Supporting Information for

Theoretical Study on the Structures, Electronic Properties, and Aromaticity of Thiophene Analogues of Anti-Kekulene

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This file includes:

1. Strain Energy Calculations

Table S1. Calculated zero-point-corrected total energies (ZPEs), ZPEs per a thiophene unit, relative strain energies per a thiophene unit, and total relative energies (E_{strain}) of **1**–**4**.

compound	ZPE value (hartree)	ZPE value per a thiophene unit (hartree)	relative strain energy per a thiophene unit (kcal/mol)	E_{strain} value (kcal/mol)
1	−3303.318346	−550.553058	4.74	28.4
2	−3853.897978	−550.556854	2.35	16.5
3	−4404.473706	−550.559213	0.87	7.0
4	−4955.045438	−550.560604	0.00	0.0

2. Molecular Planarity Analysis

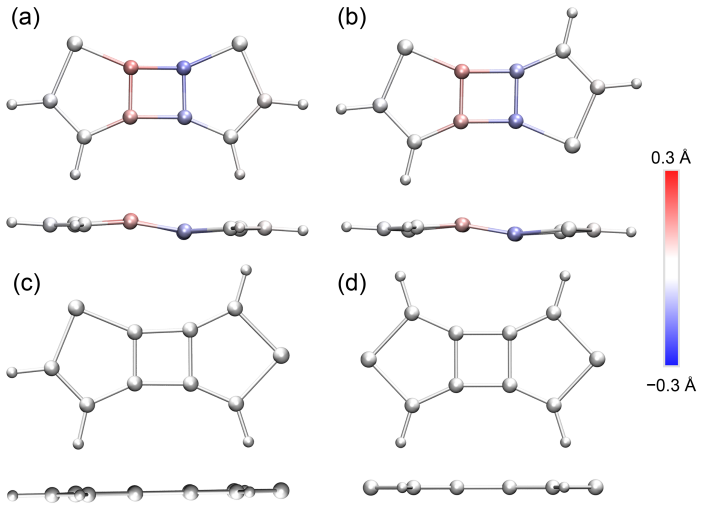

Figure S1. Results of the molecular planarity analysis for ***syn-*** (a) and ***anti-bb*CDT**s (b), ***bc*CDT** (c), and ***cc*CDT** (d). The atoms with large distance from the fitting plane are colored by red (+) or blue (–).

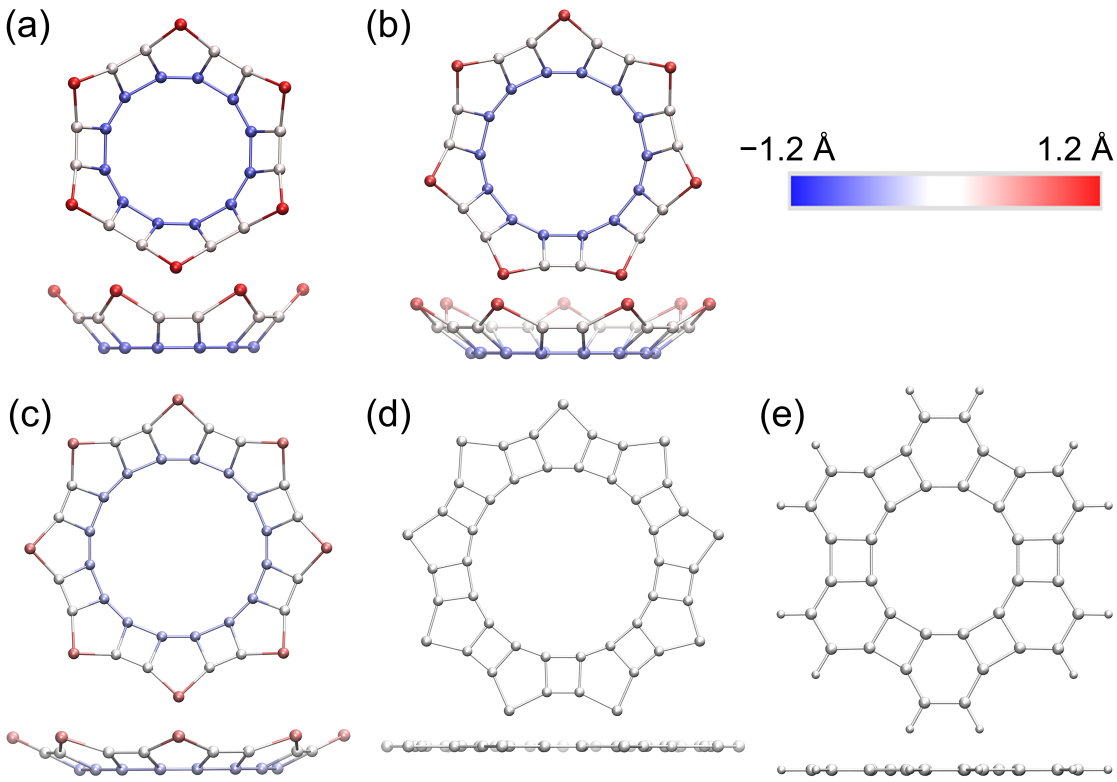

Figure S2. Results of the molecular planarity analysis for **1** (a), **2** (b), **3** (c), **4** (d), and anti-kekulene (e). The atoms with large distance from the fitting plane are colored by red (+) or blue (–).

3. Structures and Aromaticity of Benzene, Thiophene, and Cyclobutadiene

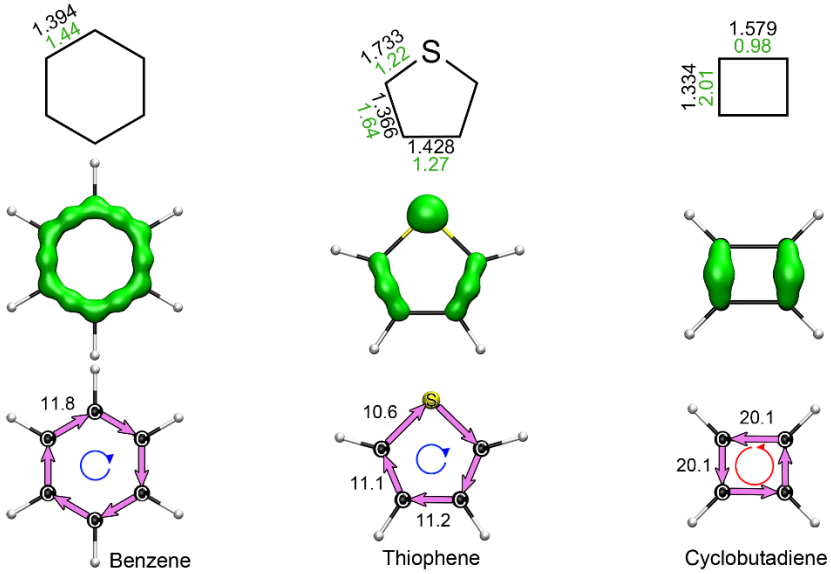

Figure S3. (Top row) Bond lengths (black numbers) and WBI values (green numbers) of benzene, thiophene, and cyclobutadiene. (Middle row) LOL-π isosurfaces (isovalue of 0.55 a.u. for benzene and 0.60 a.u. for the others, middle) of benzene, thiophene, and cyclobutadiene. (Bottom row) Paths and strengths (nA/T) of magnetically induced currents at each bond of benzene, thiophene, and cyclobutadiene.

Table S2. HOMA and MCI values of benzene and thiophene and the $NICS(1)_{zz}$ values of benzene, thiophene, and cyclobutadiene.

compound	HOMA value	MCI value	$NICS(1)_{zz}$ value (ppm)
benzene	0.991	0.0870	−29.3
thiophene	0.751	0.0750	−28.0
cyclobutadiene	---	---	55.5

4. NICS(1)$_{zz}$ Values on the Concave Face

The NICS(1)$_{zz}$ values of bowl-shaped compounds **1**–**3** calculated on the concave face of the bowl were summarized in Table S3. The results are in agreement with those on the convex face.

Table S3. NICS(1)$_{zz}$ values on the concave faces of bowl-shaped molecules **1**–**3** (ppm).

compound	4MR	thiophene ring	macrocyclic center
1	7.7	−1.3	6.8
2	9.9	−0.8	5.5
3	10.7	−0.5	5.5

5. LOL–π Isosurfaces of 1–3

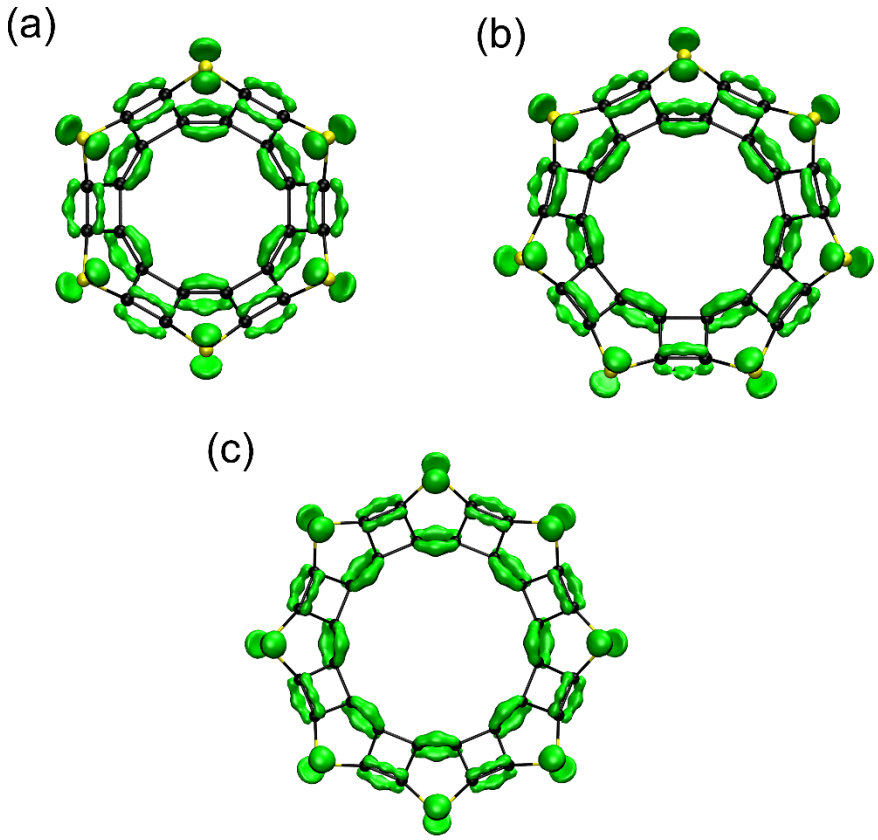

Figure S4. LOL-π isosurfaces (isovalue: 0.60 a.u.) of **1** (a), **2** (b), and **3** (c).

6. Molecular Orbital Diagrams

The HOMO and LUMO energy levels of ***bc*CDT** are decreased and increased, respectively, compared with those of ***bb*CDT**s, resulting in a larger E_{Gap} value. From the comparison between ***bc*CDT** and ***cc*CDT**, the LUMO level is almost the same, while the HOMO level of ***cc*CDT** is lower than that of ***bc*CDT**. Thus, ***cc*CDT** has the largest E_{Gap} value.

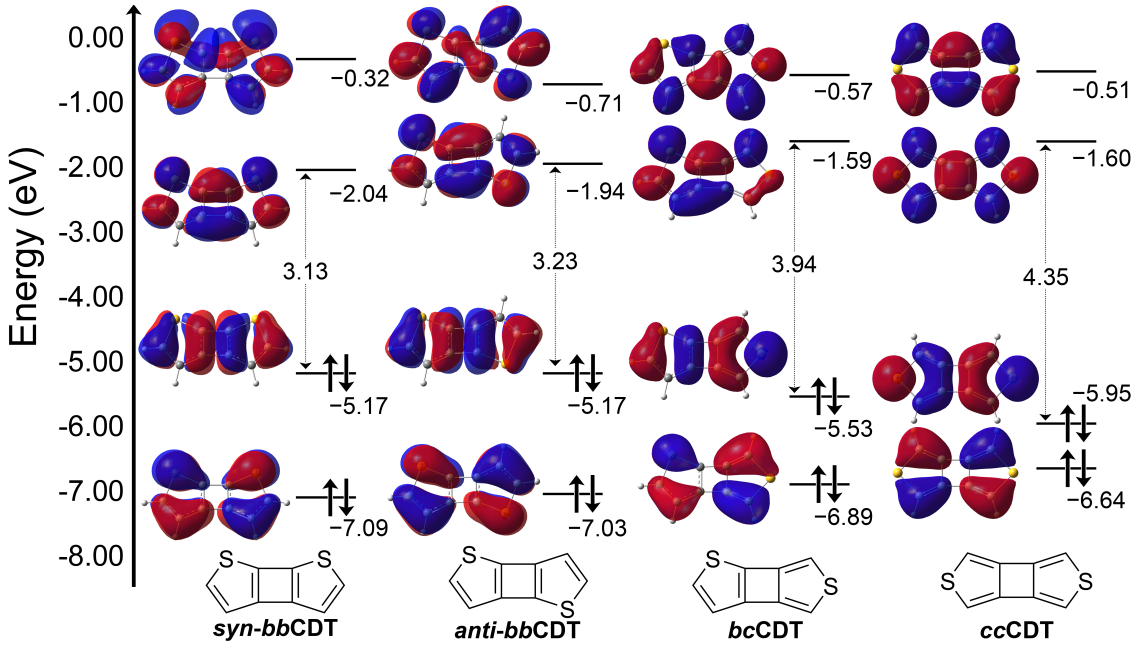

Figure S5. Molecular orbital diagrams of ***bb*CDT**, ***bc*CDT**, and ***cc*CDT** (isosurface values: 0.020 a.u.).

Compounds **2** and **4** have the doubly-degenerated LUMOs, whereas the other two compounds show no degeneracy in the LUMOs. It should be noted that there are only little differences in the energy levels of the HOMO and LUMO among the four compounds. Anti-kekulene also has the pseudo-doubly-degenerated LUMOs.

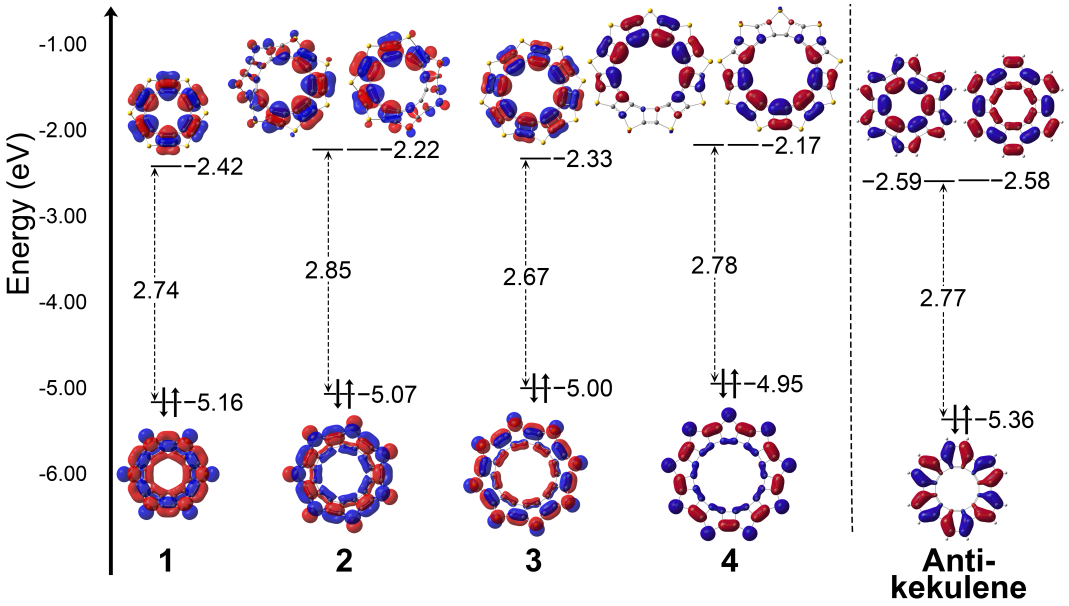

Figure S6. Molecular orbital diagrams of **1**–**4** and anti-kekulene (isosurface values: 0.020 a.u.).

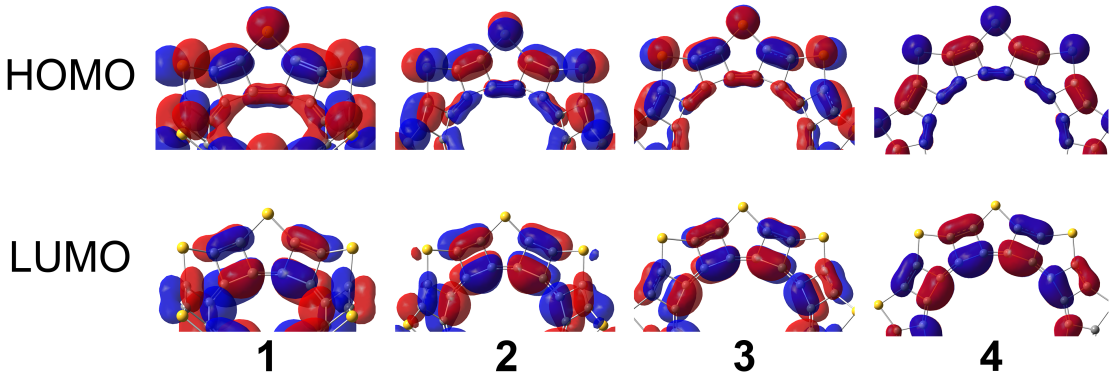

Figure S7. Zoomed frontier molecular orbital distributions for **1**–**4**.

7. Signed Modules of Current Densities

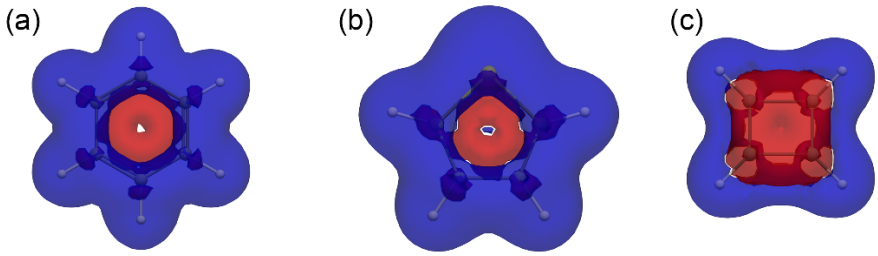

Figure S8. Signed modules of the current densities (isovalue: 0.010 a.u.) for benzene (a), thiophene (b), and cyclobutadiene (c). Diatropic and paratropic currents are shown in blue and red, respectively.

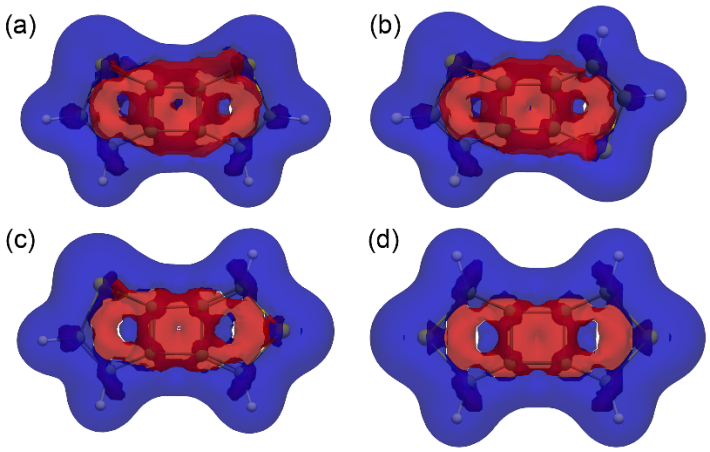

Figure S9. Signed modules of the current densities (isovalue: 0.010 a.u.) for ***syn-bb*CDT** (a), ***anti-bb*CDT** (b), ***bc*CDT** (c), and ***cc*CDT** (d). Diatropic and paratropic currents are shown in blue and red, respectively.

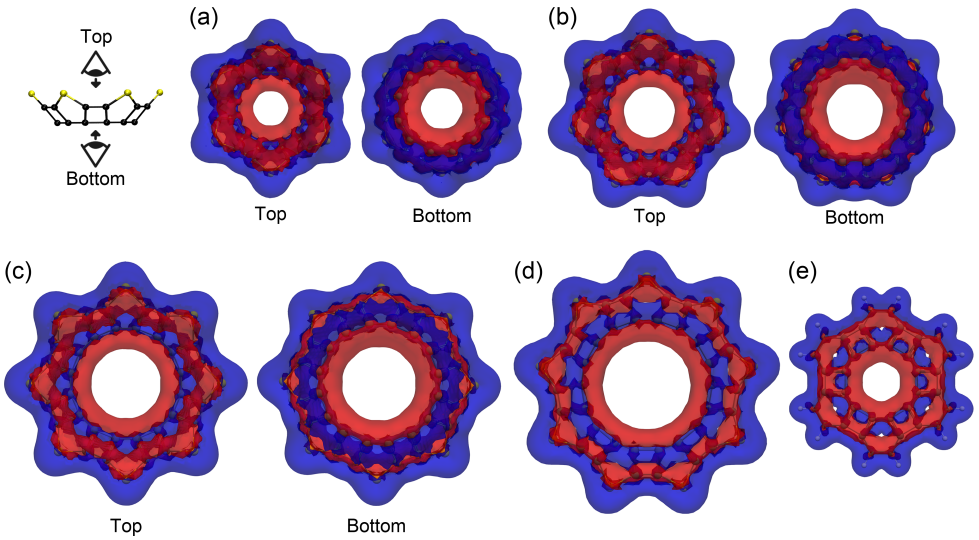

Figure S10. Signed modules of the current densities (isovalue: 0.010 a.u.) for **1** (a), **2** (b), **3** (c), **4** (d), and anti-kekulene (e). Diatropic and paratropic currents are shown in blue and red, respectively.

8. Calculated Atomic Charge

We calculated atomic charges by the Hirshfeld [101] and natural population analyses (NPA) [83] at B3LYP/6-311G(d,p) level. The calculation of Hirshfeld and NPA charge were performed using the Multiwfn program (version 3.8) [78] and NBO 3.1 program [84] implemented in the Gaussian 16 program, respectively. While the Hirshfeld method tends to give positively or negatively smaller charge values compared to those calculated by the natural population method generally [102–104], both methods qualitatively give the same results. The charges of all sulfur atoms are positive. Moreover, in the case of **1**–**4**, the carbon atoms located the macrocyclic ring inside are close to zero compared with those of outside ones.

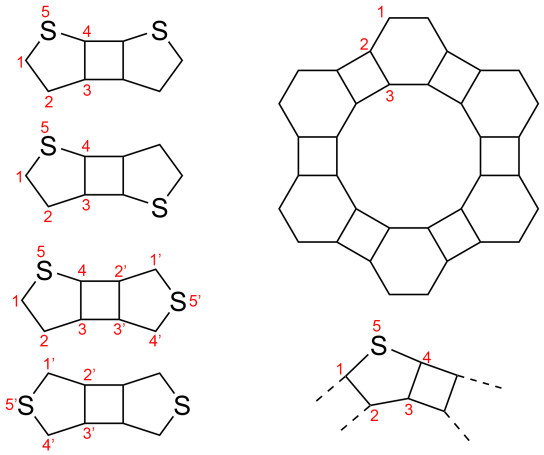

Figure S11. Atom numberings of the **CDT**s, anti-kekulene, and the thiophene analogues of anti-kekulene.

Table S4. The calculated Hirshfeld atomic charges of all atoms (a.u.).

compd.	atom positions				
	1 (1’)	2 (2’)	3 (3’)	4 (4’)	5 (5’)
***syn-bb*CDT**	–0.0754	–0.0561	–0.0240	–0.0475	0.1053
***anti-bb*CDT**	–0.0779	–0.0568	–0.0281	–0.0448	0.1067
***bc*CDT**	–0.0659 (–0.069)	–0.0539 (–0.025)	–0.0169 (–0.023)	–0.0339 (–0.069)	0.1077 (0.036)
***cc*CDT**	(–0.067)	(–0.022)	(–0.022)	(–0.067)	(0.068)
anti-kekulene	–0.0392	0.0005	–0.0059		
1	–0.0284	–0.0105	–0.0104	–0.0284	0.0776
2	–0.0291	–0.0108	–0.0108	–0.0291	0.0798
3	–0.0294	–0.0115	–0.0106	–0.0295	0.0811
4	–0.0306	–0.0107	–0.0107	–0.0306	0.0826

Table S5. The calculated NPA charges of all atoms (a.u.).

compd.	atom positions				
	1 (1’)	2 (2’)	3 (3’)	4 (4’)	5 (5’)
***syn-bb*CDT**	–0.382	–0.253	–0.043	–0.228	0.463
***anti-bb*CDT**	–0.384	–0.252	–0.067	–0.204	0.463
***bc*CDT**	–0.360 (–0.344)	–0.251 (–0.069)	–0.048 (–0.048)	–0.198 (–0.346)	0.450 (0.315)
***cc*CDT**	(–0.350)	(–0.062)	(–0.062)	(–0.350)	(0.369)
anti-kekulene	–0.197	0.007	–0.019		
1	–0.160	–0.022	–0.022	–0.160	0.363
2	–0.163	–0.023	–0.023	–0.163	0.371
3	–0.165	–0.024	–0.022	–0.166	0.376
4	–0.168	–0.022	–0.022	–0.168	0.380

9. Cartesian Coordinates

***syn-bb*CDT**

Symbol	X	Y	Z
C	-0.032016	3.006531	0.482464
C	0.000470	2.053501	1.489900
C	0.108032	0.768364	0.936366
C	0.145147	0.746047	-0.445115
S	-0.000470	2.310677	-1.119002
H	0.010378	4.080137	0.582153
H	-0.029640	2.306981	2.540194
C	-0.145147	-0.746047	-0.445115
C	-0.108032	-0.768364	0.936366
C	-0.000470	-2.053501	1.489900
C	0.032016	-3.006531	0.482464
S	0.000470	-2.310677	-1.119002
H	0.029640	-2.306981	2.540194
H	-0.010378	-4.080137	0.582153

Zero-point correction= 0.090096 (Hartree/Particle)
Thermal correction to Energy= 0.097975
Thermal correction to Enthalpy= 0.098919
Thermal correction to Gibbs Free Energy= 0.057094
Sum of electronic and zero-point Energies= -1103.555889
Sum of electronic and thermal Energies= -1103.548009
Sum of electronic and thermal Enthalpies= -1103.547065
Sum of electronic and thermal Free Energies= -1103.588891

***anti-bb*CDT**

Symbol	X	Y	Z
C	2.934550	0.711677	0.035367
C	1.838132	1.558101	-0.001993
C	0.656974	0.805891	-0.103321
C	0.841979	-0.562468	-0.134848
S	2.493026	-0.979319	0.010591
H	3.979949	0.976132	-0.000481
H	1.922776	2.635171	0.023345
C	-0.841979	0.562468	0.134848
C	-0.656974	-0.805891	0.103321
C	-1.838132	-1.558101	0.001993
C	-2.934550	-0.711677	-0.035367
S	-2.493026	0.979319	-0.010591
H	-1.922776	-2.635171	-0.023345
H	-3.979949	-0.976132	0.000481

Zero-point correction= 0.090119 (Hartree/Particle)
Thermal correction to Energy= 0.097996
Thermal correction to Enthalpy= 0.098940
Thermal correction to Gibbs Free Energy= 0.056449
Sum of electronic and zero-point Energies= -1103.556429
Sum of electronic and thermal Energies= -1103.548552
Sum of electronic and thermal Enthalpies= -1103.547607
Sum of electronic and thermal Free Energies= -1103.590098

***bc*CDT**

Symbol	X	Y	Z
C	-0.391540	2.201984	0.000000
C	0.000000	0.917753	0.000000
C	-1.085164	-0.053926	0.000000
C	-2.311876	0.490654	0.000000
S	-2.171052	2.268869	0.000000
H	0.170372	3.122674	0.000000
H	-3.293673	0.043552	0.000000
C	-0.060669	-1.164191	0.000000
C	0.380755	-2.504523	0.000000
C	0.962218	-0.228948	0.000000
C	1.759246	-2.544532	0.000000
H	-0.235496	-3.392089	0.000000
S	2.511294	-0.959166	0.000000
H	2.397118	-3.415011	0.000000

Zero-point correction= 0.090521 (Hartree/Particle)
Thermal correction to Energy= 0.098264
Thermal correction to Enthalpy= 0.099208
Thermal correction to Gibbs Free Energy= 0.057173
Sum of electronic and zero-point Energies= -1103.581040
Sum of electronic and thermal Energies= -1103.573297
Sum of electronic and thermal Enthalpies= -1103.572353
Sum of electronic and thermal Free Energies= -1103.614388

***cc*CDT**

Symbol	X	Y	Z
C	0.000000	1.283121	1.979581
C	0.000000	0.724724	0.749198
C	0.000000	-0.724724	0.749198
C	0.000000	-1.283121	1.979581
S	0.000000	0.000000	3.191769
H	0.000000	2.312598	2.301496
H	0.000000	-2.312598	2.301496
C	0.000000	-0.724724	-0.749198
C	0.000000	-1.283121	-1.979581
C	0.000000	0.724724	-0.749198
S	0.000000	0.000000	-3.191769
H	0.000000	-2.312598	-2.301496
C	0.000000	1.283121	-1.979581
H	0.000000	2.312598	-2.301496

Zero-point correction= 0.090691 (Hartree/Particle)
Thermal correction to Energy= 0.098268
Thermal correction to Enthalpy= 0.099212
Thermal correction to Gibbs Free Energy= 0.059032
Sum of electronic and zero-point Energies= -1103.592129
Sum of electronic and thermal Energies= -1103.584553
Sum of electronic and thermal Enthalpies= -1103.583609
Sum of electronic and thermal Free Energies= -1103.623788

Anti-kekulene

Symbol	X	Y	Z
C	-1.378880	3.909637	0.000111
C	-0.674199	2.643600	0.003846
C	0.674199	2.643600	-0.003846
C	1.378880	3.909637	-0.000111
C	0.722817	5.114389	0.000080
C	-0.722817	5.114389	-0.000080
H	1.249870	6.060926	0.001337
H	-1.249870	6.060926	-0.001337
C	-1.952325	1.905673	-0.003846
C	-2.696405	3.148964	-0.000111
C	-2.626524	0.737927	0.003846
C	-4.067782	3.183172	0.000080
C	-4.075285	0.760673	0.000111
C	-4.790599	1.931217	-0.000080
H	-4.623981	4.112882	0.001337
H	-5.873851	1.948044	-0.001337
C	-2.626524	-0.737927	-0.003846
C	-4.075285	-0.760673	-0.000111
C	-1.952325	-1.905673	0.003846
C	-4.790599	-1.931217	0.000080
C	-2.696405	-3.148964	0.000111
C	-4.067782	-3.183172	-0.000080
H	-5.873851	-1.948044	0.001337
H	-4.623981	-4.112882	-0.001337
C	-1.378880	-3.909637	-0.000111
C	-0.722817	-5.114389	0.000080
C	-0.674199	-2.643600	-0.003846
C	0.722817	-5.114389	-0.000080
H	-1.249870	-6.060926	0.001337
C	0.674199	-2.643600	0.003846
C	1.378880	-3.909637	0.000111
H	1.249870	-6.060926	-0.001337
C	1.952325	-1.905673	-0.003846
C	2.626524	-0.737927	0.003846
C	2.696405	-3.148964	-0.000111
C	4.075285	-0.760673	0.000111
C	4.067782	-3.183172	0.000080
C	4.790599	-1.931217	-0.000080
H	4.623981	-4.112882	0.001337
H	5.873851	-1.948044	-0.001337
C	2.626524	0.737927	-0.003846
C	4.075285	0.760673	-0.000111
C	1.952325	1.905673	0.003846
C	4.790599	1.931217	0.000080

C	2.696405	3.148964	0.000111
C	4.067782	3.183172	-0.000080
H	5.873851	1.948044	0.001337
H	4.623981	4.112882	-0.001337

Zero-point correction= 0.343179 (Hartree/Particle)
Thermal correction to Energy= 0.365095
Thermal correction to Enthalpy= 0.366039
Thermal correction to Gibbs Free Energy= 0.296343
Sum of electronic and zero-point Energies= -1378.792650
Sum of electronic and thermal Energies= -1378.770735
Sum of electronic and thermal Enthalpies= -1378.769790
Sum of electronic and thermal Free Energies= -1378.839486

Compound **1**

Symbol	X	Y	Z
C	-0.689284	3.661853	0.058999
C	-0.740550	2.617111	1.125600
S	-2.190924	3.794792	-0.888449
C	-1.896209	1.949891	1.125600
C	-2.826616	2.427864	0.058999
C	-3.515900	1.233989	0.058999
C	-2.636760	0.667220	1.125600
S	-4.381848	0.000000	-0.888449
C	-2.636760	-0.667220	1.125600
C	-3.515900	-1.233989	0.058999
C	0.689284	3.661853	0.058999
C	0.740550	2.617111	1.125600
S	2.190924	3.794792	-0.888449
C	1.896209	1.949891	1.125600
C	2.826616	2.427864	0.058999
C	-2.826616	-2.427864	0.058999
C	-1.896209	-1.949891	1.125600
S	-2.190924	-3.794792	-0.888449
C	-0.740550	-2.617111	1.125600
C	-0.689284	-3.661853	0.058999
C	0.689284	-3.661853	0.058999
C	0.740550	-2.617111	1.125600
S	2.190924	-3.794792	-0.888449
C	1.896209	-1.949891	1.125600
C	2.826616	-2.427864	0.058999
C	3.515900	-1.233989	0.058999
C	2.636760	-0.667220	1.125600
S	4.381848	0.000000	-0.888449
C	2.636760	0.667220	1.125600
C	3.515900	1.233989	0.058999

Zero-point correction= 0.143299 (Hartree/Particle)
Thermal correction to Energy= 0.163928
Thermal correction to Enthalpy= 0.164873
Thermal correction to Gibbs Free Energy= 0.096452
Sum of electronic and zero-point Energies= -3303.318346
Sum of electronic and thermal Energies= -3303.297717
Sum of electronic and thermal Enthalpies= -3303.296772
Sum of electronic and thermal Free Energies= -3303.365193

Compound **2**

Symbol	X	Y	Z
C	0.689093	4.273768	0.051217
C	0.739690	3.072343	0.936745
S	2.236946	4.645066	-0.740972
C	1.940865	2.493887	0.936745
C	2.911724	3.203405	0.051217
C	3.771009	2.125896	0.051217
C	2.863243	1.337262	0.936745
S	5.026372	1.147237	-0.740972
C	3.159909	0.037484	0.936745
C	4.319953	-0.279187	0.051217
C	-0.689093	4.273768	0.051217
C	-0.739690	3.072343	0.936745
S	-2.236946	4.645066	-0.740972
C	-1.940865	2.493887	0.936745
C	-2.911724	3.203405	0.051217
C	4.013278	-1.622819	0.051217
C	2.830716	-1.404805	0.936745
S	4.030837	-3.214485	-0.740972
C	1.999477	-2.447146	0.936745
C	2.475170	-3.551546	0.051217
C	-2.475170	-3.551546	0.051217
C	-1.999477	-2.447146	0.936745
S	-4.030837	-3.214485	-0.740972
C	-2.830716	-1.404805	0.936745
C	-4.013278	-1.622819	0.051217
C	-4.319953	-0.279187	0.051217
C	-3.159909	0.037484	0.936745
S	-5.026372	1.147237	-0.740972
C	-2.863243	1.337262	0.936745
C	-3.771009	2.125896	0.051217
C	1.233467	-4.149518	0.051217
C	0.666602	-3.089025	0.936745
S	0.000000	-5.155634	-0.740972
C	-0.666602	-3.089025	0.936745
C	-1.233467	-4.149518	0.051217

Zero-point correction= 0.166208 (Hartree/Particle)
Thermal correction to Energy= 0.191250
Thermal correction to Enthalpy= 0.192194
Thermal correction to Gibbs Free Energy= 0.114316
Sum of electronic and zero-point Energies= -3853.897978
Sum of electronic and thermal Energies= -3853.872935
Sum of electronic and thermal Enthalpies= -3853.871991
Sum of electronic and thermal Free Energies= -3853.949870

Compound **3**

Symbol	X	Y	Z
C	2.187552	4.423020	0.038034
C	1.379262	3.329834	0.655001
C	0.074735	3.600075	0.646166
C	-0.226148	4.927930	0.035460
S	1.217574	5.804583	-0.515498
C	-1.580714	4.674380	0.038034
C	-1.379262	3.329834	0.655001
S	-3.243505	4.965414	-0.515498
C	-2.492792	2.598483	0.646166
C	-3.644484	3.324662	0.035460
C	3.324662	3.644484	0.035460
C	2.598483	2.492792	0.646166
S	4.965414	3.243505	-0.515498
C	3.329834	1.379262	0.655001
C	4.674380	1.580714	0.038034
C	-4.423020	2.187552	0.038034
C	-3.329834	1.379262	0.655001
S	-5.804583	1.217574	-0.515498
C	-3.600075	0.074735	0.646166
C	-4.927930	-0.226148	0.035460
C	4.927930	0.226148	0.035460
C	3.600075	-0.074735	0.646166
S	5.804583	-1.217574	-0.515498
C	3.329834	-1.379262	0.655001
C	4.423020	-2.187552	0.038034
C	-4.674380	-1.580714	0.038034
C	-3.329834	-1.379262	0.655001
S	-4.965414	-3.243505	-0.515498
C	-2.598483	-2.492792	0.646166
C	-3.324662	-3.644484	0.035460
C	-2.187552	-4.423020	0.038034
C	-1.379262	-3.329834	0.655001
S	-1.217574	-5.804583	-0.515498
C	-0.074735	-3.600075	0.646166
C	0.226148	-4.927930	0.035460
C	1.580714	-4.674380	0.038034
C	1.379262	-3.329834	0.655001
S	3.243505	-4.965414	-0.515498
C	2.492792	-2.598483	0.646166
C	3.644484	-3.324662	0.035460

Zero-point correction= 0.189721 (Hartree/Particle)
Thermal correction to Energy= 0.218981
Thermal correction to Enthalpy= 0.219925

Thermal correction to Gibbs Free Energy= 0.132694
Sum of electronic and zero-point Energies= -4404.473706
Sum of electronic and thermal Energies= -4404.444446
Sum of electronic and thermal Enthalpies= -4404.443502
Sum of electronic and thermal Free Energies= -4404.530733

Compound **4**

Symbol	X	Y	Z
C	1.228012	5.383871	0.001056
C	0.666779	3.999920	0.006599
C	-0.666779	3.999920	-0.006599
C	-1.228012	5.383871	-0.001056
S	0.000000	6.662268	0.000000
C	-5.088836	2.144255	0.001056
C	-3.823368	1.351228	0.006599
S	-6.561053	1.156891	0.000000
C	-4.054938	0.037930	-0.006599
C	-5.515320	-0.274456	-0.001056
C	2.519974	4.913636	-0.001056
C	2.060317	3.492714	-0.006599
S	4.282423	5.103593	0.000000
C	3.081882	2.635519	0.006599
C	4.401398	3.334934	0.001056
C	-5.276575	-1.628446	0.001056
C	-3.797422	-1.422513	0.006599
S	-5.769693	-3.331134	0.000000
C	-3.130643	-2.577408	-0.006599
C	-4.048563	-3.755425	-0.001056
C	5.088836	2.144255	-0.001056
C	3.823368	1.351228	-0.006599
S	6.561053	1.156891	0.000000
C	4.054938	0.037930	0.006599
C	5.515320	-0.274456	0.001056
C	-2.995346	-4.639179	0.001056
C	-1.994621	-3.530644	0.006599
S	-2.278630	-6.260484	0.000000
C	-0.741486	-3.986748	-0.006599
C	-0.687439	-5.479189	-0.001056
C	0.687439	-5.479189	0.001056
C	0.741486	-3.986748	0.006599
S	2.278630	-6.260484	0.000000
C	1.994621	-3.530644	-0.006599
C	2.995346	-4.639179	-0.001056
C	4.048563	-3.755425	0.001056
C	3.130643	-2.577408	0.006599
S	5.769693	-3.331134	0.000000
C	3.797422	-1.422513	-0.006599
C	5.276575	-1.628446	-0.001056
C	-4.401398	3.334934	-0.001056
C	-3.081882	2.635519	-0.006599
S	-4.282423	5.103593	0.000000
C	-2.060317	3.492714	0.006599

C	-2.519974	4.913636	0.001056

Zero-point correction= 0.215163 (Hartree/Particle)
Thermal correction to Energy= 0.248079
Thermal correction to Enthalpy= 0.249024
Thermal correction to Gibbs Free Energy= 0.153444
Sum of electronic and zero-point Energies= -4955.045438
Sum of electronic and thermal Energies= -4955.012521
Sum of electronic and thermal Enthalpies= -4955.011577
Sum of electronic and thermal Free Energies= -4955.107157

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

Cyclobutadiene

Symbol	X	Y	Z
C	0.000000	0.666964	0.789636
H	0.000000	1.433422	1.551832
C	0.000000	0.666964	-0.789636
H	0.000000	1.433422	-1.551832
C	0.000000	-0.666964	-0.789636
H	0.000000	-1.433422	-1.551832
C	0.000000	-0.666964	0.789636
H	0.000000	-1.433422	1.551832

Zero-point correction= 0.060887 (Hartree/Particle)
Thermal correction to Energy= 0.064670
Thermal correction to Enthalpy= 0.065614
Thermal correction to Gibbs Free Energy= 0.036893
Sum of electronic and zero-point Energies= -154.668944
Sum of electronic and thermal Energies= -154.665161
Sum of electronic and thermal Enthalpies= -154.664217
Sum of electronic and thermal Free Energies= -154.692937