Impact of molecular and packing structure on the charge-transport properties of hetero[8]circulenes

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Electronic Supplementary Information

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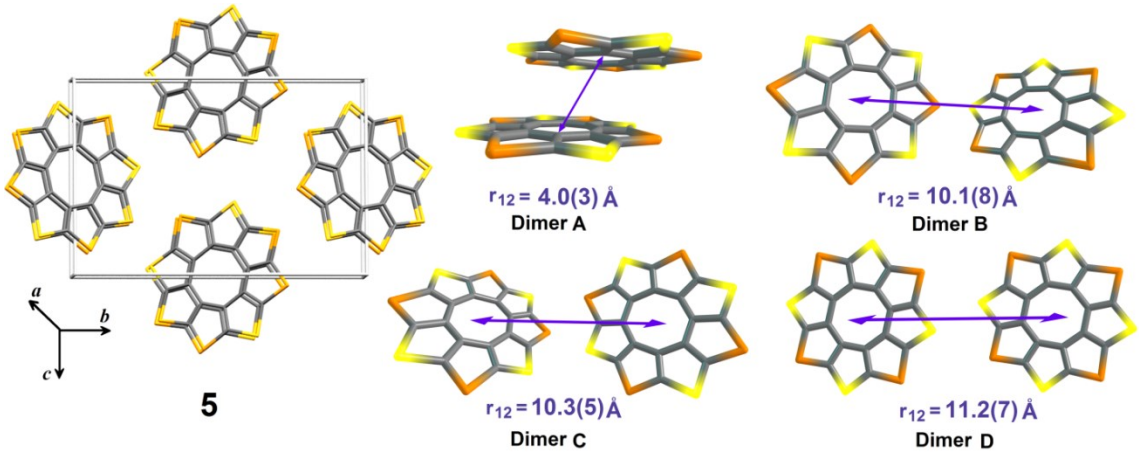

Figure S1. Crystal structure and the pertinent dimer models extracted from the crystal structure of **5** circulene. The intermolecular centroid-to-centroid distances (r_{12}) are shown by purple arrows.

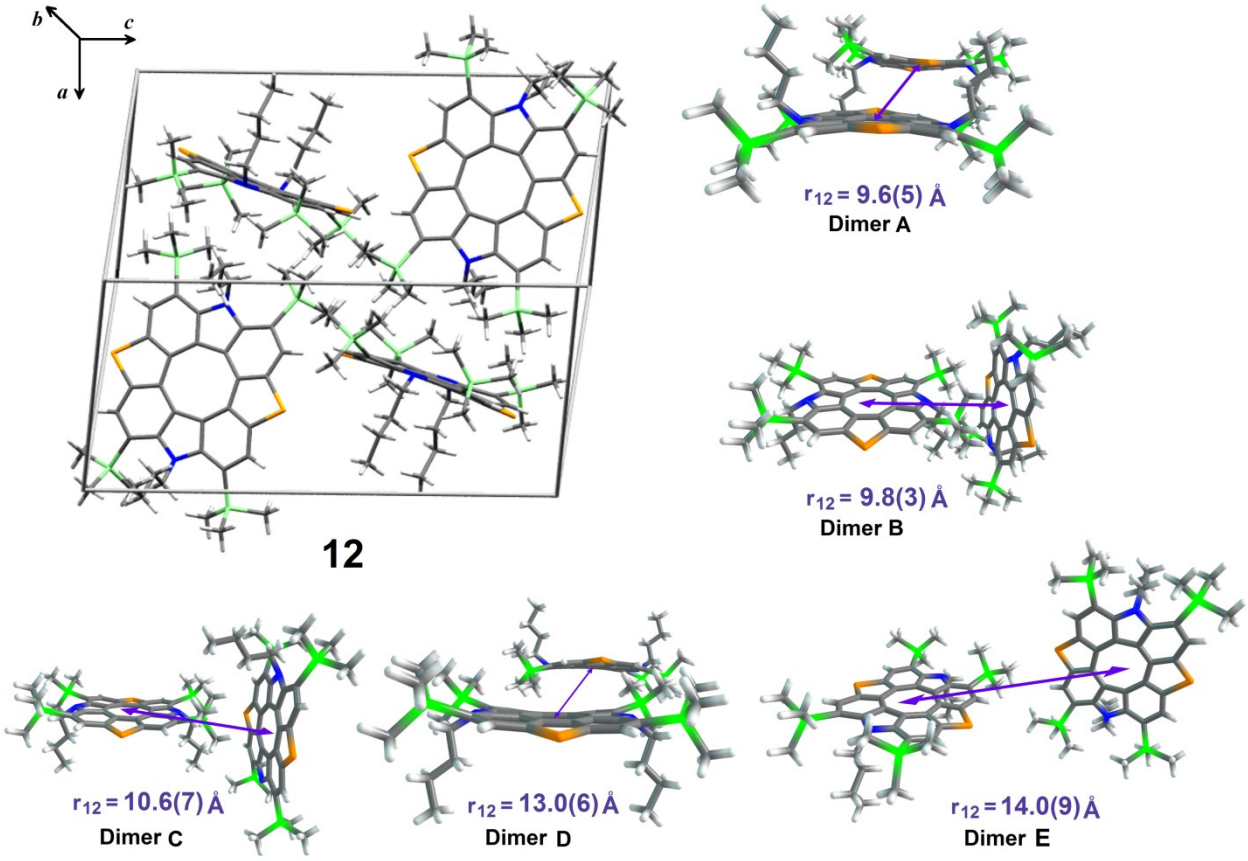

Figure S2. Crystal structure and the pertinent dimer models extracted from the crystal structure of **12** circulene. The intermolecular centroid-to-centroid distances (r_{12}) are shown by purple arrows.

Table S1. HOMO, LUMO and HOMO-LUMO gap for hetero[8]circulenes **1**–**16**

Circulene	Method	HOMO, eV	LUMO, eV	HOMO-LUMO gap, eV
1	B3LYP/6-311G(d,p) B3LYP/6-311++G(d,p)	–4.950 –5.064	–1.410 –1.540	3.540 3.524
2	B3LYP/6-311G(d,p) B3LYP/6-311++G(d,p)	–5.940 –5.718	–1.900 –1.997	4.040 3.721
3	B3LYP/6-311G(d,p), calculation in gas phase B3LYP/6-311++G(2df,2p), calculation in acetonitrile solution [41]	–5.990 –6.27 [41]	–2.350 –2.71 [41]	3.640 3.55 [41]
4	B3LYP/6-311++G(d,p)	–5.926	–1.475	4.450
5	B3LYP/6-311++G(d,p) B3P86/6-31G(d,p) [66]	–5.740 –6.19 [66]	–1.478 –1.66 [66]	4.261 4.54 [66]
6	B3LYP/6-311++G(d,p)	–0.205	–0.065	3.808
7	B3LYP/6-311++G(d,p)	–0.200	–0.055	3.936
8	B3LYP/6-31G(d) B3LYP/6-311++G(d,p)	–5.249 –5.542 [–5.96] [99]	–1.619 –1.944 [–2.97][99]	3.629 3.597 [2.99] [99]
9	B3LYP/6-31G(d) B3LYP/6-311++G(d,p)	–5.133 –5.401 [–5.87][99]	–1.642 –1.995 [–2.89][99]	3.492 3.406 [2.98] [99]
10	B3LYP/6-31G(d) B3LYP/6-311++G(d,p)	–5.373 –5.591	–1.682 –1.961	3.690 3.630
11	B3LYP/6-311++G(d,p) [100]	–5.530 [5.91] [100]	–2.180 [3.18] [100]	3.350 [2.73] [100]
12	B3LYP/6-311++G(d,p) [100]	–5.450 [5.98] [100]	–2.200 [3.06] [100]	3.250 [2.92] [100]
13	B3LYP/6-311++G(d,p)	–5.744	–2.108	3.636
14	B3LYP/6-31G(d) B3LYP/6-311++G(d,p)	–5.495 –5.780	–1.784 –2.106	3.711 3.674
15	B3LYP/6-31G(d) B3LYP/6-311++G(d,p)	–5.156 –5.431 [–5.77] [103]	–1.581 –1.909 [–2.58] [103]	3.575 3.521 [3.19] [103]
16	B3LYP/6-311++G(d,p)	–5.240	–1.642	3.598

[a] Experimental HOMO and LUMO values are given in square brackets.

The orbital energy levels of highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals were calculated for isolated molecules in gas phase with B3LYP functional and diffrent basis sets (Table S1). As one can see from the Table above the B3LYP functional and extended 6-311++G(d,p) basis set provides excellent agreement with experimental E_{HOMO} (for those hetero[8]circulenes for which these data are avaliable), while E_{LUMO} are calculated with less accuracy that is a known limitation of DFT method itself (*J. Phys. Chem. A 2007, 111,*

8, 1554–1561). For example, in the case of a pair of heterocirculenes **8** and **9** (in these molecules, sulfur heteroatoms are replaced by selenium heteroatoms) the absolute HOMO energy levels correlate well with experimental values–5.542 (exp. –5.96 eV) for **8** and –5.401 (exp. –5.87 eV) for circulene **9**, while for LUMO energy theory gives a bit worse agreement. Regarding IP and EA values for solid state circulenes, these data are not presented in any literature we know; all the experimental results correspond to solution phase. In previous report, Nguyen et. al. (*RSC Adv., 2015, **5**, 24167-24174*) have examined the reduction and oxidation potentials and energy levels of frontier orbitals for a series of O-, S-, Se- and NH-containing heterocirculenes using the SMD/IEF-PCM solvation model in acetonitrile solvent. It was found that the calculated oxidation and reduction potentials are close to the experimental values. The same patern is observed for the other hetero[8]circulenes.

Table S2. The optimized Cartesian coordinates of the tetraoxa[8]circulene **1** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.292482000	8.416185000	9.600595000
1	8.022629000	5.646576000	3.184591000
6	1.499842000	7.508997000	8.888441000
1	1.458372000	7.991049000	7.921148000
8	3.935471000	4.433845000	11.876198000
8	8.572444000	1.922457000	10.421891000
6	3.719315000	5.126851000	10.703490000
6	4.719932000	4.865502000	9.787618000
8	3.717229000	6.865449000	6.980770000
6	8.569778000	3.660192000	6.698755000
6	7.569594000	3.922141000	7.614913000
6	6.674588000	4.831822000	6.980093000
8	8.353206000	4.352692000	5.525805000
6	7.187311000	5.063380000	5.718513000
6	6.583482000	5.918086000	4.761038000
6	6.465022000	6.989349000	2.597334000
1	6.877326000	7.155487000	1.610681000
6	5.275266000	7.638590000	2.973395000
1	4.781383000	8.299974000	2.273614000
6	4.734887000	7.439125000	4.222365000
1	3.819497000	7.937208000	4.511535000
6	5.365125000	6.581125000	5.145009000
6	4.867075000	6.322104000	6.447440000
6	5.478493000	5.479283000	7.355326000
6	4.664022000	5.493210000	8.524798000
6	3.611279000	6.345295000	8.253711000
6	2.569204000	6.636628000	9.170212000
6	2.625715000	5.995777000	10.458271000
6	1.608647000	6.259083000	11.396288000
6	7.107701000	6.145593000	3.473497000
1	1.651122000	5.777073000	12.363619000
6	5.101549000	3.723425000	11.683685000
6	0.578280000	7.116151000	11.086954000
1	-0.196841000	7.309603000	11.816734000
6	5.705337000	2.868619000	12.641104000
6	0.523783000	7.743447000	9.829001000
6	5.180793000	2.640523000	13.928413000
1	4.265544000	3.139047000	14.217153000
6	5.823688000	1.796955000	14.804600000
1	5.411187000	1.630414000	15.791101000
6	7.013846000	1.148345000	14.428764000
1	7.507816000	0.487053000	15.128574000
6	7.554470000	1.348275000	13.179977000
1	8.470159000	0.850646000	12.890984000
6	6.924119000	2.206206000	12.257357000
6	7.422520000	2.465717000	10.955147000
6	6.811220000	3.308673000	10.047313000
6	7.625736000	3.294772000	8.877883000
6	8.678424000	2.442636000	9.148960000
6	9.720247000	2.150933000	8.232283000
6	9.663346000	2.791210000	6.943935000
6	10.680021000	2.527284000	6.005671000
1	10.637247000	3.008789000	5.038103000
6	5.614899000	3.955749000	10.422444000
6	11.710427000	1.670245000	6.315040000
1	12.485176000	1.476338000	5.584982000
6	11.765422000	1.043653000	7.573314000
1	12.581731000	0.371000000	7.801781000
6	10.789767000	1.278828000	8.514116000
1	10.831615000	0.797340000	9.481674000

Table S3. The optimized Cartesian coordinates of the tetraoxa[8]circulene **1** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
8	8.341465000	4.362267000	5.526544000
8	3.729265000	6.863737000	6.972710000
6	8.565243000	3.661730000	6.703776000
6	7.562490000	3.925304000	7.617931000
6	6.670885000	4.831532000	6.988372000
6	7.189938000	5.064376000	5.716454000
6	6.582563000	5.923001000	4.755641000
6	7.106763000	6.144805000	3.475837000
1	8.020817000	5.646850000	3.183966000
6	6.459216000	6.993361000	2.592951000
1	6.872786000	7.156560000	1.607101000
6	5.277932000	7.638777000	2.966095000
1	4.782424000	8.299437000	2.267912000
6	4.734844000	7.438955000	4.223773000
1	3.819716000	7.938010000	4.510536000
6	5.366062000	6.585303000	5.138876000
6	4.865176000	6.327077000	6.445883000
6	5.483010000	5.475127000	7.361177000
6	4.671326000	5.490263000	8.522799000
6	3.615879000	6.343218000	8.255219000
6	2.578102000	6.634838000	9.163499000
6	2.634462000	5.989107000	10.458585000
6	1.615783000	6.251159000	11.397443000
1	1.654741000	5.769289000	12.364226000
6	0.590269000	7.107163000	11.083737000
1	-0.186911000	7.302040000	11.810068000
6	0.536025000	7.738119000	9.822553000
1	-0.281600000	8.409835000	9.599190000
6	1.507052000	7.508866000	8.881093000
1	1.464109000	7.992844000	7.915614000
8	3.947845000	4.425018000	11.875838000
8	8.559927000	1.923405000	10.429607000
6	3.724051000	5.125566000	10.698587000
6	4.726881000	4.862128000	9.784509000
6	5.618520000	3.955923000	10.414064000
6	5.099416000	3.723005000	11.685958000
6	5.706756000	2.864323000	12.646742000
6	5.182531000	2.642482000	13.926527000
1	4.268503000	3.140469000	14.218424000
6	5.830014000	1.793833000	14.809373000
1	5.416418000	1.630614000	15.795218000
6	7.011251000	1.148345000	14.436205000
1	7.506708000	0.487609000	15.134344000
6	7.554358000	1.348202000	13.178543000
1	8.469455000	0.849097000	12.891741000
6	6.923218000	2.201960000	12.263481000
6	7.424119000	2.460211000	10.956499000
6	6.806375000	3.312293000	10.041250000
6	7.618039000	3.297116000	8.879611000
6	8.673340000	2.443941000	9.147109000
6	9.710959000	2.152122000	8.238745000
6	9.654591000	2.797882000	6.943684000
6	10.673128000	2.535647000	6.004706000
1	10.634169000	3.017563000	5.037947000
6	11.698477000	1.679400000	6.318262000
1	12.475541000	1.484355000	5.591854000
6	11.752713000	1.048391000	7.579430000
1	12.570207000	0.376473000	7.802697000
6	10.781858000	1.277845000	8.521006000
1	10.824801000	0.793830000	9.486476000

Table S4. The optimized Cartesian coordinates of the tetraoxa[8]circulene **1** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
1	-0.299150000	8.422548000	9.597379000
1	8.023760000	5.649145000	3.175553000
6	1.491874000	7.514338000	8.889712000
1	1.450176000	7.996902000	7.922246000
8	3.930321000	4.434379000	11.884297000
8	8.578566000	1.915981000	10.426171000
6	3.711631000	5.130477000	10.707763000
6	4.722677000	4.862196000	9.790589000
8	3.711045000	6.871863000	6.976443000
6	8.577474000	3.656561000	6.694469000
6	7.566756000	3.925338000	7.611875000
6	6.678005000	4.828242000	6.981555000
8	8.358401000	4.352199000	5.517718000
6	7.188209000	5.066268000	5.709404000
6	6.590144000	5.913400000	4.759894000
6	6.469840000	6.989905000	2.588877000
1	6.882775000	7.155592000	1.602220000
6	5.270449000	7.644670000	2.967924000
1	4.776295000	8.306530000	2.268501000
6	4.733317000	7.444085000	4.214250000
1	3.817716000	7.942736000	4.503304000
6	5.358057000	6.584051000	5.148073000
6	4.864752000	6.327003000	6.439278000
6	5.474666000	5.479693000	7.358981000
6	4.666207000	5.493622000	8.519978000
6	3.603084000	6.350680000	8.254405000
6	2.569945000	6.639879000	9.162657000
6	2.627242000	5.991666000	10.465246000
6	1.600888000	6.262325000	11.400284000
6	7.108635000	6.148524000	3.464684000
1	1.643166000	5.779918000	12.367877000
6	5.100647000	3.720521000	11.692767000
6	0.571971000	7.116746000	11.094377000
1	-0.203071000	7.309476000	11.824676000
6	5.698675000	2.873279000	12.642221000
6	0.517000000	7.749538000	9.826195000
6	5.179876000	2.637612000	13.937213000
1	4.264469000	3.136552000	14.226206000
6	5.818851000	1.796363000	14.813019000
1	5.405719000	1.630294000	15.799538000
6	7.018584000	1.142162000	14.434177000
1	7.512797000	0.480357000	15.133602000
6	7.555951000	1.343194000	13.188016000
1	8.471817000	0.844940000	12.899106000
6	6.931122000	2.203199000	12.254254000
6	7.424754000	2.460702000	10.963233000
6	6.814926000	3.308095000	10.043587000
6	7.623441000	3.294192000	8.882602000
6	8.686534000	2.437161000	9.148213000
6	9.719516000	2.147687000	8.239828000
6	9.661849000	2.795385000	6.936991000
6	10.687916000	2.524192000	6.001759000
1	10.645388000	3.006125000	5.033943000
6	5.611402000	3.959216000	10.420914000
6	11.716894000	1.669874000	6.307768000
1	12.491650000	1.476784000	5.577255000
6	11.772330000	1.037731000	7.576247000
1	12.588568000	0.364869000	7.805169000
6	10.797738000	1.273536000	8.512893000
1	10.839761000	0.791500000	9.480620000

Table S5. The optimized Cartesian coordinates of the tetraaza[8]circulene **2** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.890954000	-4.900935000	2.629312000
1	1.458752000	-5.503103000	1.930850000
6	0.496929000	-3.596625000	2.272385000
6	-0.253370000	-2.823818000	3.210535000
6	-0.639421000	-1.509355000	2.820679000
6	-0.327697000	-0.925806000	1.584614000
6	0.424581000	-1.695630000	0.650890000
6	0.806580000	-2.992896000	1.020499000
6	-1.524978000	0.554464000	2.830021000
6	-0.891464000	0.388223000	1.590538000
6	-0.931565000	1.472366000	0.666553000
6	-1.603932000	2.641731000	1.049487000
6	-2.256126000	2.821314000	2.302975000
6	-2.213143000	1.735327000	3.230427000
6	-2.846798000	1.885182000	4.479608000
1	-2.823783000	1.074693000	5.197672000
6	-3.500606000	3.050755000	4.811226000
1	-3.981112000	3.145821000	5.776571000
6	-3.546626000	4.116124000	3.898345000
1	-4.063509000	5.030312000	4.160889000
6	-2.934736000	3.999929000	2.670390000
1	-2.982291000	4.832881000	1.979602000
7	-1.361934000	-0.601035000	3.559765000
1	-1.721669000	-0.759893000	4.483666000
7	-1.518193000	3.548954000	0.018074000
1	-1.904892000	4.475434000	0.026496000
6	0.567959000	3.393678000	-4.459999000
1	1.134044000	2.823091000	-5.186043000
6	0.166690000	4.670867000	-4.781550000
1	0.417977000	5.089919000	-5.747481000
6	-0.568720000	5.431135000	-3.858405000
1	-0.883041000	6.435043000	-4.113986000
6	-0.890954000	4.900935000	-2.629312000
1	-1.458752000	5.503103000	-1.930850000
6	-0.496929000	3.596625000	-2.272385000
6	0.253370000	2.823818000	-3.210535000
6	0.639421000	1.509355000	-2.820679000
6	0.327697000	0.925806000	-1.584614000
6	-0.424581000	1.695630000	-0.650890000
6	-0.806580000	2.992896000	-1.020499000
6	1.524978000	-0.554464000	-2.830021000
6	0.891464000	-0.388223000	-1.590538000
6	0.931565000	-1.472366000	-0.666553000
6	1.603932000	-2.641731000	-1.049487000
6	2.256126000	-2.821314000	-2.302975000
6	2.213143000	-1.735327000	-3.230427000
6	2.846798000	-1.885182000	-4.479608000
1	2.823783000	-1.074693000	-5.197672000
6	3.500606000	-3.050755000	-4.811226000
1	3.981112000	-3.145821000	-5.776571000
6	3.546626000	-4.116124000	-3.898345000
1	4.063509000	-5.030312000	-4.160889000
6	2.934736000	-3.999929000	-2.670390000
1	2.982291000	-4.832881000	-1.979602000
7	1.361934000	0.601035000	-3.559765000
1	1.721669000	0.759893000	-4.483666000
7	1.518193000	-3.548954000	-0.018074000
1	1.904892000	-4.475434000	-0.026496000
6	-0.166690000	-4.670867000	4.781550000
1	-0.417977000	-5.089919000	5.747481000
6	0.568720000	-5.431135000	3.858405000
1	0.883041000	-6.435043000	4.113986000
6	-0.567959000	-3.393678000	4.459999000
1	-1.134044000	-2.823091000	5.186043000

Table S6. The optimized Cartesian coordinates of the tetraaza[8]circulene **2** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.898108000	-4.905673000	2.617789000
1	1.464446000	-5.507683000	1.919808000
6	0.500878000	-3.599987000	2.267263000
6	-0.249910000	-2.824899000	3.205232000
6	-0.636160000	-1.507355000	2.810843000
6	-0.324364000	-0.924466000	1.574699000
6	0.424430000	-1.689494000	0.645164000
6	0.809888000	-2.998062000	1.019212000
6	-1.522468000	0.555268000	2.820320000
6	-0.888410000	0.390041000	1.580738000
6	-0.927441000	1.468052000	0.661123000
6	-1.606796000	2.647510000	1.048176000
6	-2.257155000	2.826168000	2.298251000
6	-2.213067000	1.738642000	3.225162000
6	-2.843799000	1.888706000	4.469950000
1	-2.824789000	1.083410000	5.192259000
6	-3.496817000	3.059598000	4.796754000
1	-3.976780000	3.156131000	5.761427000
6	-3.544762000	4.124993000	3.886902000
1	-4.061167000	5.037489000	4.151671000
6	-2.933499000	4.008574000	2.659370000
1	-2.980620000	4.840532000	1.969180000
7	-1.357828000	-0.598851000	3.542484000
1	-1.719669000	-0.758947000	4.468029000
7	-1.520622000	3.554648000	0.018716000
1	-1.908309000	4.482213000	0.026778000
6	0.562942000	3.393076000	-4.450067000
1	1.128150000	2.829254000	-5.180425000
6	0.157856000	4.673432000	-4.766542000
1	0.408317000	5.092833000	-5.731742000
6	-0.576510000	5.435232000	-3.846505000
1	-0.889007000	6.437999000	-4.103948000
6	-0.898108000	4.905673000	-2.617789000
1	-1.464446000	5.507683000	-1.919808000
6	-0.500878000	3.599987000	-2.267263000
6	0.249910000	2.824899000	-3.205232000
6	0.636160000	1.507355000	-2.810843000
6	0.324364000	0.924466000	-1.574699000
6	-0.424430000	1.689494000	-0.645164000
6	-0.809888000	2.998062000	-1.019212000
6	1.522468000	-0.555268000	-2.820320000
6	0.888410000	-0.390041000	-1.580738000
6	0.927441000	-1.468052000	-0.661123000
6	1.606796000	-2.647510000	-1.048176000
6	2.257155000	-2.826168000	-2.298251000
6	2.213067000	-1.738642000	-3.225162000
6	2.843799000	-1.888706000	-4.469950000
1	2.824789000	-1.083410000	-5.192259000
6	3.496817000	-3.059598000	-4.796754000
1	3.976780000	-3.156131000	-5.761427000
6	3.544762000	-4.124993000	-3.886902000
1	4.061167000	-5.037489000	-4.151671000
6	2.933499000	-4.008574000	-2.659370000
1	2.980620000	-4.840532000	-1.969180000
7	1.357828000	0.598851000	-3.542484000
1	1.719669000	0.758947000	-4.468029000
7	1.520622000	-3.554648000	-0.018716000
1	1.908309000	-4.482213000	-0.026778000
6	-0.157856000	-4.673432000	4.766542000
1	-0.408317000	-5.092833000	5.731742000
6	0.576510000	-5.435232000	3.846505000
1	0.889007000	-6.437999000	4.103948000
6	-0.562942000	-3.393076000	4.450067000
1	-1.128150000	-2.829254000	5.180425000

Table S7. The optimized Cartesian coordinates of the tetraaza[8]circulene **2** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.892071000	-4.909191000	2.633811000
1	1.460302000	-5.512647000	1.935672000
6	0.502157000	-3.601383000	2.266956000
6	-0.257873000	-2.818988000	3.216511000
6	-0.639117000	-1.515949000	2.828484000
6	-0.329286000	-0.922418000	1.586254000
6	0.427399000	-1.696252000	0.647815000
6	0.809175000	-3.000700000	1.026682000
6	-1.530282000	0.558682000	2.837763000
6	-0.890747000	0.384487000	1.591969000
6	-0.931645000	1.474211000	0.663055000
6	-1.610640000	2.647844000	1.054584000
6	-2.257397000	2.827747000	2.297092000
6	-2.213008000	1.728772000	3.236334000
6	-2.850205000	1.889268000	4.487884000
1	-2.826283000	1.079384000	5.207723000
6	-3.504200000	3.051419000	4.821503000
1	-3.983369000	3.145800000	5.787557000
6	-3.551419000	4.125654000	3.900357000
1	-4.068425000	5.040161000	4.161521000
6	-2.941050000	4.006045000	2.674609000
1	-2.990424000	4.839530000	1.983423000
7	-1.362986000	-0.601568000	3.566902000
1	-1.724482000	-0.761426000	4.488782000
7	-1.523206000	3.554468000	0.017149000
1	-1.909756000	4.479822000	0.025162000
6	0.569256000	3.399692000	-4.467107000
1	1.135685000	2.829698000	-5.194508000
6	0.170559000	4.674732000	-4.790738000
1	0.423090000	5.092574000	-5.756851000
6	-0.570713000	5.441777000	-3.859592000
1	-0.884909000	6.446100000	-4.113553000
6	-0.892071000	4.909191000	-2.633811000
1	-1.460302000	5.512647000	-1.935672000
6	-0.502157000	3.601383000	-2.266956000
6	0.257873000	2.818988000	-3.216511000
6	0.639117000	1.515949000	-2.828484000
6	0.329286000	0.922418000	-1.586254000
6	-0.427399000	1.696252000	-0.647815000
6	-0.809175000	3.000700000	-1.026682000
6	1.530282000	-0.558682000	-2.837763000
6	0.890747000	-0.384487000	-1.591969000
6	0.931645000	-1.474211000	-0.663055000
6	1.610640000	-2.647844000	-1.054584000
6	2.257397000	-2.827747000	-2.297092000
6	2.213008000	-1.728772000	-3.236334000
6	2.850205000	-1.889268000	-4.487884000
1	2.826283000	-1.079384000	-5.207723000
6	3.504200000	-3.051419000	-4.821503000
1	3.983369000	-3.145800000	-5.787557000
6	3.551419000	-4.125654000	-3.900357000
1	4.068425000	-5.040161000	-4.161521000
6	2.941050000	-4.006045000	-2.674609000
1	2.990424000	-4.839530000	-1.983423000
7	1.362986000	0.601568000	-3.566902000
1	1.724482000	0.761426000	-4.488782000
7	1.523206000	-3.554468000	-0.017149000
1	1.909756000	-4.479822000	-0.025162000
6	-0.170559000	-4.674732000	4.790738000
1	-0.423090000	-5.092574000	5.756851000
6	0.570713000	-5.441777000	3.859592000
1	0.884909000	-6.446100000	4.113553000
6	-0.569256000	-3.399692000	4.467107000
1	-1.135685000	-2.829698000	5.194508000

Table S8. The optimized Cartesian coordinates of the tetraoxa[8]circulene **3** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.054886000	8.723389000	9.763710000
6	0.472046000	7.517028000	9.202463000
6	0.914890000	7.514127000	7.878546000
6	0.922393000	8.718177000	7.174855000
6	0.505348000	9.923107000	7.737883000
6	0.062844000	9.925899000	9.057985000
8	-0.413311000	8.914349000	11.053071000
6	-0.703991000	10.264496000	11.154124000
6	-0.427005000	10.920180000	9.955638000
8	1.326105000	8.902316000	5.863328000
6	1.158779000	10.252003000	5.602174000
6	0.659183000	10.913709000	6.722638000
6	-1.203077000	10.924731000	12.276608000
6	-1.435071000	12.298908000	12.195470000
6	-1.158391000	12.952054000	10.994955000
6	-0.658771000	12.290345000	9.874514000
6	-0.505002000	13.280999000	8.859211000
6	-0.922021000	14.485894000	9.422258000
8	-1.325667000	14.301759000	10.733813000
6	1.435233000	10.905087000	4.401599000
6	1.202976000	12.279209000	4.320348000
6	0.703926000	12.939459000	5.442850000
6	0.427228000	12.283853000	6.641459000
6	-0.062591000	13.278163000	7.539100000
6	-0.054986000	14.480596000	6.833164000
8	0.413035000	14.289564000	5.543778000
6	-0.472254000	15.686930000	7.394411000
6	-0.914913000	15.689878000	8.718404000
1	0.452971000	6.602952000	9.778964000
1	1.244334000	6.597729000	7.409760000
1	-1.407163000	10.385143000	13.190720000
1	-1.820326000	12.844287000	13.045399000
1	1.820451000	10.359690000	3.551664000
1	1.406836000	12.818751000	3.406159000
1	-0.453476000	16.600970000	6.817842000
1	-1.244446000	16.606271000	9.187136000

Table S9. The optimized Cartesian coordinates of the tetraoxa[8]circulene **3** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.051129000	8.720369000	9.772248000
6	0.468274000	7.525527000	9.207845000
6	0.915157000	7.522470000	7.872823000
6	0.926688000	8.715238000	7.166341000
6	0.508365000	9.930917000	7.729474000
6	0.058770000	9.933400000	9.065629000
8	-0.414181000	8.913105000	11.053868000
6	-0.703234000	10.255493000	11.156705000
6	-0.423384000	10.911547000	9.947826000
8	1.326679000	8.901526000	5.862288000
6	1.161844000	10.242947000	5.600343000
6	0.659505000	10.905128000	6.731330000
6	-1.199449000	10.918396000	12.267961000
6	-1.432679000	12.304356000	12.186678000
6	-1.160323000	12.961217000	10.996957000
6	-0.658383000	12.299022000	9.865899000
6	-0.507457000	13.273556000	8.867811000
6	-0.926267000	14.488886000	9.430727000
8	-1.325047000	14.302848000	10.735059000
6	1.433836000	10.899682000	4.410339000
6	1.199383000	12.284966000	4.328961000

6	0.703021000	12.948130000	5.440516000
6	0.424114000	12.292596000	6.649189000
6	-0.058328000	13.271029000	7.531604000
6	-0.051621000	14.483447000	6.824823000
8	0.411984000	14.290331000	5.542461000
6	-0.469157000	15.678589000	7.389360000
6	-0.915655000	15.681852000	8.723829000
1	0.452281000	6.606417000	9.777407000
1	1.243314000	6.601568000	7.410520000
1	-1.406294000	10.386639000	13.186626000
1	-1.817300000	12.843420000	13.041612000
1	1.818204000	10.360435000	3.555441000
1	1.404969000	12.817218000	3.410219000
1	-0.453916000	16.597179000	6.818837000
1	-1.243841000	16.602557000	9.186441000

Table S10. The optimized Cartesian coordinates of the tetraoxa[8]circulene **3** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.055809000	8.710969000	9.766118000
6	0.469080000	7.512104000	9.214393000
6	0.918580000	7.509115000	7.867375000
6	0.924985000	8.705938000	7.173958000
6	0.507744000	9.926193000	7.732418000
6	0.060416000	9.928440000	9.063617000
8	-0.414137000	8.905586000	11.062324000
6	-0.707452000	10.262831000	11.165548000
6	-0.425330000	10.913966000	9.952564000
8	1.331084000	8.893984000	5.855759000
6	1.163460000	10.250607000	5.590991000
6	0.659994000	10.907973000	6.726595000
6	-1.202386000	10.912652000	12.281550000
6	-1.438800000	12.310587000	12.198912000
6	-1.163079000	12.953449000	11.006131000
6	-0.659605000	12.296076000	9.870549000
6	-0.507418000	13.277901000	8.864670000
6	-0.924550000	14.498140000	9.423168000
8	-1.330611000	14.310097000	10.741387000
6	1.438964000	10.893416000	4.398153000
6	1.202292000	12.291298000	4.315407000
6	0.707388000	12.941128000	5.431425000
6	0.425530000	12.290061000	6.644522000
6	-0.060186000	13.275610000	7.533460000
6	-0.055981000	14.493001000	6.830741000
8	0.413799000	14.298321000	5.534511000
6	-0.469374000	15.691836000	7.382460000
6	-0.918472000	15.694914000	8.729623000
1	0.449992000	6.598720000	9.792312000
1	1.248192000	6.593073000	7.397433000
1	-1.405576000	10.372083000	13.195453000
1	-1.823574000	12.857055000	13.048548000
1	1.823700000	10.346930000	3.548511000
1	1.405252000	12.831822000	3.401428000
1	-0.450611000	16.605172000	6.804450000
1	-1.248120000	16.610956000	9.199539000

Table S11. The optimized Cartesian coordinates of the octathia[8]circulene **4** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-1.792714000	-3.811760000	0.657599000
16	-1.080076000	-3.298719000	-2.477701000
16	0.263282000	-0.852701000	-4.170702000

16	1.455004000	2.095563000	-3.415933000
6	-0.774639000	-1.407940000	0.973054000
6	-0.681741000	-1.694998000	-0.433158000
6	-0.192152000	-0.989544000	-1.586292000
6	0.411032000	0.296375000	-1.810572000
6	-1.349964000	-2.450725000	1.692686000
6	-1.189147000	-2.950279000	-0.754204000
6	-0.334904000	-1.722563000	-2.760547000
6	0.715277000	0.516355000	-3.150377000
16	1.792714000	3.811760000	-0.657599000
16	1.080076000	3.298719000	2.477701000
16	-0.263282000	0.852701000	4.170702000
16	-1.455004000	-2.095563000	3.415933000
6	0.774639000	1.407940000	-0.973054000
6	0.681741000	1.694998000	0.433158000
6	0.192152000	0.989544000	1.586292000
6	-0.411032000	-0.296375000	1.810572000
6	1.349964000	2.450725000	-1.692686000
6	1.189147000	2.950279000	0.754204000
6	0.334904000	1.722563000	2.760547000
6	-0.715277000	-0.516355000	3.150377000

Table S12. The optimized Cartesian coordinates of the octathia[8]circulene **4** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-1.791316000	-3.793887000	0.670821000
16	-1.073011000	-3.272066000	-2.443491000
16	0.269810000	-0.830773000	-4.126726000
16	1.448903000	2.097748000	-3.393493000
6	-0.760049000	-1.383374000	0.954266000
6	-0.671558000	-1.664973000	-0.419650000
6	-0.188745000	-0.970941000	-1.553735000
6	0.404766000	0.295969000	-1.773090000
6	-1.335671000	-2.431001000	1.678452000
6	-1.177984000	-2.916648000	-0.742596000
6	-0.328558000	-1.695787000	-2.715856000
6	0.706211000	0.512467000	-3.107374000
16	1.791316000	3.793887000	-0.670821000
16	1.073011000	3.272066000	2.443491000
16	-0.269810000	0.830773000	4.126726000
16	-1.448903000	-2.097748000	3.393493000
6	0.760049000	1.383374000	-0.954266000
6	0.671558000	1.664973000	0.419650000
6	0.188745000	0.970941000	1.553735000
6	-0.404766000	-0.295969000	1.773090000
6	1.335671000	2.431001000	-1.678452000
6	1.177984000	2.916648000	0.742596000
6	0.328558000	1.695787000	2.715856000
6	-0.706211000	-0.512467000	3.107374000

Table S13. The optimized Cartesian coordinates of the octathia[8]circulene **4** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	-1.792714000	-3.811760000	0.657599000
16	-1.080076000	-3.298719000	-2.477701000
16	0.263282000	-0.852701000	-4.170702000
16	1.455004000	2.095563000	-3.415933000
6	-0.774639000	-1.407940000	0.973054000
6	-0.681741000	-1.694998000	-0.433158000
6	-0.192152000	-0.989544000	-1.586292000

6	0.411032000	0.296375000	-1.810572000
6	-1.349964000	-2.450725000	1.692686000
6	-1.189147000	-2.950279000	-0.754204000
6	-0.334904000	-1.722563000	-2.760547000
6	0.715277000	0.516355000	-3.150377000
16	1.792714000	3.811760000	-0.657599000
16	1.080076000	3.298719000	2.477701000
16	-0.263282000	0.852701000	4.170702000
16	-1.455004000	-2.095563000	3.415933000
6	0.774639000	1.407940000	-0.973054000
6	0.681741000	1.694998000	0.433158000
6	0.192152000	0.989544000	1.586292000
6	-0.411032000	-0.296375000	1.810572000
6	1.349964000	2.450725000	-1.692686000
6	1.189147000	2.950279000	0.754204000
6	0.334904000	1.722563000	2.760547000
6	-0.715277000	-0.516355000	3.150377000

Table S14. The optimized Cartesian coordinates of the tetrathiatetraselena[8]circulene **5** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
34	1.618380000	2.113438000	-3.522440000
34	-1.201420000	-3.375557000	-2.582044000
16	0.294621000	-0.865427000	-4.165198000
16	1.935819000	3.743818000	-0.642081000
6	-0.204965000	-0.983790000	-1.587612000
6	0.446793000	0.276864000	-1.802732000
6	-0.739831000	-1.669547000	-0.440528000
6	1.456268000	2.407838000	-1.647120000
6	0.761074000	0.457551000	-3.137435000
6	0.839484000	1.377246000	-0.961848000
6	-0.343153000	-1.686141000	-2.770580000
6	-1.290524000	-2.902444000	-0.737355000
34	-1.618380000	-2.113438000	3.522440000
34	1.201420000	3.375557000	2.582044000
16	-0.294621000	0.865427000	4.165198000
16	-1.935819000	-3.743818000	0.642081000
6	0.204965000	0.983790000	1.587612000
6	-0.446793000	-0.276864000	1.802732000
6	0.739831000	1.669547000	0.440528000
6	-1.456268000	-2.407838000	1.647120000
6	-0.761074000	-0.457551000	3.137435000
6	-0.839484000	-1.377246000	0.961848000
6	0.343153000	1.686141000	2.770580000
6	1.290524000	2.902444000	0.737355000

Table S15. The optimized Cartesian coordinates of the tetrathiatetraselena[8]circulene **5** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
34	-0.401703000	10.453954000	-3.497244000
34	-3.224846000	4.954081000	-2.574824000
16	-1.724152000	7.468143000	-4.141652000
16	-0.075155000	12.093054000	-0.632079000
6	-2.220415000	7.357459000	-1.572428000
6	-1.570993000	8.614855000	-1.787184000
6	-2.750003000	6.678814000	-0.437733000
6	-0.560274000	10.748278000	-1.641275000
6	-1.257245000	8.794623000	-3.120240000
6	-1.180490000	9.711931000	-0.949359000
6	-2.359376000	6.653538000	-2.763839000
6	-3.309003000	5.428496000	-0.739390000

34	-3.627253000	6.226025000	3.497250000
34	-0.804225000	11.725956000	2.574815000
16	-2.304830000	9.211844000	4.141655000
16	-3.953864000	4.586956000	0.632072000
6	-1.808596000	9.322549000	1.572428000
6	-2.457974000	8.065130000	1.787185000
6	-1.279025000	10.001211000	0.437737000
6	-3.468701000	5.931705000	1.641280000
6	-2.771712000	7.885356000	3.120242000
6	-2.848470000	6.968043000	0.949361000
6	-1.669655000	10.026478000	2.763837000
6	-0.720043000	11.251535000	0.739382000

Table S16. The optimized Cartesian coordinates of the tetrathiatetraselena[8]circulene **5** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
34	-0.395514000	10.462633000	-3.535080000
34	-3.221530000	4.954525000	-2.590933000
16	-1.717287000	7.470033000	-4.183619000
16	-0.070232000	12.100354000	-0.644990000
6	-2.218622000	7.358238000	-1.584179000
6	-1.567324000	8.615585000	-1.798842000
6	-2.752292000	6.673766000	-0.439352000
6	-0.555295000	10.747945000	-1.647776000
6	-1.250897000	8.796733000	-3.138946000
6	-1.175928000	9.713929000	-0.959705000
6	-2.357379000	6.653110000	-2.772033000
6	-3.305582000	5.436067000	-0.737742000
34	-3.633553000	6.217398000	3.535070000
34	-0.807704000	11.725592000	2.590895000
16	-2.311803000	9.210007000	4.183604000
16	-3.958869000	4.579696000	0.644968000
6	-1.810295000	9.321725000	1.584194000
6	-2.461527000	8.064341000	1.798864000
6	-1.276649000	10.006217000	0.439370000
6	-3.473617000	5.932008000	1.647792000
6	-2.778032000	7.883232000	3.138954000
6	-2.852908000	6.965984000	0.959730000
6	-1.671663000	10.026912000	2.772028000
6	-0.723502000	11.243984000	0.737727000

Table S17. The optimized Cartesian coordinates of the tetrathiatetrasila[8]circulene **6** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	9.980919000	16.820883000	5.599327000
6	10.165658000	12.889276000	2.798435000
6	11.076937000	13.458024000	1.765513000
6	11.804998000	15.991583000	2.344741000
6	11.737812000	14.714569000	1.580749000
6	12.657580000	9.503483000	2.149275000
1	12.228388000	9.665819000	3.139335000
16	12.670189000	18.404821000	2.639380000
1	13.244016000	8.583236000	2.186541000
1	13.344252000	10.328696000	1.953519000
6	15.265056000	16.226453000	0.185915000
1	15.541370000	15.676497000	1.091011000
1	15.672903000	17.236512000	0.311763000
6	12.626867000	16.950001000	1.746563000
6	9.589441000	13.372206000	4.016995000

6	9.772579000	11.577474000	2.523694000
6	12.792443000	17.309016000	-1.369179000
1	13.121172000	16.765000000	-2.262115000
1	13.326339000	18.266844000	-1.395431000
6	9.639790000	14.656608000	4.770086000
6	11.566305000	9.417566000	1.074017000
1	12.017557000	9.222550000	0.093742000
1	10.913710000	8.557636000	1.269206000
6	8.494181000	12.066437000	7.738633000
1	9.586259000	11.993827000	7.734918000
1	8.124150000	11.039432000	7.634877000
6	6.105377000	13.182982000	6.079815000
1	5.761684000	13.741611000	6.958241000
1	5.668212000	12.181959000	6.178487000
6	8.008946000	12.659673000	9.070423000
1	6.919237000	12.704456000	9.120308000
1	8.348810000	12.056830000	9.915073000
1	8.390429000	13.672045000	9.221013000
6	8.200028000	11.851411000	-0.637573000
1	8.751175000	12.737156000	-0.957418000
1	7.459471000	11.623421000	-1.406855000
1	7.662869000	12.115902000	0.274717000
16	8.734545000	10.954692000	3.728267000
16	12.401602000	13.252575000	-0.438093000
16	8.936828000	16.134384000	6.763745000
14	10.863470000	18.457153000	5.405592000
14	13.384804000	16.356401000	0.147694000
14	10.463871000	10.935633000	0.910984000
14	7.981160000	13.019695000	6.195626000
6	8.869437000	14.642911000	5.935823000
6	8.783393000	12.406804000	4.625544000
6	10.288206000	15.918605000	4.577121000
6	15.896247000	15.562003000	-1.047852000
1	15.673181000	16.113268000	-1.963381000
1	16.983007000	15.513013000	-0.953845000
1	15.536151000	14.539250000	-1.180404000
6	9.745026000	19.948378000	5.128686000
1	9.074794000	19.707194000	4.297516000
1	10.372917000	20.775893000	4.776775000
6	9.142368000	10.661034000	-0.406603000
1	8.563391000	9.773934000	-0.123057000
1	9.646530000	10.394469000	-1.343253000
6	13.083866000	17.615177000	7.052151000
1	13.661982000	17.352324000	6.164742000
1	13.788480000	17.869498000	7.846596000
1	12.540554000	16.720974000	7.361839000
6	12.124476000	18.780645000	6.770482000
1	11.579352000	19.043186000	7.684573000
1	12.692808000	19.678502000	6.498708000
6	11.277641000	17.549362000	-1.432268000
1	10.930910000	18.125324000	-0.572916000
1	11.004342000	18.098918000	-2.335309000
1	10.726598000	16.607480000	-1.435609000
6	5.591802000	13.857863000	4.799901000
1	5.883826000	13.297057000	3.910754000
1	4.502353000	13.932114000	4.805424000
1	5.994366000	14.866710000	4.693793000
6	11.612252000	17.790649000	3.830824000
6	11.216962000	16.479476000	3.555702000
6	11.358665000	12.566231000	0.727553000
6	12.498540000	14.732115000	0.408633000
6	8.928118000	20.400200000	6.348554000
1	9.570751000	20.696849000	7.179922000
1	8.298685000	21.257797000	6.102057000
1	8.268698000	19.605917000	6.705579000

Table S18. The optimized Cartesian coordinates of the tetrathiatetrasila[8]circulene **6** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	9.989719000	16.825992000	5.600290000
6	10.169055000	12.896754000	2.801175000
6	11.078674000	13.463383000	1.771931000
6	11.813555000	15.981930000	2.357379000
6	11.741293000	14.710670000	1.591524000
6	12.631149000	9.445635000	2.106039000
1	12.206099000	9.608849000	3.098113000
16	12.693276000	18.409226000	2.648994000
1	13.206121000	8.515806000	2.134306000
1	13.326587000	10.265467000	1.916769000
6	15.284041000	16.235269000	0.155424000
1	15.581735000	15.681428000	1.051382000
1	15.688485000	17.247943000	0.277141000
6	12.647341000	16.939101000	1.752261000
6	9.598025000	13.375829000	4.014615000
6	9.771941000	11.578733000	2.512634000
6	12.851016000	17.324051000	-1.370405000
1	13.182438000	16.777360000	-2.261479000
1	13.402171000	18.273338000	-1.382024000
6	9.649741000	14.656044000	4.767100000
6	11.532974000	9.395798000	1.036384000
1	11.976129000	9.208941000	0.050006000
1	10.864924000	8.545100000	1.223938000
6	8.468391000	12.056277000	7.750339000
1	9.559522000	11.969643000	7.758079000
1	8.084376000	11.033902000	7.644591000
6	6.100904000	13.156566000	6.132800000
1	5.773103000	13.719310000	7.015530000
1	5.678102000	12.150205000	6.248204000
6	7.981048000	12.657907000	9.077506000
1	6.890876000	12.718203000	9.116630000
1	8.304916000	12.058703000	9.933136000
1	8.372007000	13.668062000	9.221852000
6	8.191885000	11.789430000	-0.684139000
1	8.736778000	12.678395000	-1.006857000
1	7.457572000	11.545073000	-1.456878000
1	7.648283000	12.059829000	0.223012000
16	8.721706000	10.946693000	3.724335000
16	12.404641000	13.249994000	-0.451385000
16	8.933243000	16.138427000	6.775323000
14	10.864121000	18.444526000	5.398458000
14	13.388916000	16.345511000	0.167037000
14	10.456769000	10.952864000	0.912949000
14	7.995222000	13.023520000	6.187276000
6	8.870363000	14.634618000	5.937711000
6	8.781420000	12.410782000	4.631579000
6	10.295298000	15.911255000	4.575977000
6	15.894879000	15.579120000	-1.092682000
1	15.648974000	16.133995000	-2.001060000
1	16.985358000	15.528138000	-1.027116000
1	15.528803000	14.557653000	-1.222225000
6	9.759585000	19.966292000	5.140532000
1	9.087484000	19.737140000	4.307385000
1	10.395492000	20.791988000	4.796676000
6	9.150525000	10.618777000	-0.425087000
1	8.582026000	9.727298000	-0.131104000
1	9.669189000	10.346315000	-1.353079000
6	13.079029000	17.705652000	7.106822000
1	13.671836000	17.438532000	6.230065000
1	13.768784000	17.984573000	7.908490000
1	12.546472000	16.805540000	7.419083000
6	12.098342000	18.842030000	6.786219000
1	11.532781000	19.109748000	7.687217000
1	12.650922000	19.747047000	6.502453000
6	11.342384000	17.592018000	-1.455842000
1	10.995973000	18.165344000	-0.594209000
1	11.084106000	18.151033000	-2.359627000
1	10.778590000	16.657431000	-1.466066000
6	5.548667000	13.816736000	4.862044000

1	5.834395000	13.254382000	3.971441000
1	4.457124000	13.881580000	4.885039000
1	5.943232000	14.827556000	4.742164000
6	11.619852000	17.788166000	3.844758000
6	11.225547000	16.468947000	3.559946000
6	11.350992000	12.561814000	0.726577000
6	12.507942000	14.737596000	0.412384000
6	8.943146000	20.414789000	6.361690000
1	9.588063000	20.699585000	7.196503000
1	8.313297000	21.277818000	6.127995000
1	8.284320000	19.616570000	6.712364000

Table S19. The optimized Cartesian coordinates of the tetrathiatetrasila[8]circulene **6** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	9.985497000	16.834742000	5.602295000
6	10.173498000	12.900877000	2.789246000
6	11.063901000	13.458802000	1.777234000
6	11.790045000	15.987986000	2.348151000
6	11.726735000	14.714242000	1.589672000
6	12.668949000	9.506690000	2.145864000
1	12.243862000	9.665865000	3.138068000
16	12.643557000	18.408974000	2.652121000
1	13.255750000	8.588037000	2.181893000
1	13.356484000	10.329885000	1.945562000
6	15.256317000	16.218656000	0.213102000
1	15.521830000	15.675886000	1.125648000
1	15.664945000	17.228731000	0.335399000
6	12.603237000	16.944413000	1.749838000
6	9.595100000	13.380299000	4.008159000
6	9.778098000	11.567354000	2.512698000
6	12.769824000	17.298312000	-1.367370000
1	13.098358000	16.751927000	-2.258684000
1	13.302405000	18.256225000	-1.403160000
6	9.642691000	14.660734000	4.756644000
6	11.577270000	9.407767000	1.071742000
1	12.026963000	9.208713000	0.091861000
1	10.930420000	8.544427000	1.269532000
6	8.518688000	12.078235000	7.734918000
1	9.611362000	12.016748000	7.729158000
1	8.159444000	11.047201000	7.633845000
6	6.111870000	13.188924000	6.055668000
1	5.761629000	13.749117000	6.930252000
1	5.671622000	12.189865000	6.157008000
6	8.026863000	12.667423000	9.067237000
1	6.937518000	12.697862000	9.120268000
1	8.376492000	12.064281000	9.906241000
1	8.398813000	13.682292000	9.223170000
6	8.192704000	11.864868000	-0.631610000
1	8.743887000	12.749618000	-0.954015000
1	7.450272000	11.641523000	-1.398790000
1	7.655458000	12.126562000	0.281379000
16	8.757663000	10.952299000	3.713877000
16	12.388656000	13.237378000	-0.424733000
16	8.945846000	16.151173000	6.748928000
14	10.862023000	18.494195000	5.426829000
14	13.385247000	16.361423000	0.140347000
14	10.459762000	10.900905000	0.887343000
14	7.977182000	13.016253000	6.201443000
6	8.875115000	14.647333000	5.916533000
6	8.797300000	12.417130000	4.616467000
6	10.295039000	15.920593000	4.562372000
6	15.900807000	15.545171000	-1.010355000
1	15.692815000	16.091205000	-1.931726000
1	16.984746000	15.499455000	-0.896852000
1	15.547176000	14.520209000	-1.141520000
6	9.729271000	19.961468000	5.138925000
1	9.056178000	19.714658000	4.311895000
1	10.352267000	20.789753000	4.780526000

6	9.127079000	10.665510000	-0.414819000
1	8.544782000	9.779506000	-0.135916000
1	9.623465000	10.399849000	-1.355475000
6	13.092503000	17.597845000	7.033244000
1	13.668009000	17.342106000	6.142145000
1	13.801557000	17.843548000	7.824807000
1	12.549846000	16.703189000	7.342608000
6	12.139493000	18.774043000	6.774108000
1	11.604658000	19.032008000	7.695183000
1	12.710240000	19.671926000	6.508966000
6	11.254007000	17.534284000	-1.425824000
1	10.905741000	18.118312000	-0.572550000
1	10.982305000	18.078094000	-2.331517000
1	10.701510000	16.593292000	-1.427018000
6	5.609441000	13.859889000	4.769108000
1	5.900125000	13.294607000	3.882348000
1	4.521028000	13.933730000	4.771795000
1	6.009117000	14.869529000	4.659796000
6	11.598745000	17.804462000	3.837469000
6	11.200609000	16.472074000	3.560223000
6	11.350953000	12.553604000	0.723555000
6	12.486578000	14.730315000	0.424691000
6	8.919008000	20.416701000	6.363368000
1	9.564585000	20.721590000	7.188418000
1	8.290876000	21.271493000	6.109126000
1	8.258346000	19.627379000	6.727931000

Table S20. The optimized Cartesian coordinates of the tetragermatetrathia[8]circulene **7** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	11.901086000	15.154571000	19.996011000
6	11.342601000	14.687291000	18.752023000
6	10.328457000	15.212545000	17.788329000
6	9.601129000	16.448478000	17.655764000
6	9.503846000	17.708235000	18.454862000
6	9.997791000	18.138590000	19.738238000
6	10.866660000	17.532524000	20.791830000
6	11.663342000	16.335699000	20.882478000
6	12.837451000	14.251120000	20.498693000
6	11.875521000	13.450982000	18.387848000
6	10.042706000	14.340592000	16.737246000
6	8.817203000	16.451827000	16.502091000
6	8.704980000	18.689113000	17.866897000
6	9.533472000	19.414051000	20.057802000
6	10.997795000	18.318814000	21.937402000
6	12.372022000	16.291131000	22.083247000
6	13.071543000	13.519285000	23.698608000
1	13.692766000	12.624956000	23.595945000
1	13.369255000	13.998394000	24.635313000
6	11.587097000	13.151476000	23.731857000
1	10.959059000	14.037304000	23.839553000
1	11.369403000	12.484559000	24.569600000
1	11.280512000	12.644960000	22.815562000
6	15.473621000	15.220935000	22.239843000
1	16.035900000	14.302464000	22.050731000
1	15.641976000	15.879254000	21.385110000
6	15.944837000	15.883137000	23.537530000
1	15.409646000	16.815471000	23.730266000
1	17.009193000	16.125286000	23.488441000
1	15.800266000	15.231973000	24.402058000
6	9.957611000	11.083446000	17.228881000
1	9.390274000	10.820730000	16.331785000
1	10.653590000	10.259014000	17.409267000
6	9.026001000	11.278108000	18.426300000
1	9.584574000	11.531730000	19.328643000
1	8.457849000	10.367602000	18.631410000
1	8.311655000	12.083615000	18.249567000
6	12.266083000	12.361035000	15.285052000
1	12.868844000	11.485092000	15.541941000

1	11.653375000	12.073158000	14.426237000
6	13.160553000	13.552864000	14.943917000
1	12.571291000	14.425851000	14.659304000
1	13.826437000	13.314336000	14.111212000
1	13.780764000	13.841790000	15.794006000
6	5.919856000	17.973600000	16.283162000
1	5.499641000	18.976619000	16.167005000
1	5.603133000	17.399610000	15.408081000
6	5.415860000	17.316659000	17.569437000
1	5.820001000	16.309819000	17.687422000
1	4.325972000	17.240027000	17.567116000
1	5.707836000	17.888985000	18.451112000
6	8.501567000	19.106500000	14.592666000
1	8.139793000	20.134766000	14.676424000
1	9.591404000	19.146754000	14.645641000
6	8.043275000	18.480975000	13.272424000
1	8.419780000	17.462032000	13.159195000
1	8.408135000	19.057247000	12.419073000
1	6.954698000	18.443136000	13.196708000
6	8.522341000	20.226982000	23.057658000
1	7.877731000	21.002679000	22.634804000
1	7.959720000	19.292164000	23.018167000
6	8.904206000	20.574232000	24.498393000
1	9.532769000	19.801387000	24.945936000
1	8.014633000	20.671169000	25.125271000
1	9.447544000	21.519358000	24.557561000
6	11.251645000	21.591846000	21.829766000
1	10.630213000	22.467444000	21.620356000
1	11.637288000	21.718569000	22.844756000
6	12.399012000	21.486882000	20.823781000
1	13.042778000	20.633261000	21.041959000
1	13.019731000	22.385634000	20.844699000
1	12.027065000	21.361601000	19.805781000
16	13.025186000	12.876260000	19.507673000
16	8.940463000	15.001110000	15.617106000
16	8.542327000	20.077872000	18.841762000
16	12.066649000	17.639849000	23.079276000
32	13.556041000	14.753994000	22.234347000
32	11.047418000	12.675186000	16.802439000
32	7.886502000	18.132053000	16.194155000
32	10.055361000	20.020695000	21.831597000

Table S21. The optimized Cartesian coordinates of the tetragermatetrathia[8]circulene **7** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.309322000	3.909048000	0.608261000
6	0.749374000	3.437741000	-0.626426000
6	-0.245614000	3.969894000	-1.598242000
6	-0.962780000	5.204775000	-1.732888000
6	-1.076923000	6.433692000	-0.937434000
6	-0.582448000	6.867855000	0.337790000
6	0.302208000	6.275569000	1.378609000
6	1.096144000	5.084094000	1.466503000
6	2.247771000	2.987191000	1.126743000
6	1.262780000	2.192088000	-0.978409000
6	-0.521742000	3.101837000	-2.652015000
6	-1.743113000	5.216339000	-2.913456000
6	-1.902956000	7.420474000	-1.527516000
6	-1.058542000	8.134750000	0.664338000
6	0.445649000	7.071230000	2.513722000
6	1.830437000	5.048128000	2.674182000
6	2.501330000	2.299356000	4.330924000
1	3.113279000	1.397753000	4.243861000
1	2.806964000	2.791621000	5.257626000
6	1.012681000	1.951285000	4.367784000
1	0.391823000	2.842823000	4.468408000
1	0.794484000	1.300253000	5.216341000
1	0.697396000	1.429348000	3.463329000
6	4.928780000	3.967238000	2.788877000

1	5.478593000	3.046935000	2.576146000
1	5.068281000	4.628519000	1.931497000
6	5.442927000	4.618550000	4.075708000
1	4.921015000	5.551960000	4.295880000
1	6.504093000	4.856992000	3.984210000
1	5.332179000	3.960035000	4.938739000
6	-0.690084000	-0.143422000	-2.146643000
1	-1.244203000	-0.404329000	-3.051884000
1	-0.021092000	-0.983647000	-1.941618000
6	-1.639798000	0.097027000	-0.972187000
1	-1.096968000	0.346231000	-0.059178000
1	-2.232340000	-0.797197000	-0.770047000
1	-2.334079000	0.913661000	-1.175523000
6	1.701638000	1.105953000	-4.075263000
1	2.298004000	0.227792000	-3.813245000
1	1.102370000	0.821056000	-4.943885000
6	2.600290000	2.300388000	-4.394945000
1	2.018951000	3.174931000	-4.690477000
1	3.275640000	2.059789000	-5.217953000
1	3.212544000	2.585412000	-3.538020000
6	-4.663135000	6.689300000	-3.144463000
1	-5.095622000	7.687654000	-3.250669000
1	-4.964206000	6.125810000	-4.031239000
6	-5.164386000	6.006954000	-1.871054000
1	-4.755313000	5.001069000	-1.764004000
1	-6.252235000	5.919970000	-1.888540000
1	-4.893255000	6.570536000	-0.977354000
6	-2.044890000	7.893063000	-4.796801000
1	-2.406555000	8.919283000	-4.694142000
1	-0.956466000	7.928326000	-4.722431000
6	-2.486540000	7.297128000	-6.136479000
1	-2.111198000	6.280899000	-6.272208000
1	-2.102829000	7.895325000	-6.964691000
1	-3.573029000	7.269589000	-6.232797000
6	-2.068710000	8.900150000	3.669910000
1	-2.745255000	9.646187000	3.244158000
1	-2.588330000	7.940889000	3.628030000
6	-1.705038000	9.266083000	5.110550000
1	-1.047132000	8.523377000	5.565845000
1	-2.603886000	9.321596000	5.727228000
1	-1.209063000	10.236000000	5.172078000
6	0.641129000	10.353037000	2.401938000
1	-0.001314000	11.214570000	2.200043000
1	1.037328000	10.492692000	3.410681000
6	1.773183000	10.263618000	1.377953000
1	2.439354000	9.424901000	1.585869000
1	2.374907000	11.173997000	1.392968000
1	1.391044000	10.136781000	0.364007000
16	2.419444000	1.612628000	0.149571000
16	-1.620519000	3.772228000	-3.789440000
16	-2.065879000	8.798835000	-0.556308000
16	1.529817000	6.393377000	3.659931000
32	3.018875000	3.497190000	2.856142000
32	0.454520000	1.398813000	-2.584525000
32	-2.707133000	6.893930000	-3.236684000
32	-0.532333000	8.773193000	2.444702000

Table S22. The optimized Cartesian coordinates of the tetragermatetrathia[8]circulene **7** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.222603000	4.803956000	13.807099000
6	2.786985000	4.335361000	15.039202000
6	3.775683000	4.871611000	16.017913000
6	4.509130000	6.095774000	16.146812000
6	4.622454000	7.345962000	15.341438000
6	4.104308000	7.788963000	14.079428000
6	3.195580000	7.208365000	13.049139000
6	2.415485000	6.009902000	12.950253000
6	1.304974000	3.881478000	13.278457000

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6        2.282977000      3.072341000     15.389896000
6        4.040504000      3.996886000     17.085446000
6        5.294412000      6.106259000     17.310915000
6        5.458869000      8.313121000     15.921671000
6        4.580022000      9.067175000     13.748062000
6        3.022204000      8.031986000     11.923669000
6        1.668867000      5.977872000     11.761168000
6        1.087993000      3.228086000     10.048793000
1        0.491308000      2.312545000     10.112162000
1        0.788658000      3.734855000      9.126342000
6        2.582431000      2.902477000     10.019603000
1        3.181863000      3.812523000      9.956406000
1        2.838019000      2.271176000      9.163119000
1        2.890692000      2.379272000     10.926364000
6       -1.385966000      4.709701000     11.514051000
1       -1.878522000      3.742669000     11.655650000
1       -1.634316000      5.325160000     12.381238000
6       -1.870927000      5.373927000     10.222228000
1       -1.408177000      6.353842000     10.082513000
1       -2.954805000      5.523901000     10.229723000
1       -1.633131000      4.770150000      9.343150000
6        4.102183000      0.688118000     16.777371000
1        4.587647000      0.468446000     17.733718000
1        3.392541000     -0.125208000     16.594363000
6        5.133631000      0.767714000     15.651324000
1        4.656233000      0.980865000     14.693078000
1        5.687446000     -0.170583000     15.549815000
1        5.855834000      1.565500000     15.833327000
6        1.747164000      2.043976000     18.489397000
1        1.156106000      1.162397000     18.220986000
1        2.319745000      1.775347000     19.382605000
6        0.836944000      3.241338000     18.765483000
1        1.417388000      4.118838000     19.055834000
1        0.125876000      3.027272000     19.569059000
1        0.266221000      3.515269000     17.876259000
6        8.240029000      7.579408000     17.560878000
1        8.665735000      8.581298000     17.676750000
1        8.530046000      7.010689000     18.449496000
6        8.772409000      6.904960000     16.295601000
1        8.357959000      5.901577000     16.180983000
1        9.862883000      6.817640000     16.317774000
1        8.497805000      7.468155000     15.402157000
6        5.723265000      8.787369000     19.193118000
1        6.125306000      9.799684000     19.088945000
1        4.634859000      8.870614000     19.160083000
6        6.176671000      8.164023000     20.516735000
1        5.766776000      7.159077000     20.642769000
1        5.847709000      8.758602000     21.374350000
1        7.264876000      8.085121000     20.574996000
6        5.467052000      9.940777000     10.713358000
1        6.125103000     10.720468000     11.109722000
1        6.039027000      9.010576000     10.719336000
6        5.017464000     10.292607000      9.293234000
1        4.376315000      9.513422000      8.874300000
1        5.871842000     10.407438000      8.619060000
1        4.456257000     11.229700000      9.267594000
6        2.879271000     11.344584000     12.060891000
1        3.557313000     12.186946000     12.233207000
1        2.448914000     11.486873000     11.065282000
6        1.780390000     11.307313000     13.123789000
1        1.089562000     10.480944000     12.946988000
1        1.200201000     12.234758000     13.131541000
1        2.200639000     11.164737000     14.120934000
16       1.141266000      2.473320000     14.252235000
16       5.152898000      4.654229000     18.220569000
16       5.621469000      9.720709000     14.948271000
16       1.926568000      7.364300000     10.778190000
32       0.574637000      4.399961000     11.573182000
32       3.038121000      2.351728000     17.011085000
32       6.259150000      7.752876000     17.583106000
32       3.991461000      9.697280000     12.023572000
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Table S23. The optimized Cartesian coordinates of the tetrathia[8]circulene **8** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	12.253500000	13.801000000	9.153200000
16	12.604700000	7.680300000	9.040800000
16	15.432600000	7.785200000	14.479500000
16	15.849900000	13.882200000	14.112700000
8	11.053300000	12.146900000	7.149100000
8	11.301700000	9.270500000	7.038900000
8	13.351800000	5.344600000	10.527000000
8	14.599600000	5.397000000	13.131800000
8	16.698600000	9.375400000	16.389300000
8	17.142100000	12.277300000	16.148700000
8	14.946900000	16.222000000	12.730500000
8	13.175900000	16.184100000	10.444300000
6	13.085300000	11.478200000	10.204600000
6	12.349300000	12.073100000	9.145300000
6	11.736700000	11.406600000	8.082800000
6	11.836800000	10.041400000	8.041700000
6	12.533800000	9.409500000	9.073800000
6	13.158800000	10.042300000	10.182400000
6	13.698100000	9.016200000	11.092700000
6	13.415200000	7.726000000	10.569700000
6	13.690800000	6.502100000	11.184000000
6	14.299300000	6.526800000	12.410000000
6	14.616000000	7.772900000	12.955600000
6	14.373100000	9.040700000	12.362600000
6	14.946600000	10.096300000	13.216300000
6	15.555700000	9.507300000	14.353200000
6	16.285400000	10.163000000	15.355300000
6	16.464700000	11.517400000	15.218500000
6	15.817300000	12.149500000	14.147500000
6	15.048000000	11.528100000	13.128600000
6	14.474300000	12.554700000	12.239800000
6	14.853800000	13.842900000	12.700300000
6	14.479700000	15.069000000	12.148300000
6	13.630000000	15.051400000	11.074200000
6	13.255700000	13.807200000	10.563800000
6	13.641200000	12.535200000	11.068300000
6	9.859300000	9.244600000	7.026400000
1	9.579400000	8.577800000	6.215700000
1	9.456000000	10.240900000	6.851400000
1	9.484100000	8.854000000	7.973500000
6	12.278600000	4.610000000	11.152600000
1	12.077300000	3.763700000	10.501900000
1	11.390200000	5.238500000	11.228600000
1	12.572600000	4.264300000	12.142500000
6	15.664400000	4.606300000	12.563900000
1	15.831600000	3.787900000	13.258500000
1	16.570600000	5.207100000	12.475000000
1	15.379400000	4.219400000	11.586400000
6	18.012200000	9.563700000	16.932500000
1	18.182900000	8.707500000	17.579700000
1	18.070000000	10.481700000	17.510500000
1	18.755700000	9.565900000	16.134300000
6	18.460300000	12.701100000	15.750600000
1	18.778500000	13.428400000	16.492700000
1	18.447600000	13.166300000	14.765500000
1	19.151400000	11.857100000	15.741500000
6	15.859300000	16.966000000	11.897500000
1	16.182300000	17.816600000	12.491200000
1	15.364300000	17.306700000	10.989100000
1	16.719400000	16.346700000	11.638600000
6	12.270600000	16.974000000	11.242500000
1	11.961300000	17.803000000	10.612100000
1	12.767800000	17.345900000	12.137300000
1	11.401600000	16.377400000	11.523000000
6	11.698400000	12.198000000	5.859800000
1	11.084000000	12.848200000	5.243500000
1	11.756800000	11.204100000	5.417900000
1	12.699500000	12.619600000	5.958900000

Table S24. The optimized Cartesian coordinates of the tetrathia[8]circulene **8** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	12.213950000	13.775195000	9.180550000
16	12.543873000	7.676624000	9.064035000
16	15.744569000	7.783327000	14.275371000
16	15.913862000	13.902237000	14.076226000
8	10.951650000	12.157146000	7.225856000
8	11.148267000	9.243046000	7.150322000
8	13.390198000	5.353428000	10.476518000
8	14.890651000	5.403671000	12.981266000
8	17.090803000	9.400003000	16.121183000
8	17.326822000	12.321589000	15.980451000
8	14.965480000	16.207485000	12.713809000
8	13.112341000	16.128620000	10.469447000
6	13.090373000	11.464748000	10.202674000
6	12.315243000	12.062250000	9.160969000
6	11.650403000	11.398883000	8.120399000
6	11.728280000	10.032850000	8.093860000
6	12.480996000	9.401712000	9.101955000
6	13.162880000	10.030551000	10.174144000
6	13.757204000	9.010974000	11.043942000
6	13.454862000	7.722441000	10.537094000
6	13.785058000	6.490621000	11.117749000
6	14.501607000	6.511378000	12.286414000
6	14.831034000	7.766061000	12.815602000
6	14.512735000	9.037298000	12.265060000
6	15.095524000	10.088012000	13.104435000
6	15.789257000	9.499321000	14.188020000
6	16.517233000	10.173681000	15.196541000
6	16.601443000	11.555254000	15.109443000
6	15.886892000	12.175290000	14.098785000
6	15.106557000	11.532856000	13.063559000
6	14.506001000	12.535971000	12.218654000
6	14.878037000	13.847734000	12.687571000
6	14.488826000	15.059872000	12.155424000
6	13.598786000	15.033904000	11.082514000
6	13.246601000	13.783814000	10.562679000
6	13.654379000	12.513646000	11.047064000
6	9.700012000	9.303624000	7.093868000
1	9.411651000	8.609340000	6.311575000
1	9.361275000	10.309165000	6.855571000
1	9.284085000	8.986108000	8.049606000
6	12.422167000	4.554614000	11.202582000
1	12.176706000	3.725368000	10.547081000
1	11.531377000	5.149349000	11.404204000
1	12.844681000	4.189087000	12.136371000
6	15.828294000	4.545625000	12.282877000
1	16.058084000	3.741295000	12.973968000
1	16.732386000	5.105715000	12.044376000
1	15.385319000	4.150125000	11.371485000
6	17.267836000	9.880874000	17.480843000
1	17.345716000	8.980238000	18.080486000
1	16.405804000	10.468331000	17.782172000
1	18.175619000	10.468429000	17.565256000
6	18.731746000	12.420840000	15.636566000
1	19.174272000	13.075403000	16.380606000
1	18.849502000	12.851374000	14.642157000
1	19.205562000	11.439460000	15.667906000
6	15.877959000	16.955186000	11.866612000
1	16.191854000	17.809741000	12.456834000
1	15.378736000	17.285550000	10.957599000
1	16.738101000	16.335115000	11.615531000
6	12.423281000	17.111956000	11.293204000
1	12.180870000	17.925158000	10.618503000
1	13.056051000	17.456593000	12.104916000
1	11.512452000	16.662502000	11.685108000
6	11.472202000	12.129107000	5.873038000
1	10.844429000	12.806816000	5.303713000
1	11.418724000	11.124000000	5.459449000
1	12.504245000	12.479361000	5.866546000

Table S25. The optimized Cartesian coordinates of the tetrathia[8]circulene **8** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
16	12.110905000	13.812952000	9.226777000
16	12.852640000	7.702246000	8.966046000
16	15.176238000	7.876934000	14.671972000
16	15.917739000	13.954061000	14.062499000
8	10.987353000	12.106578000	7.171187000
8	11.457925000	9.281674000	6.968810000
8	13.527307000	5.359100000	10.543024000
8	14.464037000	5.441514000	13.252910000
8	16.556548000	9.539856000	16.563680000
8	17.194261000	12.315485000	16.148707000
8	14.945637000	16.299100000	12.671002000
8	13.093032000	16.236808000	10.481021000
6	13.066530000	11.511658000	10.239151000
6	12.285071000	12.082208000	9.179686000
6	11.729518000	11.407913000	8.110455000
6	11.946326000	10.041917000	8.020768000
6	12.660121000	9.431553000	9.032500000
6	13.211184000	10.068147000	10.194621000
6	13.734000000	9.064525000	11.110856000
6	13.537963000	7.751824000	10.565975000
6	13.773648000	6.551732000	11.206036000
6	14.238287000	6.591489000	12.511690000
6	14.493795000	7.827963000	13.070886000
6	14.320746000	9.103998000	12.437475000
6	14.864750000	10.156753000	13.282979000
6	15.410998000	9.591875000	14.481815000
6	16.153591000	10.248436000	15.445274000
6	16.422928000	11.595268000	15.246609000
6	15.819495000	12.217733000	14.166350000
6	15.013275000	11.594187000	13.156166000
6	14.463313000	12.599932000	12.256115000
6	14.874646000	13.908501000	12.673614000
6	14.473716000	15.112861000	12.130633000
6	13.563540000	15.082910000	11.086844000
6	13.169178000	13.849174000	10.607478000
6	13.593609000	12.566740000	11.094093000
6	10.041722000	9.063272000	7.049539000
1	9.779666000	8.420898000	6.210875000
1	9.500800000	10.007830000	6.978391000
1	9.786301000	8.564725000	7.987066000
6	12.327328000	4.709424000	10.989125000
1	12.206041000	3.825051000	10.366317000
1	11.466927000	5.369625000	10.860169000
1	12.412686000	4.418782000	12.036986000
6	15.649058000	4.739618000	12.849075000
1	15.757340000	3.899069000	13.532169000
1	16.522620000	5.390404000	12.928028000
1	15.552567000	4.377527000	11.824736000
6	17.950719000	9.232866000	16.622284000
1	18.067806000	8.471380000	17.391681000
1	18.534357000	10.112081000	16.897051000
1	18.302398000	8.837227000	15.666776000
6	18.506202000	12.632356000	15.664555000
1	19.002159000	13.183095000	16.461897000
1	18.464817000	13.252935000	14.768188000
1	19.070541000	11.724801000	15.438153000
6	15.899717000	16.958582000	11.827133000
1	16.237259000	17.838453000	12.371665000
1	15.440955000	17.257986000	10.883771000
1	16.749949000	16.302297000	11.627322000
6	12.160830000	16.959711000	11.297543000
1	11.826405000	17.809097000	10.704797000
1	12.638633000	17.309903000	12.213376000
1	11.306010000	16.328397000	11.549576000
6	11.669873000	12.269523000	5.919120000
1	11.018411000	12.873903000	5.290709000
1	11.850305000	11.302382000	5.448333000
1	12.619425000	12.788135000	6.068087000

Table S26. The optimized Cartesian coordinates of the tetraselena[8]circulene **9** in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
34	1.372865000	2.909599000	-14.658941000
34	2.753746000	1.660619000	-8.504805000
8	0.439649000	1.378861000	-16.977805000
8	3.168543000	4.412744000	-12.899782000
8	4.018201000	3.648648000	-10.239821000
8	1.331393000	0.569554000	-6.184813000
6	0.206171000	0.655028000	-15.832775000
6	0.499343000	1.235420000	-14.602597000
6	0.336553000	0.637810000	-13.326660000
6	1.033523000	1.419830000	-12.278671000
6	1.683847000	2.551879000	-12.831442000
6	2.642510000	3.346504000	-12.209369000
6	3.031804000	2.995403000	-10.941237000
6	2.355734000	1.945302000	-10.327911000
6	1.302387000	1.176839000	-10.882972000
6	0.599868000	0.399154000	-9.835687000
6	1.179526000	0.618483000	-8.559870000
6	0.632055000	0.268479000	-7.329444000
6	-0.749472000	1.655899000	-17.745670000
1	-0.425946000	2.254296000	-18.592747000
1	-1.211030000	0.732215000	-18.092026000
1	-1.460521000	2.221030000	-17.141543000
6	4.555463000	4.249033000	-13.265559000
1	4.817294000	5.129578000	-13.845509000
1	5.183431000	4.181316000	-12.378523000
1	4.676928000	3.353321000	-13.875944000
6	3.652188000	4.983789000	-9.829843000
1	4.485099000	5.353557000	-9.238372000
1	3.491647000	5.623440000	-10.696805000
1	2.748872000	4.952790000	-9.219423000
6	1.718230000	-0.587340000	-5.415007000
1	2.282355000	-0.207930000	-4.567715000
1	0.841825000	-1.133683000	-5.069360000
1	2.348880000	-1.242583000	-6.017285000
34	-1.372865000	-2.909599000	-14.658941000
34	-2.753746000	-1.660619000	-8.504805000
8	-0.439649000	-1.378861000	-16.977805000
8	-3.168543000	-4.412744000	-12.899782000
8	-4.018201000	-3.648648000	-10.239821000
8	-1.331393000	-0.569554000	-6.184813000
6	-0.206171000	-0.655028000	-15.832775000
6	-0.499343000	-1.235420000	-14.602597000
6	-0.336553000	-0.637810000	-13.326660000
6	-1.033523000	-1.419830000	-12.278671000
6	-1.683847000	-2.551879000	-12.831442000
6	-2.642510000	-3.346504000	-12.209369000
6	-3.031804000	-2.995403000	-10.941237000
6	-2.355734000	-1.945302000	-10.327911000
6	-1.302387000	-1.176839000	-10.882972000
6	-0.599868000	-0.399154000	-9.835687000
6	-1.179526000	-0.618483000	-8.559870000
6	-0.632055000	-0.268479000	-7.329444000
6	0.749472000	-1.655899000	-17.745670000
1	0.425946000	-2.254296000	-18.592747000
1	1.211030000	-0.732215000	-18.092026000
1	1.460521000	-2.221030000	-17.141543000
6	-4.555463000	-4.249033000	-13.265559000
1	-4.817294000	-5.129578000	-13.845509000
1	-5.183431000	-4.181316000	-12.378523000
1	-4.676928000	-3.353321000	-13.875944000
6	-3.652188000	-4.983789000	-9.829843000
1	-4.485099000	-5.353557000	-9.238372000
1	-3.491647000	-5.623440000	-10.696805000
1	-2.748872000	-4.952790000	-9.219423000
6	-1.718230000	0.587340000	-5.415007000
1	-2.282355000	0.207930000	-4.567715000
1	-0.841825000	1.133683000	-5.069360000
1	-2.348880000	1.242583000	-6.017285000

Table S27. The optimized Cartesian coordinates of the tetraselena[8]circulene **9** cation in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
34	1.347383000	2.923403000	-14.666799000
34	2.841609000	1.534066000	-8.558851000
8	0.418419000	1.395909000	-16.977986000
8	3.118906000	4.404148000	-12.891120000
8	4.047103000	3.581245000	-10.255419000
8	1.376259000	0.459378000	-6.260162000
6	0.193611000	0.662247000	-15.850873000
6	0.485584000	1.247520000	-14.620245000
6	0.333562000	0.645766000	-13.343766000
6	1.019554000	1.414461000	-12.309858000
6	1.653546000	2.561294000	-12.842604000
6	2.633599000	3.335158000	-12.216074000
6	3.060025000	2.946071000	-10.954497000
6	2.405374000	1.883555000	-10.356167000
6	1.312938000	1.138389000	-10.909469000
6	0.623158000	0.382788000	-9.890207000
6	1.229120000	0.549424000	-8.608384000
6	0.665079000	0.221819000	-7.390456000
6	-0.746301000	1.608327000	-17.815356000
1	-0.399476000	2.204913000	-18.652756000
1	-1.149871000	0.660908000	-18.165823000
1	-1.504364000	2.154152000	-17.254148000
6	4.548875000	4.416897000	-13.153442000
1	4.727126000	5.325058000	-13.718972000
1	5.116797000	4.422433000	-12.227864000
1	4.811359000	3.544050000	-13.749708000
6	3.690288000	4.909256000	-9.788931000
1	4.543124000	5.256561000	-9.214703000
1	3.501950000	5.575588000	-10.628690000
1	2.807382000	4.852556000	-9.152719000
6	1.608018000	-0.693039000	-5.405175000
1	2.167230000	-0.314873000	-4.556323000
1	0.667979000	-1.130574000	-5.078704000
1	2.199581000	-1.429373000	-5.947619000
34	-1.347254000	-2.923438000	-14.666911000
34	-2.841535000	-1.533962000	-8.559035000
8	-0.418429000	-1.395800000	-16.978028000
8	-3.118855000	-4.404227000	-12.891136000
8	-4.047040000	-3.581215000	-10.255585000
8	-1.376419000	-0.459025000	-6.260319000
6	-0.193432000	-0.662244000	-15.850889000
6	-0.485360000	-1.247595000	-14.620287000
6	-0.333244000	-0.645940000	-13.343804000
6	-1.019258000	-1.414648000	-12.309904000
6	-1.653385000	-2.561379000	-12.842701000
6	-2.633459000	-3.335224000	-12.216158000
6	-3.059845000	-2.946149000	-10.954601000
6	-2.405111000	-1.883679000	-10.356250000
6	-1.312628000	-1.138593000	-10.909524000
6	-0.622839000	-0.383020000	-9.890221000
6	-1.228958000	-0.549461000	-8.608494000
6	-0.665053000	-0.221706000	-7.390536000
6	0.746128000	-1.608163000	-17.815639000
1	0.399093000	-2.204510000	-18.653120000
1	1.149764000	-0.660715000	-18.165942000
1	1.504205000	-2.154220000	-17.254676000
6	-4.548922000	-4.417066000	-13.152876000
1	-4.727333000	-5.325189000	-13.718418000
1	-5.116445000	-4.422765000	-12.227046000
1	-4.811753000	-3.544186000	-13.748942000
6	-3.690607000	-4.909497000	-9.789584000
1	-4.543448000	-5.256679000	-9.215290000
1	-3.502680000	-5.575635000	-10.629588000
1	-2.807548000	-4.853307000	-9.153539000
6	-1.608056000	0.693495000	-5.405435000
1	-2.167154000	0.315436000	-4.556461000
1	-0.667971000	1.131071000	-5.079161000
1	-2.199696000	1.429753000	-5.947899000

Table S28. The optimized Cartesian coordinates of the tetraselena[8]circulene **9** anion in the ground singlet state calculated at the B3LYP/DZP level of theory

Atomic Number	Coordinates (Angstroms) X	Y	Z
34	1.283716000	2.968308000	-14.637521000
34	2.826359000	1.568185000	-8.521381000
8	0.410376000	1.373839000	-16.991939000
8	3.151500000	4.448240000	-12.865602000
8	4.057185000	3.632622000	-10.263164000
8	1.321512000	0.551964000	-6.163189000
6	0.194745000	0.666789000	-15.818577000
6	0.461644000	1.256626000	-14.604045000
6	0.331873000	0.647618000	-13.313337000
6	1.019338000	1.416696000	-12.279870000
6	1.654377000	2.582834000	-12.816412000
6	2.615038000	3.354417000	-12.201849000
6	3.045611000	2.966138000	-10.940063000
6	2.393421000	1.915038000	-10.336337000
6	1.303840000	1.159190000	-10.876101000
6	0.611023000	0.394126000	-9.843501000
6	1.204126000	0.582798000	-8.552539000
6	0.643487000	0.261184000	-7.337389000
6	-0.807290000	1.703292000	-17.674984000
1	-0.523421000	2.298307000	-18.541038000
1	-1.327142000	0.800744000	-17.998617000
1	-1.461622000	2.288382000	-17.024954000
6	4.481442000	4.210938000	-13.354469000
1	4.769960000	5.103969000	-13.905584000
1	5.171732000	4.044854000	-12.526604000
1	4.491609000	3.348076000	-14.023180000
6	3.637408000	4.908253000	-9.751579000
1	4.481375000	5.308791000	-9.193316000
1	3.376566000	5.582849000	-10.567967000
1	2.781688000	4.786521000	-9.084514000
6	1.791919000	-0.621038000	-5.485717000
1	2.341634000	-0.273790000	-4.612851000
1	0.956735000	-1.249268000	-5.172818000
1	2.457605000	-1.194107000	-6.134927000
34	-1.283716000	-2.968308000	-14.637521000
34	-2.826359000	-1.568185000	-8.521381000
8	-0.410376000	-1.373839000	-16.991939000
8	-3.151500000	-4.448240000	-12.865602000
8	-4.057185000	-3.632622000	-10.263164000
8	-1.321512000	-0.551964000	-6.163189000
6	-0.194745000	-0.666789000	-15.818577000
6	-0.461644000	-1.256626000	-14.604045000
6	-0.331873000	-0.647618000	-13.313337000
6	-1.019338000	-1.416696000	-12.279870000
6	-1.654377000	-2.582834000	-12.816412000
6	-2.615038000	-3.354417000	-12.201849000
6	-3.045611000	-2.966138000	-10.940063000
6	-2.393421000	-1.915038000	-10.336337000
6	-1.303840000	-1.159190000	-10.876101000
6	-0.611023000	-0.394126000	-9.843501000
6	-1.204126000	-0.582798000	-8.552539000
6	-0.643487000	-0.261184000	-7.337389000
6	0.807290000	-1.703292000	-17.674984000
1	0.523421000	-2.298307000	-18.541038000
1	1.327142000	-0.800744000	-17.998617000
1	1.461622000	-2.288382000	-17.024954000
6	-4.481442000	-4.210938000	-13.354469000
1	-4.769960000	-5.103969000	-13.905584000
1	-5.171732000	-4.044854000	-12.526604000
1	-4.491609000	-3.348076000	-14.023180000
6	-3.637408000	-4.908253000	-9.751579000
1	-4.481375000	-5.308791000	-9.193316000
1	-3.376566000	-5.582849000	-10.567967000
1	-2.781688000	-4.786521000	-9.084514000
6	-1.791919000	0.621038000	-5.485717000
1	-2.341634000	0.273790000	-4.612851000
1	-0.956735000	1.249268000	-5.172818000
1	-2.457605000	1.194107000	-6.134927000