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Supporting Information

Rubrenes. Planar and Twisted

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Cyclic Voltammetry Measurements.

Representative cyclic voltammograms of various substituted rubrenes are shown in Figure S1.

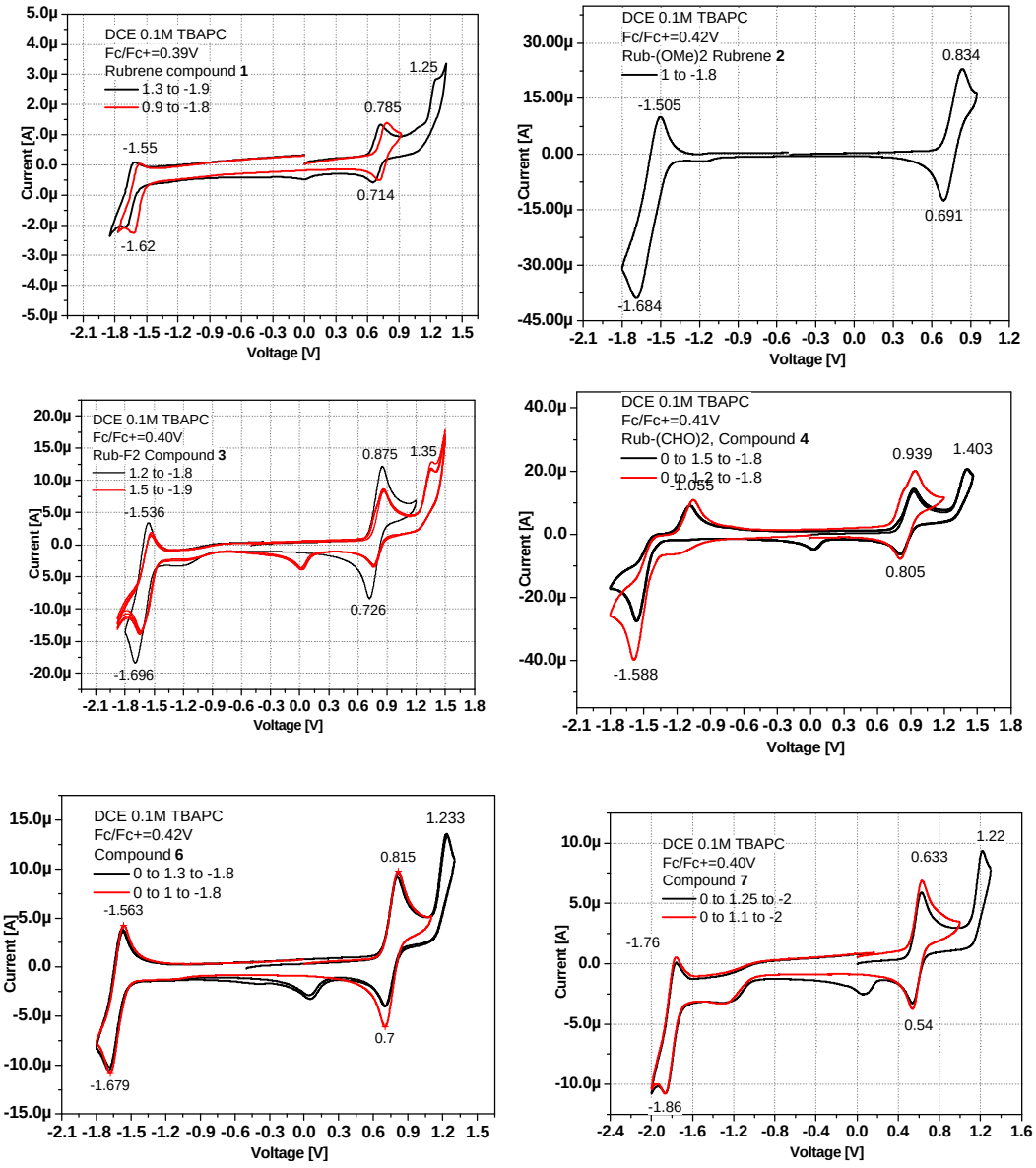


Figure S1: Cyclic voltammograms spectra of rubrenes **1**-**4**, **6** and **7**.

General X-ray Procedures:

The X-ray diffraction data were collected on a Nonius KappaCCD diffractometer, MoKα (l = 0.71073 Å), a graphite monochromator, T=120(2)K. The data were processed with Denzo-Scalepack. The structures were refined by full matrix least-squares based on F^2 with SHELXL-97.

X-ray Structural Analysis of 2. Compound **2** was crystallized from a solution of DCM/Ethanol to give orange crystals. Crystal data: $C_{44}H_{32}O_2$, 0.5 x 0.5 x 0.3 mm^3, Orthorhombic, space group Pbca, a=15.766(3) Å, b=13.859(3) Å, c=28.351(6) Å, from 20 degrees of data, V=6195(1) $Å^3$, Z=8, fw=592.70, Dc=1.271 Mg/m^3, m=0.076 mm^{-1}. Data collection and treatment: 34854 reflections collected, 0 = h = 14, 0 = k = 12, 0 = l = 25, frame scan width = 1.0°, scan speed 1.0° per 40 s, typical peak mosaicity 0.68°, 6953 independent reflections (R_{int} =0.095). Solution and refinement: 417 parameters with no restraints, final R_1= 0.0415 for data with $I>2s(I)$ and R_1= 0.0569 on 2417 reflections, wR_2=0.1075, goodness-of-fit on F^2 = 1.086, largest electron density peak = 0.145 e/$Å^3$ and hole=-0.155 e/$Å^3$. CCDC-671889 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray Structural Analysis of 3. Compound **3** was crystallized from a solution of DCM/Ethanol to give orange prism crystals. Crystal data: $C_{42}H_{26}F_2$ prism, 0.1 x 0.1 x 0.1 mm^3, Orthorhombic , Cmca a=27.450(6)Å, b=7.102(1)Å, c=14.327(3) Å, from 16 degrees of data, T=120(2)K, V=2793.0(10)$Å^3$, Z=4, Fw=568.63, Dc=1.347$Mg.m^{-3}$, μ=0.086mm^1**.**

Data collection and processing: 0=h=26, 0=k=6, 0=l=13, frame scan width = 2.0°, scan speed 1.0° per 300 sec, typical peak mosaicity 0.72°, 11396 reflections collected, 1826 independent reflections (R-int =0.081). Solution and refinement: Structure solved by Patterson method with SHELXS-97. Refined 106 parameters with 0 restraints, final R_1= 0.0563 (based on F^2) for data with I>2σ(I) and, R_1= 0.0573 on 655 reflections, goodness-of-fit on F^2 = 1.429, largest electron density peak = 0.20 e/$Å^3$ and hole -0.178 e/$Å^3$. CCDC-671890 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray Structural Analysis of 4. Compound **4** was crystallized from a solution of DCM/Ethanol to give red prismatic crystals. Crystal data: $C_{44}H_{28}O_2$ +0.25(O) 0.50x0.30x0.10 mm^3, Orthorhombic, $Pna2_1$, a=15.320(3), b=13.661(3), c=14.250(3) A from 20 degrees of data, T=120(2) K, V=2982(1) $Å^3$, Z=4, Fw=592.66, Dc=1.320 $Mg.m^{-3}$, μ=0.080 mm^{-1}. Data

collection and processing: 21191 reflections collected, -17=h=18, -16=k=16, -16=l=16, frame scan width = 1.0°, scan speed 1.0° per 400 sec, typical peak mosaicity 0.643°, 4883 independent reflections (R-int =0.059). Solution and refinement: Structure solved by direct methods with SHELXS. Refine 421 parameters with 1 restraint, final R_1= 0.0393 (based on F^2) for data with I>2s (I) and, R_1= 0.0512 on 4855 reflections, goodness-of-fit on F^2 = 1.040, largest electron density peak =0.177 e/Å^3. CCDC-671892 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

X-ray Structural Analysis of 6. Compound **6** was crystallized from a solution of DCM/Ethanol to give orange plate-like crystals. Crystal data: $C_{43}H_{28}OF_2$, 0.8 x 0.4 x 0.2 mm^3, Monoclinic, P2(1)/n, a=17.677(4)Å, b=9.424(2)Å, c=18.571(4) Å, β= 103.79°(3) from 20 degrees of data, T=120(2)K, V=3004.5(10)Å^3, Z=4, Fw=598.65, Dc=1.323Mg.m^{-3}, μ=0.086mm^1. Data collection and processing: 0=h=19, 0=k=10, -20=l=12, frame scan width = 1.5°, scan speed 1.0° per 120 sec, typical peak mosaicity 0.54°, 16323 reflections collected, 4618 independent reflections (R-int =0.065). Solution and refinement: Structure solved by Patterson method with SHELXS-97. Refined 415 parameters with 0 restraints, final R_1= 0.0559 (based on F^2) for data with I>2σ(I) and, R_1= 0.0815 on 4310 reflections, goodness-of-fit on F^2 = 1.020, largest electron density peak = 0.93 e/Å^3 and hole -0.28 e/Å^3. CCDC-671891 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

In order to clarify the packing density, Cremer–Pople puckering parameters[S1] were calculated and estimation of the packing index was made using PLATON (December, 2006)[S2]. The results are summarized in the Table S1.

Table S1. Calculated densities and packing indexes.

Compound	*V*/*Z*	Calculated density, g/cm^3	Packing index, %
1	685	1.291	70.3
2	774	1.271	68.4
4	745	1.311	69.7
6	751	1.323	68.7

Table S2: Distribution of twist through tetracene core.

Compound	Degree of Twist (degrees)				Total twist (degrees)
	1st ring	2nd ring	3rd ring	4th ring	
2	7.4	16.2	15.6	4.8	44.0
4	5.2	13.4	12.5	4.1	35.2
5	5.4	13.5	13.0	5.7	37.6

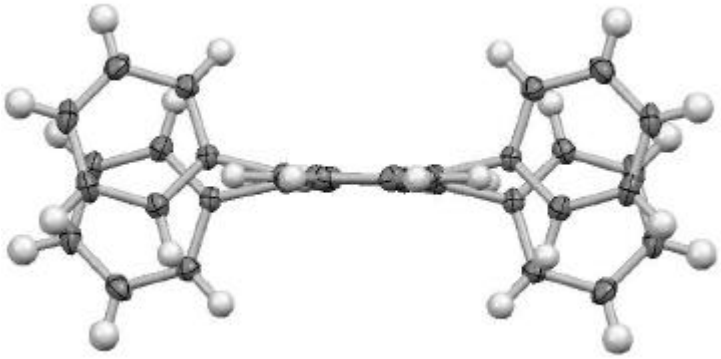
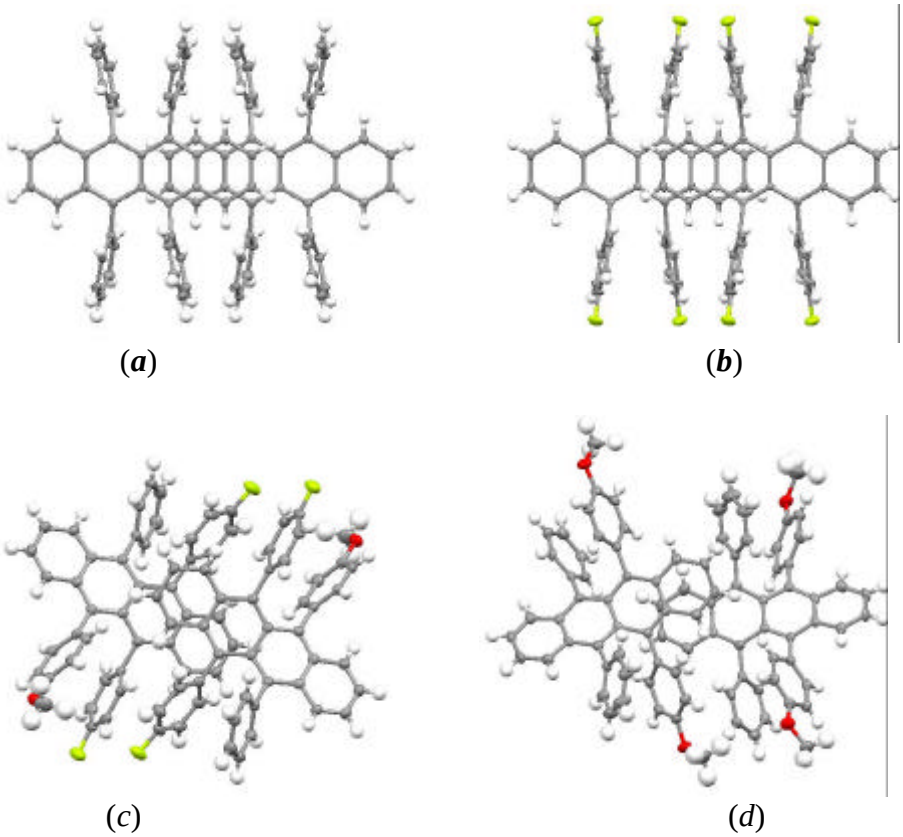


Figure S2. X ray structure of rubrene **1**.



(***a***) (***b***)

(*c*) (*d*)

Figure. S3. p-p contacts in (*a*) **1**, (*b*) **3**, (*c*) **6** and (*d*). **2.** A view parallel to the mean plane of the side aromatic ring.

Details of DFT calculations

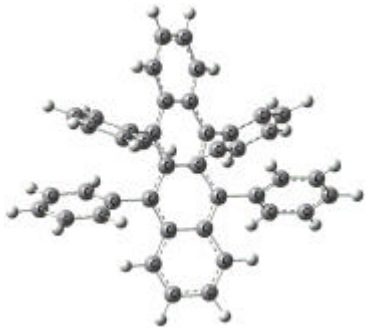


Figure S4: Calculated (B3LYP/6-31G(d)) geometries of rubrene **1**.

Table S3: Absolute energies of the optimized structures (B3LYP/6-31G(d)).

Compound	Number of imaginary frequencies (NIMAG)	Energy at B3LYP/6-31G(d) (Hartree)
1 (D_2 symmetry)	0	-1617.3354858
1 (C_{2h} symmetry)	1	-1617.3294631
1 (D_{2h} symmetry)	2	-1617.3251840
2 (C_2 symmetry)	0	-1846.3811626
2 (C_s symmetry)	1	-1846.3747893
5 (C_2 symmetry)	0	-1801.8244396
5 (C_s symmetry)	1	-1801.8186880

9,10-diphenylanthracene

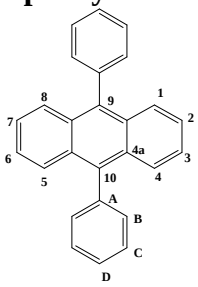


Table S4. Calculated (GIAO-B3LYP/6-311G(2df,p)//B3LYP/6-31G(d)) and measured ^{13}C NMR chemical shifts for 9,10-diphenylanthracene.

Carbon	Calculated values (ppm)	Measured values (ppm)[a]	Difference
1	133.0	126.9	6.1

2	129.5	125.0	4.5
4a	136.0	129.9	6.1
9	145.5	137.1	8.4
A	149.1	139.1	10.0
B	137.1	128.4	8.7
C	133.1	131.3	1.8
D	132.4	127.4	5.0

[a] The values are from the Spectral Database for Organic Compounds (SDBS) at http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/direct_frame_top.cgi

Rubrene

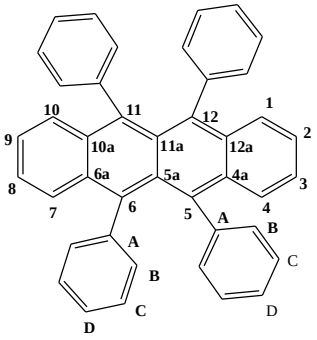


Table S5. Calculated (as planar C_{2h} and twisted D_2 structures at GIAO-B3LYP/6-311G(2df,p)//B3LYP/6-31G(d)) and measured ^{13}C NMR chemical shifts for rubrene **1**.

Carbon	Twisted	Planar	Measured	Ref C[a]	**Difference Twisted[b]**	**Difference Planar[c]**
1	132.5	133.5	127.1	1	**-0.6**	**0.4**
2	129.8	129.2	125.4	2	**-0.2**	**-0.7**
4a	136.8	138.6	131.1	4a	**-0.5**	**1.4**
5	145.1	148.6	137.5	9	**-0.7**	**2.7**
5a	136.1	131.7	129.6	4a	**0.3**	**-4.0**
A	151.3	153.0	142.4	A	**-1.1**	**0.6**
B	139.2	141.2	132.6	B	**0.6**	**2.6**
C	132.4	132.4	127.6	C	**3.0**	**3.0**
D	130.9	131.7	126	D	**0.0**	**0.7**

[a] Carbon from 9,10-diphenyanthracene for comparison.

[b] Difference between the ^{13}C NMR chemical shifts for rubrene **1** as measured (in benzene) and as estimated (based on GIAO-B3LYP/6-311G(2df,p)//B3LYP/6-31G(d) calculations of rubrene **1** in a twisted D_2 symmetry, corrected for the measured and calculated difference of the corresponding carbon atom of 9,10-diphenylanthracene, see Table S4). For example, the "difference twisted" for carbon C1 is 132.548–(132.97-126.94)–127.1 = -0.6 ppm. We note

that 4 digits after the decimal point were used to obtain the “difference twisted”, while only one digit after the decimal point is given in the Table.

[c] Difference between the ^{13}C NMR chemical shifts for rubrene **1** as measured (in benzene) and as estimated (based on GIAO-B3LYP/6-311G(2df,p)//B3LYP/6-31G(d) calculations of rubrene **1** keeping a planar C_{2h} symmetry, corrected for the measured and calculated difference of the corresponding carbon atom of 9,10-diphenylanthracene, see Table S4). For example, “difference planar” for carbon C1 is 133.5 – (132.97-126.94)– 127.1 = 0.4 ppm. We note that 4 digits after the decimal point were used to obtain the “difference twisted”, while only one digit after the decimal point is given in the Table.

Cartesian coordinates for the optimized geometries

Compound **1** D_2 symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471919	3.715397	-1.320111
2	6	0	-0.193120	2.448688	-0.699122
3	6	0	0.193120	2.448688	0.699122
4	6	0	0.471919	3.715397	1.320111
5	6	0	0.256625	4.895230	0.664748
6	6	0	-0.256625	4.895230	-0.664748
7	1	0	-0.844073	3.725627	-2.337171
8	1	0	0.844073	3.725627	2.337171
9	6	0	0.250330	1.234676	1.408185
10	6	0	-0.250330	1.234676	-1.408185
11	6	0	0.000000	0.000000	0.727869
12	6	0	0.000000	0.000000	-0.727869
13	6	0	-0.250330	-1.234676	1.408185
14	6	0	0.250330	-1.234676	-1.408185
15	6	0	-0.193120	-2.448688	0.699122
16	6	0	0.193120	-2.448688	-0.699122
17	6	0	-0.471919	-3.715397	1.320111
18	1	0	-0.844073	-3.725627	2.337171
19	6	0	0.471919	-3.715397	-1.320111
20	1	0	0.844073	-3.725627	-2.337171
21	6	0	-0.256625	-4.895230	0.664748
22	6	0	0.256625	-4.895230	-0.664748
23	6	0	-0.743138	-1.256325	2.822159
24	6	0	-0.017277	-1.840061	3.871248
25	6	0	-2.027294	-0.758690	3.096117
26	6	0	-0.551353	-1.908395	5.157755
27	1	0	0.978037	-2.228373	3.676597
28	6	0	-2.566120	-0.833374	4.380482
29	1	0	-2.607023	-0.318231	2.289413
30	6	0	-1.828376	-1.406788	5.417227
31	1	0	0.032306	-2.354305	5.958927
32	1	0	-3.564825	-0.447651	4.569365
33	1	0	-2.245458	-1.464797	6.419201
34	6	0	0.743138	-1.256325	-2.822159
35	6	0	0.017277	-1.840061	-3.871248

36	6	0	2.027294	-0.758690	-3.096117
37	6	0	0.551353	-1.908395	-5.157755
38	1	0	-0.978037	-2.228373	-3.676597
39	6	0	2.566120	-0.833374	-4.380482
40	1	0	2.607023	-0.318231	-2.289413
41	6	0	1.828376	-1.406788	-5.417227
42	1	0	-0.032306	-2.354305	-5.958927
43	1	0	3.564825	-0.447651	-4.569365
44	1	0	2.245458	-1.464797	-6.419201
45	6	0	0.743138	1.256325	2.822159
46	6	0	2.027294	0.758690	3.096117
47	6	0	0.017277	1.840061	3.871248
48	6	0	2.566120	0.833374	4.380482
49	1	0	2.607023	0.318231	2.289413
50	6	0	0.551353	1.908395	5.157755
51	1	0	-0.978037	2.228373	3.676597
52	6	0	1.828376	1.406788	5.417227
53	1	0	3.564825	0.447651	4.569365
54	1	0	-0.032306	2.354305	5.958927
55	1	0	2.245458	1.464797	6.419201
56	6	0	-0.743138	1.256325	-2.822159
57	6	0	-0.017277	1.840061	-3.871248
58	6	0	-2.027294	0.758690	-3.096117
59	6	0	-0.551353	1.908395	-5.157755
60	1	0	0.978037	2.228373	-3.676597
61	6	0	-2.566120	0.833374	-4.380482
62	1	0	-2.607023	0.318231	-2.289413
63	6	0	-1.828376	1.406788	-5.417227
64	1	0	0.032306	2.354305	-5.958927
65	1	0	-3.564825	0.447651	-4.569365
66	1	0	-2.245458	1.464797	-6.419201
67	1	0	0.465003	-5.838702	-1.162322
68	1	0	-0.465003	-5.838702	1.162322
69	1	0	0.465003	5.838702	1.162322
70	1	0	-0.465003	5.838702	-1.162322

Compound **1** C_{2h} symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.693165	0.564481	1.398395
2	6	0	-2.437170	0.369603	0.723230
3	6	0	-2.437170	0.369603	-0.723230
4	6	0	-3.693165	0.564481	-1.398395
5	6	0	-4.853858	0.781158	-0.711828
6	6	0	-4.853858	0.781158	0.711828
7	1	0	-3.709418	0.549627	2.480401
8	1	0	-3.709418	0.549627	-2.480401
9	1	0	-5.782321	0.943606	-1.252819
10	1	0	-5.782321	0.943606	1.252819
11	6	0	-1.248423	0.099546	-1.428991
12	6	0	-1.248423	0.099546	1.428991
13	6	0	0.000000	0.000000	-0.737009
14	6	0	0.000000	0.000000	0.737009
15	6	0	1.248423	-0.099546	-1.428991
16	6	0	1.248423	-0.099546	1.428991
17	6	0	2.437170	-0.369603	-0.723230
18	6	0	2.437170	-0.369603	0.723230
19	6	0	3.693165	-0.564481	-1.398395

20	1	0	3.709418	-0.549627	-2.480401
21	6	0	3.693165	-0.564481	1.398395
22	1	0	3.709418	-0.549627	2.480401
23	6	0	4.853858	-0.781158	-0.711828
24	1	0	5.782321	-0.943606	-1.252819
25	6	0	4.853858	-0.781158	0.711828
26	1	0	5.782321	-0.943606	1.252819
27	6	0	1.409665	0.274229	-2.875314
28	6	0	1.619007	-0.669252	-3.890825
29	6	0	1.490901	1.636272	-3.203169
30	6	0	1.879106	-0.263144	-5.199644
31	1	0	1.566706	-1.727428	-3.652781
32	6	0	1.752277	2.044851	-4.511357
33	1	0	1.353366	2.377922	-2.420604
34	6	0	1.946331	1.095413	-5.515450
35	1	0	2.029263	-1.010852	-5.974049
36	1	0	1.812346	3.105342	-4.743077
37	1	0	2.152436	1.410205	-6.535090
38	6	0	1.409665	0.274229	2.875314
39	6	0	1.490901	1.636272	3.203169
40	6	0	1.619007	-0.669252	3.890825
41	6	0	1.752277	2.044851	4.511357
42	1	0	1.353366	2.377922	2.420604
43	6	0	1.879106	-0.263144	5.199644
44	1	0	1.566706	-1.727428	3.652781
45	6	0	1.946331	1.095413	5.515450
46	1	0	1.812346	3.105342	4.743077
47	1	0	2.029263	-1.010852	5.974049
48	1	0	2.152436	1.410205	6.535090
49	6	0	-1.409665	-0.274229	-2.875314
50	6	0	-1.490901	-1.636272	-3.203169
51	6	0	-1.619007	0.669252	-3.890825
52	6	0	-1.752277	-2.044851	-4.511357
53	1	0	-1.353366	-2.377922	-2.420604
54	6	0	-1.879106	0.263144	-5.199644
55	1	0	-1.566706	1.727428	-3.652781
56	6	0	-1.946331	-1.095413	-5.515450
57	1	0	-1.812346	-3.105342	-4.743077
58	1	0	-2.029263	1.010852	-5.974049
59	1	0	-2.152436	-1.410205	-6.535090
60	6	0	-1.409665	-0.274229	2.875314
61	6	0	-1.490901	-1.636272	3.203169
62	6	0	-1.619007	0.669252	3.890825
63	6	0	-1.752277	-2.044851	4.511357
64	1	0	-1.353366	-2.377922	2.420604
65	6	0	-1.879106	0.263144	5.199644
66	1	0	-1.566706	1.727428	3.652781
67	6	0	-1.946331	-1.095413	5.515450
68	1	0	-1.812346	-3.105342	4.743077
69	1	0	-2.029263	1.010852	5.974049
70	1	0	-2.152436	-1.410205	6.535090

Compound **1** D_{2h} symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.397259	-3.747360	0.000000
2	6	0	-0.721415	-2.473613	0.000000
3	6	0	0.721415	-2.473613	0.000000

4	6	0	1.397259	-3.747360	0.000000
5	6	0	0.711489	-4.927811	0.000000
6	6	0	-0.711489	-4.927811	0.000000
7	1	0	-2.478194	-3.766937	0.000000
8	1	0	2.478194	-3.766937	0.000000
9	1	0	1.253813	-5.869636	0.000000
10	1	0	-1.253813	-5.869636	0.000000
11	6	0	1.431608	-1.257298	0.000000
12	6	0	-1.431608	-1.257298	0.000000
13	6	0	0.741217	0.000000	0.000000
14	6	0	-0.741217	0.000000	0.000000
15	6	0	1.431608	1.257298	0.000000
16	6	0	-1.431608	1.257298	0.000000
17	6	0	0.721415	2.473613	0.000000
18	6	0	-0.721415	2.473613	0.000000
19	6	0	1.397259	3.747360	0.000000
20	1	0	2.478194	3.766937	0.000000
21	6	0	-1.397259	3.747360	0.000000
22	1	0	-2.478194	3.766937	0.000000
23	6	0	0.711489	4.927811	0.000000
24	1	0	1.253813	5.869636	0.000000
25	6	0	-0.711489	4.927811	0.000000
26	1	0	-1.253813	5.869636	0.000000
27	6	0	2.926204	1.428293	0.000000
28	6	0	3.618512	1.620307	1.203675
29	6	0	3.618512	1.620307	-1.203675
30	6	0	4.968443	1.971576	1.205762
31	1	0	3.087674	1.504191	2.144906
32	6	0	4.968443	1.971576	-1.205762
33	1	0	3.087674	1.504191	-2.144906
34	6	0	5.648905	2.150028	0.000000
35	1	0	5.486320	2.114540	2.150806
36	1	0	5.486320	2.114540	-2.150806
37	1	0	6.699008	2.430151	0.000000
38	6	0	-2.926204	1.428293	0.000000
39	6	0	-3.618512	1.620307	-1.203675
40	6	0	-3.618512	1.620307	1.203675
41	6	0	-4.968443	1.971576	-1.205762
42	1	0	-3.087674	1.504191	-2.144906
43	6	0	-4.968443	1.971576	1.205762
44	1	0	-3.087674	1.504191	2.144906
45	6	0	-5.648905	2.150028	0.000000
46	1	0	-5.486320	2.114540	-2.150806
47	1	0	-5.486320	2.114540	2.150806
48	1	0	-6.699008	2.430151	0.000000
49	6	0	2.926204	-1.428293	0.000000
50	6	0	3.618512	-1.620307	1.203675
51	6	0	3.618512	-1.620307	-1.203675
52	6	0	4.968443	-1.971576	1.205762
53	1	0	3.087674	-1.504191	2.144906
54	6	0	4.968443	-1.971576	-1.205762
55	1	0	3.087674	-1.504191	-2.144906
56	6	0	5.648905	-2.150028	0.000000
57	1	0	5.486320	-2.114540	2.150806
58	1	0	5.486320	-2.114540	-2.150806
59	1	0	6.699008	-2.430151	0.000000
60	6	0	-2.926204	-1.428293	0.000000
61	6	0	-3.618512	-1.620307	1.203675
62	6	0	-3.618512	-1.620307	-1.203675
63	6	0	-4.968443	-1.971576	1.205762
64	1	0	-3.087674	-1.504191	2.144906

65	6	0	-4.968443	-1.971576	-1.205762
66	1	0	-3.087674	-1.504191	-2.144906
67	6	0	-5.648905	-2.150028	0.000000
68	1	0	-5.486320	-2.114540	2.150806
69	1	0	-5.486320	-2.114540	-2.150806
70	1	0	-6.699008	-2.430151	0.000000

Compound **2** C_2 symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.323432	0.634994	-4.727137
2	6	0	-0.669169	1.231662	-3.546922
3	6	0	-0.394154	0.608803	-2.280767
4	6	0	0.394154	-0.608803	-2.280767
5	6	0	0.669169	-1.231662	-3.546922
6	6	0	0.323432	-0.634994	-4.727137
7	6	0	-0.890537	1.120618	-1.067106
8	6	0	0.890537	-1.120618	-1.067106
9	6	0	0.547264	-0.479758	0.166440
10	6	0	-0.547264	0.479758	0.166440
11	6	0	-1.227041	0.735532	1.400623
12	6	0	-0.655038	0.311900	2.614515
13	6	0	0.655038	-0.311900	2.614515
14	6	0	1.227041	-0.735532	1.400623
15	1	0	-0.553055	1.123254	-5.670630
16	1	0	-1.176850	2.188480	-3.555569
17	1	0	1.176850	-2.188480	-3.555569
18	1	0	0.553055	-1.123254	-5.670630
19	6	0	1.307103	-0.506486	3.881366
20	6	0	-1.307103	0.506486	3.881366
21	6	0	-0.670650	0.240846	5.061249
22	6	0	0.670650	-0.240846	5.061249
23	1	0	2.320107	-0.889530	3.891647
24	1	0	1.183426	-0.408613	6.004704
25	1	0	-1.183426	0.408613	6.004704
26	1	0	-2.320107	0.889530	3.891647
27	6	0	-1.629779	2.420019	-1.080311
28	6	0	-2.885524	2.580223	-1.675663
29	6	0	-1.007581	3.565903	-0.551195
30	6	0	-3.519082	3.823575	-1.730367
31	1	0	-3.390725	1.713530	-2.091593
32	6	0	-1.619387	4.810944	-0.603049
33	1	0	-0.024823	3.472858	-0.097076
34	6	0	-2.885524	4.948159	-1.189530
35	1	0	-4.499024	3.898991	-2.187739
36	1	0	-1.135412	5.694839	-0.198789
37	6	0	1.629779	-2.420019	-1.080311
38	6	0	2.885524	-2.580223	-1.675663
39	6	0	1.007581	-3.565903	-0.551195
40	6	0	3.519082	-3.823575	-1.730367
41	1	0	3.390725	-1.713530	-2.091593
42	6	0	1.619387	-4.810944	-0.603049
43	1	0	0.024823	-3.472858	-0.097076
44	6	0	2.885524	-4.948159	-1.189530
45	1	0	4.499024	-3.898991	-2.187739
46	1	0	1.135412	-5.694839	-0.198789
47	6	0	2.620583	-1.284835	1.421260
48	6	0	3.664761	-0.491839	0.918413

49	6	0	2.945233	-2.515986	2.010665
50	6	0	4.990567	-0.918523	0.994058
51	1	0	3.429812	0.471271	0.473389
52	6	0	4.269695	-2.947817	2.080317
53	1	0	2.150655	-3.143027	2.403844
54	6	0	5.297982	-2.150024	1.574576
55	1	0	5.783522	-0.284956	0.604452
56	1	0	4.497621	-3.909558	2.532724
57	1	0	6.330406	-2.484583	1.635371
58	6	0	-2.620583	1.284835	1.421260
59	6	0	-3.664761	0.491839	0.918413
60	6	0	-2.945233	2.515986	2.010665
61	6	0	-4.990567	0.918523	0.994058
62	1	0	-3.429812	-0.471271	0.473389
63	6	0	-4.269695	2.947817	2.080317
64	1	0	-2.150655	3.143027	2.403844
65	6	0	-5.297982	2.150024	1.574576
66	1	0	-5.783522	0.284956	0.604452
67	1	0	-4.497621	3.909558	2.532724
68	1	0	-6.330406	2.484583	1.635371
69	8	0	3.408739	-6.210219	-1.186426
70	8	0	-3.408739	6.210219	-1.186426
71	6	0	-4.690324	6.405020	-1.760777
72	1	0	-5.459051	5.815892	-1.243135
73	1	0	-4.912282	7.467725	-1.645730
74	1	0	-4.699336	6.147263	-2.828404
75	6	0	4.690324	-6.405020	-1.760777
76	1	0	4.912282	-7.467725	-1.645730
77	1	0	4.699336	-6.147263	-2.828404
78	1	0	5.459051	-5.815892	-1.243135

Compound **2** C_s symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.868732	0.712550	1.398382
2	6	0	-2.636517	0.399995	0.723225
3	6	0	-2.636517	0.399995	-0.723225
4	6	0	-3.868732	0.712550	-1.398382
5	6	0	-5.004171	1.036500	-0.711880
6	6	0	-5.004171	1.036500	0.711880
7	1	0	-3.885759	0.700349	2.480431
8	1	0	-3.885759	0.700349	-2.480431
9	1	0	-5.913346	1.285249	-1.252920
10	1	0	-5.913346	1.285249	1.252920
11	6	0	-1.478080	0.021723	-1.429292
12	6	0	-1.478080	0.021723	1.429292
13	6	0	-0.244385	-0.196271	-0.737223
14	6	0	-0.244385	-0.196271	0.737223
15	6	0	0.989054	-0.413790	-1.429896
16	6	0	0.989054	-0.413790	1.429896
17	6	0	2.145844	-0.796004	-0.722959
18	6	0	2.145844	-0.796004	0.722959
19	6	0	3.376623	-1.111747	-1.398616
20	1	0	3.392988	-1.098541	-2.480779
21	6	0	3.376623	-1.111747	1.398616
22	1	0	3.392988	-1.098541	2.480779
23	6	0	4.510829	-1.440264	-0.711932
24	1	0	5.419179	-1.692544	-1.252762

25	6	0	4.510829	-1.440264	0.711932
26	1	0	5.419179	-1.692544	1.252762
27	6	0	1.181066	-0.069139	-2.878605
28	6	0	1.284370	-1.034704	-3.894215
29	6	0	1.407183	1.266326	-3.226959
30	6	0	1.573625	-0.675398	-5.203451
31	1	0	1.125170	-2.081406	-3.653109
32	6	0	1.698165	1.647345	-4.540094
33	1	0	1.358981	2.030911	-2.455927
34	6	0	1.779001	0.671223	-5.538067
35	1	0	1.641470	-1.421272	-5.989250
36	1	0	1.865620	2.694865	-4.764531
37	6	0	1.181066	-0.069139	2.878605
38	6	0	1.407183	1.266326	3.226959
39	6	0	1.284370	-1.034704	3.894215
40	6	0	1.698165	1.647345	4.540094
41	1	0	1.358981	2.030911	2.455927
42	6	0	1.573625	-0.675398	5.203451
43	1	0	1.125170	-2.081406	3.653109
44	6	0	1.779001	0.671223	5.538067
45	1	0	1.865620	2.694865	4.764531
46	1	0	1.641470	-1.421272	5.989250
47	6	0	-1.675747	-0.326399	-2.878002
48	6	0	-1.906013	-1.669405	-3.213097
49	6	0	-1.783012	0.639631	-3.888504
50	6	0	-2.212752	-2.039922	-4.523012
51	1	0	-1.849577	-2.425908	-2.434745
52	6	0	-2.087990	0.271469	-5.198739
53	1	0	-1.617879	1.684814	-3.644344
54	6	0	-2.303527	-1.069947	-5.521777
55	1	0	-2.388345	-3.086315	-4.760051
56	1	0	-2.158486	1.035034	-5.969133
57	1	0	-2.543367	-1.354815	-6.542774
58	6	0	-1.675747	-0.326399	2.878002
59	6	0	-1.906013	-1.669405	3.213097
60	6	0	-1.783012	0.639631	3.888504
61	6	0	-2.212752	-2.039922	4.523012
62	1	0	-1.849577	-2.425908	2.434745
63	6	0	-2.087990	0.271469	5.198739
64	1	0	-1.617879	1.684814	3.644344
65	6	0	-2.303527	-1.069947	5.521777
66	1	0	-2.388345	-3.086315	4.760051
67	1	0	-2.158486	1.035034	5.969133
68	1	0	-2.543367	-1.354815	6.542774
69	8	0	2.055704	0.920861	6.853223
70	8	0	2.055704	0.920861	-6.853223
71	6	0	2.273260	2.265067	-7.246400
72	1	0	3.138740	2.703396	-6.731428
73	1	0	2.470398	2.236118	-8.319809
74	1	0	1.390021	2.890141	-7.057243
75	6	0	2.273260	2.265067	7.246400
76	1	0	2.470398	2.236118	8.319809
77	1	0	3.138740	2.703396	6.731428
78	1	0	1.390021	2.890141	7.057243

Compound **5** C_2 symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.253481	-0.665922	-4.774750
2	6	0	-0.466212	-1.322124	-3.595210
3	6	0	-0.190354	-0.699989	-2.328315
4	6	0	0.190354	0.699989	-2.328315
5	6	0	0.466212	1.322124	-3.595210
6	6	0	0.253481	0.665922	-4.774750
7	6	0	-0.245864	-1.405160	-1.112563
8	6	0	0.245864	1.405160	-1.112563
9	6	0	-0.000718	0.727615	0.124796
10	6	0	0.000718	-0.727615	0.124796
11	6	0	0.245864	-1.409542	1.358680
12	6	0	0.189755	-0.699901	2.572995
13	6	0	-0.189755	0.699901	2.572995
14	6	0	-0.245864	1.409542	1.358680
15	1	0	-0.459129	-1.164378	-5.718005
16	1	0	-0.835200	-2.340286	-3.609030
17	1	0	0.835200	2.340286	-3.609030
18	1	0	0.459129	1.164378	-5.718005
19	6	0	-0.463622	1.323511	3.838911
20	6	0	0.463622	-1.323511	3.838911
21	6	0	0.252158	-0.666299	5.018526
22	6	0	-0.252158	0.666299	5.018526
23	1	0	-0.829362	2.342809	3.849319
24	1	0	-0.456936	1.164960	5.961982
25	1	0	0.456936	-1.164960	5.961982
26	1	0	0.829362	-2.342809	3.849319
27	6	0	-0.737830	-2.818705	-1.136140
28	6	0	-0.005605	-3.868194	-1.713222
29	6	0	-2.026692	-3.092414	-0.648163
30	6	0	-0.528911	-5.154357	-1.781650
31	1	0	0.991431	-3.674517	-2.095283
32	6	0	-2.566492	-4.371705	-0.718904
33	1	0	-2.611692	-2.286649	-0.214845
34	6	0	-1.816564	-5.415926	-1.284075
35	1	0	0.051945	-5.960989	-2.217159
36	1	0	-3.565704	-4.569428	-0.343844
37	6	0	0.737830	2.818705	-1.136140
38	6	0	0.005605	3.868194	-1.713222
39	6	0	2.026692	3.092414	-0.648163
40	6	0	0.528911	5.154357	-1.781650
41	1	0	-0.991431	3.674517	-2.095283
42	6	0	2.566492	4.371705	-0.718904
43	1	0	2.611692	2.286649	-0.214845
44	6	0	1.816564	5.415926	-1.284075
45	1	0	-0.051945	5.960989	-2.217159
46	1	0	3.565704	4.569428	-0.343844
47	6	0	-0.724948	2.827951	1.378551
48	6	0	-2.004204	3.115243	0.875213
49	6	0	0.012545	3.870623	1.960005
50	6	0	-2.525741	4.407367	0.939688
51	1	0	-2.594285	2.313457	0.439451
52	6	0	-0.503662	5.165154	2.016809
53	1	0	1.002332	3.664773	2.357145
54	6	0	-1.774942	5.438235	1.507113
55	1	0	-3.521002	4.607105	0.550928
56	1	0	0.088247	5.961528	2.459910
57	1	0	-2.177734	6.446255	1.556082
58	6	0	0.724948	-2.827951	1.378551
59	6	0	2.004204	-3.115243	0.875213
60	6	0	-0.012545	-3.870623	1.960005
61	6	0	2.525741	-4.407367	0.939688

62	1	0	2.594285	-2.313457	0.439451
63	6	0	0.503662	-5.165154	2.016809
64	1	0	-1.002332	-3.664773	2.357145
65	6	0	1.774942	-5.438235	1.507113
66	1	0	3.521002	-4.607105	0.550928
67	1	0	-0.088247	-5.961528	2.459910
68	1	0	2.177734	-6.446255	1.556082
69	6	0	2.360884	6.740096	-1.353126
70	6	0	-2.360884	-6.740096	-1.353126
71	7	0	2.801948	7.815601	-1.406810
72	7	0	-2.801948	-7.815601	-1.406810

Compound **5** C_s symmetry

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.858181	-0.627396	1.399030
2	6	0	2.614293	-0.370150	0.723077
3	6	0	2.614293	-0.370150	-0.723077
4	6	0	3.858181	-0.627396	-1.399030
5	6	0	5.006682	-0.899938	-0.711787
6	6	0	5.006682	-0.899938	0.711787
7	1	0	3.875152	-0.614080	2.480958
8	1	0	3.875152	-0.614080	-2.480958
9	1	0	5.926175	-1.107448	-1.252309
10	1	0	5.926175	-1.107448	1.252309
11	6	0	1.440169	-0.043295	-1.429285
12	6	0	1.440169	-0.043295	1.429285
13	6	0	0.199906	0.125258	-0.736773
14	6	0	0.199906	0.125258	0.736773
15	6	0	-1.042837	0.295682	-1.425373
16	6	0	-1.042837	0.295682	1.425373
17	6	0	-2.217031	0.629018	-0.723317
18	6	0	-2.217031	0.629018	0.723317
19	6	0	-3.460450	0.892518	-1.398388
20	1	0	-3.480207	0.882328	-2.480381
21	6	0	-3.460450	0.892518	1.398388
22	1	0	-3.480207	0.882328	2.480381
23	6	0	-4.608024	1.169703	-0.711782
24	1	0	-5.526086	1.382250	-1.252539
25	6	0	-4.608024	1.169703	0.711782
26	1	0	-5.526086	1.382250	1.252539
27	6	0	-1.227098	-0.061675	-2.872568
28	6	0	-1.366152	0.899524	-3.884877
29	6	0	-1.407852	-1.413973	-3.205093
30	6	0	-1.646534	0.525359	-5.194166
31	1	0	-1.240905	1.949955	-3.643624
32	6	0	-1.692325	-1.803047	-4.509571
33	1	0	-1.327890	-2.166864	-2.426365
34	6	0	-1.809945	-0.832328	-5.517234
35	1	0	-1.740218	1.276735	-5.971527
36	1	0	-1.830735	-2.851532	-4.753998
37	6	0	-1.227098	-0.061675	2.872568
38	6	0	-1.407852	-1.413973	3.205093
39	6	0	-1.366152	0.899524	3.884877
40	6	0	-1.692325	-1.803047	4.509571
41	1	0	-1.327890	-2.166864	2.426365
42	6	0	-1.646534	0.525359	5.194166
43	1	0	-1.240905	1.949955	3.643624

44	6	0	-1.809945	-0.832328	5.517234
45	1	0	-1.830735	-2.851532	4.753998
46	1	0	-1.740218	1.276735	5.971527
47	6	0	1.615466	0.302725	-2.880630
48	6	0	1.774724	1.652756	-3.229423
49	6	0	1.759634	-0.667057	-3.883075
50	6	0	2.044645	2.025367	-4.546777
51	1	0	1.691839	2.412894	-2.456935
52	6	0	2.027199	-0.296832	-5.201199
53	1	0	1.654436	-1.717339	-3.627059
54	6	0	2.168444	1.051128	-5.538496
55	1	0	2.166176	3.076524	-4.795621
56	1	0	2.126169	-1.062750	-5.965729
57	1	0	2.379854	1.337626	-6.565098
58	6	0	1.615466	0.302725	2.880630
59	6	0	1.774724	1.652756	3.229423
60	6	0	1.759634	-0.667057	3.883075
61	6	0	2.044645	2.025367	4.546777
62	1	0	1.691839	2.412894	2.456935
63	6	0	2.027199	-0.296832	5.201199
64	1	0	1.654436	-1.717339	3.627059
65	6	0	2.168444	1.051128	5.538496
66	1	0	2.166176	3.076524	4.795621
67	1	0	2.126169	-1.062750	5.965729
68	1	0	2.379854	1.337626	6.565098
69	6	0	-2.096531	-1.222948	-6.866230
70	7	0	-2.325878	-1.540098	-7.962108
71	6	0	-2.096531	-1.222948	6.866230
72	7	0	-2.325878	-1.540098	7.962108

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