612132	-0.477117
7	6	-0.000000	0.724969	-1.572213
8	6	-0.000000	-3.000176	-0.653941
9	6	-0.000000	-1.272794	-2.859983
10	6	-0.000000	1.272794	-2.859983
11	6	-0.000000	3.000176	-0.653941
12	6	0.000000	2.294938	1.787362
13	6	0.000000	0.000000	2.858578
14	6	0.000000	-2.294938	1.787362
15	6	-0.000000	-2.669860	-3.049359
16	6	-0.000000	-3.534907	-1.954613
17	1	-0.000000	-3.086927	-4.049135
18	1	-0.000000	-4.604845	-2.123568
19	16	0.000000	3.848471	0.933456
20	16	0.000000	1.683819	3.464882
21	16	0.000000	-1.683819	3.464882
22	16	0.000000	-3.848471	0.933456
23	6	-0.000000	2.669860	-3.049359
24	6	-0.000000	3.534907	-1.954613
25	16	-0.000000	-0.000000	-4.098460
26	1	-0.000000	3.086927	-4.049135
27	1	-0.000000	4.604845	-2.123568

Table 20. The optimized Cartesian coordinates of the thia[7]circulene **16** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.595951	-0.237624	-0.704273
2	6	-0.457661	-0.329367	-1.560051
3	6	0.918289	-0.405707	-1.256510
4	6	1.538672	-0.440985	0.000000
5	6	0.918289	-0.405707	1.256510
6	6	-0.457661	-0.329367	1.560051
7	6	-1.595951	-0.237624	0.704273
8	6	-0.694606	-0.036089	-2.875070
9	6	-2.762049	0.085810	-1.404426
10	6	-3.957110	0.331800	-0.698962
11	6	-3.957110	0.331800	0.698962
12	6	-2.762049	0.085810	1.404426
13	16	-2.416466	0.270327	3.159723
14	6	-0.694606	-0.036089	2.875070
15	6	1.766607	-0.132440	2.290158
16	6	2.875892	-0.176616	0.000000
17	16	3.441240	0.079591	1.682878
18	6	1.766607	-0.132440	-2.290158
19	1	-4.874819	0.568283	-1.223691
20	1	-4.874819	0.568283	1.223691
21	16	0.828130	0.165193	3.782322
22	16	3.441240	0.079591	-1.682878
23	16	0.828130	0.165193	-3.782322
24	16	-2.416466	0.270327	-3.159723

Table 21. The optimized Cartesian coordinates of the thia[7]circulene **17** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.363428	1.592284	-0.593010
2	6	-1.018304	1.276913	-0.593010
3	6	-1.633233	0.000000	-0.593010
4	6	-1.018304	-1.276913	-0.593010
5	6	0.363428	-1.592284	-0.593010
6	6	1.471492	-0.708633	-0.593010
7	6	1.471492	0.708633	-0.593010
8	6	-1.816908	2.278331	-0.110224
9	6	0.648447	2.841032	-0.110224
10	6	2.625508	1.264378	-0.110224
11	16	3.815888	-0.000000	0.307739
12	6	2.625508	-1.264378	-0.110224
13	6	0.648447	-2.841032	-0.110224
14	6	-1.816908	-2.278331	-0.110224
15	16	-0.849115	-3.720215	0.307739
16	6	-2.914094	0.000000	-0.110224
17	16	-3.437996	-1.655652	0.307739
18	16	2.379167	-2.983381	0.307739
19	16	2.379167	2.983381	0.307739
20	16	-0.849115	3.720215	0.307739
21	16	-3.437996	1.655652	0.307739

Table 22. The optimized Cartesian coordinates of the octathia[8]circulene **18** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	16	3.003592	-3.003592	0.000000
2	6	-0.711673	1.718131	0.000000
3	6	0.711673	1.718131	0.000000
4	6	-1.718131	-0.711673	0.000000
5	6	-1.718131	0.711673	0.000000
6	6	1.718131	0.711673	0.000000
7	6	1.718131	-0.711673	0.000000
8	6	-0.711673	-1.718131	0.000000
9	16	-3.003592	3.003592	0.000000
10	16	0.000000	4.247720	0.000000
11	16	3.003592	3.003592	0.000000
12	16	4.247720	-0.000000	0.000000
13	16	-3.003592	-3.003592	0.000000
14	16	-4.247720	0.000000	0.000000
15	6	-2.992161	-1.239394	0.000000
16	6	-2.992161	1.239394	0.000000
17	6	-1.239394	2.992161	0.000000
18	6	1.239394	2.992161	0.000000
19	6	2.992161	1.239394	0.000000
20	6	2.992161	-1.239394	0.000000
21	6	-1.239394	-2.992161	0.000000
22	6	0.711673	-1.718131	0.000000
23	6	1.239394	-2.992161	0.000000
24	16	-0.000000	-4.247720	-0.000000

Table 23. The optimized Cartesian coordinates of the tetrathiatetraselena[8]circulene **19** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	34	0.826816	4.332608	-0.000000
2	34	-4.332608	0.826816	-0.000000
3	16	-2.400275	3.532451	-0.000000
4	16	3.532451	2.400275	-0.000000
5	6	-1.571775	1.033555	-0.000000
6	6	-0.382098	1.841932	-0.000000
7	6	-1.841932	-0.382098	-0.000000
8	6	1.815006	2.714295	-0.000000
9	6	-0.687886	3.191936	-0.000000
10	6	1.033555	1.571775	-0.000000
11	6	-2.714295	1.815006	-0.000000
12	6	-3.191936	-0.687886	-0.000000
13	34	-0.826816	-4.332608	-0.000000
14	34	4.332608	-0.826816	-0.000000

15	16	2.400275	-3.532451	-0.000000
16	16	-3.532451	-2.400275	-0.000000
17	6	1.571775	-1.033555	-0.000000
18	6	0.382098	-1.841932	-0.000000
19	6	1.841932	0.382098	-0.000000
20	6	-1.815006	-2.714295	-0.000000
21	6	0.687886	-3.191936	-0.000000
22	6	-1.033555	-1.571775	-0.000000
23	6	2.714295	-1.815006	-0.000000
24	6	3.191936	0.687886	-0.000000

Table 24. The optimized Cartesian coordinates of the hetero[8]circulene **20** in the ground singlet state calculated by the DFT/B3LYP method using the 6-311++G(d,p) basis set for the light atoms and the effective core potential Lanl2DZ basis set for the heavy Te atoms

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	52	-3.284505	3.284505	-0.000000
2	6	-1.215924	3.065998	-0.000000
3	6	-0.728209	1.763416	-0.000000
4	6	-1.763416	0.728209	-0.000000
5	6	-3.065998	1.215924	-0.000000
6	16	-4.291472	-0.000000	-0.000000
7	6	-3.065998	-1.215924	-0.000000
8	6	-1.763416	-0.728209	-0.000000
9	6	-0.728209	-1.763416	0.000000
10	6	-1.215924	-3.065998	0.000000
11	52	-3.284505	-3.284505	0.000000
12	6	0.728209	1.763416	0.000000
13	6	1.215924	3.065998	0.000000
14	16	-0.000000	4.291472	-0.000000
15	52	3.284505	3.284505	0.000000
16	6	3.065998	1.215924	0.000000
17	6	1.763416	0.728209	0.000000
18	6	1.763416	-0.728209	0.000000
19	6	0.728209	-1.763416	0.000000
20	6	1.215924	-3.065998	0.000000
21	16	0.000000	-4.291472	0.000000
22	52	3.284505	-3.284505	0.000000
23	6	3.065998	-1.215924	0.000000
24	16	4.291472	0.000000	0.000000

Table 25. The optimized Cartesian coordinates of the hetero[8]circulene **21** in the ground singlet state calculated at the B3LYP/6-311++G(d,p) level of theory

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	1.757638	0.728038	0.000000
2	6	0.728038	1.757638	0.000000
3	6	-0.728038	1.757638	-0.000000
4	6	-1.757638	0.728038	0.000000
5	6	-1.757638	-0.728038	0.000000
6	6	-0.728038	-1.757638	0.000000
7	6	1.757638	-0.728038	0.000000
8	6	0.728038	-1.757638	0.000000
9	6	3.039869	1.259155	0.000000
10	34	3.136219	3.136219	-0.000000
11	6	1.259155	3.039869	-0.000000
12	34	-0.000000	4.435284	-0.000000
13	6	-1.259155	3.039869	-0.000000
14	34	-3.136219	3.136219	-0.000000
15	6	-3.039869	1.259155	-0.000000
16	34	-4.435284	-0.000000	0.000000
17	6	-3.039869	-1.259155	0.000000
18	6	-1.259155	-3.039869	0.000000
19	34	-3.136219	-3.136219	0.000000
20	6	1.259155	-3.039869	0.000000
21	34	0.000000	-4.435284	0.000000
22	6	3.039869	-1.259155	0.000000
23	34	3.136219	-3.136219	0.000000
24	34	4.435284	0.000000	0.000000

Table 26. The optimized Cartesian coordinates of the hetero[8]circulene **22** in the ground singlet state calculated by the DFT/B3LYP method using the 6-311++G(d,p) basis set for the light atoms and the effective core potential Lanl2DZ basis set for the heavy Te atoms

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	52	-3.304994	3.304994	0.000000
2	6	-1.251225	3.078950	0.000000
3	6	-0.737728	1.784350	0.000000
4	6	-1.784350	0.737728	0.000000
5	6	-3.078950	1.251225	0.000000
6	34	-4.459248	-0.000000	-0.000000
7	6	-3.078950	-1.251225	0.000000
8	6	-1.784350	-0.737728	0.000000
9	6	-0.737728	-1.784350	0.000000
10	6	-1.251225	-3.078950	0.000000
11	52	-3.304994	-3.304994	0.000000
12	6	0.737728	1.784350	0.000000
13	6	1.251225	3.078950	0.000000
14	34	-0.000000	4.459248	0.000000
15	52	3.304994	3.304994	0.000000
16	6	3.078950	1.251225	0.000000
17	6	1.784350	0.737728	0.000000
18	6	1.784350	-0.737728	0.000000
19	6	0.737728	-1.784350	0.000000
20	6	1.251225	-3.078950	0.000000
21	34	0.000000	-4.459248	0.000000
22	52	3.304994	-3.304994	0.000000

23	6	3.078950	-1.251225	0.000000
24	34	4.459248	0.000000	0.000000

Table 27. The optimized Cartesian coordinates of the hetero[8]circulene **23** in the ground singlet state calculated by the DFT/B3LYP method using the 6-311++G(d,p) basis set for the light atoms and the effective core potential Lanl2DZ basis set for the heavy Te atoms

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.023103	1.178370	-0.565147
2	6	1.756613	0.703925	-0.241382
3	6	1.756613	-0.703925	0.241382
4	6	0.703925	-1.756613	0.241382
5	6	-0.703925	-1.756613	-0.241382
6	6	-1.756613	-0.703925	-0.241382
7	6	-1.756613	0.703925	0.241382
8	6	-0.703925	1.756613	0.241382
9	6	0.703925	1.756613	-0.241382
10	52	3.161065	3.161065	-1.119994
11	6	1.178370	3.023103	-0.565147
12	52	4.619378	0.000000	0.000000
13	6	3.023103	-1.178370	0.565147
14	52	3.161065	-3.161065	1.119994
15	6	1.178370	-3.023103	0.565147
16	52	-0.000000	-4.619378	0.000000
17	6	-1.178370	-3.023103	-0.565147
18	52	-3.161065	-3.161064	-1.119994
19	6	-3.023103	-1.178370	-0.565147
20	52	-4.619378	-0.000000	0.000000
21	6	-3.023103	1.178370	0.565147
22	6	-1.178370	3.023103	0.565147
23	52	-3.161065	3.161065	1.119994
24	52	0.000000	4.619378	0.000000