Electronic Supplementary Information (ESI) for

Theoretical study on the structures, electronic properties, and aromaticity of thia[4]circulenes

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1. Geometry Optimization Using Various Density Functionals and Diradical Character

The geometry optimizations of **4** were performed in a singlet or triplet state using different density functional theories with 6-311+G(d, p) basis set[1–3] to compare their geometries and total energies. We used six different functionals, B3LYP[4–6]-D3BJ,[7,8] BLYP[5,9]-D3BJ, M06,[10] BHandHLYP,[11] CAM-B3LYP,[12] and ωB97-XD.[13] For the calculations in an open-shell state, a spin-unrestricted method was employed.[14] The bond lengths and the degree of non-planarity (DNP)[15] of the optimized geometries are summarized in Figure S1 and Table S1.

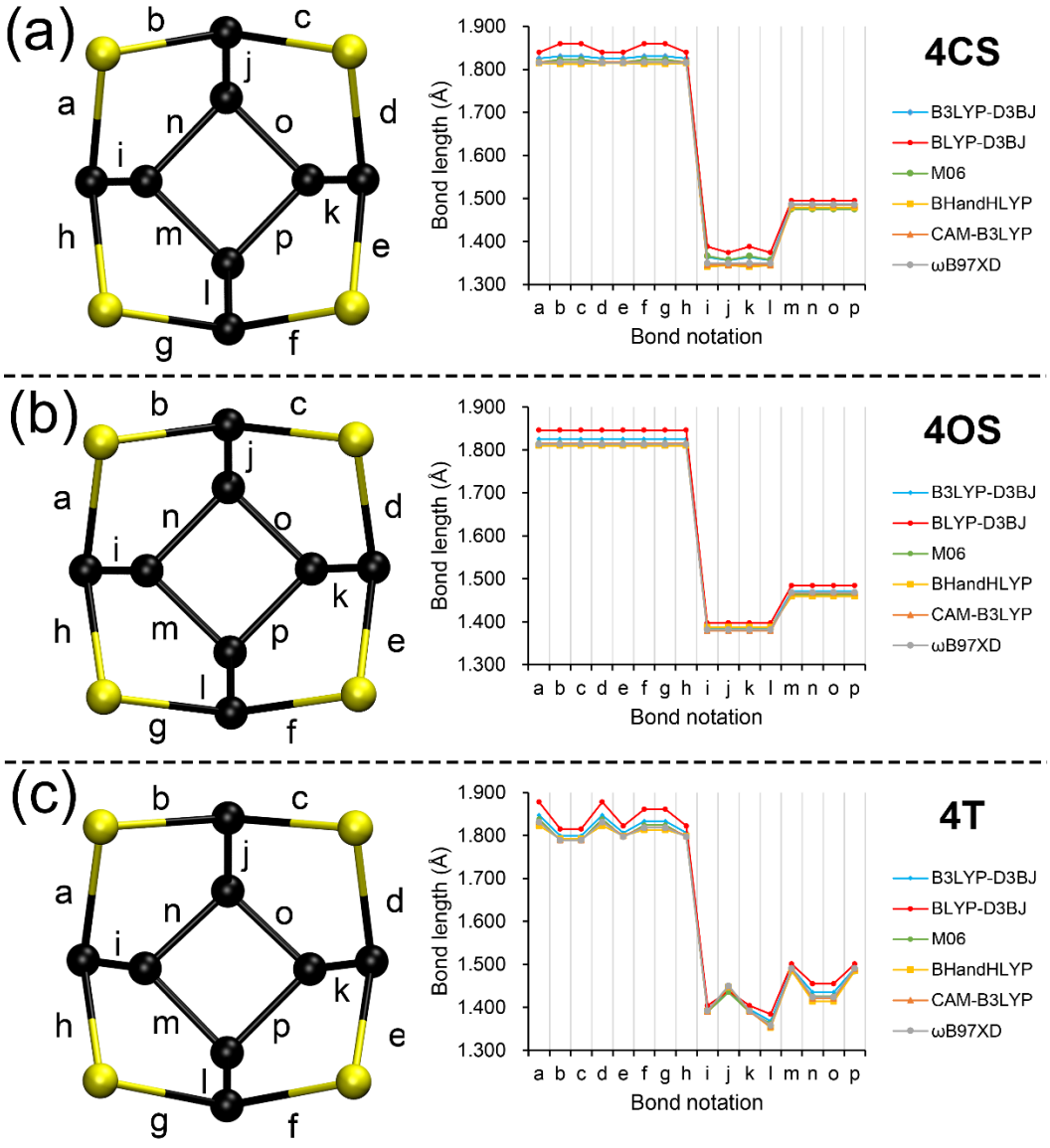

Figure S1. The bond lengths of optimized geometries of **4CS** (a), **4OS** (b) and **4T** (c).

Table S1. DNP and $<S^2>$ values of the optimized geometries of **4** using six different DFT methods.

DFT methods	DNP (°)			$<S^2>$	
	at closed-shell singlet geometries	at open-shell singlet geometries	at triplet geometries	at open-shell singlet geometries	at triplet geometries
B3LYP-D3BJ	55.53	55.84	55.67	1.09	2.08
BLYP-D3BJ	55.69	55.69	55.55	0.97	2.03
M06	55.70	55.95	55.74	1.11	2.09
BHandHLYP	55.47	55.94	55.52	1.54	2.31
CAM-B3LYP	55.49	55.93	55.73	1.20	2.17
ωB97-XD	55.62	56.06	55.90	1.15	2.15

Table S2. The total energies (hartree), relative energies (kcal/mol) of **4** with different spin solutions, and ΔE_{ST} values (kcal/mol) using six different DFT methods.

DFT methods	E_{CS}[a,d] (hartree)	E_{OS}[b,d] (hartree)	E_{T}[c,d] (hartree)	ΔE_{ST}[e] (kcal/mol)
B3LYP-D3BJ	−1897.411921 (0.00)	−1897.422240 (−6.48)	−1897.418523 (−4.14)	−2.33
BLYP-D3BJ	−1897.298368 (0.00)	−1897.304278 (−3.71)	−1897.304058 (−3.57)	−0.14
M06	−1897.027263 (0.00)	−1897.036500 (−5.80)	−1897.032462 (−3.26)	−2.53
BHandHLYP	−1897.071366 (0.00)	−1897.096812 (−15.97)	−1897.084033 (−7.95)	−8.02
CAM-B3LYP	−1897.160567 (0.00)	−1897.173354 (−8.02)	−1897.164018 (−2.17)	−5.86
ωB97-XD	−1897.169053 (0.00)	−1897.179981 (−6.86)	−1897.171779 (−1.71)	−5.15

[a]Zero-point-corrected energies at a closed-shell singlet geometry. [b]Zero-point-corrected energies at an open-shell singlet geometry. [c]Zero-point-corrected energies at a triplet geometry. [d]The relative total energies with respect to the closed-shell singlet geometry are in parentheses. [e]$\Delta E_{ST} = E_{OS} - E_{T}$.

In the case of hybrid functionals (B3LYP, M06, BHandHLYP, CAM-B3LYP, and ωB97-XD), the bond lengths of the optimized geometries were virtually identical. In the case of BLYP, which is the pure DFT, those become slightly longer (Figure S1). The DNP values of all optimized geometries are virtually identical (Table S1).

In all cases, the total energies obtained by the unrestricted method are lower than those by the restricted method. Moreover, the energies of the lowest open-shell singlet geometries are lower than those of the lowest triplet geometries in all cases. The relative energies of the open-shell singlet geometries to the closed-shell singlet geometries are −6.48 kcal/mol, −3.71 kcal/mol, −5.80 kcal/mol, −15.97 kcal/mol, −8.02 kcal/mol, and −6.86 kcal/mol for the B3LYP, BLYP, M06, BHandHLYP, CAM-B3LYP, and ωB97-XD calculations (Table S2). The ΔE_{ST} values are −2.33 kcal/mol, −0.14 kcal/mol, −2.53 kcal/mol, −8.02 kcal/mol, −5.86 kcal/mol, and −5.15 kcal/mol for the B3LYP, BLYP, M06, BHandHLYP, CAM-B3LYP, and ωB97-XD calculations (Table S2). These energy differences are less than 10 kcal/mol. Note that the $<S^2>$ values by the BHandHLYP calculation are the highest (1.54 and 2.31 for the singlet and triplet solutions), indicating a large spin-contamination due to the high percentage of the Hartree-Fock exchange (50%) of this functional.[16–18]

It is worth mentioning that diradical character y_0 of the open-shell singlet geometry of **4** (optimized at UB3LYP-D3BJ/6-311+G(d, p)) is 0.751, while those of [4]circulene and thia[4]circulenes **1**–**3** are 0.000. Those were calculated using Yamaguchi's spin-projected formalism at the unrestricted Hartree-Fock level of theory (PUHF) with 6-311+G(d, p) basis set.[19]

2. Method Dependent Singlet-Triplet Energy Gaps of 4

Since the calculation result of ΔE_{ST} of **4** depends on the choice of exchange-correlation functional, we further investigated dependence of theoretically predicted ΔE_{ST} on the levels of theory and approximation. At first, by using the B3LYP-D3BJ geometries, we performed the single point calculations at the spin-flip non-collinear time-dependent DFT (SF-NC-TDDFT)[20–23] level of theory along with the PBE5050 functional and 6-311G* basis set. This method is known to be useful to estimate ΔE_{ST} values of several fused-ring conjugated molecules having several different open-shell characters.[24] SF-NC-TDDFT calculations were performed using Q-Chem 6.0 program package.[25] Since we have not performed the geometry optimizations at this level, zero-point vibrational energy (ZPVE) corrections were estimated from those at the B3LYP-D3BJ level. The results of adiabatic ΔE_{ST} of **1-3** at the SF-NC-TDDFT level summarized in Table S3 are qualitative and (semi-)quantitatively in nice agreement with those at the B3LYP-D3BJ level given in Table 1 in the main text. Unfortunately, a meaningful solution was not obtained for **4T** due to the spin-contamination errors in the SF-NC-TDDFT solution (i.e., $<\hat{S}^2> \sim 1$),[26] the feature of which may suggest multi-reference character of **4T**. When we estimate the triplet state energy of **4T** at the restricted open-shell (RO)PBE5050/6-311G* level, which is used as the reference state of SF-NC-TDDFT, adiabatic ΔE_{ST} is calculated to be –3.1 kcal/mol. SF-NC-TDDFT calculations suggest that **4** may have a singlet ground state.

Table S3. ΔE_{ST} values (kcal/mol) of thia[4]circulenes **1**–**4** at the SF-NC-TDDFT level.

	1	**2**	**2'**	**3**	**4CS/4T**	**4OS/4T**
vertical ΔE_{ST}	–65.4	–46.7	–64.4	–36.6	–12.5	–5.2
adiabatic ΔE_{ST} (+ ZPVE)	–46.6	–27.1	–43.4	–18.1	(–3.1)[a]	(–4.1)[a]

[a]We could not obtain physically meaningful solution for the triplet state due to the spin-contamination errors in the SF-NC-TDDFT solution. Therefore, for reference, we employed total energy of the spin-restricted open-shell (RO)DFT triplet solution, which is used as the reference state of SF-NC-TDDFT calculations, to estimate adiabatic ΔE_{ST}.

Since SF-NC-TDDFT of **4** suggests multi-reference character of wavefunction, we have also tried to perform *ab initio* multi-reference calculations. The *ab initio* calculations were performed using ORCA 4.2 and 5.0 program packages.[27–29] To determine the active orbital space, we at first performed RMP2/def2-SVP calculations for **4CS**, **4OS** and **4T** (treated as a singlet state) to obtain the natural orbitals (NOs). To reduce the computational efforts, we employed the resolution-of-the-identity (RI) approximation for the integral transformation in the MP2[30] using def2-SVP/C auxiliary basis set. Figure S2 shows the frontier NOs and their occupation numbers. Judging from the topologies of these NOs, we may choose the CAS(2,2), CAS(6,6) and CAS(8,8) orbital spaces

as the reference active spaces.

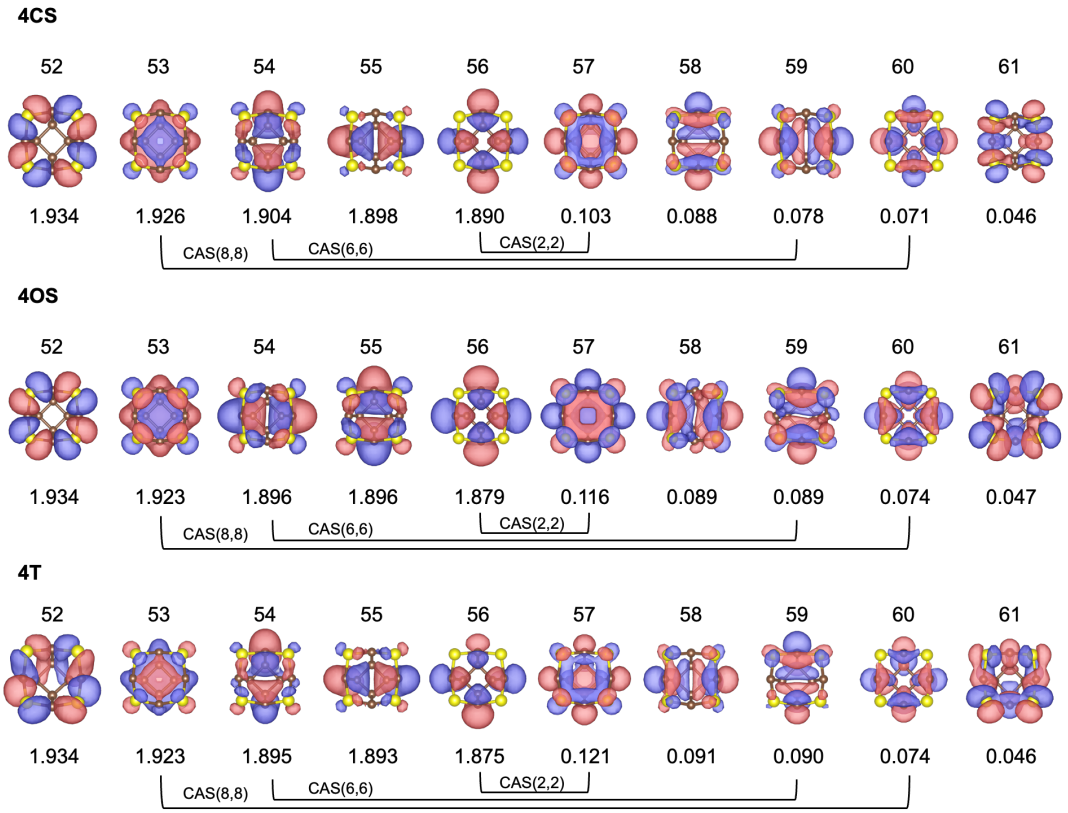

Figure S2. RI-RMP2 natural orbitals and occupation numbers of **4CS**, **4OS**, and **4T** (treated as a singlet state). Note that the 56th orbital is HOMO of the singlet state.

We also performed the Iterative Configuration Expansion-Configuration Interaction (ICE-CI) calculations,[31,32] which is based on the framework of Configuration Interaction by Perturbation with multiconfigurational zeroth-order wave functions Selected by Iterative process (CIPSI)[33] and can offer an approximate full-CI calculations in the target active subspace, just to check the multi-reference characters of **4**. We employed the auto-ICE procedure implemented in ORCA 5.0 where RMP2 natural orbitals and occupation number are used to determine the active subspace automatically. Here, we set *nmin* and *nmax* (thresholds for occupation numbers) to be 1.96 and 0.04, respectively, resulting in CAS(38e,28o) as the active subspace (this condition may be somewhat loose when we need to discuss energies, but would be sufficient for our purpose). We employed default settings for other parameters. Results of occupation numbers of NOs obtained from (RI-based) ICE-CI [approximate CASCI(38e,28o)] calculations using def2-SVP basis set are summarized in Table S4. We should note that topologies of the frontier NOs (from the 53rd to 60th) are similar with those of RI-RMP2 NOs. Occupation numbers of the 58th (0.173) and 59th (0.142) NOs of **4T** (treated as a triplet state) are found to be comparable to that of the

57th (0.156/0.201) NO of **4CS**/**4OS**. These results suggest that we may at least need CAS(6,6) active space when we want to discuss energy of the triplet state of **4**. We also should note that electron correlations within the CAS(6,6) space may not be so strong (suggested from the results that the occupation numbers of 58th and 59th NOs are less than 0.2), but appropriate treatment of dynamical correlations along with sufficiently large active space may be needed.

Table S4. Occupation numbers of NOs obtained from ICE-CI [approximate CASCI(38e,28o)/def2-SVP] calculations.

# NO	52	53	54	55	56	57	58	59	60	61
4CS	1.976	1.939	1.894	1.891	1.861	0.156	0.116	0.099	0.088	0.031
4OS	1.981	1.934	1.877	1.877	1.818	0.201	0.121	0.121	0.093	0.027
4T[a]	1.979	1.935	1.858	1.834	1.066	0.945	0.173	0.142	0.088	0.027

[a]In this calculation, **4T** is treated as a triplet state.

Then, we tried to estimate adiabatic ΔE_{ST} of **4** at the *n*-electron valence state perturbation theory (NEVPT2) level.[34,35] Here, we performed fully-internally-contracted (FIC-)NEVPT2 calculations based on the CASSCF(2,2), CASSCF(6,6) and CASSCF(8,8) reference space. During these CASSCF/NEVPT2 calculations, the RI-RMP2 NOs are used as the initial orbitals, and state-specific calculations are performed. Calculation results for different basis set (def2-SVP and def2-TZVP) are summarized in Table S5. When we take the minimal CAS(2,2) active space as the reference, the singlet state becomes lower than the triplet state. However, the results with CAS(6,6) reference predict that the triplet is lower than the singlet. With the CAS(8,8) active space, again the singlet becomes the ground spin state.

These results suggest that it is highly difficult to determine the ground spin state of **4**. Further careful investigations of the convergence behavior of ΔE_{ST} against the level of theory/approximation (choice of active space, treatment of dynamical correlation and choice of basis set as well as quality of geometry optimization) are needed in order to determine the ground spin state. Since such a detailed discussion on the accuracy of calculated ΔE_{ST} of **4** is far beyond the scope of this study, we focus mainly on the aromatic characters of thia[4]circulenes in the remaining part of this paper. Regardless of difficulty in the treatment of electron correlation effects during the discussion of energy difference between **4S** and **4T**, usual DFT approximation is expected to work efficiently for prediction of their aromatic characters. Indeed, UDFT calculations can usually give reliable results for magnetic responses that are comparable to the experimental results (such as $^{1}H/^{13}C$ NMR chemical shifts) even for the systems with multi-reference characters.[36,37]

Table S5. Adiabatic ΔE_{ST} (+ ZPVE from UB3LYP-D3BJ) values (kcal/mol) of **4OS/4T** calculated at the (RI-Based) FIC-NEVPT2 level based on different active spaces/basis sets.

	CAS(2,2)	CAS(6,6)	CAS(8,8)
def2-SVP	–7.4 (–4.2)	+0.6 (+2.9)	–5.3 (–2.3)
def2-TZVP	–3.7 (–1.7)	–[b] (+5.5)[c]	–1.8 (–0.02)

[a] Values in parenthesis are ΔE_{ST} calculated for **4CS**. [b]We could not obtain well converged CASSCF results. [b]In the log file of the singlet state calculation, there are warning messages indicating negative eigenvalues of Koopmans matrices.

3. Excitation Energies Calculated by TDDFT

Table S6. Vertical S_0–S_1 and S_0–T_1 excitation energies evaluated at the SF-NC-TDDFT PBE5050/6-311G(d) level.

compound	**[4]circulene**	**1**	**2**	**2'**	**3**	**4CS**	**4OS**
S_0–S_1 (eV)	4.81[a]	3.68[a]	2.43	3.20	2.19	1.26	1.24
S_0–T_1 (eV)	3.26	2.84	2.03	2.79	1.59	0.54	0.23

[a] $\langle S^2 \rangle$ of S_1 state was relatively large (~0.61 for [4]circulene and **1**).

4. LUMO Distributions of Planar and Distorted Thiophenes

To investigate the effect of a ring distortion on the HOMO and LUMO distributions and their energy levels in thiophene, we conducted the single point calculation of a distorted thiophene at the B3LYP-D3BJ/6-311+G(d, p) level of theory (Figure S3). The atomic coordinates of carbon and sulfur frameworks of the distorted thiophene is identical to the ring D of **4** (optimized at a singlet state). Four hydrogen atoms are substituted to the five membered ring. The LUMO energy level of planar thiophene is −0.70 eV. On the other hand, that of the distorted thiophene is −2.68 eV. The LUMO energy level is significantly lowered. Moreover, there exist antrafacial bonding-like orbital interaction along the C–S bonds. This would stabilize the LUMO energy level. In contrast to the LUMO level, the difference in the energy levels of HOMO between planar and distorted thiophene is small (−6.69 and −6.17 eV for planar thiophene and distorted one, respectively).

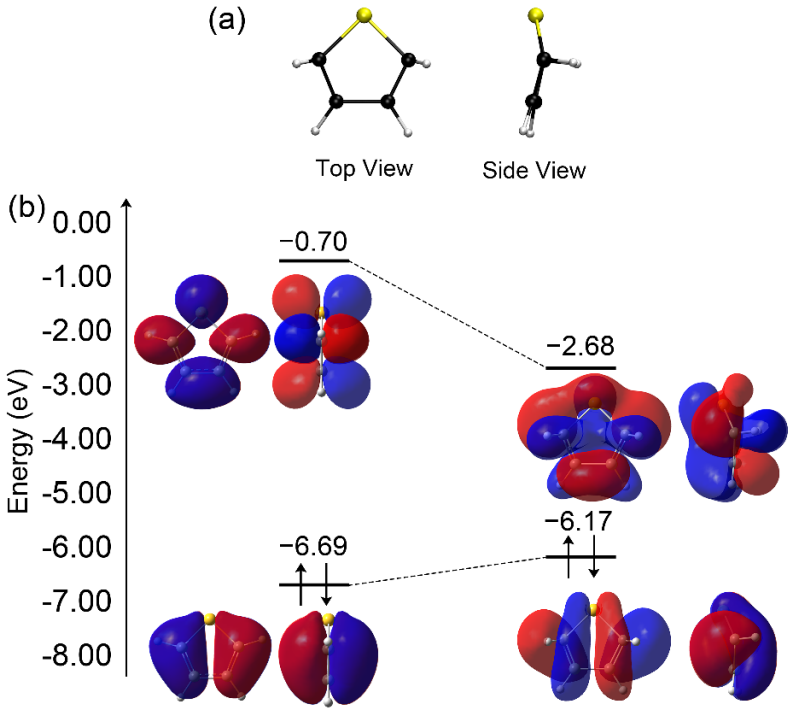

Figure S3. (a) The geometry of a distorted thiophene (top and side views). (b) The HOMO and LUMO distributions and their energy levels of the planar (left) and distorted thiophene (right).

5. Molecular Geometries

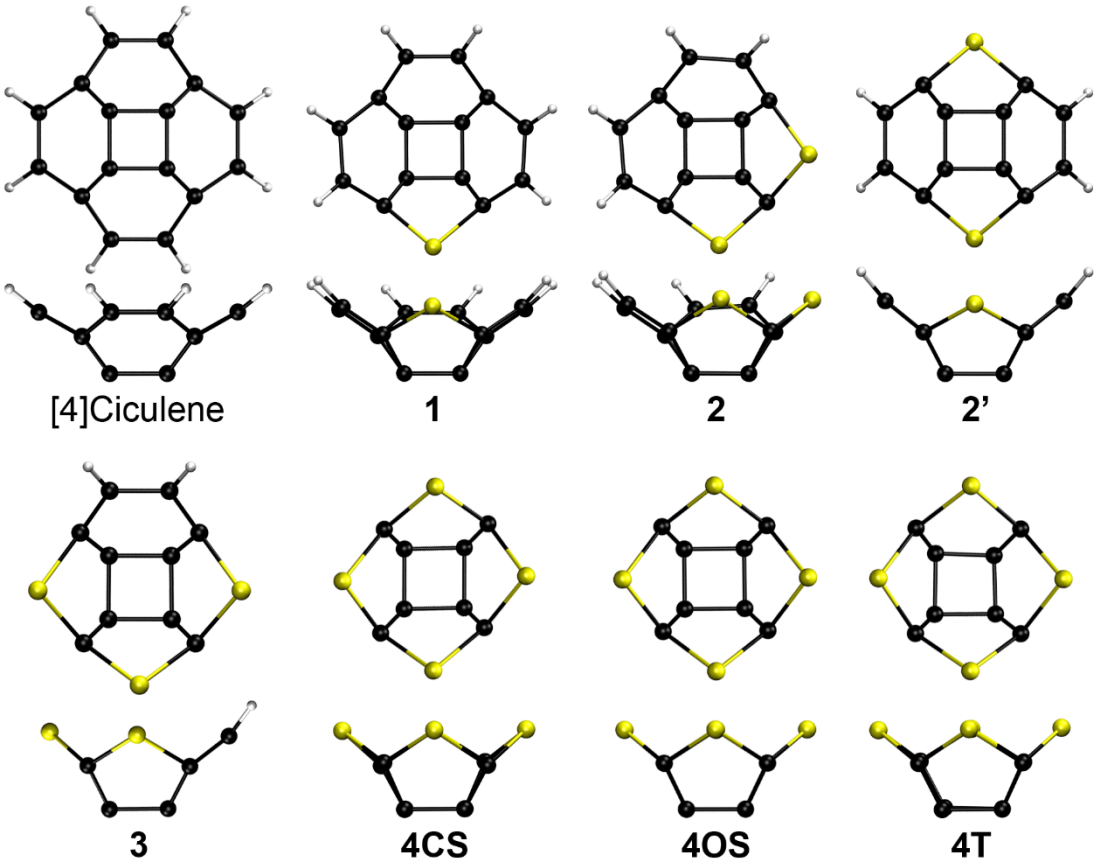

Figure S4. Top and side views of each optimized geometry of [4]circulene, and thia[4]circulenes **1**, **2**, **2'**, **3**, **4CS**, **4OS**, and **4T**.

6. Bond Lengths and WBI Values of Benzene, Thiophene, and [4]Radialene

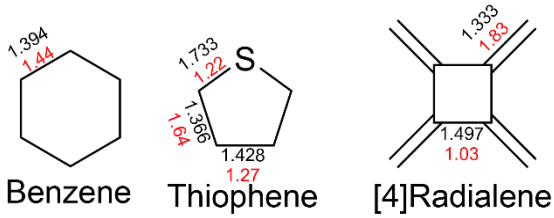

Figure S5. Bond lengths (Å, black) and WBI values (red) of benzene, thiophene, and [4]radialene.

7. Calculated π-Electron Densities and LOL-π

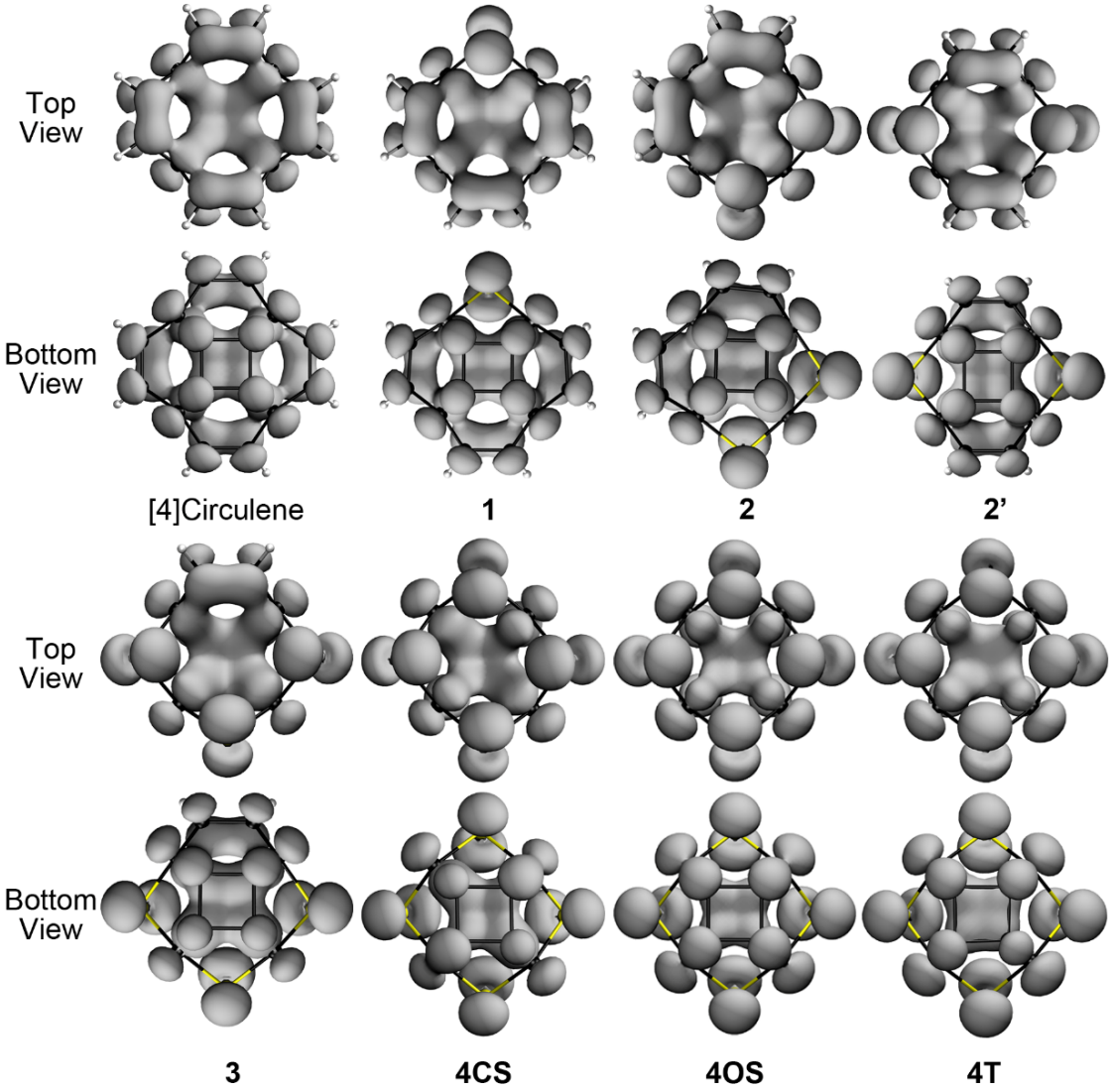

Figure S6. Calculated π-electron density (isosurface value: 0.03 a.u.) of [4]circulene, and thia[4]circulenes **1**, **2**, **2'**, **3**, **4CS**, **4OS**, and **4T**.

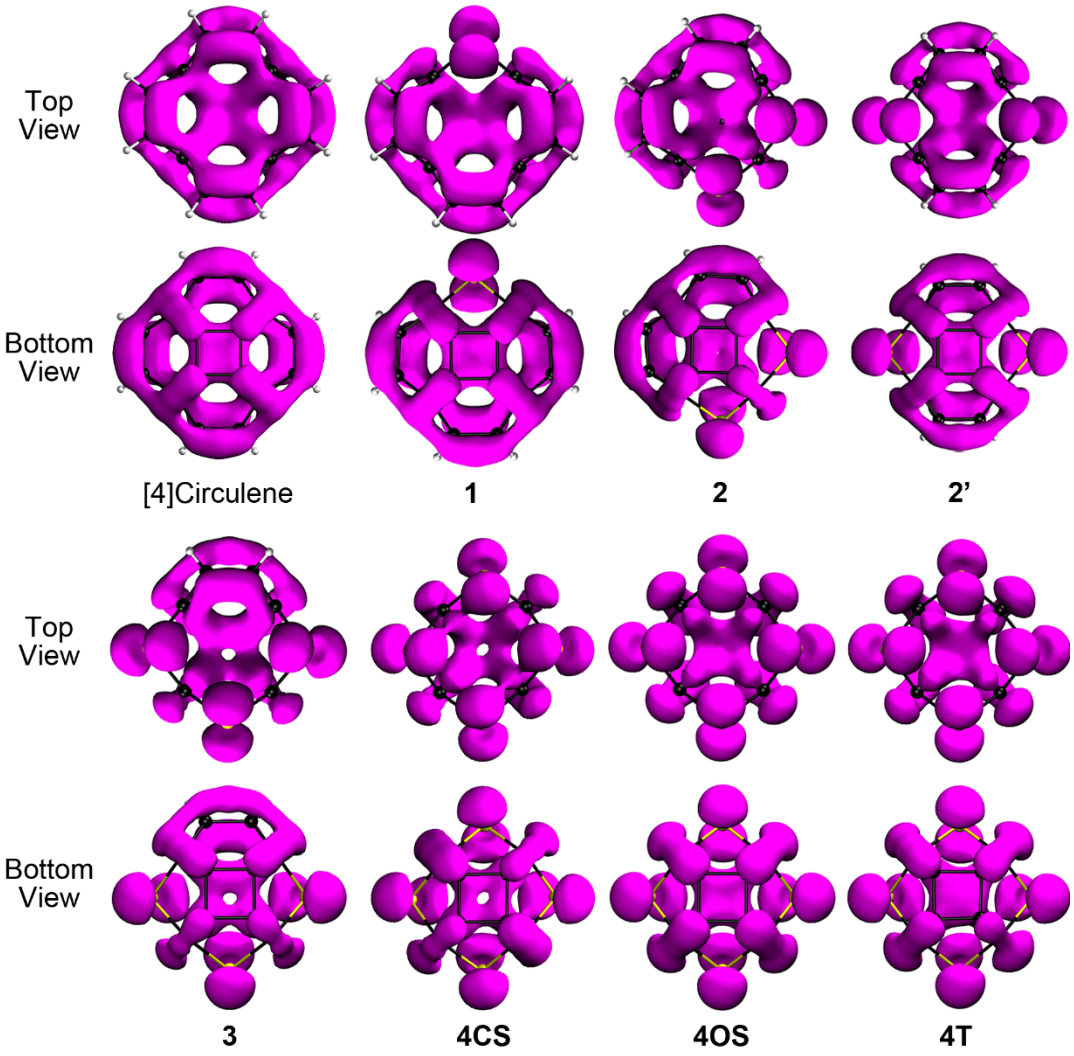

Figure S7. Calculated LOL-π (isosurface value: 0.35 a.u.) of [4]circulene, and thia[4]circulenes **1**, **2**, **2'**, **3**, **4CS**, **4OS**, and **4T**

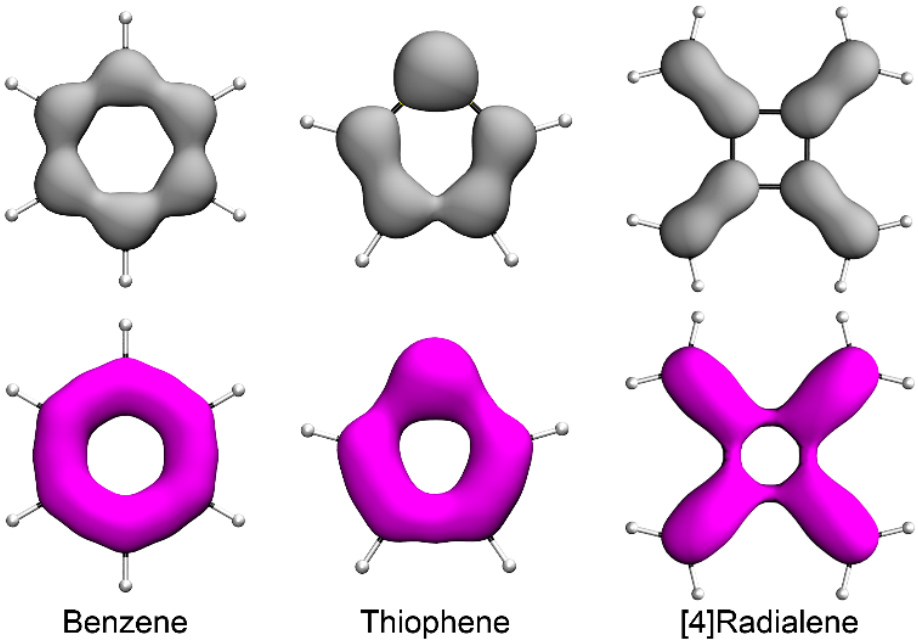

Figure S8. Calculated π-electron densities (top, isosurface value: 0.03 a.u.) and LOL-π (bottom, isosurface value: 0.35 a.u.) of benzene, thiophene, and [4]radialene.

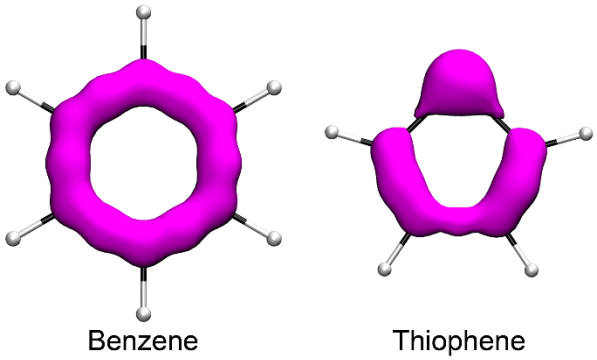

Figure S9. Calculated LOL-π (isosurface value: 0.47 a.u.) for benzene and thiophene. The π-electron density at C–S bond of thiophene is lower than that at C–C bond of benzene.

8. Additional ICSS Analyses

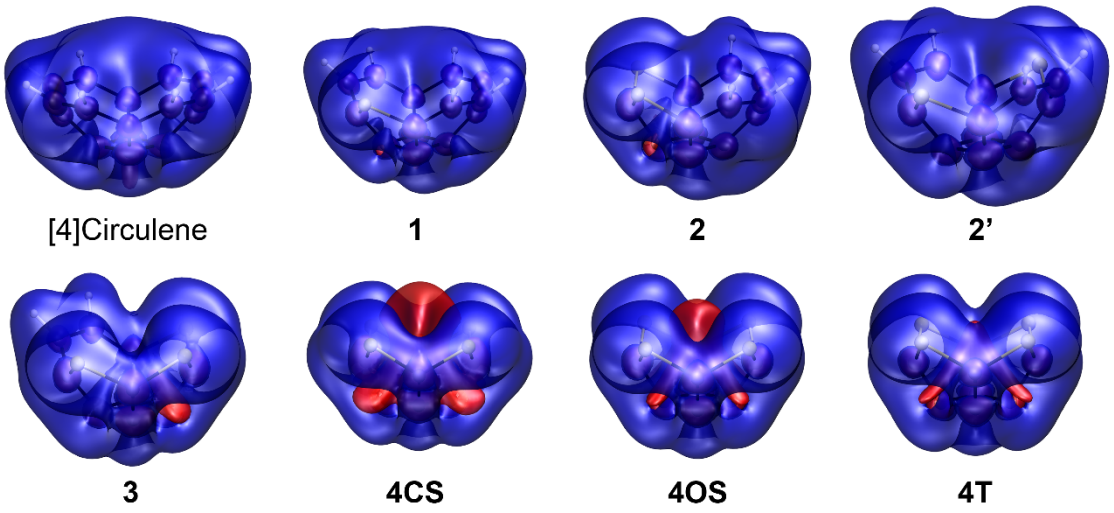

Figure S10. Side views of calculated ICSS maps (isosurface value: ±3 ppm) of [4]circulene and thia[4]circulenes **1**–**4**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

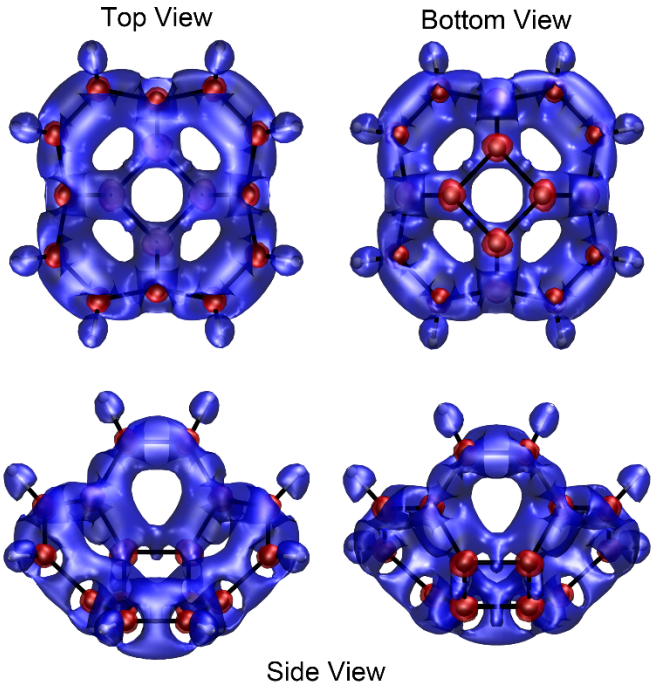

Figure S11. Calculated ICSS maps (isosurface value: ±19 ppm) of [4]circulene. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

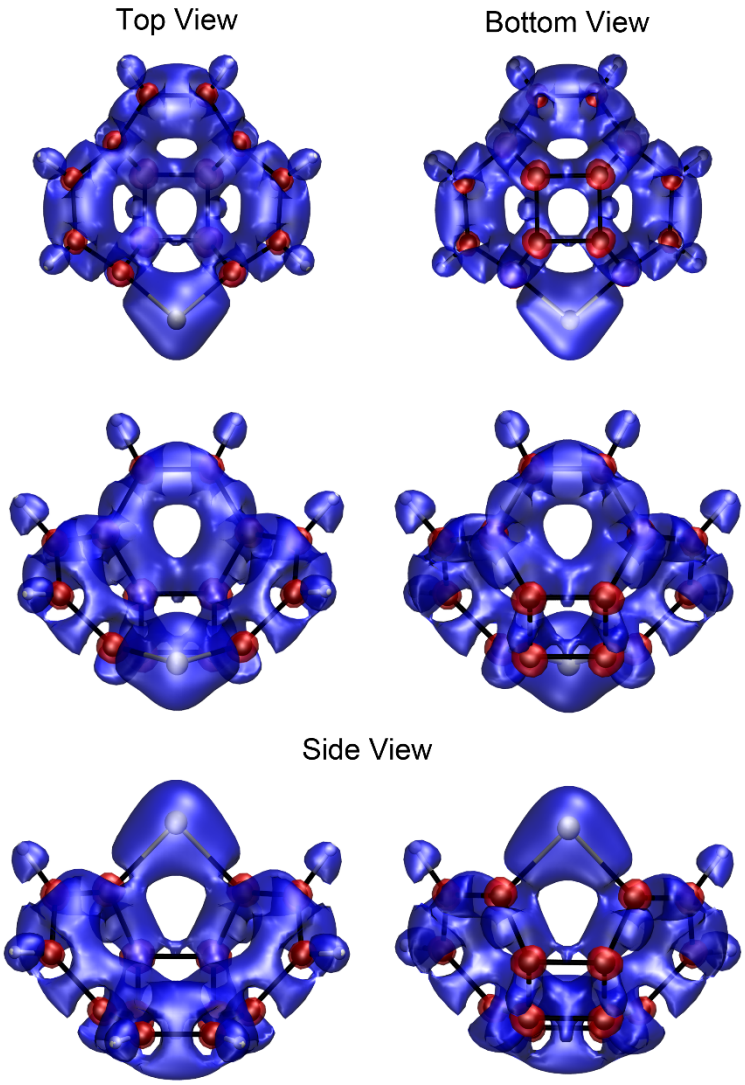

Figure S12. Calculated ICSS maps (isosurface value: ±19 ppm) of **1**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

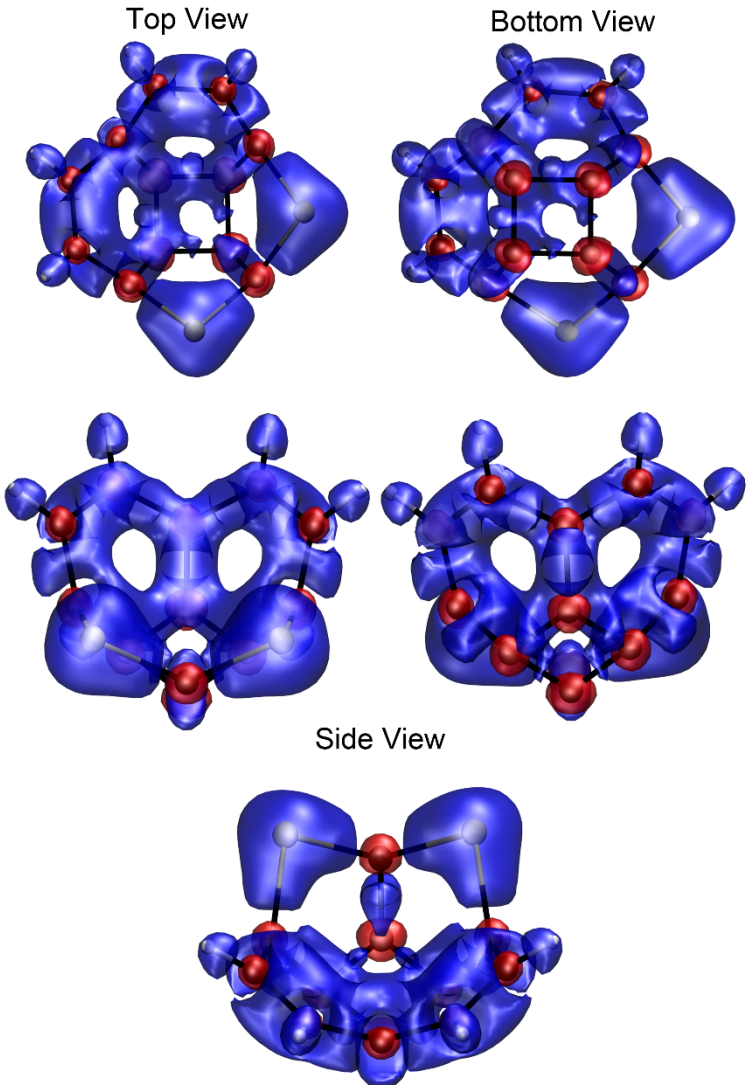

Figure S13. Calculated ICSS maps (isosurface value: ±19 ppm) of **2**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

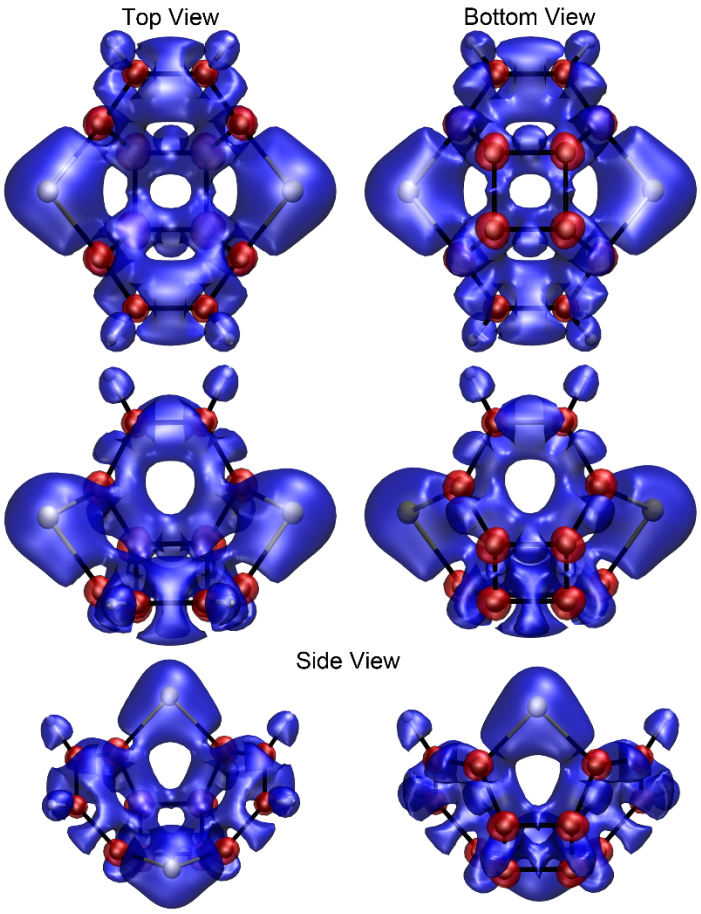

Figure S14. Calculated ICSS maps (isosurface value: ±19 ppm) of **2'**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

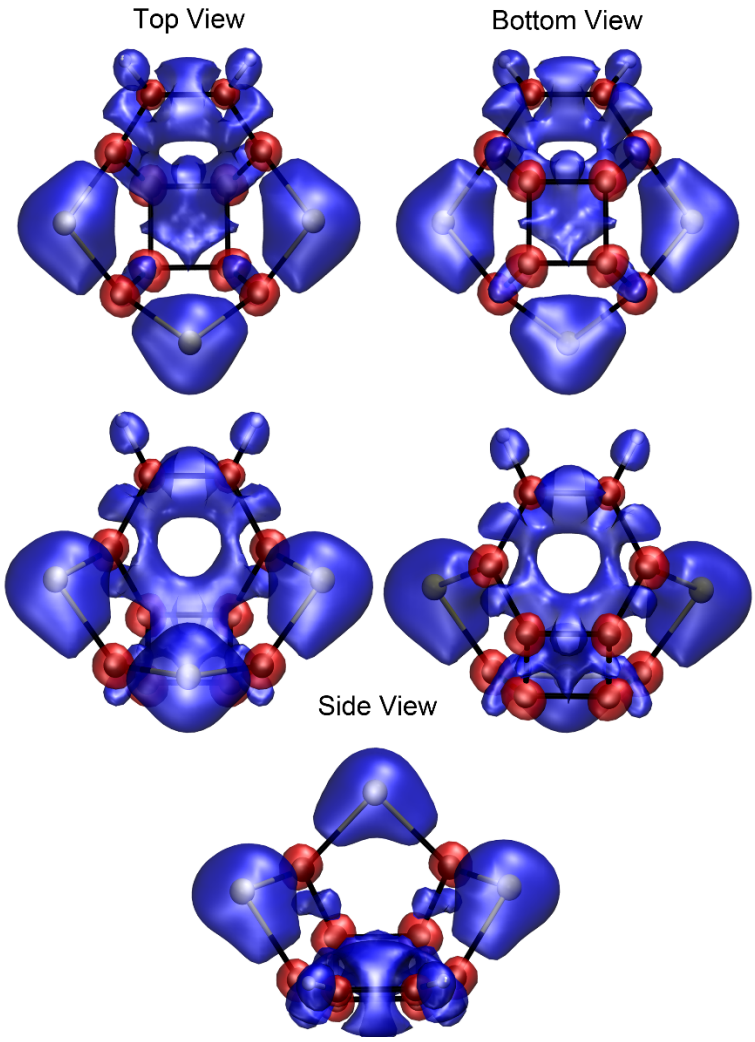

Figure S15. Calculated ICSS maps (isosurface value: ±19 ppm) of **3**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

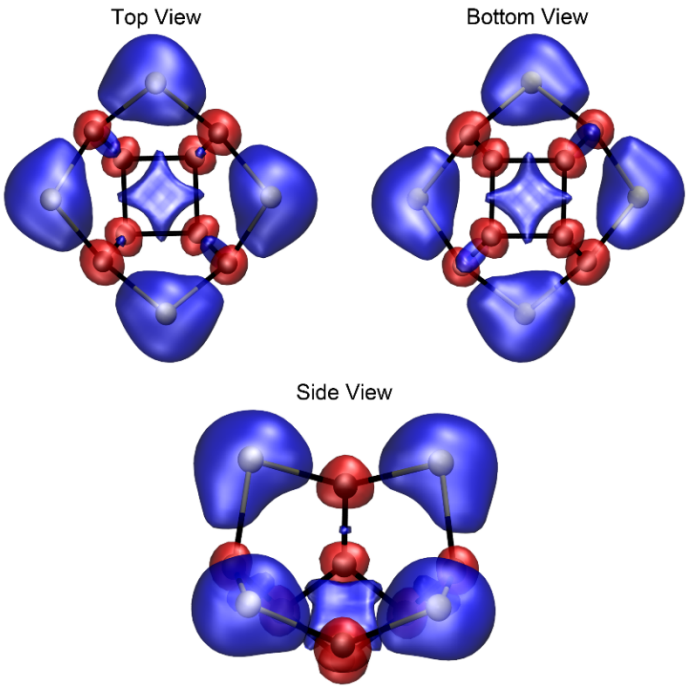

Figure S16. Calculated ICSS maps (isosurface value: ±19 ppm) of **4CS**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

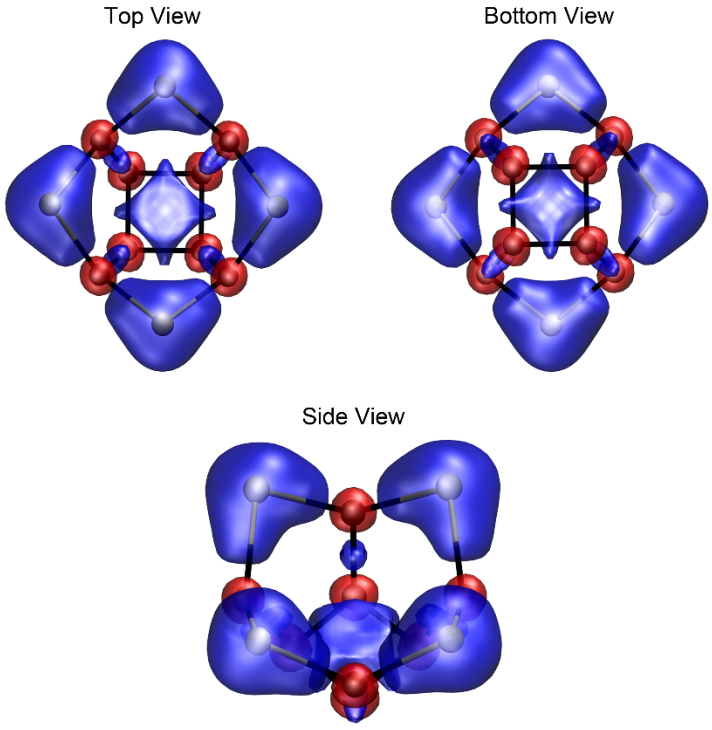

Figure S17. Calculated ICSS maps (isosurface value: ±19 ppm) of **4OS**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

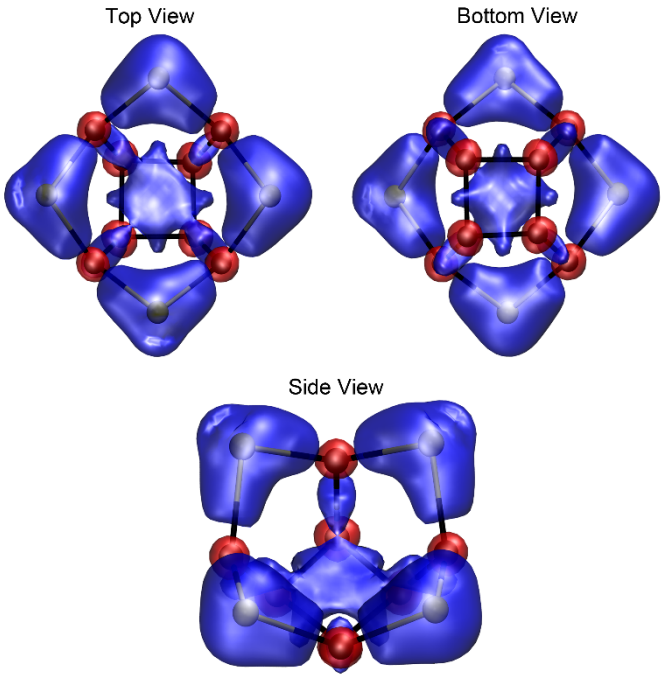

Figure S18. Calculated ICSS maps (isosurface value: ±19 ppm) of **4T**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

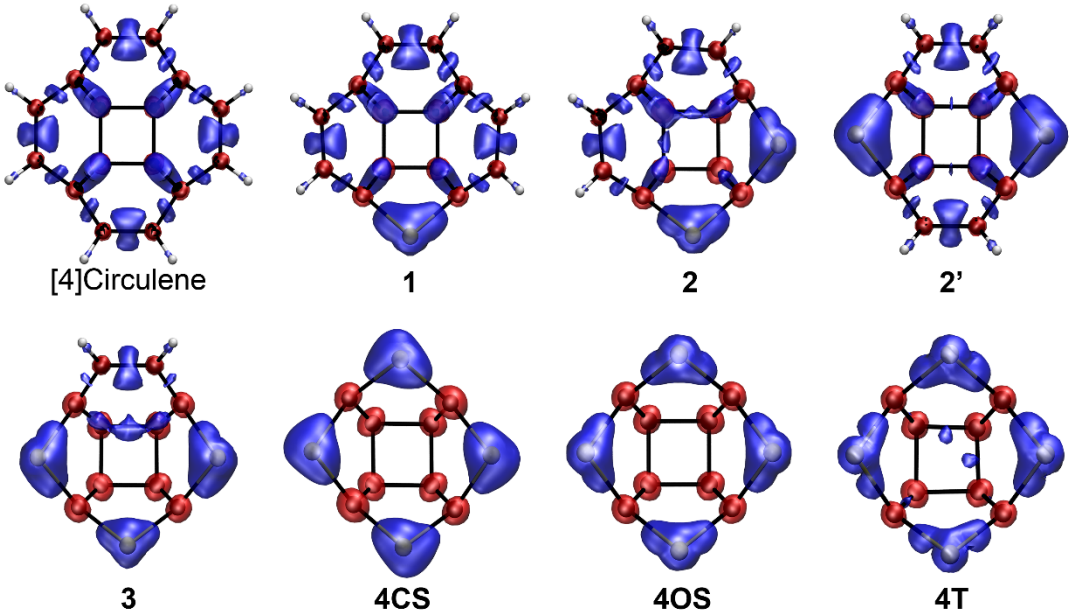

Figure S19. Calculated ICSS maps (isosurface value: ±28 ppm) of [4]circulene and thia[4]circulenes **1**–**4**. Blue and red colored regions correspond to spaces with negative and positive NICS values, respectively.

The ICSS maps (Figures S11–S18) with the isosurface value of ±19 ppm show all carbon atoms are surrounded by red-colored deshielding regions, which is the typical feature of sp^2 hybridized carbon atoms.[38–41] On the other hand, the sulfur atoms in the fused thiophene rings are surrounded by blue-colored shielding region.[42,43] The fused benzene rings are surrounded by thicker shielding regions compared to the thiophene rings, showing weak diatropic character for the latter. In the case of [4]circulene and compounds **1**, **2**, the *rim* bonds of the benzene ring and *spoke* bonds shared by the benzene rings are well-shielded, showing strong bonding interaction (Figures S11–S13). However, the shielding of the *spoke* bond of **2** shared by the thiophene rings is weaker than those shared by the benzene rings (Figure S13). In addition, at the isosurface value of ±28 ppm, the *spoke* bonds in ring E of **3** are covered almost no shielding region, which indicates weak bonding interactions (Figure S19). The shielding region still covers the *hub* bonds in its benzene ring for **3**. In the case of **4CS**, **4OS**, and **4T**, there are the shielding regions at the middle of the *spoke* bonds with the isosurface value of ±19 ppm (Figures S16–18). These regions were not observed with the isosurface value of ±28 ppm (Figure S19). The *spoke* bonds shared by the thiophene rings are weaker than the other *spoke* bonds. In all cases, the bonding interaction of the carbon–sulfur bond is weak. These results are in line with the WBI values in the case of the benzene rings, while not in the thiophene rings.

9. NICS Scans

The NICS scan calculations[44–47] were performed using the Aroma program at GIAO-B3LYP/6-311+G(d,p) level of theory (Figure S20).[48] The BQs were placed at a step size of 0.1 Å.

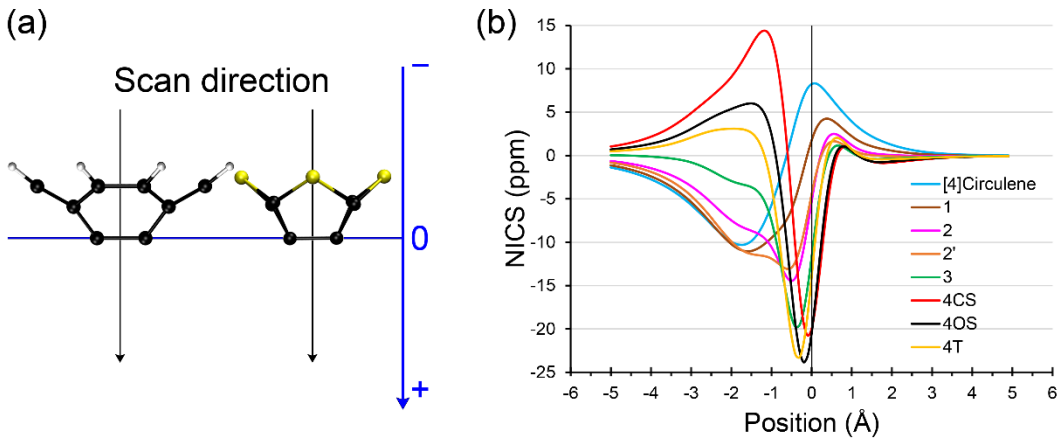

Figure S20. (a) The direction of NICS scan. (b) The results of NICS scan.

10. The Signed Modules of Current Densities

The grid information for the calculations of the signed modulus of the current densities (Figure S21) was obtained by the use of the Multiwfn program.[49] The current densities were visualized using the ParaView (ver. 5.8.1) application.[50]

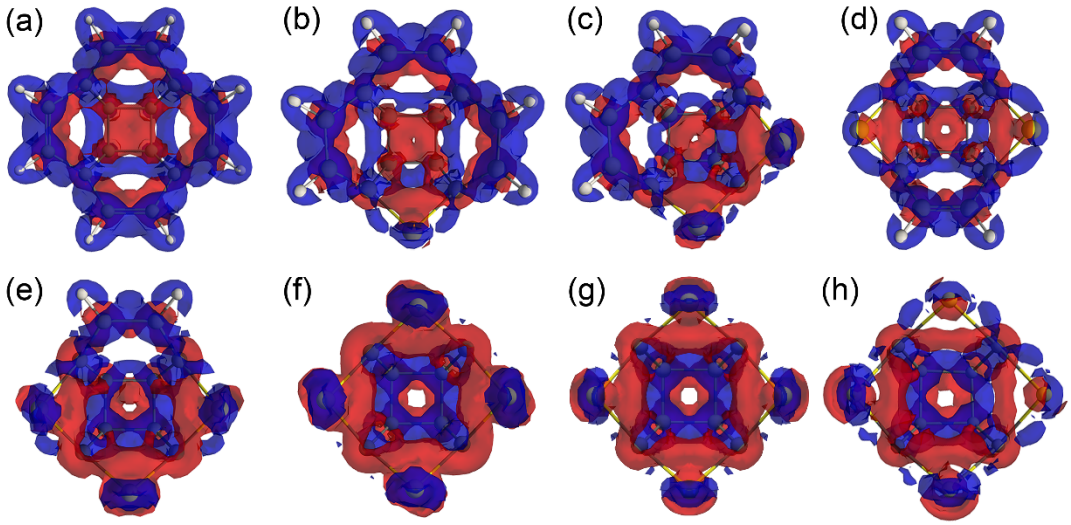

Figure S21. The signed modules of the current densities (isosurface values: 0.05 a.u.; red and blue regions are indicate paratropic and diatropic current densities, respectively) for [4]circulene (a), **1** (b), **2** (c), **.2'** (d), **3** (e), **4CS** (f), **4OS** (g) and **4T** (h).

11. AICD analyses

The anisotropy of the induced current density (AICD) analyses for [4]circulene and thia[4]circulenes were carried out using AICD program (ver 3.0.4).[51,52] The magnetic shielding calculation were performed at the B3LYP/6-311+G(d, p) level of theory employing the continuous set of the gauge transformation (CSGT) method.[53] Calculated AICD isosurfaces with current density vectors were visualized by POV-Ray (ver. 3.7; Figures S22–S29).[54] The clockwise or counter clockwise vector indicate diatropic or paratropic current flow, respectively.

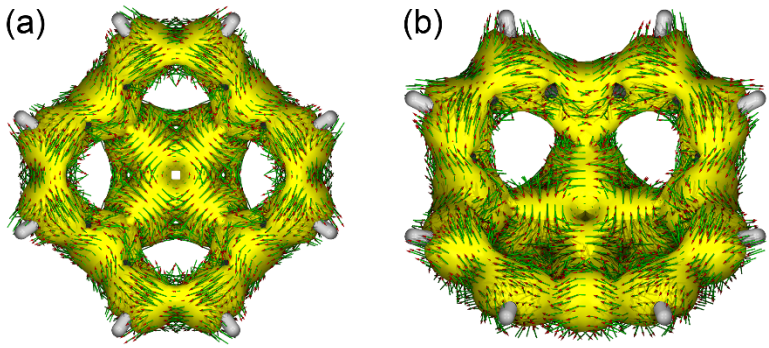

Figure S22. Top view (a) and side view (b) of the calculated AICD plots for [4]circulene (isovalues: 0.055).

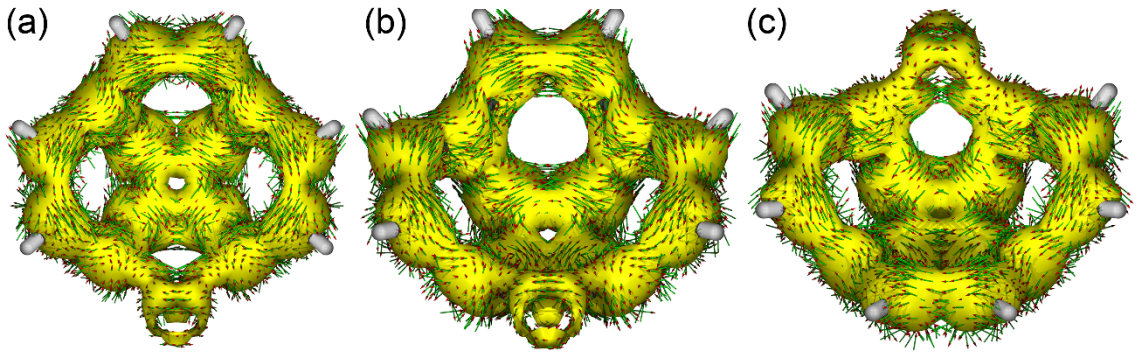

Figure S23. Top view (a) and side views (b, c) of the calculated AICD plots for **1** (isovalues: 0.055).

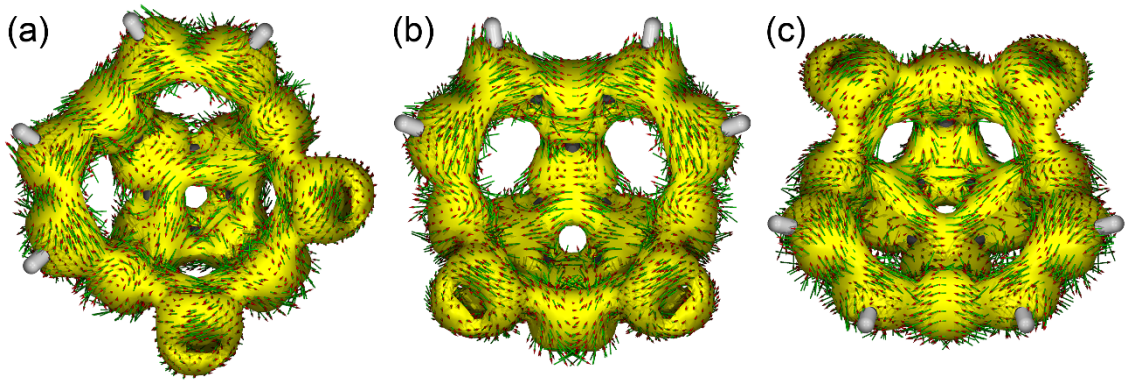

Figure S24. Top view (a) and side views (b, c) of the calculated AICD plots for **2** (isovalues: 0.055).

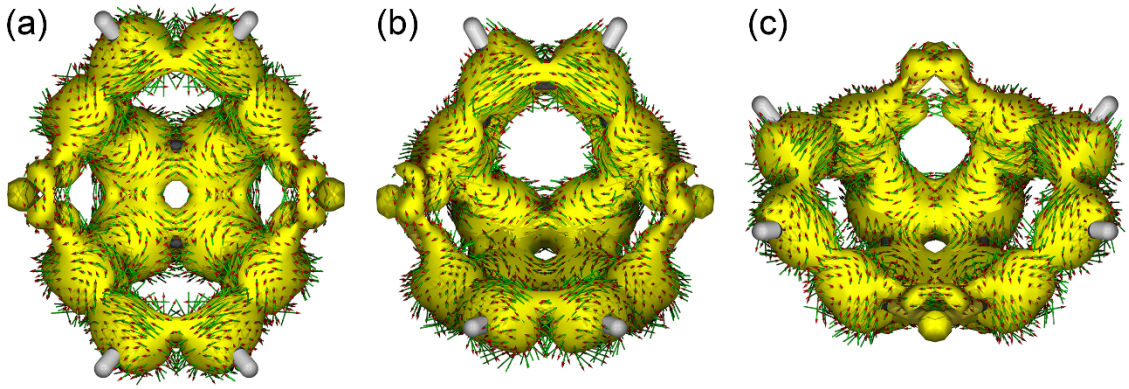

Figure S25. Top view (a) and side views (b, c) of the calculated AICD plots for **2'** (isovalues: 0.055).

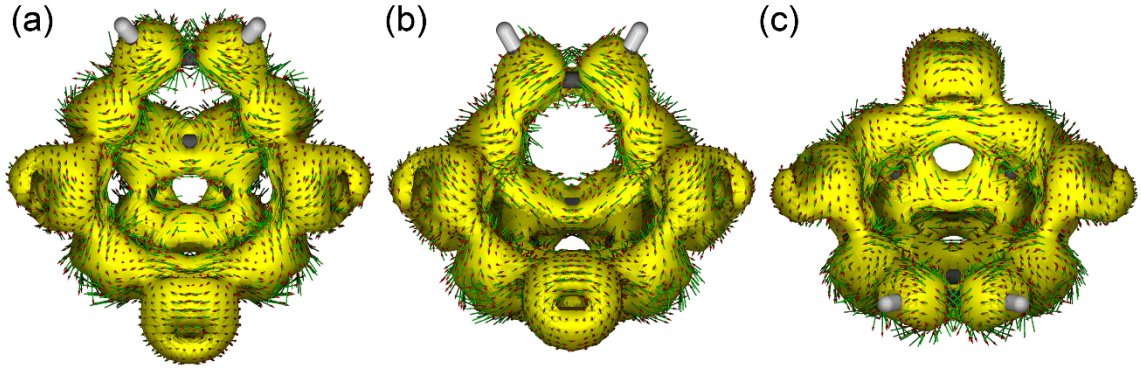

Figure S26. Top view (a) and side views (b, c) of the calculated AICD plots for **3** (isovalues: 0.055).

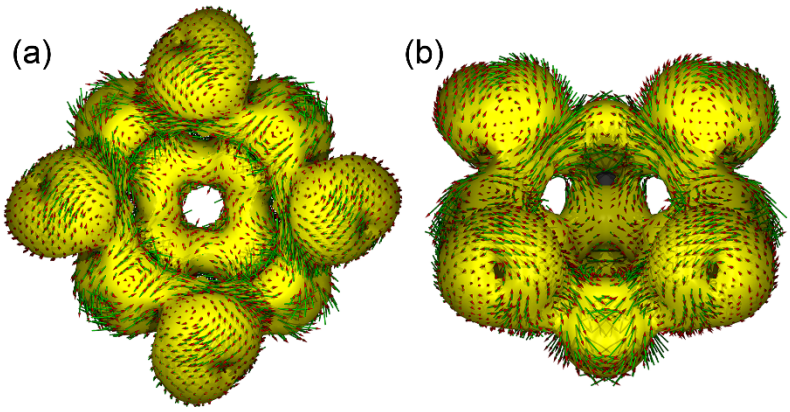

Figure S27. Top view (a) and side view (b) of the calculated AICD plots for **4CS** (isovalues: 0.055).

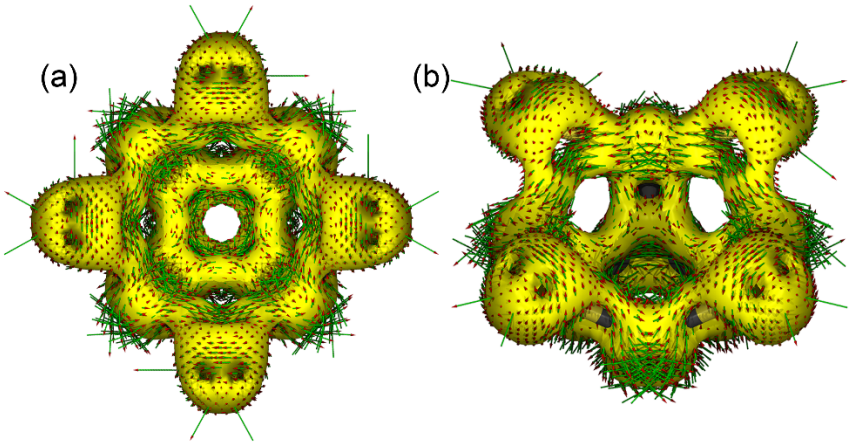

Figure S28. Top view (a) and side view (b) of the calculated AICD plots for **4OS** (isovalues: 0.055).

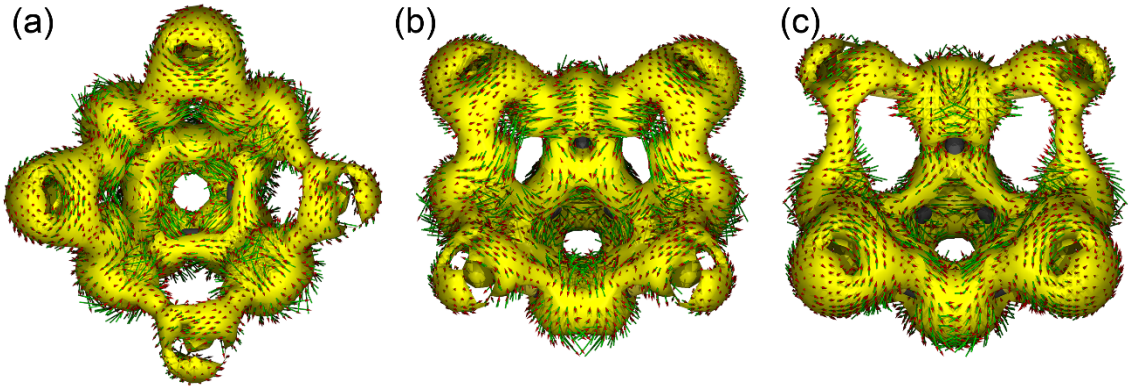

Figure S29. Top view (a) and side views (b, c) of the calculated AICD plots for **4T** (isovalues: 0.055).

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13. Optimized Cartesian Coordinates

[4]Circulene (singlet)

Symbol	X	Y	Z
C	-1.030295	0.000000	1.104475
C	0.000000	1.030295	1.104475
C	0.000000	2.023237	0.158471
C	-1.297831	2.272020	-0.456680
C	-2.272020	1.297831	-0.456680
C	-2.023237	0.000000	0.158471
H	-1.457086	3.167745	-1.048758
H	-3.167745	1.457086	-1.048758
C	1.297831	-2.272020	-0.456680
C	2.272020	-1.297831	-0.456680
C	2.023237	0.000000	0.158471
C	1.030295	0.000000	1.104475
C	0.000000	-1.030295	1.104475
C	0.000000	-2.023237	0.158471
H	1.457086	-3.167745	-1.048758
H	3.167745	-1.457086	-1.048758
C	2.272020	1.297831	-0.456680
H	3.167745	1.457086	-1.048758
C	1.297831	2.272020	-0.456680
H	1.457086	3.167745	-1.048758
C	-1.297831	-2.272020	-0.456680
H	-1.457086	-3.167745	-1.048758
C	-2.272020	-1.297831	-0.456680
H	-3.167745	-1.457086	-1.048758

Zero-point correction= 0.181571 (Hartree/Particle)
Thermal correction to Energy= 0.190819
Thermal correction to Enthalpy= 0.191763
Thermal correction to Gibbs Free Energy= 0.148780
Sum of electronic and zero-point Energies= -614.370113
Sum of electronic and thermal Energies= -614.360864
Sum of electronic and thermal Enthalpies= -614.359920
Sum of electronic and thermal Free Energies= -614.402903

[4]Circulene (triplet)

Symbol	X	Y	Z
C	-0.684314	1.093966	0.731361
C	-0.684314	1.093966	-0.731361
C	-1.418697	0.153086	-1.455223
C	-2.413602	-0.522980	-0.714834
C	-2.413602	-0.522980	0.714834
C	-1.418697	0.153086	1.455223
H	-3.035209	-1.265350	-1.205126
H	-3.035209	-1.265350	1.205126
C	2.394087	-0.552253	0.736288
C	2.394087	-0.552253	-0.736288
C	1.421110	0.145159	-1.457077
C	0.731980	1.157886	-0.760006
C	0.731980	1.157886	0.760006
C	1.421110	0.145159	1.457077
H	2.941598	-1.357679	1.214835
H	2.941598	-1.357679	-1.214835
C	0.677418	-0.375816	-2.620197
H	1.207028	-0.892360	-3.413937
C	-0.689795	-0.367683	-2.625013
H	-1.222536	-0.872801	-3.423706
C	0.677418	-0.375816	2.620197
H	1.207028	-0.892360	3.413937
C	-0.689795	-0.367683	2.625013
H	-1.222536	-0.872801	3.423706

Zero-point correction= 0.176581 (Hartree/Particle)
Thermal correction to Energy= 0.186829
Thermal correction to Enthalpy= 0.187774
Thermal correction to Gibbs Free Energy= 0.140497
Sum of electronic and zero-point Energies= -614.290614
Sum of electronic and thermal Energies= -614.280366
Sum of electronic and thermal Enthalpies= -614.279422
Sum of electronic and thermal Free Energies= -614.326698

1 (singlet)

Symbol	X	Y	Z
C	1.164113	0.803659	0.734330
C	1.164113	0.803659	-0.734330
C	0.169780	1.462151	-1.421846
C	-0.476869	2.539504	-0.688509
C	-0.476869	2.539504	0.688509
C	0.169780	1.462151	1.421846
H	-1.113753	3.246417	-1.210438
H	-1.113753	3.246417	1.210438
C	0.205189	-1.367022	-1.296226
C	1.218277	-0.648346	-0.735613
C	1.218277	-0.648346	0.735613
C	0.205189	-1.367022	1.296226
C	-0.530853	-0.710152	-2.352484
H	-1.207794	-1.261206	-2.995702
C	-0.505684	0.669025	-2.437500
H	-1.157369	1.149855	-3.160116
C	-0.530853	-0.710152	2.352484
H	-1.207794	-1.261206	2.995702
C	-0.505684	0.669025	2.437500
H	-1.157369	1.149855	3.160116
S	-0.498100	-2.453497	0.000000

Zero-point correction= 0.148521 (Hartree/Particle)
Thermal correction to Energy= 0.157567
Thermal correction to Enthalpy= 0.158511
Thermal correction to Gibbs Free Energy= 0.114430
Sum of electronic and zero-point Energies= -935.137588
Sum of electronic and thermal Energies= -935.128542
Sum of electronic and thermal Enthalpies= -935.127598
Sum of electronic and thermal Free Energies= -935.171679

1 (triplet)

Symbol	X	Y	Z
C	-0.805221	-0.710703	1.148386
C	-0.862101	0.724684	1.196137
C	-1.538664	1.377200	0.194753
C	-2.634554	0.616961	-0.402370
C	-2.605935	-0.756573	-0.410554
C	-1.458248	-1.442241	0.169641
H	-3.385132	1.130009	-0.994837
H	-3.336349	-1.301370	-0.999092
C	1.359020	1.314374	0.134267
C	0.657419	0.782164	1.317621
C	0.648636	-0.644599	1.203952
C	1.412286	-1.217778	0.187539
C	0.626581	2.111777	-0.728061
H	1.090617	2.466325	-1.643820
C	-0.777445	2.340785	-0.578732
H	-1.275710	2.969707	-1.307627
C	0.762233	-2.199809	-0.597952
H	1.305441	-2.721457	-1.378103
C	-0.631305	-2.363267	-0.555408
H	-1.080991	-3.026186	-1.287642
S	2.610370	0.055320	-0.379012

Zero-point correction= 0.144722 (Hartree/Particle)
Thermal correction to Energy= 0.154364
Thermal correction to Enthalpy= 0.155308
Thermal correction to Gibbs Free Energy= 0.109111
Sum of electronic and zero-point Energies= -935.070349
Sum of electronic and thermal Energies= -935.060708
Sum of electronic and thermal Enthalpies= -935.059764
Sum of electronic and thermal Free Energies= -935.105961

2 (singlet)

Symbol	X	Y	Z
C	1.255095	0.103436	1.033664
C	1.211882	1.134553	0.000000
C	1.255095	0.103436	-1.033664
C	1.308163	-0.942703	0.000000
C	0.259093	-1.799019	0.000000
S	-0.552520	-1.674977	1.627027
S	-0.552520	-1.674977	-1.627027
C	0.191036	-0.011134	-1.885242
C	-0.550850	1.188672	-2.165574
H	-1.279199	1.228546	-2.967620
C	-0.500493	2.234933	-1.261249
H	-1.183742	3.065737	-1.403934
C	0.199041	2.077139	0.000000
C	-0.500493	2.234933	1.261249
C	0.191036	-0.011134	1.885242
C	-0.550850	1.188672	2.165574
H	-1.279199	1.228546	2.967620
H	-1.183742	3.065737	1.403934

Zero-point correction= 0.115353 (Hartree/Particle)
Thermal correction to Energy= 0.124233
Thermal correction to Enthalpy= 0.125177
Thermal correction to Gibbs Free Energy= 0.081221
Sum of electronic and zero-point Energies= -1255.899590
Sum of electronic and thermal Energies= -1255.890710
Sum of electronic and thermal Enthalpies= -1255.889766
Sum of electronic and thermal Free Energies= -1255.933722

2 (triplet)

Symbol	X	Y	Z
C	-0.116291	-1.037350	1.274378
C	-1.150161	0.000045	1.196376
C	-0.116209	1.037356	1.274378
C	0.902183	-0.000036	1.365526
C	1.834246	-0.000072	0.198846
S	1.677920	-1.639626	-0.553263
S	1.678052	1.639497	-0.553259
C	0.008777	1.905027	0.220843
C	-1.181977	2.160751	-0.551844
H	-1.214722	2.984120	-1.256472
C	-2.228760	1.265067	-0.524688
H	-3.066749	1.417184	-1.197407
C	-2.071463	0.000082	0.170553
C	-2.228863	-1.264892	-0.524686
C	0.008625	-1.905029	0.220843
C	-1.182151	-2.160659	-0.551843
H	-1.214964	-2.984027	-1.256468
H	-3.066865	-1.416943	-1.197404

Zero-point correction= 0.112400 (Hartree/Particle)
Thermal correction to Energy= 0.121887
Thermal correction to Enthalpy= 0.122831
Thermal correction to Gibbs Free Energy= 0.076498
Sum of electronic and zero-point Energies= -1255.856519
Sum of electronic and thermal Energies= -1255.847032
Sum of electronic and thermal Enthalpies= -1255.846088
Sum of electronic and thermal Free Energies= -1255.892421

2’ (singlet)

Symbol	X	Y	Z
C	-0.742290	0.724719	1.261609
C	0.742290	0.724719	1.261609
C	0.742290	-0.724719	1.261609
C	-0.742290	-0.724719	1.261609
C	1.290754	1.403587	0.209196
C	-1.290754	-1.403587	0.209196
S	0.000000	2.486007	-0.504085
S	0.000000	-2.486007	-0.504085
C	1.290754	-1.403587	0.209196
C	2.265635	-0.693730	-0.579715
H	2.878159	-1.205042	-1.313864
C	2.265635	0.693730	-0.579715
H	2.878159	1.205042	-1.313864
C	-1.290754	1.403587	0.209196
C	-2.265635	0.693730	-0.579715
H	-2.878159	1.205042	-1.313864
C	-2.265635	-0.693730	-0.579715
H	-2.878159	-1.205042	-1.313864

Zero-point correction= 0.115309 (Hartree/Particle)
Thermal correction to Energy= 0.124167
Thermal correction to Enthalpy= 0.125112
Thermal correction to Gibbs Free Energy= 0.081874
Sum of electronic and zero-point Energies= -1255.907610
Sum of electronic and thermal Energies= -1255.898751
Sum of electronic and thermal Enthalpies= -1255.897807
Sum of electronic and thermal Free Energies= -1255.941045

2’ (triplet)

Symbol	X	Y	Z
C	-0.809319	-0.714214	1.298405
C	-0.714284	0.747467	1.250791
C	0.736068	0.654912	1.253005
C	0.690430	-0.776865	1.325652
C	-1.362474	1.334406	0.189885
C	1.348484	-1.320541	0.110189
S	-2.540807	0.106487	-0.457393
S	2.635358	-0.115678	-0.385618
C	1.489084	1.203295	0.207723
C	0.804971	2.115846	-0.640720
H	1.338906	2.612526	-1.443399
C	-0.590125	2.214741	-0.636580
H	-1.062955	2.787268	-1.426443
C	-1.518445	-1.239675	0.270504
C	-0.849386	-2.183638	-0.620191
H	-1.408986	-2.762945	-1.343835
C	0.546261	-2.045187	-0.777019
H	0.992635	-2.433075	-1.688016

Zero-point correction= 0.111214 (Hartree/Particle)
Thermal correction to Energy= 0.120857
Thermal correction to Enthalpy= 0.121801
Thermal correction to Gibbs Free Energy= 0.075318
Sum of electronic and zero-point Energies= -1255.842829
Sum of electronic and thermal Energies= -1255.833187
Sum of electronic and thermal Enthalpies= -1255.832242
Sum of electronic and thermal Free Energies= -1255.878725

3 (singlet)

Symbol	X	Y	Z
C	0.683001	1.330771	0.740278
C	-0.796567	1.295403	0.726360
C	-0.796567	1.295403	-0.726360
C	0.683001	1.330771	-0.740278
C	-1.334456	0.218920	1.390024
C	1.246416	0.235049	1.305569
C	1.246416	0.235049	-1.305569
S	2.220370	-0.606027	0.000000
S	0.012648	-0.558700	2.375244
S	0.012648	-0.558700	-2.375244
C	-1.334456	0.218920	-1.390024
C	-2.313213	-0.559187	-0.697318
H	-2.876410	-1.338316	-1.198504
C	-2.313213	-0.559187	0.697318
H	-2.876410	-1.338316	1.198504

Zero-point correction= 0.082054 (Hartree/Particle)
Thermal correction to Energy= 0.090807
Thermal correction to Enthalpy= 0.091751
Thermal correction to Gibbs Free Energy= 0.047831
Sum of electronic and zero-point Energies= -1576.661800
Sum of electronic and thermal Energies= -1576.653047
Sum of electronic and thermal Enthalpies= -1576.652103
Sum of electronic and thermal Free Energies= -1576.696022

3 (triplet)

Symbol	X	Y	Z
C	-0.791587	-0.602312	1.378731
C	-0.711412	0.894312	1.288999
C	0.756575	0.817043	1.309540
C	0.616655	-0.644685	1.343228
C	-1.316388	1.415170	0.187033
C	-1.399321	-1.198364	0.256388
C	1.207622	-1.321610	0.198657
S	-0.106914	-2.266240	-0.577043
S	-2.319518	0.084236	-0.591853
S	2.363627	-0.160200	-0.535111
C	1.463495	1.269007	0.229733
C	0.823280	2.277705	-0.598519
H	1.401471	2.877876	-1.292227
C	-0.543336	2.356308	-0.614561
H	-1.030083	3.021931	-1.319028

Zero-point correction= 0.079223 (Hartree/Particle)
Thermal correction to Energy= 0.088554
Thermal correction to Enthalpy= 0.089498
Thermal correction to Gibbs Free Energy= 0.043346
Sum of electronic and zero-point Energies= -1576.636697
Sum of electronic and thermal Energies= -1576.627366
Sum of electronic and thermal Enthalpies= -1576.626422
Sum of electronic and thermal Free Energies= -1576.672575

4 (singlet, B3LYP-D3BJ)

Symbol	X	Y	Z
C	0.000000	1.063408	1.355187
C	-1.039571	0.000000	1.357570
C	0.000000	-1.063408	1.355187
C	1.039571	0.000000	1.357570
C	0.000000	-1.899676	0.279297
C	-1.739902	0.000000	0.196188
C	0.000000	1.899676	0.279297
C	1.739902	0.000000	0.196188
S	1.580537	1.641981	-0.597795
S	-1.580537	1.641981	-0.597795
S	-1.580537	-1.641981	-0.597795
S	1.580537	-1.641981	-0.597795

Zero-point correction= 0.048286 (Hartree/Particle)
Thermal correction to Energy= 0.057193
Thermal correction to Enthalpy= 0.058137
Thermal correction to Gibbs Free Energy= 0.014045
Sum of electronic and zero-point Energies= -1897.411921
Sum of electronic and thermal Energies= -1897.403015
Sum of electronic and thermal Enthalpies= -1897.402071
Sum of electronic and thermal Free Energies= -1897.446163

4 (triplet, B3LYP-D3BJ)

Symbol	X	Y	Z
C	-1.719771	0.426624	0.000000
C	-0.876923	1.078248	1.043270
C	-0.075760	1.651198	0.000000
C	-0.876923	1.078248	-1.043270
C	1.307297	1.254541	0.000000
C	-0.147859	0.182501	1.824795
C	-1.601957	-0.936352	0.000000
C	-0.147859	0.182501	-1.824795
S	-0.876923	-1.454828	-1.602193
S	-0.876923	-1.454828	1.602193
S	1.653127	0.532795	1.610765
S	1.653127	0.532795	-1.610765

Zero-point correction= 0.045996 (Hartree/Particle)
Thermal correction to Energy= 0.055086
Thermal correction to Enthalpy= 0.056030
Thermal correction to Gibbs Free Energy= 0.010048
Sum of electronic and zero-point Energies= -1897.418523
Sum of electronic and thermal Energies= -1897.409433
Sum of electronic and thermal Enthalpies= -1897.408489
Sum of electronic and thermal Free Energies= -1897.454471

4 (open-shell singlet, B3LYP-D3BJ)

Symbol	X	Y	Z
S	-1.609647	1.609647	-0.603290
S	-1.609647	-1.609647	-0.603290
S	1.609647	-1.609647	-0.603290
S	1.609647	1.609647	-0.603290
C	-1.040406	0.000000	1.377936
C	0.000000	-1.040406	1.377936
C	1.040406	0.000000	1.377936
C	0.000000	1.040406	1.377936
C	1.818859	0.000000	0.230838
C	0.000000	-1.818859	0.230838
C	-1.818859	0.000000	0.230838
C	0.000000	1.818859	0.230838

Zero-point correction= 0.046043 (Hartree/Particle)
Thermal correction to Energy= 0.054929
Thermal correction to Enthalpy= 0.055873
Thermal correction to Gibbs Free Energy= 0.012128
Sum of electronic and zero-point Energies= -1897.422240
Sum of electronic and thermal Energies= -1897.413354
Sum of electronic and thermal Enthalpies= -1897.412409
Sum of electronic and thermal Free Energies= -1897.456155

4 (singlet, BLYP-D3BJ)

Symbol	X	Y	Z
C	0.000000	1.078959	1.376526
C	-1.035093	0.000000	1.368363
C	0.000000	-1.078959	1.376526
C	1.035093	0.000000	1.368363
C	0.000000	-1.952225	0.297516
C	-1.714551	0.000000	0.173935
C	0.000000	1.952225	0.297516
C	1.714551	0.000000	0.173935
S	1.582511	1.684691	-0.603064
S	-1.582511	1.684691	-0.603064
S	-1.582511	-1.684691	-0.603064
S	1.582511	-1.684691	-0.603064

Zero-point correction= 0.044858 (Hartree/Particle)
Thermal correction to Energy= 0.054327
Thermal correction to Enthalpy= 0.055271
Thermal correction to Gibbs Free Energy= 0.010106
Sum of electronic and zero-point Energies= -1897.298368
Sum of electronic and thermal Energies= -1897.288899
Sum of electronic and thermal Enthalpies= -1897.287955
Sum of electronic and thermal Free Energies= -1897.333121

4 (triplet, BLYP-D3BJ)

Symbol	X	Y	Z
C	-1.734373	0.433443	0.000000
C	-0.884642	1.084988	1.051672
C	-0.069048	1.673612	0.000000
C	-0.884642	1.084988	-1.051672
C	1.309174	1.262381	0.000000
C	-0.157405	0.183256	1.845502
C	-1.625791	-0.946422	0.000000
C	-0.157405	0.183256	-1.845502
S	-0.884642	-1.472020	-1.623944
S	-0.884642	-1.472020	1.623944
S	1.672917	0.542114	1.626299
S	1.672917	0.542114	-1.626299

Zero-point correction= 0.043176 (Hartree/Particle)
Thermal correction to Energy= 0.052920
Thermal correction to Enthalpy= 0.053864
Thermal correction to Gibbs Free Energy= 0.006644
Sum of electronic and zero-point Energies= -1897.304058
Sum of electronic and thermal Energies= -1897.294314
Sum of electronic and thermal Enthalpies= -1897.293370
Sum of electronic and thermal Free Energies= -1897.340590

4 (open-shell singlet, BLYP-D3BJ)

Symbol	X	Y	Z
C	0.000000	1.078959	1.376526
C	-1.035093	0.000000	1.368363
C	0.000000	-1.078959	1.376526
C	1.035093	0.000000	1.368363
C	0.000000	-1.952225	0.297516
C	-1.714551	0.000000	0.173935
C	0.000000	1.952225	0.297516
C	1.714551	0.000000	0.173935
S	1.582511	1.684691	-0.603064
S	-1.582511	1.684691	-0.603064
S	-1.582511	-1.684691	-0.603064
S	1.582511	-1.684691	-0.603064

Zero-point correction= 0.044858 (Hartree/Particle)
Thermal correction to Energy= 0.054327
Thermal correction to Enthalpy= 0.055271
Thermal correction to Gibbs Free Energy= 0.010106
Sum of electronic and zero-point Energies= -1897.298368
Sum of electronic and thermal Energies= -1897.288899
Sum of electronic and thermal Enthalpies= -1897.287955
Sum of electronic and thermal Free Energies= -1897.333121

4 (singlet, M06)

Symbol	X	Y	Z
C	0.000000	1.057232	1.343435
C	-1.028216	0.000000	1.358105
C	0.000000	-1.057232	1.343435
C	1.028216	0.000000	1.358105
C	0.000000	-1.930855	0.293848
C	-1.682782	0.000000	0.168921
C	0.000000	1.930855	0.293848
C	1.682782	0.000000	0.168921
S	1.560649	1.650941	-0.593308
S	-1.560649	1.650941	-0.593308
S	-1.560649	-1.650941	-0.593308
S	1.560649	-1.650941	-0.593308

Zero-point correction= 0.048324 (Hartree/Particle)
Thermal correction to Energy= 0.057180
Thermal correction to Enthalpy= 0.058124
Thermal correction to Gibbs Free Energy= 0.014249
Sum of electronic and zero-point Energies= -1897.027263
Sum of electronic and thermal Energies= -1897.018407
Sum of electronic and thermal Enthalpies= -1897.017463
Sum of electronic and thermal Free Energies= -1897.061338

4 (triplet, M06)

Symbol	X	Y	Z
C	-1.709798	0.427905	0.000000
C	-0.874739	1.076173	1.040764
C	-0.075384	1.635373	0.000000
C	-0.874739	1.076173	-1.040764
C	1.304151	1.238511	0.000000
C	-0.145303	0.181791	1.813837
C	-1.598816	-0.930016	0.000000
C	-0.145303	0.181791	-1.813837
S	-0.874739	-1.445011	-1.593394
S	-0.874739	-1.445011	1.593394
S	1.647226	0.528567	1.605629
S	1.647226	0.528567	-1.605629

Zero-point correction= 0.046792 (Hartree/Particle)
Thermal correction to Energy= 0.055754
Thermal correction to Enthalpy= 0.056698
Thermal correction to Gibbs Free Energy= 0.011052
Sum of electronic and zero-point Energies= -1897.032462
Sum of electronic and thermal Energies= -1897.023500
Sum of electronic and thermal Enthalpies= -1897.022556
Sum of electronic and thermal Free Energies= -1897.068202

4 (open-shell singlet, M06)

Symbol	X	Y	Z
S	-1.602933	-1.602933	-0.600329
S	1.602933	-1.602933	-0.600329
S	1.602933	1.602933	-0.600329
S	-1.602933	1.602933	-0.600329
C	0.000000	-1.034582	1.372891
C	1.034582	0.000000	1.372891
C	0.000000	1.034582	1.372891
C	-1.034582	0.000000	1.372891
C	0.000000	1.808180	0.227987
C	1.808180	0.000000	0.227987
C	0.000000	-1.808180	0.227987
C	-1.808180	0.000000	0.227987

Zero-point correction= 0.046622 (Hartree/Particle)
Thermal correction to Energy= 0.055464
Thermal correction to Enthalpy= 0.056408
Thermal correction to Gibbs Free Energy= 0.013378
Sum of electronic and zero-point Energies= -1897.036500
Sum of electronic and thermal Energies= -1897.027659
Sum of electronic and thermal Enthalpies= -1897.026715
Sum of electronic and thermal Free Energies= -1897.069745

4 (singlet, BHandHLYP)

Symbol	X	Y	Z
C	0.000000	1.052553	1.332260
C	-1.039447	0.000000	1.343646
C	0.000000	-1.052553	1.332260
C	1.039447	0.000000	1.343646
C	0.000000	-1.874086	0.268431
C	-1.737981	0.000000	0.199130
C	0.000000	1.874086	0.268431
C	1.737981	0.000000	0.199130
S	1.578498	1.626604	-0.589400
S	-1.578498	1.626604	-0.589400
S	-1.578498	-1.626604	-0.589400
S	1.578498	-1.626604	-0.589400

Zero-point correction= 0.051447 (Hartree/Particle)
Thermal correction to Energy= 0.059902
Thermal correction to Enthalpy= 0.060846
Thermal correction to Gibbs Free Energy= 0.017595
Sum of electronic and zero-point Energies= -1897.071366
Sum of electronic and thermal Energies= -1897.062911
Sum of electronic and thermal Enthalpies= -1897.061967
Sum of electronic and thermal Free Energies= -1897.105217

4 (triplet, BHandHLYP)

Symbol	X	Y	Z
C	-1.709792	0.413075	0.000000
C	-0.872037	1.069557	1.035570
C	-0.088815	1.629794	0.000000
C	-0.872037	1.069557	-1.035570
C	1.311061	1.263629	0.000000
C	-0.138365	0.181320	1.815354
C	-1.574602	-0.933488	0.000000
C	-0.138365	0.181320	-1.815354
S	-0.872037	-1.445561	-1.590747
S	-0.872037	-1.445561	1.590747
S	1.637590	0.531543	1.602646
S	1.637590	0.531543	-1.602646

Zero-point correction= 0.048983 (Hartree/Particle)
Thermal correction to Energy= 0.057401
Thermal correction to Enthalpy= 0.058346
Thermal correction to Gibbs Free Energy= 0.013746
Sum of electronic and zero-point Energies= -1897.084033
Sum of electronic and thermal Energies= -1897.075615
Sum of electronic and thermal Enthalpies= -1897.074671
Sum of electronic and thermal Free Energies= -1897.119270

4 (open-shell singlet, BHandHLYP)

Symbol	X	Y	Z
S	-1.599767	-1.599767	-0.597992
S	1.599767	-1.599767	-0.597992
S	1.599767	1.599767	-0.597992
S	-1.599767	1.599767	-0.597992
C	0.000000	-1.031884	1.371845
C	1.031884	0.000000	1.371845
C	0.000000	1.031884	1.371845
C	-1.031884	0.000000	1.371845
C	0.000000	1.808786	0.222800
C	1.808786	0.000000	0.222800
C	0.000000	-1.808786	0.222800
C	-1.808786	0.000000	0.222800

Zero-point correction= 0.049075 (Hartree/Particle)
Thermal correction to Energy= 0.057341
Thermal correction to Enthalpy= 0.058285
Thermal correction to Gibbs Free Energy= 0.016307
Sum of electronic and zero-point Energies= -1897.096812
Sum of electronic and thermal Energies= -1897.088547
Sum of electronic and thermal Enthalpies= -1897.087602
Sum of electronic and thermal Free Energies= -1897.129580

4 (singlet, CAM-B3LYP)

Symbol	X	Y	Z
C	0.000000	1.050382	1.344872
C	-1.050382	0.000000	1.344872
C	0.000000	-1.050382	1.344872
C	1.050382	0.000000	1.344872
C	0.000000	-1.812587	0.236314
C	-1.812586	0.000000	0.236313
C	0.000000	1.812587	0.236314
C	1.812586	0.000000	0.236313
S	1.604268	1.604269	-0.592945
S	-1.604268	1.604269	-0.592945
S	-1.604268	-1.604269	-0.592945
S	1.604268	-1.604269	-0.592945

Zero-point correction= 0.050569 (Hartree/Particle)
Thermal correction to Energy= 0.059197
Thermal correction to Enthalpy= 0.060141
Thermal correction to Gibbs Free Energy= 0.016349
Sum of electronic and zero-point Energies= -1897.160563
Sum of electronic and thermal Energies= -1897.151935
Sum of electronic and thermal Enthalpies= -1897.150991
Sum of electronic and thermal Free Energies= -1897.194783

4 (triplet, CAM-B3LYP)

Symbol	X	Y	Z
C	-1.713258	0.415127	0.000000
C	-0.874409	1.073359	1.040501
C	-0.085193	1.634501	0.000000
C	-0.874409	1.073359	-1.040501
C	1.312600	1.252224	0.000000
C	-0.141802	0.181664	1.814437
C	-1.584665	-0.933339	0.000000
C	-0.141802	0.181664	-1.814437
S	-0.874409	-1.446288	-1.594151
S	-0.874409	-1.446288	1.594151
S	1.643710	0.531558	1.603655
S	1.643710	0.531558	-1.603655

Zero-point correction= 0.048121 (Hartree/Particle)
Thermal correction to Energy= 0.056744
Thermal correction to Enthalpy= 0.057688
Thermal correction to Gibbs Free Energy= 0.012665
Sum of electronic and zero-point Energies= -1897.164018
Sum of electronic and thermal Energies= -1897.155395
Sum of electronic and thermal Enthalpies= -1897.154451
Sum of electronic and thermal Free Energies= -1897.199473

4 (open-shell singlet, CAM-B3LYP)

Symbol	X	Y	Z
S	-1.602986	-1.602986	-0.598385
S	1.602986	-1.602986	-0.598385
S	1.602986	1.602986	-0.598385
S	-1.602986	1.602986	-0.598385
C	0.000000	-1.037220	1.369186
C	1.037220	0.000000	1.369186
C	0.000000	1.037220	1.369186
C	-1.037220	0.000000	1.369186
C	0.000000	1.809911	0.226508
C	1.809911	0.000000	0.226508
C	0.000000	-1.809911	0.226508
C	-1.809911	0.000000	0.226508

Zero-point correction= 0.048029 (Hartree/Particle)
Thermal correction to Energy= 0.056491
Thermal correction to Enthalpy= 0.057435
Thermal correction to Gibbs Free Energy= 0.015108
Sum of electronic and zero-point Energies= -1897.173354
Sum of electronic and thermal Energies= -1897.164892
Sum of electronic and thermal Enthalpies= -1897.163947
Sum of electronic and thermal Free Energies= -1897.206275

4 (singlet, ωB97-XD)

Symbol	X	Y	Z
C	-0.743127	0.743127	1.347291
C	-0.743127	-0.743127	1.347291
C	0.743127	-0.743127	1.347291
C	0.743127	0.743127	1.347291
C	1.281701	-1.281701	0.234089
C	-1.281701	-1.281701	0.234089
C	-1.281701	1.281701	0.234089
C	1.281701	1.281701	0.234089
S	0.000000	2.267969	-0.593017
S	-2.267967	0.000000	-0.593018
S	0.000000	-2.267969	-0.593017
S	2.267967	0.000000	-0.593018

Zero-point correction= 0.050202 (Hartree/Particle)
Thermal correction to Energy= 0.058978
Thermal correction to Enthalpy= 0.059922
Thermal correction to Gibbs Free Energy= 0.015242
Sum of electronic and zero-point Energies= -1897.169052
Sum of electronic and thermal Energies= -1897.160277
Sum of electronic and thermal Enthalpies= -1897.159332
Sum of electronic and thermal Free Energies= -1897.204012

4 (triplet, ωB97-XD)

Symbol	X	Y	Z
C	-1.715140	0.418461	0.000000
C	-0.875458	1.075797	1.041970
C	-0.083401	1.636581	0.000000
C	-0.875458	1.075797	-1.041970
C	1.313606	1.249672	0.000000
C	-0.140222	0.179887	1.812676
C	-1.584601	-0.933525	0.000000
C	-0.140222	0.179887	-1.812676
S	-0.875458	-1.445266	-1.593783
S	-0.875458	-1.445266	1.593783
S	1.644376	0.529786	1.603715
S	1.644376	0.529786	-1.603715

Zero-point correction= 0.047811 (Hartree/Particle)
Thermal correction to Energy= 0.056510
Thermal correction to Enthalpy= 0.057454
Thermal correction to Gibbs Free Energy= 0.012283
Sum of electronic and zero-point Energies= -1897.171779
Sum of electronic and thermal Energies= -1897.163080
Sum of electronic and thermal Enthalpies= -1897.162136
Sum of electronic and thermal Free Energies= -1897.207307

4 (open-shell singlet, ωB97-XD)

Symbol	X	Y	Z
S	-1.602547	-1.602547	-0.598319
S	1.602547	-1.602547	-0.598319
S	1.602547	1.602547	-0.598319
S	-1.602547	1.602547	-0.598319
C	0.000000	-1.038285	1.370548
C	1.038285	0.000000	1.370548
C	0.000000	1.038285	1.370548
C	-1.038285	0.000000	1.370548
C	0.000000	1.809385	0.224969
C	1.809385	0.000000	0.224969
C	0.000000	-1.809385	0.224969
C	-1.809385	0.000000	0.224969

Zero-point correction= 0.047651 (Hartree/Particle)
Thermal correction to Energy= 0.056181
Thermal correction to Enthalpy= 0.057126
Thermal correction to Gibbs Free Energy= 0.014700
Sum of electronic and zero-point Energies= -1897.179981
Sum of electronic and thermal Energies= -1897.171451
Sum of electronic and thermal Enthalpies= -1897.170507
Sum of electronic and thermal Free Energies= -1897.212933

Benzene

Symbol	X	Y	Z
C	0.000000	1.394084	0.000000
C	1.207312	0.697042	0.000000
C	1.207312	-0.697042	0.000000
C	0.000000	-1.394084	0.000000
C	-1.207312	-0.697042	0.000000
C	-1.207312	0.697042	0.000000
H	0.000000	2.478099	0.000000
H	2.146096	1.239049	0.000000
H	2.146096	-1.239049	0.000000
H	0.000000	-2.478099	0.000000
H	-2.146096	-1.239049	0.000000
H	-2.146096	1.239049	0.000000

Zero-point correction= 0.100196 (Hartree/Particle)
Thermal correction to Energy= 0.104594
Thermal correction to Enthalpy= 0.105538
Thermal correction to Gibbs Free Energy= 0.075078
Sum of electronic and zero-point Energies= -232.229965
Sum of electronic and thermal Energies= -232.225567
Sum of electronic and thermal Enthalpies= -232.224623
Sum of electronic and thermal Free Energies= -232.255083

Thiophene

Symbol	X	Y	Z
C	0.000000	1.240808	-0.011488
C	0.000000	0.713872	-1.271779
C	0.000000	-0.713872	-1.271779
C	0.000000	-1.240808	-0.011488
S	0.000000	0.000000	1.198239
H	0.000000	2.278766	0.282133
H	0.000000	1.318698	-2.168442
H	0.000000	-1.318698	-2.168442
H	0.000000	-2.278766	0.282133

Zero-point correction= 0.066406 (Hartree/Particle)
Thermal correction to Energy= 0.070488
Thermal correction to Enthalpy= 0.071432
Thermal correction to Gibbs Free Energy= 0.039823
Sum of electronic and zero-point Energies= -553.022090
Sum of electronic and thermal Energies= -553.018008
Sum of electronic and thermal Enthalpies= -553.017064
Sum of electronic and thermal Free Energies= -553.048673

Distorted Thiophene

Symbol	X	Y	Z
C	1.294162	-0.694804	-0.125008
C	1.199543	0.788772	-0.085041
C	-0.044232	1.304986	0.123361
C	0.101798	-1.267769	0.173740
S	-1.236243	-0.055086	-0.127846
H	2.067420	1.421230	-0.213886
H	2.195217	-1.244459	-0.361219
H	-0.015211	1.827432	1.066643
H	0.224835	-1.909929	1.031682

SCF Done: E(RB3LYP) = -552.970257899 A.U. after 14 cycles
NFock= 14 Conv=0.30D-08 -V/T= 2.0024
KE= 5.516596056456D+02 PE=-1.701342683608D+03
EE= 3.989366916523D+02

[4]Radialene

Symbol	X	Y	Z
C	0.000000	1.058230	0.000000
C	1.058230	0.000000	0.000000
C	0.000000	-1.058230	0.000000
C	-1.058230	0.000000	0.000000
C	2.391412	0.000000	0.000000
H	2.955264	0.925642	0.000000
H	2.955264	-0.925642	0.000000
C	0.000000	-2.391412	0.000000
H	-0.925642	-2.955264	0.000000
H	0.925642	-2.955264	0.000000
C	-2.391412	0.000000	0.000000
H	-2.955264	0.925642	0.000000
H	-2.955264	-0.925642	0.000000
C	0.000000	2.391412	0.000000
H	-0.925642	2.955264	0.000000
H	0.925642	2.955264	0.000000

Zero-point correction= 0.127965 (Hartree/Particle)
Thermal correction to Energy= 0.135803
Thermal correction to Enthalpy= 0.136747
Thermal correction to Gibbs Free Energy= 0.097953
Sum of electronic and zero-point Energies= -309.534968
Sum of electronic and thermal Energies= -309.527131
Sum of electronic and thermal Enthalpies= -309.526187
Sum of electronic and thermal Free Energies= -309.564980

[5]Circulene

Symbol	X	Y	Z
C	0.000000	2.476194	0.102772
C	1.304155	2.973353	-0.270146
C	2.424821	2.159141	-0.270146
C	2.355000	0.765186	0.102772
C	1.148529	0.373180	0.655132
C	0.000000	1.207635	0.655132
C	-1.304155	2.973353	-0.270146
C	3.230833	-0.321508	-0.270146
C	2.802777	-1.638930	-0.270146
C	1.455470	-2.003283	0.102772
C	0.709830	-0.976997	0.655132
C	-0.709830	-0.976997	0.655132
C	-1.148529	0.373180	0.655132
C	-2.355000	0.765186	0.102772
C	-2.424821	2.159141	-0.270146
C	-3.230833	-0.321508	-0.270146
C	-2.802777	-1.638930	-0.270146
C	-1.455470	-2.003283	0.102772
C	-0.692610	-3.172056	-0.270146
C	0.692610	-3.172056	-0.270146
H	-3.472746	-2.401737	-0.652835
H	-4.221216	-0.098182	-0.652835
H	3.472746	-2.401737	-0.652835
H	1.397804	3.984275	-0.652835
H	4.221216	-0.098182	-0.652835
H	3.357325	2.560600	-0.652835
H	-1.211051	-4.044955	-0.652835
H	1.211051	-4.044955	-0.652835
H	-3.357325	2.560600	-0.652835
H	-1.397804	3.984275	-0.652835

Zero-point correction= 0.231236 (Hartree/Particle)
Thermal correction to Energy= 0.242705
Thermal correction to Enthalpy= 0.243650
Thermal correction to Gibbs Free Energy= 0.196060
Sum of electronic and zero-point Energies= -768.174716
Sum of electronic and thermal Energies= -768.163247
Sum of electronic and thermal Enthalpies= -768.162302
Sum of electronic and thermal Free Energies= -768.209892