Electronic Supplementary Material for PCCP

Shedding light on sulflower and some of its plate-like derivatives

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Supplementary Material

I. Figures

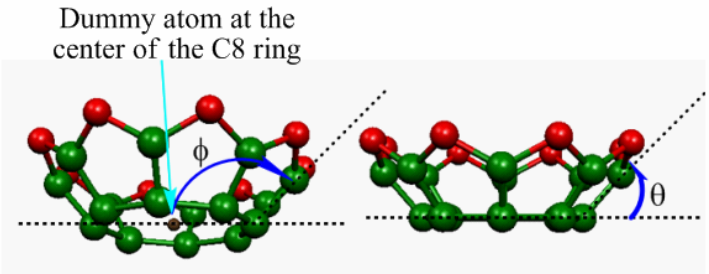

Figure S1. Description of the twist angle in non-planar derivatives.

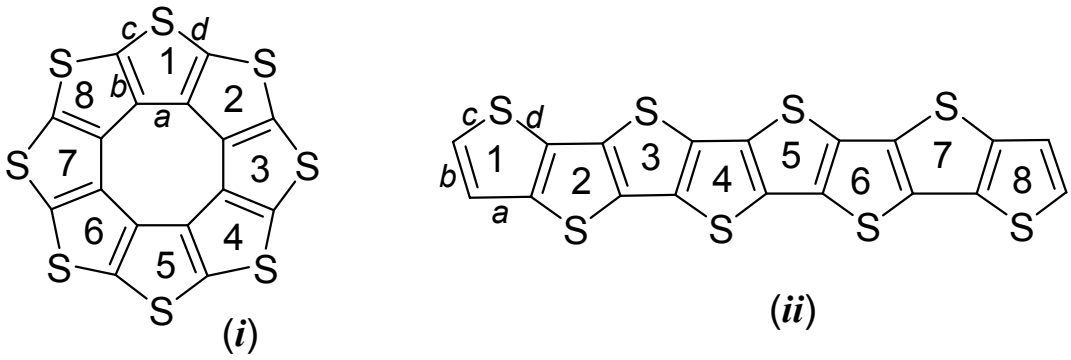

Figure S2. Labeling scheme used for sulflower and its linear homologue.

II. Tables

Table S1. Optimized parameters for **1** and **2** in both the neutral and cationic forms.
S1a. Optimized parameters for **1**.

Bond[a]	Neutral	Cation	Diff.[b]	Neutral	Cation	Diff. [b]
	BPE0/6-31G(d,p)			B3P866-31G(d,p)		
a1	1.418	1.413	-0.005	1.418	1.404	-0.014
b1	1.377	1.376	-0.001	1.378	1.397	0.019
c1	1.752	1.753	0.001	1.755	1.752	-0.003
d1	1.752	1.734	-0.018	1.755	1.767	0.012
a2	1.418	1.404	-0.014	1.418	1.413	-0.005
b2	1.377	1.385	0.008	1.378	1.389	0.011
c2	1.752	1.766	0.014	1.755	1.736	-0.019
d2	1.752	1.745	-0.007	1.755	1.76	0.005
a3	1.418	1.404	-0.014	1.418	1.415	-0.003
b3	1.377	1.396	0.019	1.378	1.377	-0.001
c3	1.752	1.746	-0.006	1.755	1.753	-0.002
d3	1.752	1.765	0.013	1.755	1.738	-0.017
a4	1.418	1.413	-0.005	1.418	1.406	-0.012
b4	1.377	1.386	0.009	1.378	1.384	0.006
c4	1.752	1.734	-0.018	1.755	1.769	0.014
d4	1.752	1.754	0.002	1.755	1.745	-0.01
a5	1.418	1.413	-0.005	1.418	1.404	-0.014
b5	1.377	1.376	-0.001	1.378	1.397	0.019
c5	1.752	1.753	0.001	1.755	1.752	-0.003
d5	1.752	1.734	-0.018	1.755	1.767	0.012
a6	1.418	1.404	-0.014	1.418	1.413	-0.005
b6	1.377	1.385	0.008	1.378	1.389	0.011
c6	1.752	1.766	0.014	1.755	1.736	-0.019
d6	1.752	1.745	-0.007	1.755	1.76	0.005
a7	1.418	1.404	-0.014	1.418	1.415	-0.003
b7	1.377	1.396	0.019	1.378	1.377	-0.001
c7	1.752	1.746	-0.006	1.755	1.753	-0.002
d7	1.752	1.765	0.013	1.755	1.738	-0.017
a8	1.418	1.413	-0.005	1.418	1.406	-0.012
b8	1.377	1.386	0.009	1.378	1.384	0.006
c8	1.752	1.734	-0.018	1.755	1.769	0.014
d8	1.752	1.754	0.002	1.755	1.745	-0.01

[a] See scheme 1 for labeling. [b] Calculated difference between cationic and neutral forms.

S1b. Optimized parameters for **2**.

	BPE0//6-31G(d,p)			B3P86//6-31G(d,p)		
Bond [a]	Neutral	Cation	Diff. [b]	Neutral	Cation	Diff. [b]
a1	1.419	1.409	-0.010	1.419	1.409	-0.010
b1	1.365	1.372	0.007	1.366	1.373	0.007
c1	1.735	1.728	-0.008	1.739	1.730	-0.008
d1	1.726	1.728	0.002	1.729	1.731	0.002
a2	1.416	1.398	-0.018	1.415	1.398	-0.017
b2	1.391	1.405	0.014	1.392	1.406	0.014
c2	1.745	1.742	-0.002	1.748	1.745	-0.003
d2	1.740	1.740	0.000	1.743	1.743	0.000
a3	1.414	1.391	-0.023	1.414	1.392	-0.022
b3	1.392	1.414	0.022	1.393	1.415	0.021
c3	1.740	1.739	-0.001	1.744	1.742	-0.001
d3	1.740	1.742	0.002	1.744	1.745	0.001
a4	1.414	1.388	-0.026	1.413	1.388	-0.025
b4	1.393	1.418	0.025	1.394	1.418	0.024
c4	1.741	1.741	0.001	1.744	1.744	0.000
d4	1.741	1.742	0.001	1.744	1.745	0.001
a5	1.414	1.388	-0.026	1.413	1.388	-0.025
b5	1.393	1.420	0.027	1.394	1.420	0.026
c5	1.741	1.742	0.001	1.744	1.745	0.001
d5	1.741	1.741	0.001	1.744	1.744	0.000
a6	1.414	1.391	-0.023	1.414	1.392	-0.022
b6	1.393	1.418	0.025	1.394	1.418	0.024
c6	1.740	1.742	0.002	1.744	1.745	0.001
d6	1.740	1.739	-0.001	1.744	1.742	-0.001
a7	1.416	1.398	-0.018	1.415	1.398	-0.017
b7	1.392	1.414	0.022	1.393	1.415	0.021
c7	1.740	1.740	0.000	1.743	1.743	0.000
d7	1.745	1.742	-0.002	1.748	1.745	-0.003
a8	1.419	1.409	-0.010	1.419	1.409	-0.010
b8	1.391	1.405	0.014	1.392	1.406	0.014
c8	1.726	1.728	0.002	1.729	1.731	0.002
d8	1.735	1.728	-0.008	1.739	1.731	-0.008
a9	1.365	1.372	0.007	1.366	1.373	0.007

[a] See Figure S1 for labeling scheme. [b] Calculated difference between cationic and neutral forms.

Table S2. The FMO energies E_{HOMO} and E_{LUMO} (eV) and Ionization potential (IP in eV) at different levels of theory.

	PBE0/6-31G(d,p)			B3LYP// PBE0/6-31G(d,p)		
Molecule	E_{HOMO}	E_{LUMO}	IP	E_{HOMO}	E_{LUMO}	IP
1	-6.02	-0.94	7.17	-5.72	-1.01	7.00
2	-5.36	-1.78	6.29	-5.08	-1.81	6.14
3	-5.61	-0.93	6.71	-5.32	-0.98	6.57
4	-5.80	-0.91	6.92	-5.50	-0.97	6.76
5	-4.71	-1.03	5.93	-4.44	-1.15	5.81
6	-4.11	-0.30	5.20	-3.84	-0.40	5.15
7	-6.15	-2.47	7.48	-5.88	-2.57	7.40
Tetracene	-5.10	-2.03	6.38	-4.86	-2.08	6.28
Pentacene	-4.83	-2.36	5.99	-4.60	-2.39	5.90
DT-TTF	-5.10	-1.01	6.33	-4.85	-1.11	6.30

Table S3. Energetics of the neutral and charged species at both the PBE0/6-31G(d,p) and B3P86/6-31G(d,p) levels of theory.

Molecule	E	E^*_+	E_+	E^*
PBE0/6-31G(d,p)//PBE0/6-31G(d,p)				
1	-3793.309272	-3793.043374	-3793.045759	-3793.306773
2	-3871.846192	-3871.609825	-3871.614886	-3871.841138
3	-19801.47732	-19801.22842	-19801.23058	-19801.47516
4	-11797.39862	-11797.14142	-11797.14420	-11797.39635
5	-922.949329	-922.7288488	-922.7314411	-922.9470351
6	-1051.143817	-1050.941177	-1050.952675	-1051.133873
7	-1209.784058	-1209.490787	-1209.509235	-1209.780338
Pentacene	-845.8259886	-845.6041097	-845.6057348	-845.8244998
Tetracene	-692.3666461	-692.1303188	-692.1323321	-692.3646859
DT-TTF	-2771.213804	-2770.976546	-2770.981091	-2771.209042
B3LYP/6-31G(d,p)//PBE0/6-31G(d,p)				
1	-3795.164241	-3794.90536	-3794.907032	-3795.161523
2	-3873.805406	-3873.574856	-3873.579696	-3873.800357
3	-19804.70054	-19804.45806	-19804.45927	-19804.69775
4	-11799.93784	-11799.68794	-11799.6893	-11799.93501
5	-923.9954318	-923.7800609	-923.7818648	-923.9925763
6	-1052.269939	-1052.072464	-1052.080644	-1052.257494
7	-1211.03586	-1210.747678	-1210.763955	-1211.031413
Pentacene	-846.8216612	-846.6032888	-846.6048837	-846.8198101
Tetracene	-693.1845071	-692.9516155	-692.9536319	-693.182297
DT-TTF	-2772.548871	-2772.315782	-2772.317306	-2772.541461
B3P86/6-31G(d,p)//B3P86/6-31G(d,p)				
1	−3799. 346805	−3799. 062478	−3799. 064829	−3799. 344567
2	−3878. 275935	−3878. 020412	−3878. 025158	−3878. 271247
3	−19812. 70112	−19812. 43322	−19812. 43539	−19812. 69898
4	−11806. 02909	−11805. 7539	−11805. 75601	−11806. 02684
5	−926. 9114731	−926. 671405	−926. 6740609	−926. 9094799
6	−1055. 181373	−1054. 958639	−1054. 96959	−1055. 171434
7	−1213. 908429	−1213. 60459	−1213. 612375	−1213. 90537
Pentacene	−695. 3470475	−695. 0896671	−695. 0915616	−695. 3452805
Tetracene	−849. 4533223	−849. 2103973	−849. 2118795	−849. 4519673
DT-TTF	−2775. 536038	−2775. 278613	−2775. 282839	−2775. 5314

III. Cartesian coordinates

Sulflower (1)

C	0.00000000	1.85246100	0.00000000
C	1.30988700	1.30988700	0.00000000
C	1.85246100	0.00000000	0.00000000
C	1.30988700	-1.30988700	0.00000000
C	0.00000000	-1.85246100	0.00000000
C	-1.30988700	-1.30988700	0.00000000
C	-1.85246100	0.00000000	0.00000000
C	-1.30988700	1.30988700	0.00000000
C	0.00000000	3.22970700	0.00000000
C	2.28374800	2.28374800	0.00000000
C	3.22970700	0.00000000	0.00000000
C	2.28374800	-2.28374800	0.00000000
C	0.00000000	-3.22970700	0.00000000
C	-2.28374800	-2.28374800	0.00000000
C	-3.22970700	0.00000000	0.00000000
C	-2.28374800	2.28374800	0.00000000
S	1.61725500	3.90439900	0.00000000
S	3.90439900	1.61725500	0.00000000
S	3.90439900	-1.61725500	0.00000000
S	1.61725500	-3.90439900	0.00000000
S	-1.61725500	-3.90439900	0.00000000
S	-3.90439900	-1.61725500	0.00000000
S	-3.90439900	1.61725500	0.00000000
S	-1.61725500	3.90439900	0.00000000

Sulflinear (2)

C	6.05537000	-0.89155800	-0.00000100
S	4.76892000	-2.07023800	-0.00001100
C	3.58762000	-0.79227800	0.00002500
C	4.16415000	0.47463200	0.00004400
C	5.57878000	0.41525200	0.00002900
C	2.17442000	-0.73365800	-0.00002600
C	1.70140000	0.57628200	-0.00001900
S	2.98331900	1.75326200	0.00005100
S	0.89291000	-1.91165800	-0.00002700
C	-0.28892000	-0.63371900	0.00000000
C	0.28883000	0.63367200	0.00000900
C	-1.70146900	-0.57628800	-0.00005200
C	-2.17450000	0.73365100	-0.00006400
S	-0.89297000	1.91163200	-0.00005500
S	-2.98333000	-1.75331900	-0.00002200
C	-4.16417000	-0.47472900	0.00001500
C	-3.58769000	0.79220100	0.00000400
C	-5.57879000	-0.41518800	0.00000200
C	-6.05538000	0.89166200	-0.00003000
S	-4.76878000	2.07026100	-0.00005900
S	-6.88241000	-1.54681900	0.00002200
C	-8.04271000	-0.25663900	0.00016900
C	-7.47157000	0.98302200	0.00003800
S	6.88241000	1.54689300	0.00003800
C	8.04288000	0.25662200	0.00000100
C	7.47157000	-0.98291800	-0.00001700
H	9.09706000	0.49769200	-0.00000400
H	8.03809000	-1.90589700	-0.00004100
H	-8.03835000	1.90580100	0.00003600
H	-9.09683000	-0.49795800	0.00022300

Sulflower-Se (3)

C	0.72069600	1.74007900	0.00098200
C	1.74003000	0.72081200	0.00098200
C	1.74007900	-0.72069600	0.00098200
C	0.72081200	-1.74003000	0.00098200
C	-0.72069600	-1.74007900	0.00098200
C	-1.74003000	-0.72081200	0.00098200
C	-1.74007900	0.72069600	0.00098200
C	-0.72081200	1.74003000	0.00098200
C	1.25064300	3.01931900	0.00081300
C	3.01931900	1.25064300	0.00081300
C	3.01931900	-1.25064300	0.00081300
C	1.25064300	-3.01931900	0.00081300
C	-1.25064300	-3.01931900	0.00081300
C	-3.01931900	-1.25064300	0.00081300
C	-3.01931900	1.25064300	0.00081300
C	-1.25064300	3.01931900	0.00081300
Se	3.09862500	3.09874400	-0.00031700
Se	4.38220100	0.00008400	-0.00031700
Se	3.09874400	-3.09862500	-0.00031700
Se	0.00008400	-4.38220100	-0.00031700
Se	-3.09862500	-3.09874400	-0.00031700
Se	-4.38220100	-0.00008400	-0.00031700
Se	-3.09874400	3.09862500	-0.00031700
Se	-0.00008400	4.38220100	-0.00031700

Sulflower-SSe (4)

C	-0.00056900	-1.72609600	-0.71434300
C	-0.00056900	-1.72609600	0.71434300
C	-0.00057000	-0.71434300	1.72609600
C	-0.00056900	0.71434300	1.72609600
C	-0.00056900	1.72609600	0.71434300
C	-0.00056800	1.72609600	-0.71434300
C	-0.00056800	0.71434300	-1.72609600
C	-0.00056900	-0.71434300	-1.72609600
C	0.00006400	-3.01119300	-1.22111900
C	0.00006300	-3.01119300	1.22112000
C	0.00006300	-1.22111900	3.01119300
C	0.00006100	1.22112000	3.01119300
C	0.00006400	3.01119300	1.22111900
C	0.00006200	3.01119300	-1.22112000
C	0.00006500	1.22111900	-3.01119300
C	0.00006200	-1.22112000	-3.01119300
S	0.00039200	-4.24390400	0.00000000
Se	-0.00000400	-3.08570500	3.08570500
S	0.00038700	0.00000000	4.24390400
Se	-0.00000600	3.08570500	3.08570500
S	0.00039000	4.24390400	0.00000000
Se	-0.00000400	3.08570500	-3.08570500
S	0.00039000	0.00000000	-4.24390400
Se	-0.00000500	-3.08570500	-3.08570500

Sulflower-CH_2 (5)

C	1.54893400	1.05277400	-0.55750100
C	1.84649300	-0.34973300	-0.57303200
C	1.05373200	-1.54463100	-0.55211400
C	-0.34976500	-1.83811400	-0.55534500
C	-1.55031400	-1.05449000	-0.56208300
C	-1.84208800	0.34909800	-0.56258600
C	-1.05485800	1.54739900	-0.55960000
C	0.34920900	1.83809700	-0.55635700
C	2.57131400	1.74876000	-0.00697900
C	3.06917600	-0.58202500	-0.03808300
C	1.74804200	-2.56409500	0.00536100
C	-0.58073300	-3.05494400	-0.00857000
C	-2.57613500	-1.75289400	-0.02029800
C	-3.06025600	0.58030400	-0.01846900
C	-1.75251500	2.57176400	-0.01415500
C	0.57984600	3.05472500	-0.00862600
C	3.68453500	0.76397900	0.35526900
H	3.88202200	0.79008200	1.43628400
H	4.64631800	0.97724000	-0.13182600
C	3.14945800	-2.05966400	0.35435400
H	3.95363500	-2.61255700	-0.15174000
H	3.34510200	-2.15901800	1.43100400
C	0.76527300	-3.68067600	0.36370700
H	0.80512600	-3.91166300	1.43702900
H	0.97040900	-4.62691400	-0.15726900
C	-2.06359600	-3.14447100	0.35876200
H	-2.18743500	-3.32175600	1.43609700
H	-2.59425900	-3.96513100	-0.14477800
C	-3.68426600	-0.76620800	0.35548600
H	-3.88963100	-0.80963200	1.43408200
H	-4.64420800	-0.96492000	-0.14211700
C	-3.14688700	2.06160700	0.35702500
H	-3.32554000	2.17600200	1.43526000
H	-3.96461200	2.60004500	-0.14274800
C	-0.76675700	3.68088100	0.36078100
H	-0.81398300	3.89147900	1.43833300
H	-0.96320000	4.63834600	-0.14214300
C	2.06222900	3.14415200	0.36189000
H	2.18209000	3.33060400	1.43824600
H	2.59771900	3.95821200	-0.14673900

Sulflower-NH (6)

C	0.71149200	1.71769400	0.84876200
C	-0.71149200	1.71769400	0.84876200
C	-1.71769400	0.71149200	0.84876200
C	-1.71769400	-0.71149200	0.84876200
C	-0.71149200	-1.71769400	0.84876200
C	0.71149200	-1.71769400	0.84876200
C	1.71769400	-0.71149200	0.84876200
C	1.71769400	0.71149200	0.84876200
C	1.12357200	2.71300300	-0.01107300
C	-1.12389700	2.71286800	-0.01107300
C	-2.71300300	1.12357200	-0.01107300
C	-2.71286800	-1.12389700	-0.01107300
C	-1.12357200	-2.71300300	-0.01107300
C	1.12389700	-2.71286800	-0.01107300
C	2.71300300	-1.12357200	-0.01107300
C	2.71286800	1.12389700	-0.01107300
N	0.00009100	3.34078100	-0.59375200
N	-2.36222400	2.36235300	-0.59375200
N	-3.34078100	0.00009100	-0.59375200
N	-2.36235300	-2.36222400	-0.59375200
N	-0.00009100	-3.34078100	-0.59375200
N	2.36222400	-2.36235300	-0.59375200
N	3.34078100	-0.00009100	-0.59375200
N	2.36235300	2.36222400	-0.59375200
H	-0.00025100	4.31334500	-0.86986800
H	-3.05017300	3.04981800	-0.86986800
H	-4.31334500	-0.00025100	-0.86986800
H	-3.04981800	-3.05017300	-0.86986800
H	0.00025100	-4.31334500	-0.86986800
H	3.05017300	-3.04981800	-0.86986800
H	4.31334500	0.00025100	-0.86986800
H	3.04981800	3.05017300	-0.86986800

Sulflower-O (7)

C	-0.00003700	1.87156900	0.97531900
C	-1.32342500	1.32337300	0.97531900
C	-1.87156900	-0.00003700	0.97531900
C	-1.32337300	-1.32342500	0.97531900
C	0.00003700	-1.87156900	0.97531900
C	1.32342500	-1.32337300	0.97531900
C	1.87156900	0.00003700	0.97531900
C	1.32337300	1.32342500	0.97531900
C	-0.00003400	2.77950600	-0.04657700
C	-1.96543100	1.96538400	-0.04657700
C	-2.77950600	-0.00003400	-0.04657700
C	-1.96538400	-1.96543100	-0.04657700
C	0.00003400	-2.77950600	-0.04657700
C	1.96543100	-1.96538400	-0.04657700
C	2.77950600	0.00003400	-0.04657700
C	1.96538400	1.96543100	-0.04657700
O	-1.20138200	2.90039200	-0.69655600
O	-2.90039200	1.20138200	-0.69655600
O	-2.90039200	-1.20138200	-0.69655600
O	-1.20138200	-2.90039200	-0.69655600
O	1.20138200	-2.90039200	-0.69655600
O	2.90039200	-1.20138200	-0.69655600
O	2.90039200	1.20138200	-0.69655600
O	1.20138200	2.90039200	-0.69655600

Tetracene

C	0.00000000	0.71315100	-4.87317600
C	0.00000000	-0.71315100	-4.87317600
C	0.00000000	1.40579400	-3.69885000
C	0.00000000	-1.40579400	-3.69885000
C	0.00000000	-0.72281300	-2.44242000
C	0.00000000	0.72281300	-2.44242000
C	0.00000000	1.40274900	-1.23118000
H	0.00000000	2.49061300	-1.23184800
C	0.00000000	0.72314700	-0.00014500
C	0.00000000	-0.72314700	-0.00014500
C	0.00000000	-1.40274900	-1.23118000
H	0.00000000	2.49272600	-3.69628700
H	0.00000000	-2.49272600	-3.69628700
H	0.00000000	-2.49061300	-1.23184800
C	0.00000000	-1.40284900	1.23146900
C	0.00000000	-0.72299800	2.44221400
C	0.00000000	1.40284900	1.23146900
C	0.00000000	0.72299800	2.44221400
H	0.00000000	-2.49072100	1.23121800
H	0.00000000	2.49072100	1.23121800
C	0.00000000	-1.40563700	3.69892300
C	0.00000000	-0.71353900	4.87326000
H	0.00000000	-1.24542500	5.82017200
C	0.00000000	1.40563700	3.69892300
H	0.00000000	2.49266100	3.69612500
C	0.00000000	0.71353900	4.87326000
H	0.00000000	1.24542500	5.82017200
H	0.00000000	-2.49266100	3.69612500
H	0.00000000	1.24567700	-5.81995200
H	0.00000000	-1.24567700	-5.81995200

Pentacene

C	0.00000000	0.71464000	-6.09783200
C	0.00000000	1.40680200	-4.92508400
C	0.00000000	0.72469400	-3.66616100
C	0.00000000	-0.72469400	-3.66616100
C	0.00000000	-1.40680200	-4.92508400
C	0.00000000	-0.71464000	-6.09783200
C	0.00000000	1.40441600	-2.45933900
C	0.00000000	-1.40441600	-2.45933900
C	0.00000000	-0.72559700	-1.22228500
C	0.00000000	0.72559700	-1.22228500
C	0.00000000	1.40510100	0.00000800
H	0.00000000	2.49281100	-0.00000500
C	0.00000000	0.72560100	1.22226800
C	0.00000000	-0.72560100	1.22226800
C	0.00000000	-1.40510100	0.00000800
H	0.00000000	2.49224900	-2.45978200
H	0.00000000	1.24582400	-7.04508700
H	0.00000000	2.49380000	-4.92261400
H	0.00000000	-2.49380000	-4.92261400
H	0.00000000	-1.24582400	-7.04508700
H	0.00000000	-2.49224900	-2.45978200
H	0.00000000	-2.49281100	-0.00000500
C	0.00000000	-1.40441700	2.45935400
C	0.00000000	-0.72470400	3.66614900
C	0.00000000	1.40441700	2.45935400
C	0.00000000	0.72470400	3.66614900
H	0.00000000	-2.49225100	2.45977200
H	0.00000000	2.49225100	2.45977200
C	0.00000000	-1.40680800	4.92509600
C	0.00000000	-0.71465100	6.09782900
H	0.00000000	-1.24581700	7.04509400
C	0.00000000	1.40680800	4.92509600
H	0.00000000	2.49380500	4.92260900
C	0.00000000	0.71465100	6.09782900
H	0.00000000	1.24581700	7.04509400
H	0.00000000	-2.49380500	4.92260900

DT-TTF

C	1.24547600	-4.43148500	0.00000000
C	0.71461000	-3.17547200	0.00000000
C	-0.71417000	-3.17571800	0.00000000
C	-1.24454800	-4.43188100	0.00000000
S	0.00064800	-5.62274600	0.00000000
S	1.50463500	-1.61252600	0.00000000
C	0.00009800	-0.67379800	0.00000000
S	-1.50433700	-1.61281500	0.00000000
C	0.00000000	0.67379600	0.00000000
S	1.50440400	1.61288400	0.00000000
C	0.71415200	3.17572300	0.00000000
C	-0.71464500	3.17544600	0.00000000
S	-1.50459300	1.61246400	0.00000000
C	-1.24550500	4.43143900	0.00000000
S	-0.00072900	5.62274900	0.00000000
C	1.24447700	4.43191800	0.00000000
H	2.28419100	4.72598400	0.00000000
H	-2.28532000	4.72513400	0.00000000
H	-2.28428400	-4.72587500	0.00000000
H	2.28528400	-4.72521700	0.00000000