Supplementary Information

Sulfinfinitenes: Infinitenes of Fused Thiophene Rings

Peter B. Karadakov[a]* and Edward Cummings[a]
[a]Department of Chemistry, University of York, Heslington, York YO10 5DD, UK
E-mail: peter.karadakov@york.ac.uk

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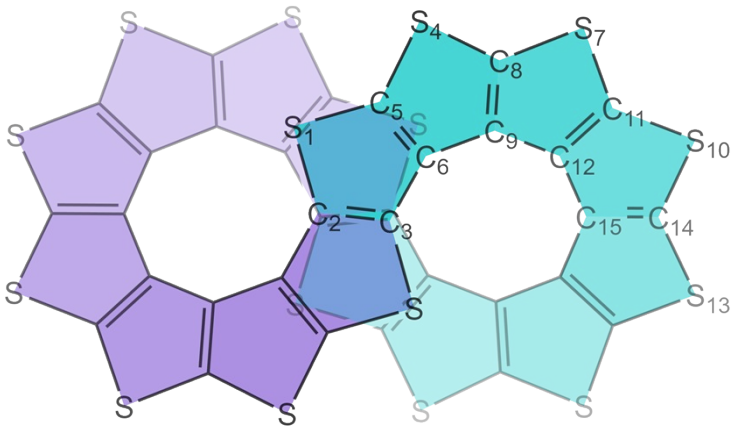
1. Additional Computational Details

All DFT calculations reported in this paper made use of the GAUSSIAN "SuperFine" integration grid. All geometry optimizations were carried out under the GAUSSIAN "VeryTight" convergence criteria and were combined with analytical harmonic frequency calculations to confirm that the optimized geometries were local minima.

NICS(0) and NICS(1) values at planar geometries (thiophene, [8]sulflower and [9]sulflower]) were calculated according to the standard definitions, as $-\sigma_{iso}$(at the ring centre) and $-\sigma_{iso}$(at 1 Å above the ring centre), respectively. The optimized geometries of all other molecules studied in this paper are non-planar. The NICS(0) positions at these geometries were chosen as the averages of the coordinates of the ring atoms; in order to calculate NICS(±1) values, a plane was fitted to the coordinates of the ring atoms and the NICS(0) position, and the NICS(±1) positions were taken as the points 1 Å above and below that plane along the normal passing through the NICS(0) position following the procedure outlined in refs. S1 and S2. NICS positions were specified in the GAUSSIAN input files as ghost atoms without basis functions (symbol "Bq"). To improve accuracy, the GAUSSIAN "CPHF(Separate)" option was used in all NMR calculations.

2. NICS Values and Isotropic Nuclear Shieldings

The following tables contain the NICS values and isotropic nuclear shieldings (in ppm) for thiophene and the symmetry-unique thiophene rings in the [*n*]sulflowers and [2*n*]sulfinfiniteness with $n = 5-10$. The atom numbering scheme uses the consecutive numbers of the C_2S units (i), as illustrated on the example of the [16]sulfinfinitene (**10**, D_2 point group) shown below.



We assume that the first C_2S unit ($i = 1$) is the one involving the central carbon-carbon double bond in the top thieno[3,2-*b*]thiophene junction; the numbers of the atoms in this unit are S_1, C_2 and C_3. We continue counting the C_2S units clockwise, with the second one ($i = 2$) comprised of S_4, C_5 and C_6. The NICS values associated with a C_2S unit are those for the thiophene ring including the atoms from this unit and the carbon atoms from the next C_2S unit; for the first C_2S unit these are S_1, C_2, C_3, C_6 and C_5. Due to its D_2 symmetry, [16]sulfinfinitene has four symmetry-unique thiophene rings. Thiophene and the [*n*]sulflowers with $n = 5-9$ have only one symmetry-unique thiophene ring. For all [*n*]sulflowers we also include the NICS values for the central C_n ring formed by the carbon-carbon hub bonds; these values are denoted by "c". The NICS(+1) and NICS(−1) values for the planar thiophene, [8]sulflower and [9]sulflower are identical and we provide the NICS(+1) value only.

thiophene (C_{2v})

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−10.4	−13.0	=	246.0	50.1	53.6

[5]sulflower (**1**, C_{5v})

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−0.4	−2.3	−3.9	200.3	−31.7	−2.1
c	0.9	−7.6	−7.9			

[6]sulflower (**2**, C_{6v})

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−2.6	−7.0	−7.2	191.2	0.3	26.6
c	3.0	0.8	−6.9			

[7]sulflower (**3**, C_{7v})

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−4.6	−8.6	−7.8	234.5	20.0	44.2
c	4.7	6.4	−0.6			

[8]sulflower (**4**, D_{8h})

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−6.9	−9.7	=	278.1	29.9	50.6
c	5.4	2.6	=			

[9]sulflower (**5**, D_{9h})

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−6.5	−9.3	=	316.9	32.1	49.5
c	2.9	4.8	=			

[10]sulflower (**6**, C_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−5.5	−8.8	−6.5	329.1	31.3	45.7
2	−5.8	−9.0	−6.4	326.5	31.3	47.8
3	−6.4	−9.0	−5.8	326.5	31.3	45.7
4	−6.5	−8.8	−6.6	329.1	31.2	47.0
5	−6.2	−9.1	−6.2	324.9	31.2	47.0
c	3.1	4.7	3.1			

[10]sulfinfinitene (**7**, C_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−7.3	−8.2	−6.5	222.2	39.4	24.9
2	−5.6	−5.9	−4.5	221.3	26.5	57.2
3	−7.2	−9.2	−6.5	190.9	32.0	34.8
4	−3.0	−0.6	0.5	165.7	39.7	7.0
5	−4.7	−5.6	−4.2	89.5	−0.3	43.9

[12]sulfinfinitene (**8**, C_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−7.5	−8.6	−7.0	203.5	33.0	42.5
2	−4.4	−7.3	−6.4	220.9	18.8	47.2
3	−4.1	−6.8	−6.1	200.2	18.2	39.5
4	−5.7	−9.1	−7.3	211.9	31.9	39.0
5	−5.7	−8.6	−7.3	232.5	35.5	44.7
6	−5.8	−8.3	−7.3	236.3	26.3	52.5

[14]sulfinfinitene (**9**, D_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−7.6	−9.3	−6.8	266.4	39.8	39.8
2	−6.8	−9.5	−6.9	270.6	27.7	48.8
3	−6.4	−9.0	−6.5	260.7	29.9	49.4
4	−6.4	−9.1	−6.4	257.3	32.8	49.4

[16]sulfinfinitene (**10**, D_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−7.6	−9.8	−7.5	283.2	42.4	42.4
2	−6.8	−10.0	−7.4	301.1	31.8	47.3
3	−6.5	−9.1	−6.2	299.9	30.8	48.1
4	−6.5	−9.0	−6.3	299.3	31.4	48.6
5	−6.3	−9.0	−6.5	299.3	31.4	49.6

[18]sulfinfinitene (**11**, D_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−7.4	−10.1	−8.1	297.3	44.5	44.5
2	−6.5	−9.7	−7.0	305.5	33.5	48.1
3	−6.6	−9.3	−6.0	319.8	33.4	46.2
4	−6.4	−8.9	−5.9	320.7	32.2	45.8
5	−6.0	−8.7	−6.0	317.7	30.1	47.1

[20]sulfinfinitene (**12**, D_2)

i	NICS(+1)	NICS(0)	NICS(−1)	$^{33}S_{(i-1)+1}$	$^{13}C_{(i-1)+2}$	$^{13}C_{(i-1)+3}$
1	−7.1	−10.0	−8.3	306.6	45.8	45.8
2	−6.3	−9.8	−7.9	307.5	31.5	48.5
3	−6.3	−9.4	−6.0	324.3	31.3	46.3
4	−6.2	−8.7	−5.2	330.7	34.0	41.4
5	−5.9	−8.2	5.3	324.2	30.6	41.7
6	−5.3	−8.2	5.9	324.2	29.1	43.9

3. Optimized Geometries and Other Computational Data

The geometries at which NICS were calculated include the coordinates of the respective ghost atoms; all coordinates are given in Å. Further computational data include the molecular point group, the total energy (E) and the lowest vibrational frequency (ν_1) with its symmetry at the optimised geometry.

3.1. B3LYP-D3(BJ)/def2-TZVP Optimised Geometries

Thiophene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_{2v} point group).
E = −553.113580 Ha, ν_1 = 465.2 cm^{-1} (b_1).

C 1.234850 -0.005850 0.000000
C 0.711130 -1.266520 0.000000
C -0.711130 -1.266520 0.000000
C -1.234850 -0.005850 0.000000
S 0.000000 1.188910 0.000000
H 2.272260 0.284860 0.000000
H 1.315590 -2.161900 0.000000
H -1.315590 -2.161900 0.000000
H -2.272260 0.284860 0.000000
Bq 0.000000 -0.271166 0.000000
Bq 0.000000 -0.271166 1.000000

[5]sulflower, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_{5v} point group).
E = −2372.098463 Ha, ν_1 = 82.6 cm^{-1} (e_2).

C 1.170693 0.380381 1.218791
C 0.723528 -0.995851 1.218791
C -0.723528 -0.995851 1.218791
C -1.170693 0.380381 1.218791
C 0.000000 1.230940 1.218791
S 0.000000 -2.741272 -0.547433
S 2.607104 -0.847100 -0.547433
S 1.611279 2.217735 -0.547433
S -1.611279 2.217735 -0.547433
S -2.607104 -0.847100 -0.547433
C 0.000000 2.177140 0.241029
C -2.070583 0.672773 0.241029
C -1.279691 -1.761343 0.241029
C 1.279691 -1.761343 0.241029
C 2.070583 0.672773 0.241029
Bq 0.000000 0.000000 1.218791
Bq 0.000000 0.000000 0.218791
Bq 0.000000 0.000000 2.218791
Bq 0.970511 1.335794 0.474441
Bq 0.548087 0.754378 -0.220910
Bq 1.392935 1.917210 1.169793

[6]sulflower, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_{6v} point group).
E = −2846.663611 Ha, ν_1 = 97.6 cm^{-1} (e_2).

C 1.233526 0.712177 1.004855
C 1.233526 -0.712177 1.004855
C 0.000000 -1.424353 1.004855
C -1.233526 -0.712177 1.004855
C -1.233526 0.712177 1.004855
C 0.000000 1.424353 1.004855
S -1.627145 -2.818297 -0.455542
S 1.627145 -2.818297 -0.455542
S 3.254289 0.000000 -0.455542
S 1.627145 2.818297 -0.455542
S -1.627145 2.818297 -0.455542
S -3.254289 0.000000 -0.455542
C 0.000000 2.536776 0.209924
C -2.196913 1.268388 0.209924
C -2.196913 -1.268388 0.209924
C 0.000000 -2.536776 0.209924
C 2.196913 -1.268388 0.209924
C 2.196913 1.268388 0.209924
Bq 0.000000 0.000000 1.004855
Bq 0.000000 0.000000 0.004855
Bq 0.000000 0.000000 2.004855
Bq 1.011517 1.751998 0.394803
Bq 0.715437 1.239173 -0.411017
Bq 1.307597 2.264824 1.200624

[7]sulflower, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_{7v} point group).
E = −3321.211101 Ha, ν_1 = 90.4 cm^{-1} (e_2).

C 0.000000 1.628511 0.648445
C 0.000000 2.901099 0.139123
C 1.273221 1.015360 0.648445
C 2.268170 1.808805 0.139123
C 1.587681 -0.362378 0.648445
C 2.828362 -0.645555 0.139123
C 1.258739 -2.613799 0.139123
C 0.706585 -1.467238 0.648445
C -0.706585 -1.467238 0.648445
C -1.258739 -2.613799 0.139123
C -1.587681 -0.362378 0.648445
C -2.828362 -0.645555 0.139123
C -1.273221 1.015360 0.648445
C -2.268170 1.808805 0.139123
S 0.000000 -3.781591 -0.295338
S -2.956567 -2.357783 -0.295338
S -3.686779 0.841483 -0.295338
S -1.640771 3.407096 -0.295338
S 1.640771 3.407096 -0.295338
S 3.686779 0.841483 -0.295338
S 2.956567 -2.357783 -0.295338
Bq 0.000000 0.000000 0.648445
Bq 0.000000 0.000000 -0.351555
Bq 0.000000 0.000000 1.648445
Bq 1.036432 2.152174 0.255960
Bq 0.870869 1.808378 -0.668374
Bq 1.201996 2.495971 1.180293

[8]sulflower, B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_{8h} point group).
E = −3795.743630 Ha, ν_1 = 59.6 cm^{-1} (a_{2u}).

C 0.000000 1.851928 0.000000
C 0.000000 -1.851928 0.000000
C 1.851928 0.000000 0.000000
C -1.851928 0.000000 0.000000
C 1.309511 1.309511 0.000000
C -1.309511 1.309511 0.000000
C 1.309511 -1.309511 0.000000
C -1.309511 -1.309511 0.000000
C -2.285849 2.285849 0.000000
C 0.000000 3.232679 0.000000
C 2.285849 2.285849 0.000000
C 3.232679 0.000000 0.000000
C 2.285849 -2.285849 0.000000
C 0.000000 -3.232679 0.000000
C -2.285849 -2.285849 0.000000
C -3.232679 0.000000 0.000000
S -3.905585 1.617746 0.000000
S -1.617746 3.905585 0.000000
S 1.617746 3.905585 0.000000
S 3.905585 1.617746 0.000000
S 3.905585 -1.617746 0.000000
S 1.617746 -3.905585 0.000000
S -1.617746 -3.905585 0.000000
S -3.905585 -1.617746 0.000000
Bq 0.000000 0.000000 0.000000
Bq 0.000000 0.000000 1.000000
Bq -1.042621 2.517110 0.000000
Bq -1.042621 2.517110 1.000000

[9]sulflower, B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_{9h} point group).
E = −4270.213348 Ha, ν_1 = 44.2 cm^{-1} (e_2'').

C	0.000000	2.114995	0.000000
C	0.000000	3.511508	0.000000
C	1.359492	1.620180	0.000000
S	-1.551686	4.263223	0.000000
S	1.551686	4.263223	0.000000
C	-1.359492	1.620180	0.000000
C	2.082863	0.367265	0.000000
C	2.257154	2.689971	0.000000
C	-2.257154	2.689971	0.000000
C	-2.082863	0.367265	0.000000
C	1.831639	-1.057497	0.000000
C	3.458161	0.609767	0.000000
S	3.929007	2.268413	0.000000
S	-3.929007	2.268413	0.000000
C	-1.831639	-1.057497	0.000000
C	-3.458161	0.609767	0.000000
C	0.723371	-1.987445	0.000000
C	3.041055	-1.755754	0.000000
S	4.467902	-0.787812	0.000000
C	-3.041055	-1.755754	0.000000
C	-0.723371	-1.987445	0.000000
S	-4.467902	-0.787812	0.000000
C	1.201007	-3.299738	0.000000
S	2.916216	-3.475411	0.000000
S	-2.916216	-3.475411	0.000000
C	-1.201007	-3.299738	0.000000
S	0.000000	-4.536827	0.000000
Bq	0.000000	0.000000	0.000000
Bq	0.000000	0.000000	1.000000
Bq	-1.033666	2.839975	0.000000
Bq	-1.033666	2.839975	1.000000

[10]sulflower, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_2 point group).
$E = -4744.620767$ Ha, $\nu_1 = 0.9$ cm^{-1} (*a*).

C	0.000035	2.366634	-0.000281
C	0.000035	3.770145	-0.000567
S	-1.451934	4.569724	0.417246
C	-1.374351	1.903131	0.263643
C	-2.175681	3.023440	0.534457
S	-3.863787	2.783481	0.678023
C	-2.247129	0.718810	0.163295
C	-3.577506	1.133936	0.330236
C	-2.247199	-0.718725	-0.162841
S	-4.814720	0.000053	0.000718
C	-3.577642	-1.133823	-0.329315
S	-3.864044	-2.783244	-0.677574
C	-1.374461	-1.903021	-0.263816
C	-2.175871	-3.023229	-0.534810
C	-0.000035	-2.366634	-0.000281
S	-1.452085	-4.569558	-0.418413
C	-0.000035	-3.770145	-0.000567
C	1.374351	-1.903131	0.263643
S	1.451934	-4.569724	0.417246
C	2.175681	-3.023440	0.534457
C	2.247129	-0.718810	0.163295
S	3.863787	-2.783481	0.678023
C	3.577506	-1.133936	0.330236
S	4.814720	-0.000053	0.000718
C	2.247199	0.718725	-0.162841
C	3.577642	1.133823	-0.329315
C	1.374461	1.903021	-0.263816
S	3.864044	2.783244	-0.677574
C	2.175871	3.023229	-0.534810
S	1.452085	4.569558	-0.418413

Bq	0.000000	0.000000	0.000000
Bq	0.000000	0.000000	-1.000000
Bq	0.000000	0.000000	1.000000
Bq	-3.292839	0.000050	0.000419
Bq	-3.293020	0.262966	-0.964400
Bq	-3.292659	-0.262865	0.965237
Bq	-2.647691	1.912560	0.393931
Bq	-2.743733	2.083199	-0.586711
Bq	-2.551649	1.741920	1.374573
Bq	-1.000379	3.126615	0.242900
Bq	-1.237087	3.164355	-0.727948
Bq	-0.763671	3.088874	1.213747
Bq	1.000497	3.126517	-0.243577
Bq	0.763988	3.088401	-1.214459
Bq	1.237007	3.164634	0.727304
Bq	2.647843	1.912408	-0.393671
Bq	2.552189	1.741433	-1.374292
Bq	2.743498	2.083384	0.586950

[10]sulfinfinitene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_2 point group).
E = −4744.241584 Ha, ν_1 = 43.7 cm^{-1} (*a*).

C	-2.658210	-0.374978	-1.479881
C	-3.504215	1.871177	-0.708880
C	-2.248020	3.662707	0.555213
C	-1.438677	2.792011	-0.165217
C	-2.166364	1.619766	-0.457070
C	-1.894084	0.218273	-0.495410
C	-1.160153	-0.769807	0.251409
C	-0.924411	-1.873442	-0.521811
C	0.018143	-2.755812	0.120395
C	-0.018143	-2.715845	1.486917
C	1.438677	-2.792011	-0.165217
C	2.248020	-3.662707	0.555213
C	2.166364	-1.619766	-0.457070
C	3.504215	-1.871177	-0.708880
C	1.894084	-0.218273	-0.495410
C	2.658210	0.374978	-1.479881
C	1.160153	0.769807	0.251409
C	0.924411	1.873442	-0.521811
C	-0.018143	2.755812	0.120395
C	0.018143	2.715845	1.486917
S	-3.959428	3.341251	0.124703
S	-1.400882	3.668380	2.158111
S	-4.094905	0.617590	-1.829567
S	-2.007363	-1.948729	-1.909704
S	0.869607	1.246195	1.986833
S	-0.869607	-1.246195	1.986833
S	1.400882	-3.668380	2.158111
S	3.959428	-3.341251	0.124703
S	4.094905	-0.617590	-1.829567
S	2.007363	1.948729	-1.909704
Bq	-1.728844	-0.949737	-0.831079
Bq	-1.005863	-0.567754	-1.406743
Bq	-2.451825	-1.331719	-0.255416
Bq	-2.863556	0.790366	-0.994162
Bq	-2.405697	1.148161	-1.808009
Bq	-3.321414	0.432570	-0.180314
Bq	-2.663341	2.657382	-0.130250
Bq	-2.597956	3.118852	-1.014993
Bq	-2.728725	2.195912	0.754493
Bq	-1.017516	3.118951	0.831084
Bq	-0.661203	3.982680	0.474693
Bq	-1.373828	2.255222	1.187474
Bq	0.590834	1.872220	0.664749
Bq	-0.241749	1.370399	0.430269

Bq 1.423418 2.374041 0.899228

[12]sulfinfinitene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (C_2 point group).
E = −5693.375549 Ha, ν_1 = 40.5 cm^{-1} (a).

C 1.808128 1.211768 1.838846
C 1.405559 3.705992 1.714866
C -0.005030 4.925241 -0.026681
C -1.570084 3.799024 -1.673709
C -0.822740 2.953696 -0.894708
C 0.238694 3.595506 -0.242413
C 1.250994 3.013982 0.543107
C 1.696209 1.669012 0.541926
C 1.716679 0.612040 -0.426112
C 1.392540 -0.592029 0.150636
C 1.345901 -1.643187 -0.816113
C 2.086153 -1.345124 -1.940036
C 0.822740 -2.953696 -0.894708
C 1.570084 -3.799024 -1.673709
C -0.238694 -3.595506 -0.242413
C 0.005030 -4.925241 -0.026681
C -1.250994 -3.013982 0.543107
C -1.405559 -3.705992 1.714866
C -1.696209 -1.669012 0.541926
C -1.808128 -1.211768 1.838846
C -1.716679 -0.612040 -0.426112
C -1.392540 0.592029 0.150636
C -1.345901 1.643187 -0.816113
C -2.086153 1.345124 -1.940036
S 0.704623 5.349539 1.552930
S -1.274810 5.474198 -1.156829
S -2.548028 2.829674 -2.795924
S 1.784492 2.553931 3.005840
S 1.570084 -0.528487 1.913782
S -2.364883 -0.390583 -2.058402
S 2.364883 0.390583 -2.058402
S 2.548028 -2.829674 -2.795924
S 1.274810 -5.474198 -1.156829
S -0.704623 -5.349539 1.552930
S -1.784492 -2.553931 3.005840
S -1.570084 0.528487 1.913782
Bq 1.636728 0.474461 0.803816
Bq 2.607973 0.342079 0.605930
Bq 0.665483 0.606843 1.001701
Bq 1.589076 2.430937 1.528917
Bq 2.555892 2.620673 1.357840
Bq 0.622261 2.241201 1.699994
Bq 0.718968 4.118052 0.708362
Bq 1.516373 4.464160 0.214039
Bq -0.078437 3.771944 1.202684
Bq -0.686794 4.149533 -0.798868
Bq -0.046112 4.236717 -1.561709
Bq -1.327476 4.062349 -0.036027
Bq -1.674581 2.514141 -1.624098
Bq -0.914381 2.364681 -2.256361
Bq -2.434782 2.663601 -0.991835
Bq -1.781231 0.515543 -1.018005
Bq -0.878173 0.337864 -1.409051
Bq -2.684289 0.693223 -0.626960

[14]sulfinfinitene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_2 point group).
E = −6642.461401 Ha, ν_1 = 37.6 cm^{-1} (b_2).

C -1.790783 2.111801 0.870351
C -1.568527 2.463766 3.317832
C 0.642515 -1.072564 5.170748

C 1.568527 -2.463766 3.317832
C 1.161706 -1.213814 2.899778
C 0.451166 -0.539751 3.916461
C -1.161706 1.213814 2.899778
C -1.478975 0.940148 1.542222
C -1.515598 -0.186183 0.664954
C -1.515598 0.186183 -0.664954
C -1.478975 -0.940148 -1.542222
C -1.790783 -2.111801 -0.870351
C -1.161706 -1.213814 -2.899778
C -1.568527 -2.463766 -3.317832
C 0.451166 0.539751 -3.916461
C 0.642515 1.072564 -5.170748
C 1.161706 1.213814 -2.899778
C 1.568527 2.463766 -3.317832
C 1.478975 0.940148 -1.542222
C 1.790783 2.111801 -0.870351
C 1.515598 -0.186183 -0.664954
C 1.515598 0.186183 0.664954
C 1.478975 -0.940148 1.542222
C 1.790783 -2.111801 0.870351
S -1.413924 2.652856 5.064294
S 1.413924 -2.652856 5.064294
S 2.024335 -3.471227 1.955329
S -2.024335 3.471227 1.955329
S -1.779892 1.911557 -0.864601
S 1.779892 -1.911557 -0.864601
S -1.779892 -1.911557 0.864601
S -2.024335 -3.471227 -1.955329
S -1.413924 -2.652856 -5.064294
S 1.413924 2.652856 -5.064294
S 2.024335 3.471227 -1.955329
S 1.779892 1.911557 0.864601
C -0.451166 -0.539751 -3.916461
C -0.642515 -1.072564 -5.170748
S 0.000000 0.000000 -6.416951
C -0.451166 0.539751 3.916461
C -0.642515 1.072564 5.170748
S 0.000000 0.000000 6.416951
Bq 1.616169 0.992701 -0.309594
Bq 2.600485 0.865684 -0.432027
Bq 0.631854 1.119718 -0.187161
Bq 1.604865 2.040151 -2.117102
Bq 2.552413 1.779080 -2.301477
Bq 0.657317 2.301223 -1.932728
Bq 1.047568 1.588550 -4.073823
Bq 1.924302 1.143753 -4.256833
Bq 0.170834 2.033348 -3.890812
Bq 0.000000 0.000000 -4.918274
Bq -0.839630 0.543159 -4.918274
Bq 0.839630 -0.543159 -4.918274
Bq -1.047568 -1.588550 -4.073823
Bq -1.924302 -1.143753 -4.256833
Bq -0.170834 -2.033348 -3.890812
Bq -1.604865 -2.040151 -2.117102
Bq -2.552413 -1.779080 -2.301477
Bq -0.657317 -2.301223 -1.932728
Bq -1.616169 -0.992701 -0.309594
Bq -2.600485 -0.865684 -0.432027
Bq -0.631854 -1.119718 -0.187161

[16]sulfinfinitene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_2 point group).
$E = -7591.464772$ Ha, $\nu_1 = 35.7$ cm^{-1} (*a*).

C -1.704767 2.217862 0.491074
C -1.476735 3.020889 2.783768

C	0.000000	0.000000	5.834711
C	1.476735	-3.020889	2.783768
C	1.189829	-1.663987	2.696135
C	0.000000	0.000000	4.443654
C	-1.189829	1.663987	2.696135
C	-1.474355	1.171628	1.380723
C	-1.541302	-0.073549	0.690238
C	-1.541302	0.073549	-0.690238
C	-1.474355	-1.171628	-1.380723
C	-1.704767	-2.217862	-0.491074
C	-1.189829	-1.663987	-2.696135
C	-1.476735	-3.020889	-2.783768
C	0.659247	1.173540	-3.937605
C	0.848520	2.106127	-4.952343
C	1.189829	1.663987	-2.696135
C	1.476735	3.020889	-2.783768
C	1.474355	1.171628	-1.380723
C	1.704767	2.217862	-0.491074
C	1.541302	-0.073549	-0.690238
C	1.541302	0.073549	0.690238
C	1.474355	-1.171628	1.380723
C	1.704767	-2.217862	0.491074
S	-1.390902	3.661088	4.396679
S	1.390902	-3.661088	4.396679
S	1.810256	-3.774730	1.252782
S	-1.810256	3.774730	1.252782
S	-1.763334	1.736306	-1.174164
S	1.763334	-1.736306	-1.174164
S	-1.763334	-1.736306	1.174164
S	-1.810256	-3.774730	-1.252782
S	-1.390902	-3.661088	-4.396679
S	1.390902	3.661088	-4.396679
S	1.810256	3.774730	-1.252782
S	1.763334	1.736306	1.174164
C	0.000000	0.000000	-4.443654
C	0.000000	0.000000	-5.834711
S	0.518195	1.498354	-6.546717
C	-0.659247	1.173540	3.937605
C	-0.848520	2.106127	4.952343
S	-0.518195	1.498354	6.546717
C	0.659247	-1.173540	3.937605
C	0.848520	-2.106127	4.952343
S	0.518195	-1.498354	6.546717
C	-0.659247	-1.173540	-3.937605
C	-0.848520	-2.106127	-4.952343
S	-0.518195	-1.498354	-6.546717
Bq	1.605012	1.025159	-0.139527
Bq	2.596611	0.945140	-0.241160
Bq	0.613413	1.105178	-0.037893
Bq	1.531188	2.369819	-1.720896
Bq	2.503261	2.229689	-1.909147
Bq	0.559116	2.509950	-1.532646
Bq	1.113047	2.325126	-3.753306
Bq	2.050353	2.039938	-3.953617
Bq	0.175740	2.610314	-3.552995
Bq	0.405192	0.955604	-5.143006
Bq	1.324885	0.577802	-5.249921
Bq	-0.514500	1.333407	-5.036091
Bq	-0.405192	-0.955604	-5.143006
Bq	-1.324885	-0.577802	-5.249921
Bq	0.514500	-1.333407	-5.036091
Bq	-1.113047	-2.325126	-3.753306
Bq	-2.050353	-2.039938	-3.953617
Bq	-0.175740	-2.610314	-3.552995
Bq	-1.531188	-2.369819	-1.720896
Bq	-2.503261	-2.229689	-1.909147
Bq	-0.559116	-2.509950	-1.532646

Bq -1.605012 -1.025159 -0.139527
Bq -2.596611 -0.945140 -0.241160
Bq -0.613413 -1.105178 -0.037893

[18]sulfinfinitene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_2 point group).
E = −8540.390054 Ha, ν_1 = 29.7 cm^{-1} (b_2).

C -1.713641 2.255598 0.122952
C -1.418248 3.426872 2.213527
C 0.241834 -1.167775 5.940893
C 1.418248 -3.426872 2.213527
C 1.213612 -2.060113 2.408654
C 0.230810 -0.703343 4.618588
C -1.213612 2.060113 2.408654
C -1.504490 1.369703 1.181640
C -1.579729 0.037280 0.694154
C -1.579729 -0.037280 -0.694154
C -1.504490 -1.369703 -1.181640
C -1.713641 -2.255598 -0.122952
C -1.213612 -2.060113 -2.408654
C -1.418248 -3.426872 -2.213527
C 0.726135 1.789742 -3.754589
C 0.808469 2.977772 -4.489801
C 1.213612 2.060113 -2.408654
C 1.418248 3.426872 -2.213527
C 1.504490 1.369703 -1.181640
C 1.713641 2.255598 -0.122952
C 1.579729 0.037280 -0.694154
C 1.579729 -0.037280 0.694154
C 1.504490 -1.369703 1.181640
C 1.713641 -2.255598 0.122952
S -1.229639 4.405598 3.617459
S 1.229639 -4.405598 3.617459
S 1.767954 -3.916342 0.590820
S -1.767954 3.916342 0.590820
S -1.806182 1.516692 -1.437658
S 1.806182 -1.516692 -1.437658
S -1.806182 -1.516692 1.437658
S -1.767954 -3.916342 -0.590820
S -1.229639 -4.405598 -3.617459
S 1.229639 4.405598 -3.617459
S 1.767954 3.916342 -0.590820
S 1.806182 1.516692 1.437658
C 0.230810 0.703343 -4.618588
C 0.241834 1.167775 -5.940893
S 0.558650 2.840994 -6.184535
C -0.726135 1.789742 3.754589
C -0.808469 2.977772 4.489801
S -0.558650 2.840994 6.184535
C 0.726135 -1.789742 3.754589
C 0.808469 -2.977772 4.489801
S 0.558650 -2.840994 6.184535
C -0.726135 -1.789742 -3.754589
C -0.808469 -2.977772 -4.489801
S -0.558650 -2.840994 -6.184535
C -0.230810 0.703343 4.618588
C -0.241834 1.167775 5.940893
S 0.000000 0.000000 7.177716
C -0.230810 -0.703343 -4.618588
C -0.241834 -1.167775 -5.940893
S 0.000000 0.000000 -7.177716
Bq 1.636754 1.028399 0.026613
Bq 2.628796 0.968938 -0.084369
Bq 0.644712 1.087859 0.137595
Bq 1.523589 2.605726 -1.303519
Bq 2.499304 2.535597 -1.511035

Bq 0.547874 2.675854 -1.096003
Bq 1.079221 2.932019 -3.296806
Bq 2.033834 2.777057 -3.551170
Bq 0.124608 3.086982 -3.042442
Bq 0.513180 1.895925 -4.997681
Bq 1.474808 1.669189 -5.152155
Bq -0.448448 2.122662 -4.843207
Bq 0.000000 0.000000 -5.659336
Bq 0.969849 -0.243706 -5.659336
Bq -0.969849 0.243706 -5.659336
Bq -0.513180 -1.895925 -4.997681
Bq -1.474808 -1.669189 -5.152155
Bq 0.448448 -2.122662 -4.843207
Bq -1.079221 -2.932019 -3.296806
Bq -2.033834 -2.777057 -3.551170
Bq -0.124608 -3.086982 -3.042442
Bq -1.523589 -2.605726 -1.303519
Bq -2.499304 -2.535597 -1.511035
Bq -0.547874 -2.675854 -1.096003
Bq -1.636754 -1.028399 0.026613
Bq -2.628796 -0.968938 -0.084369
Bq -0.644712 -1.087859 0.137595

[20]sulfinfinitene, B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_2 point group). $E = -9489.266271$ Ha, $\nu_1 = 20.1$ cm^{-1} (b_3).

C -1.768008 2.236268 -0.249180
C -1.378216 3.732607 1.591318
C -0.018537 -2.251059 5.604451
C 1.378216 -3.732607 1.591318
C 1.215508 -2.415166 2.033433
C 0.189543 -1.445546 4.473110
C -1.215508 2.415166 2.033433
C -1.549618 1.540254 0.942157
C -1.617159 0.149920 0.677998
C -1.617159 -0.149920 -0.677998
C -1.549618 -1.540254 -0.942157
C -1.768008 -2.236268 0.249180
C -1.215508 -2.415166 -2.033433
C -1.378216 -3.732607 -1.591318
C 0.639895 2.368624 -3.382520
C 0.524301 3.697742 -3.815143
C 1.215508 2.415166 -2.033433
C 1.378216 3.732607 -1.591318
C 1.549618 1.540254 -0.942157
C 1.768008 2.236268 0.249180
C 1.617159 0.149920 -0.677998
C 1.617159 -0.149920 0.677998
C 1.549618 -1.540254 0.942157
C 1.768008 -2.236268 -0.249180
S -0.952468 4.951970 2.717770
S 0.952468 -4.951970 2.717770
S 1.782036 -3.948756 -0.073885
S -1.782036 3.948756 -0.073885
S -1.848062 1.252513 -1.666989
S 1.848062 -1.252513 -1.666989
S -1.848062 -1.252513 1.666989
S -1.782036 -3.948756 0.073885
S -0.952468 -4.951970 -2.717770
S 0.952468 4.951970 -2.717770
S 1.782036 3.948756 0.073885
S 1.848062 1.252513 1.666989
C 0.189543 1.445546 -4.473110
C -0.018537 2.251059 -5.604451
S 0.063881 3.954974 -5.440845
C -0.639895 2.368624 3.382520

C -0.524301 3.697742 3.815143
S -0.063881 3.954974 5.440845
C 0.639895 -2.368624 3.382520
C 0.524301 -3.697742 3.815143
S 0.063881 -3.954974 5.440845
C -0.639895 -2.368624 -3.382520
C -0.524301 -3.697742 -3.815143
S -0.063881 -3.954974 -5.440845
C 0.000000 0.000000 4.898160
C 0.000000 0.000000 6.302856
S -0.129691 -1.489420 7.129392
C -0.189543 -1.445546 -4.473110
C 0.018537 -2.251059 -5.604451
S 0.129691 -1.489420 -7.129392
C 0.000000 0.000000 -4.898160
C 0.000000 0.000000 -6.302856
S -0.129691 1.489420 -7.129392
S 0.129691 1.489420 7.129392
C -0.189543 1.445546 4.473110
C 0.018537 2.251059 5.604451
Bq 1.680001 1.005807 0.194802
Bq 2.671788 0.954011 0.077858
Bq 0.688214 1.057603 0.311747
Bq 1.538677 2.774610 -0.848769
Bq 2.509500 2.767346 -1.088458
Bq 0.567855 2.781874 -0.609079
Bq 0.942078 3.433222 -2.708037
Bq 1.871716 3.421949 -3.076337
Bq 0.012439 3.444494 -2.339736
Bq 0.279817 2.743589 -4.543214
Bq 1.236999 2.696433 -4.828832
Bq -0.677366 2.790745 -4.257595
Bq 0.008263 1.037205 -5.681594
Bq 1.000268 1.030700 -5.807621
Bq -0.983742 1.043710 -5.555567
Bq -0.008263 -1.037205 -5.681594
Bq -1.000268 -1.030700 -5.807621
Bq 0.983742 -1.043710 -5.555567
Bq -0.279817 -2.743589 -4.543214
Bq -1.236999 -2.696433 -4.828832
Bq 0.677366 -2.790745 -4.257595
Bq -0.942078 -3.433222 -2.708037
Bq -1.871716 -3.421949 -3.076337
Bq -0.012439 -3.444494 -2.339736
Bq -1.538677 -2.774610 -0.848769
Bq -2.509500 -2.767346 -1.088458
Bq -0.567855 -2.781874 -0.609079
Bq -1.680001 -1.005807 0.194802
Bq -2.671788 -0.954011 0.077858
Bq -0.688214 -1.057603 0.311747

Coronene B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_{6h} point group).
$E = -922.314589$ Ha, $\nu_1 = 88.3$ cm^{-1} (e_{2u}).

C 1.243391 3.519811 0.000000
C 0.000000 2.837004 0.000000
C 0.000000 1.421690 0.000000
C 1.231219 0.710845 0.000000
C 2.456917 1.418502 0.000000
C 2.426550 2.836714 0.000000
C -1.231219 0.710845 0.000000
C 1.231219 -0.710845 0.000000
C 0.000000 -1.421690 0.000000
C -1.231219 -0.710845 0.000000
C 0.000000 -2.837004 0.000000
C 1.243391 -3.519811 0.000000

C 2.426550 -2.836714 0.000000
C 2.456917 -1.418502 0.000000
C 3.669941 -0.683097 0.000000
C 3.669941 0.683097 0.000000
H 4.606336 1.227561 0.000000
H 4.606336 -1.227561 0.000000
H 1.240069 4.602984 0.000000
H 3.366267 3.375423 0.000000
H 1.240069 -4.602984 0.000000
H 3.366267 -3.375423 0.000000
C -1.243391 3.519811 0.000000
C -2.426550 2.836714 0.000000
C -2.456917 1.418502 0.000000
H -1.240069 4.602984 0.000000
H -3.366267 3.375423 0.000000
C -3.669941 0.683097 0.000000
C -3.669941 -0.683097 0.000000
C -2.456917 -1.418502 0.000000
H -4.606336 1.227561 0.000000
H -4.606336 -1.227561 0.000000
C -1.243391 -3.519811 0.000000
H -1.240069 -4.602984 0.000000
C -2.426550 -2.836714 0.000000
H -3.366267 -3.375423 0.000000

Infinitene B3LYP-D3(BJ)/def2-TZVP optimised geometry (D_2 point group).
$E = -1844.504076$ Ha, $\nu_1 = 44.9$ cm^{-1} (*a*).

C -1.751819 1.321321 -1.284340
C -1.882779 2.419774 -0.497760
C -1.573082 2.364814 0.887153
C -1.580643 3.553715 1.651948
C -1.310672 3.504761 2.980415
C -0.891356 2.298477 3.597920
C -0.670568 2.309784 4.998240
C -0.334106 1.166862 5.639257
C 0.000000 0.000000 4.903416
C 0.334106 -1.166862 5.639257
C 0.670568 -2.309784 4.998240
C 0.891356 -2.298477 3.597920
C 0.717872 -1.105283 2.837502
C 0.000000 0.000000 3.478873
C -0.717872 1.105283 2.837502
C -1.257210 1.123468 1.496551
C -1.479497 -0.055250 0.705390
C -1.751819 -1.321321 1.284340
C -1.479497 0.055250 -0.705390
C -1.882779 -2.419774 0.497760
C -1.257210 -1.123468 -1.496551
C -1.573082 -2.364814 -0.887153
C -0.717872 -1.105283 -2.837502
C -1.580643 -3.553715 -1.651948
C -0.891356 -2.298477 -3.597920
C 0.000000 0.000000 -3.478873
C -1.310672 -3.504761 -2.980415
C -0.670568 -2.309784 -4.998240
C 0.000000 0.000000 -4.903416
C 0.717872 1.105283 -2.837502
C -0.334106 -1.166862 -5.639257
C 0.334106 1.166862 -5.639257
C 0.891356 2.298477 -3.597920
C 1.257210 1.123468 -1.496551
C 0.670568 2.309784 -4.998240
C 1.310672 3.504761 -2.980415
C 1.573082 2.364814 -0.887153
C 1.580643 3.553715 -1.651948

C 1.479497 -0.055250 -0.705390
C 1.479497 0.055250 0.705390
C 1.310672 -3.504761 2.980415
C 1.751819 1.321321 1.284340
C 1.882779 2.419774 0.497760
C 1.257210 -1.123468 1.496551
C 1.882779 -2.419774 -0.497760
C 1.751819 -1.321321 -1.284340
C 1.580643 -3.553715 1.651948
C 1.573082 -2.364814 0.887153
H -2.163029 3.373338 -0.926233
H -1.840292 4.486125 1.166842
H -1.386217 4.392137 3.596320
H -0.840828 3.230133 5.542218
H -0.264847 1.128860 6.718953
H 0.264847 -1.128860 6.718953
H 0.840828 -3.230133 5.542218
H -2.163029 -3.373338 0.926233
H -1.840292 -4.486125 -1.166842
H -1.386217 -4.392137 -3.596320
H -0.840828 -3.230133 -5.542218
H -0.264847 -1.128860 -6.718953
H 0.264847 1.128860 -6.718953
H 0.840828 3.230133 -5.542218
H 1.386217 4.392137 -3.596320
H 1.840292 4.486125 -1.166842
H -1.901703 -1.390447 2.350576
H -1.901703 1.390447 -2.350576
H 1.901703 1.390447 2.350576
H 2.163029 3.373338 0.926233
H 1.901703 -1.390447 -2.350576
H 1.386217 -4.392137 3.596320
H 1.840292 -4.486125 1.166842
H 2.163029 -3.373338 -0.926233

3.2. M06-2X/def2-TZVP Optimised Geometries

Thiophene, M06-2X/def2-TZVP optimised geometry (C_{2v} point group).
E = −552.993191 Ha, ν_1 = 469.9 cm^{-1} (b_1).

C 1.229244 -0.003225 0.000000
C 0.710926 -1.262019 0.000000
C -0.710926 -1.262019 0.000000
C -1.229244 -0.003225 0.000000
S -0.000000 1.182270 0.000000
H 2.266430 0.289121 0.000000
H 1.317306 -2.155819 0.000000
H -1.317306 -2.155819 0.000000
H -2.266430 0.289121 0.000000

[5]sulflower, M06-2X/def2-TZVP optimised geometry (C_{5v} point group).
E = −2371.753340 Ha, ν_1 = 93.7 cm^{-1} (e_2).

C 1.170445 0.380301 1.211550
C 0.723375 -0.995640 1.211550
C -0.723375 -0.995640 1.211550
C -1.170445 0.380301 1.211550
C 0.000000 1.230678 1.211550
S 0.000000 -2.734283 -0.541997
S 2.600457 -0.844940 -0.541997
S 1.607171 2.212081 -0.541997
S -1.607171 2.212081 -0.541997
S -2.600457 -0.844940 -0.541997
C 0.000000 2.165889 0.233775
C -2.059883 0.669297 0.233775

C -1.273078 -1.752241 0.233775
C 1.273078 -1.752241 0.233775
C 2.059883 0.669297 0.233775

[6]sulflower, M06-2X/def2-TZVP optimised geometry (C_{6v} point group).
E = −2846.253198 Ha, ν_1 = 102.2 cm^{-1} (e_2).

C 1.233429 0.712121 0.995820
C 1.233429 -0.712121 0.995820
C 0.000000 -1.424241 0.995820
C -1.233429 -0.712121 0.995820
C -1.233429 0.712121 0.995820
C 0.000000 1.424241 0.995820
S -1.622857 -2.810871 -0.449032
S 1.622857 -2.810871 -0.449032
S 3.245714 0.000000 -0.449032
S 1.622857 2.810871 -0.449032
S -1.622857 2.810871 -0.449032
S -3.245714 0.000000 -0.449032
C 0.000000 2.526987 0.201599
C -2.188435 1.263494 0.201599
C -2.188435 -1.263494 0.201599
C 0.000000 -2.526987 0.201599
C 2.188435 -1.263494 0.201599
C 2.188435 1.263494 0.201599

[7]sulflower, M06-2X/def2-TZVP optimised geometry (C_{7v} point group).
E = −3320.736133 Ha, ν_1 = 93.0 cm^{-1} (e_2).

C 0.000000 1.628107 0.638331
C 0.000000 2.892795 0.132061
C 1.272905 1.015108 0.638331
C 2.261678 1.803628 0.132061
C 1.587287 -0.362288 0.638331
C 2.820267 -0.643707 0.132061
C 1.255137 -2.606318 0.132061
C 0.706409 -1.466874 0.638331
C -0.706409 -1.466874 0.638331
C -1.255137 -2.606318 0.132061
C -1.587287 -0.362288 0.638331
C -2.820267 -0.643707 0.132061
C -1.272905 1.015108 0.638331
C -2.261678 1.803628 0.132061
S 0.000000 -3.769394 -0.288897
S -2.947031 -2.350179 -0.288897
S -3.674888 0.838769 -0.288897
S -1.635479 3.396107 -0.288897
S 1.635479 3.396107 -0.288897
S 3.674888 0.838769 -0.288897
S 2.947031 -2.350179 -0.288897

[8]sulflower, M06-2X/def2-TZVP optimised geometry (D_{8h} point group).
E = −3795.203337 Ha, ν_1 = 59.8 cm^{-1} (a_{2u}).

C 0.000000 1.851648 0.000000
C 0.000000 -1.851648 0.000000
C 1.851648 0.000000 0.000000
C -1.851648 0.000000 0.000000
C 1.309313 1.309313 0.000000
C -1.309313 1.309313 0.000000
C 1.309313 -1.309313 0.000000
C -1.309313 -1.309313 0.000000
C -2.279098 2.279098 0.000000
C 0.000000 3.223131 0.000000
C 2.279098 2.279098 0.000000

C 3.223131 0.000000 0.000000
C 2.279098 -2.279098 0.000000
C 0.000000 -3.223131 0.000000
C -2.279098 -2.279098 0.000000
C -3.223131 0.000000 0.000000
S -3.889742 1.611184 0.000000
S -1.611184 3.889742 0.000000
S 1.611184 3.889742 0.000000
S 3.889742 1.611184 0.000000
S 3.889742 -1.611184 0.000000
S 1.611184 -3.889742 0.000000
S -1.611184 -3.889742 0.000000
S -3.889742 -1.611184 0.000000

[9]sulflower, M06-2X/def2-TZVP optimised geometry (D_{9h} point group).
E = −4269.607518 Ha, ν_1 = 46.3 cm^{-1} (e_2'').

C 0.000000 2.114329 0.000000
C 0.000000 3.499683 0.000000
C 1.359064 1.619670 0.000000
S -1.546052 4.247744 0.000000
S 1.546052 4.247744 0.000000
C -1.359064 1.619670 0.000000
C 2.082208 0.367149 0.000000
C 2.249553 2.680913 0.000000
C -2.249553 2.680913 0.000000
C -2.082208 0.367149 0.000000
C 1.831063 -1.057164 0.000000
C 3.446515 0.607714 0.000000
S 3.914742 2.260177 0.000000
S -3.914742 2.260177 0.000000
C -1.831063 -1.057164 0.000000
C -3.446515 0.607714 0.000000
C 0.723143 -1.986819 0.000000
C 3.030814 -1.749842 0.000000
S 4.451680 -0.784951 0.000000
C -3.030814 -1.749842 0.000000
C -0.723143 -1.986819 0.000000
S -4.451680 -0.784951 0.000000
C 1.196962 -3.288626 0.000000
S 2.905628 -3.462792 0.000000
S -2.905628 -3.462792 0.000000
C -1.196962 -3.288626 0.000000
S 0.000000 -4.520355 0.000000

[10]sulflower, M06-2X/def2-TZVP optimised geometry (D_2 point group).
E = −4743.949806 Ha, ν_1 = 1.6 cm^{-1} (b_3).

C 0.000000 0.000000 2.389710
C 0.000000 0.000000 3.783102
S -0.162939 1.487242 4.592571
C -0.100929 1.402209 1.931631
C -0.205073 2.217727 3.056635
S -0.263830 3.903148 2.832213
C -0.062155 2.272238 0.736648
C -0.126090 3.596755 1.164567
C 0.062155 2.272238 -0.736648
S 0.000000 4.830429 0.000000
C 0.126090 3.596755 -1.164567
S 0.263830 3.903148 -2.832213
C 0.100929 1.402209 -1.931631
C 0.205073 2.217727 -3.056635
C 0.000000 0.000000 -2.389710
S 0.162939 1.487242 -4.592571
C 0.000000 0.000000 -3.783102
C -0.100929 -1.402209 -1.931631

S -0.162939 -1.487242 -4.592571
C -0.205073 -2.217727 -3.056635
C -0.062155 -2.272238 -0.736648
S -0.263830 -3.903148 -2.832213
C -0.126090 -3.596755 -1.164567
S 0.000000 -4.830429 0.000000
C 0.062155 -2.272238 0.736648
C 0.126090 -3.596755 1.164567
C 0.100929 -1.402209 1.931631
S 0.263830 -3.903148 2.832213
C 0.205073 -2.217727 3.056635
S 0.162939 -1.487242 4.592571

[10]sulfinfinitene, M06-2X/def2-TZVP optimised geometry (C_2 point group).
E = −4743.549160 Ha, ν_1 = 32.7 cm^{-1} (*a*).

C 1.971651 -2.075895 -1.465812
C 0.432421 -3.991630 -0.981757
C -1.426121 -3.740607 0.770988
C -1.399636 -2.739278 -0.145233
C -0.096947 -2.754076 -0.729787
C 0.940776 -1.794184 -0.600176
C 1.249559 -0.618169 0.177608
C 1.964412 0.261486 -0.564981
C 2.071091 1.513831 0.159289
C 2.052475 1.376794 1.516269
C 1.399636 2.739278 -0.145233
C 1.426121 3.740607 0.770988
C 0.096947 2.754076 -0.729787
C -0.432421 3.991630 -0.981757
C -0.940776 1.794184 -0.600176
C -1.971651 2.075895 -1.465812
C -1.249559 0.618169 0.177608
C -1.964412 -0.261486 -0.564981
C -2.071091 -1.513831 0.159289
C -2.052475 -1.376794 1.516269
S -0.320932 -5.064601 0.226048
S -1.874582 -2.980129 2.307997
S 1.971651 -3.790320 -1.833275
S 2.750352 -0.554889 -1.923955
S -1.537164 0.255095 1.922032
S 1.537164 -0.255095 1.922032
S 1.874582 2.980129 2.307997
S 0.320932 5.064601 0.226048
S -1.971651 3.790320 -1.833275
S -2.750352 0.554889 -1.923955

[12]sulfinfinitene, M06-2X/def2-TZVP optimised geometry (C_2 point group).
E = −5692.552118 Ha, ν_1 = 41.3 cm^{-1} (*a*).

C 1.800857 1.207381 1.831157
C 1.417539 3.696439 1.706820
C -0.001464 4.915214 -0.015473
C -1.555489 3.801466 -1.673127
C -0.824367 2.957561 -0.892613
C 0.235563 3.594005 -0.231590
C 1.247700 3.004632 0.546978
C 1.683876 1.655618 0.541694
C 1.715218 0.596881 -0.427491
C 1.403445 -0.595818 0.157813
C 1.354634 -1.649416 -0.809865
C 2.089455 -1.357333 -1.927791
C 0.824367 -2.957561 -0.892613
C 1.555489 -3.801466 -1.673127
C -0.235563 -3.594005 -0.231590
C 0.001464 -4.915214 -0.015473

C	-1.247700	-3.004632	0.546978
C	-1.417539	-3.696439	1.706820
C	-1.683876	-1.655618	0.541694
C	-1.800857	-1.207381	1.831157
C	-1.715218	-0.596881	-0.427491
C	-1.403445	0.595818	0.157813
C	-1.354634	1.649416	-0.809865
C	-2.089455	1.357333	-1.927791
S	0.739846	5.337820	1.539708
S	-1.247700	5.467006	-1.155782
S	-2.537243	2.836751	-2.781336
S	1.811545	2.548425	2.985434
S	1.582670	-0.526530	1.909765
S	-2.358402	-0.370660	-2.050231
S	2.358402	0.370660	-2.050231
S	2.537243	-2.836751	-2.781336
S	1.247700	-5.467006	-1.155782
S	-0.739846	-5.337820	1.539708
S	-1.811545	-2.548425	2.985434
S	-1.582670	0.526530	1.909765

[14]sulfinfinitene, M06-2X/def2-TZVP optimised geometry (D_2 point group).
$E = -6641.504344$ Ha, $\nu_1 = 37.8$ cm^{-1} (b_2).

C	-1.786176	2.100434	0.878390
C	-1.570955	2.449354	3.317792
C	0.645417	-1.066645	5.166658
C	1.570955	-2.449354	3.317792
C	1.161973	-1.209620	2.900625
C	0.452565	-0.538493	3.920548
C	-1.161973	1.209620	2.900625
C	-1.475738	0.934919	1.540992
C	-1.514642	-0.190756	0.658601
C	-1.514642	0.190756	-0.658601
C	-1.475738	-0.934919	-1.540992
C	-1.786176	-2.100434	-0.878390
C	-1.161973	-1.209620	-2.900625
C	-1.570955	-2.449354	-3.317792
C	0.452565	0.538493	-3.920548
C	0.645417	1.066645	-5.166658
C	1.161973	1.209620	-2.900625
C	1.570955	2.449354	-3.317792
C	1.475738	0.934919	-1.540992
C	1.786176	2.100434	-0.878390
C	1.514642	-0.190756	-0.658601
C	1.514642	0.190756	0.658601
C	1.475738	-0.934919	1.540992
C	1.786176	-2.100434	0.878390
S	-1.422302	2.633796	5.055963
S	1.422302	-2.633796	5.055963
S	2.028914	-3.448486	1.961665
S	-2.028914	3.448486	1.961665
S	-1.774874	1.907632	-0.848966
S	1.774874	-1.907632	-0.848966
S	-1.774874	-1.907632	0.848966
S	-2.028914	-3.448486	-1.961665
S	-1.422302	-2.633796	-5.055963
S	1.422302	2.633796	-5.055963
S	2.028914	3.448486	-1.961665
S	1.774874	1.907632	0.848966
C	-0.452565	-0.538493	-3.920548
C	-0.645417	-1.066645	-5.166658
S	0.000000	0.000000	-6.403661
C	-0.452565	0.538493	3.920548
C	-0.645417	1.066645	5.166658
S	0.000000	0.000000	6.403661

[16]sulfinfinitene, M06-2X/def2-TZVP optimised geometry (D_2 point group).
E = −7590.371755 Ha, ν_1 = 35.4 cm^{-1} (a).

C	-1.701299	2.206021	0.504592
C	-1.494370	2.998284	2.793346
C	0.000000	0.000000	5.834030
C	1.494370	-2.998284	2.793346
C	1.199363	-1.653865	2.702900
C	0.000000	0.000000	4.453645
C	-1.199363	1.653865	2.702900
C	-1.473061	1.164196	1.382755
C	-1.540445	-0.079513	0.684370
C	-1.540445	0.079513	-0.684370
C	-1.473061	-1.164196	-1.382755
C	-1.701299	-2.206021	-0.504592
C	-1.199363	-1.653865	-2.702900
C	-1.494370	-2.998284	-2.793346
C	0.671679	1.165815	-3.947033
C	0.873208	2.087274	-4.955200
C	1.199363	1.653865	-2.702900
C	1.494370	2.998284	-2.793346
C	1.473061	1.164196	-1.382755
C	1.701299	2.206021	-0.504592
C	1.540445	-0.079513	-0.684370
C	1.540445	0.079513	0.684370
C	1.473061	-1.164196	1.382755
C	1.701299	-2.206021	0.504592
S	-1.424595	3.630477	4.401771
S	1.424595	-3.630477	4.401771
S	1.825364	-3.751374	1.270819
S	-1.825364	3.751374	1.270819
S	-1.763008	1.736239	-1.156206
S	1.763008	-1.736239	-1.156206
S	-1.763008	-1.736239	1.156206
S	-1.825364	-3.751374	-1.270819
S	-1.424595	-3.630477	-4.401771
S	1.424595	3.630477	-4.401771
S	1.825364	3.751374	-1.270819
S	1.763008	1.736239	1.156206
C	0.000000	0.000000	-4.453645
C	0.000000	0.000000	-5.834030
S	0.536623	1.484593	-6.541443
C	-0.671679	1.165815	3.947033
C	-0.873208	2.087274	4.955200
S	-0.536623	1.484593	6.541443
C	0.671679	-1.165815	3.947033
C	0.873208	-2.087274	4.955200
S	0.536623	-1.484593	6.541443
C	-0.671679	-1.165815	-3.947033
C	-0.873208	-2.087274	-4.955200
S	-0.536623	-1.484593	-6.541443

[18]sulfinfinitene, M06-2X/def2-TZVP optimised geometry (D_2 point group).
E = −8539.161274 Ha, ν_1 = 28.7 cm^{-1} (b_2).

C	-1.701164	2.246099	0.136589
C	-1.452660	3.402134	2.232175
C	0.278910	-1.154170	5.947530
C	1.452660	-3.402134	2.232175
C	1.231480	-2.048548	2.420171
C	0.248986	-0.696922	4.634970
C	-1.231480	2.048548	2.420171
C	-1.497046	1.363052	1.183582
C	-1.572974	0.031215	0.688935
C	-1.572974	-0.031215	-0.688935

C -1.497046 -1.363052 -1.183582
C -1.701164 -2.246099 -0.136589
C -1.231480 -2.048548 -2.420171
C -1.452660 -3.402134 -2.232175
C 0.759636 1.776595 -3.771576
C 0.877546 2.948713 -4.506404
C 1.231480 2.048548 -2.420171
C 1.452660 3.402134 -2.232175
C 1.497046 1.363052 -1.183582
C 1.701164 2.246099 -0.136589
C 1.572974 0.031215 -0.688935
C 1.572974 -0.031215 0.688935
C 1.497046 -1.363052 1.183582
C 1.701164 -2.246099 0.136589
S -1.310174 4.368784 3.641912
S 1.310174 -4.368784 3.641912
S 1.786882 -3.896543 0.615192
S -1.786882 3.896543 0.615192
S -1.798757 1.518440 -1.421620
S 1.798757 -1.518440 -1.421620
S -1.798757 -1.518440 1.421620
S -1.786882 -3.896543 -0.615192
S -1.310174 -4.368784 -3.641912
S 1.310174 4.368784 -3.641912
S 1.786882 3.896543 -0.615192
S 1.798757 1.518440 1.421620
C 0.248986 0.696922 -4.634970
C 0.278910 1.154170 -5.947530
S 0.637480 2.811013 -6.195487
C -0.759636 1.776595 3.771576
C -0.877546 2.948713 4.506404
S -0.637480 2.811013 6.195487
C 0.759636 -1.776595 3.771576
C 0.877546 -2.948713 4.506404
S 0.637480 -2.811013 6.195487
C -0.759636 -1.776595 -3.771576
C -0.877546 -2.948713 -4.506404
S -0.637480 -2.811013 -6.195487
C -0.248986 0.696922 4.634970
C -0.278910 1.154170 5.947530
S 0.000000 0.000000 7.179681
C -0.248986 -0.696922 -4.634970
C -0.278910 -1.154170 -5.947530
S 0.000000 0.000000 -7.179681

[20]sulfinfinitene, M06-2X/def2-TZVP optimised geometry (D_2 point group).
E = −9487.903140 Ha, ν_1 = 11.7 cm^{-1} (b_1).

C -1.729757 2.228072 -0.247418
C -1.392941 3.715988 1.599059
C 0.097175 -2.240770 5.629548
C 1.392941 -3.715988 1.599059
C 1.221153 -2.410841 2.036634
C 0.244483 -1.440802 4.498326
C -1.221153 2.410841 2.036634
C -1.525148 1.537503 0.935883
C -1.600312 0.146596 0.672718
C -1.600312 -0.146596 -0.672718
C -1.525148 -1.537503 -0.935883
C -1.729757 -2.228072 0.247418
C -1.221153 -2.410841 -2.036634
C -1.392941 -3.715988 -1.599059
C 0.691357 2.362488 -3.403959
C 0.631903 3.679956 -3.846306
C 1.221153 2.410841 -2.036634
C 1.392941 3.715988 -1.599059

C	1.525148	1.537503	-0.935883
C	1.729757	2.228072	0.247418
C	1.600312	0.146596	-0.672718
C	1.600312	-0.146596	0.672718
C	1.525148	-1.537503	0.935883
C	1.729757	-2.228072	-0.247418
S	-1.045193	4.930238	2.748891
S	1.045193	-4.930238	2.748891
S	1.775662	-3.934263	-0.064180
S	-1.775662	3.934263	-0.064180
S	-1.817922	1.248589	-1.659806
S	1.817922	-1.248589	-1.659806
S	-1.817922	-1.248589	1.659806
S	-1.775662	-3.934263	0.064180
S	-1.045193	-4.930238	-2.748891
S	1.045193	4.930238	-2.748891
S	1.775662	3.934263	0.064180
S	1.817922	1.248589	1.659806
C	0.244483	1.440802	-4.498326
C	0.097175	2.240770	-5.629548
S	0.231088	3.936056	-5.481211
C	-0.691357	2.362488	3.403959
C	-0.631903	3.679956	3.846306
S	-0.231088	3.936056	5.481211
C	0.691357	-2.362488	3.403959
C	0.631903	-3.679956	3.846306
S	0.231088	-3.936056	5.481211
C	-0.691357	-2.362488	-3.403959
C	-0.631903	-3.679956	-3.846306
S	-0.231088	-3.936056	-5.481211
C	0.000000	0.000000	4.919388
C	0.000000	0.000000	6.313174
S	-0.043844	-1.483467	7.146203
C	-0.244483	-1.440802	-4.498326
C	-0.097175	-2.240770	-5.629548
S	0.043844	-1.483467	-7.146203
C	0.000000	0.000000	-4.919388
C	0.000000	0.000000	-6.313174
S	-0.043844	1.483467	-7.146203
S	0.043844	1.483467	7.146203
C	-0.244483	1.440802	4.498326
C	-0.097175	2.240770	5.629548

Coronene M06-2X/def2-TZVP optimised geometry (D_{6h} point group).
E = −921.846239 Ha, ν_1 = 88.9 cm^{-1} (e_{2u}).

C	0.680898	-3.666347	0.000000
C	1.414687	-2.450310	0.000000
C	0.711094	-1.231651	0.000000
C	-0.711094	-1.231651	0.000000
C	-1.414687	-2.450310	0.000000
C	-0.680898	-3.666347	0.000000
C	1.422188	0.000000	0.000000
C	-1.422188	0.000000	0.000000
C	-0.711094	1.231651	0.000000
C	0.711094	1.231651	0.000000
C	-1.414687	2.450310	0.000000
C	-2.834701	2.422849	0.000000
C	-3.515599	1.243498	0.000000
C	-2.829375	0.000000	0.000000
C	-3.515599	-1.243498	0.000000
C	-2.834701	-2.422849	0.000000
H	-3.370948	-3.364289	0.000000
H	-4.599034	-1.237182	0.000000
H	1.228085	-4.601471	0.000000
H	-1.228085	-4.601471	0.000000

H	-3.370948	3.364289	0.000000
H	-4.599034	1.237182	0.000000
C	2.834701	-2.422849	0.000000
C	3.515599	-1.243498	0.000000
C	2.829375	0.000000	0.000000
H	3.370948	-3.364289	0.000000
H	4.599034	-1.237182	0.000000
C	3.515599	1.243498	0.000000
C	2.834701	2.422849	0.000000
C	1.414687	2.450310	0.000000
H	4.599034	1.237182	0.000000
H	3.370948	3.364289	0.000000
C	-0.680898	3.666347	0.000000
H	-1.228085	4.601471	0.000000
C	0.680898	3.666347	0.000000
H	1.228085	4.601471	0.000000

Infinitene M06-2X/def2-TZVP optimised geometry (D_2 point group).
$E = -1843.558127$ Ha, $\nu_1 = 43.5$ cm^{-1} (*a*).

C	-1.755744	1.323672	-1.284589
C	-1.886496	2.418500	-0.499224
C	-1.572341	2.359082	0.887711
C	-1.581088	3.551113	1.652638
C	-1.318672	3.499528	2.978703
C	-0.897918	2.289402	3.593383
C	-0.679988	2.303489	4.996884
C	-0.343348	1.164054	5.635317
C	0.000000	0.000000	4.894315
C	0.343348	-1.164054	5.635317
C	0.679988	-2.303489	4.996884
C	0.897918	-2.289402	3.593383
C	0.721951	-1.104917	2.836847
C	0.000000	0.000000	3.478518
C	-0.721951	1.104917	2.836847
C	-1.260221	1.124597	1.492900
C	-1.481966	-0.055599	0.701114
C	-1.755744	-1.323672	1.284589
C	-1.481966	0.055599	-0.701114
C	-1.886496	-2.418500	0.499224
C	-1.260221	-1.124597	-1.492900
C	-1.572341	-2.359082	-0.887711
C	-0.721951	-1.104917	-2.836847
C	-1.581088	-3.551113	-1.652638
C	-0.897918	-2.289402	-3.593383
C	0.000000	0.000000	-3.478518
C	-1.318672	-3.499528	-2.978703
C	-0.679988	-2.303489	-4.996884
C	0.000000	0.000000	-4.894315
C	0.721951	1.104917	-2.836847
C	-0.343348	-1.164054	-5.635317
C	0.343348	1.164054	-5.635317
C	0.897918	2.289402	-3.593383
C	1.260221	1.124597	-1.492900
C	0.679988	2.303489	-4.996884
C	1.318672	3.499528	-2.978703
C	1.572341	2.359082	-0.887711
C	1.581088	3.551113	-1.652638
C	1.481966	-0.055599	-0.701114
C	1.481966	0.055599	0.701114
C	1.318672	-3.499528	2.978703
C	1.755744	1.323672	1.284589
C	1.886496	2.418500	0.499224
C	1.260221	-1.124597	1.492900
C	1.886496	-2.418500	-0.499224

C	1.755744	-1.323672	-1.284589
C	1.581088	-3.551113	1.652638
C	1.572341	-2.359082	0.887711
H	-2.172169	3.373269	-0.923160
H	-1.842280	4.482894	1.166194
H	-1.395242	4.384692	3.598200
H	-0.856538	3.223879	5.539367
H	-0.273301	1.122737	6.715129
H	0.273301	-1.122737	6.715129
H	0.856538	-3.223879	5.539367
H	-2.172169	-3.373269	0.923160
H	-1.842280	-4.482894	-1.166194
H	-1.395242	-4.384692	-3.598200
H	-0.856538	-3.223879	-5.539367
H	-0.273301	-1.122737	-6.715129
H	0.273301	1.122737	-6.715129
H	0.856538	3.223879	-5.539367
H	1.395242	4.384692	-3.598200
H	1.842280	4.482894	-1.166194
H	-1.913440	-1.388707	2.352293
H	-1.913440	1.388707	-2.352293
H	1.913440	1.388707	2.352293
H	2.172169	3.373269	0.923160
H	1.913440	-1.388707	-2.352293
H	1.395242	-4.384692	3.598200
H	1.842280	-4.482894	1.166194
H	2.172169	-3.373269	-0.923160

4. Additional References

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