Photochromic Oligothienoacene Derivatives with Photo-Switchable Luminescene Properties and Computational Studies

Chi-Chiu Ko, Wai Han Lam and Vivian Wing-Wah Yam*

Department of Chemistry, and HKU-CAS Joint Laboratory on New Materials, The University of Hong Kong, Pokfulam Road, Hong Kong, PR China.

Supplementary Information

General Experimental Procedures for 1 – 3

The tetrabromodithieno[3,2-b:2',3'-d]thiophene, 2,3,5-tribromo- and tetrabromo-thieno[3,2-b]thiophene, and were prepared according to the procedure reported by Iddon and coworkers[1] as well as Frey, Holmes and coworkers.[2] All reactions were performed under strictly anaerobic conditions in an inert atmosphere of nitrogen using standard Schlenk technique.

2,5-Dimethylthien-3-ylboronic acid.[3] To a stirred solution of anhydrous 3-bromo-2,5-dimethylthiophene (2.7 g, 14.1 mmol) in anhydrous THF (40 ml) at –78°C was slowly added *n*-butyllithium (1.6 M in hexane, 9.7 ml, 15.6 mmol) and the reaction mixture was then stirred at this temperature for 90 minutes. A solution of tri-*n*-butyl borate (3.85 ml, 14.2 mmol) in THF (10 ml) was then added over a period of 15 min. After stirring for 5 hours, aqueous HCl (2 M) solution was added and the mixture was stirred at room temperature for 10 hours. This was followed by extraction with diethyl ether and the combined extracts were then washed with copious amounts of water. The product was then obtained by extracting the ethereal layer with aqueous sodium hydroxide solution (2 M, 20 ml), followed by acidification with HCl (12 M) to commence the precipitation of 2,5-dimethylthien-3-yl boronic acid as an analytically pure white powder. Yield: 1.9 g, 7.8 mmol; 87 %. ^{1}H NMR (300 MHz, d^6-DMSO, 298 K): δ 2.33 (s, 3H, 5-Me), 2.50 (s, 3H, 2-Me), 6.85 (s, 1H, thienyl proton at 4-position), 7.72 (br, s, 2H, -B(OH)$_2$).

Diarylethene-containing thieno[3,2-b]thiophenes and dithieno[3,2-b:2',3'-d]thiophene (1 – 3). The target compounds were synthesized by the bis-coupling reaction of 2,5-dimethylthien-3-yl boronic acid with the corresponding the bromo-derivatives of thieno[3,2-b]thiophene and dithieno[3,2-b:2',3'-d]thiophene according to standard Suzuki coupling procedure in a heterogeneous mixture of water and 1,4-dioxane.

To the solution of bromo- derivatives of thieno[3,2-b]thiophene and dithieno[3,2-b:2',3'-d]thiophene, 2,5-dimethylthien-3-yl boronic acid (4 – 6 mol equiv.), tetrakis(triphenylphosphine)palladium(0) (0.1 mol equiv.) in 1,4-dioxane was added aqueous sodium carbonate solution (2 M, 8 mol equiv.). The resulting heterogeneous mixture was vigorously stirred and heated under reflux and the course of reaction monitored by TLC. It was then extracted with dichloromethane, and the combined extracts were dried over anhydrous magnesium sulfate. After filtration and removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel (70–230 mesh) with *n*-hexane-chloroform (1:1 v/v) as eluent. Further purification was achieved by slowly diffusion of diethyl ether vapor into a concentrated chloroform solution to give the target compounds as white to pale yellow crystalline solid.

Experimental Details for Luminescence Quantum Yield Determinations

The quantum yields of luminescence were determined according to the method described by Crosby *et al.*[4] utilizing quinine sulfate in aqueous sulfuric acid (0.5 M) as reference standard.

Computational Details

Calculations were carried out using Gaussian03 software package.[5] Density functional theory (DFT) at the hybrid Perdew, Burke, and Ernzerhof functional (PBE1PBE)[6] level of theory with a larger grid size (99590) was used to optimize the ground-state geometries of the open forms **1**–**3** and closed forms **1'**–**3'**. Based on the ground state optimized geometries in the gas phase, non-equilibrium time-dependent (TDDFT) method[7] at the same level associated with conductor-like polarizable continuum model (CPCM)[8] using benzene as a solvent (ofac = 0.8 and rmin = 0.5) was employed to study the nature of the singlet-singlet transitions in the electronic absorption spectra of the open forms **1**–**3** and closed forms **1'**–**3'**. The first singlet excited state (S_1) of the open forms **1**–**3** was optimized using the configuration interaction singles (CIS) method.[9] Since CIS method is the Hartree-Fock (HF) analogue for the excited state, the open forms were also optimized at the HF level of theory in order to compare the ground-state and excited-state structures of the open forms. On the basis of the S_1 optimized geometries, the emission energies of the open forms **1**–**3** were computed at the TD-PBE1PBE/CPCM calculation (benzene as the solvent). Except for the geometry optimizations of the ground and first singlet excited states of the open forms **2** and **3**, in which they were performed with the constraint of C_2 symmetry, all the geometry optimizations were performed with no symmetry restriction. For all the calculations, the 6-31Gd(p) basis set[10] was employed to describe the S, C and H atoms. Vibrational frequencies were calculated for all stationary points to verify that each was a minimum (NIMAG = 0) on the potential energy surface.

PBE1PBE Ground-State Geometries

The PBE1PBE optimized ground-state structures of the open forms **1**–**3** and closed forms **1'**–**3'** are shown in Figure S1. For the open forms, the oligothienoacene core is essentially planar in the calculated structures of **1**–**3**, with the interplanar angles between the core and the peripheral thiophene rings in the ranges of 35.5–51.2, 48.8–51.3, and 49.2–51.4° for **1**, **2** and **3**, respectively. The average C=C and C–C bond distances are 1.382 and 1.423 Å for **1**, 1.384 and 1.429 Å for **2**, 1.386 and 1.424 Å for **3,** respectively, in the oligothienoacene core as well as 1.370 and 1.435 Å for **1**, 1.370 and 1.436 Å for **2**, 1.370 and 1.436 Å for **3** in the peripheral thiophene rings. Different from the symmetric S–C bond distances found in the peripheral thiophene rings [**1** (1.731–1.735 Å), **2** (1.732–1.735 Å) and **3** (1.732–1.735 Å)], the calculated C–S bond distances in the oligothienoacene core are rather unsymmetric, in which the average exterior C–S bond distances [**1** (1.756 Å), **2** (1.755 Å) and **3** (1.756 Å)] are slightly longer than the average interior S–C bonds [**1** (1.729 Å), **2** (1.728 Å) and **3** (1.735 Å)]. The distance between the two reacting carbon atoms is 3.576, 3.578 and 3.580 Å for **l**, **2** and **3**, respectively. This distance is decreased to 1.534 Å for the *trans* configuration of the closed forms **1'**–**3'**. In addition, the bond lengths of inner C–S bonds (1.853–1.854 Å) are longer than outer C–S bonds (1.758–1.762 Å) in the condensed ring for **1'**–**3'**. The difference between the C–S bond lengths is due to the hybridization of the carbon atoms.

References

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Table S1. The first singlet excited state (S_1) computed by TD-PBE1PBE/CPCM using benzene as a solvent based on PBE1PBE ground-state optimized geometry of the open forms **1**–**3**, with the orbitals involved in the excitations (H = HOMO and L = LUMO), transition coefficients, vertical excitation wavelengths (nm), oscillator strengths (*f*) and the λ_{max} observed from the electronic absorption spectra of the open forms **1**–**3**

Compound	S_n	Excitation	Transition Coefficient	*f*	Vertical excitation wavelength (nm)	Experimental λ_{max} (nm)
1 (open form)	S_1	H → L	0.66	0.881	336	334
2 (open form)	S_1	H → L	0.66	0.654	334	332
3 (open form)	S_1	H → L	0.66	0.970	353	350

Table S2. The first three singlet excited states computed by TD-PBE1PBE/CPCM using benzene as a solvent based on PBE1PBE ground-state optimized geometry of the closed forms **1'**–**3'**, with the orbitals involved in the excitations (H = HOMO and L = LUMO), transition coefficients, vertical excitation wavelengths (nm), oscillator strengths (*f*) and λ_{max} observed from the UV electronic absorption spectra of the closed forms **1'**–**3'**

Compound	S_n	Excitation[a]	Transition Coefficient	*f*	Vertical excitation wavelength (nm)	Experimental λ_{max} (nm)
1' (closed form)	S_1	H → L	0.63	0.187	585	560
	S_2	H–1 → L	0.42	0.005	389	
		H → L+1	0.55			
	S_3	H–1 → L	0.52	1.025	377	378
		H → L+1	–0.40			
2' (closed form)	S_1	H → L	0.63	0.189	582	560
	S_2	H–1 → L	–0.46	0.006	390	
		H → L+1	0.51			
	S_3	H–1 → L	0.48	0.776	378	370
		H → L+1	0.46			
3' (closed form)	S_1	H → L	0.63	0.224	589	564
	S_2	H–1 → L	–0.38	0.008	402	
		H → L+1	0.57			
	S_3	H–1 → L	0.54	1.067	392	386
		H → L+1	0.37			

[a]The excitation with the absolute value of transition coefficients less than 0.2 were not shown.

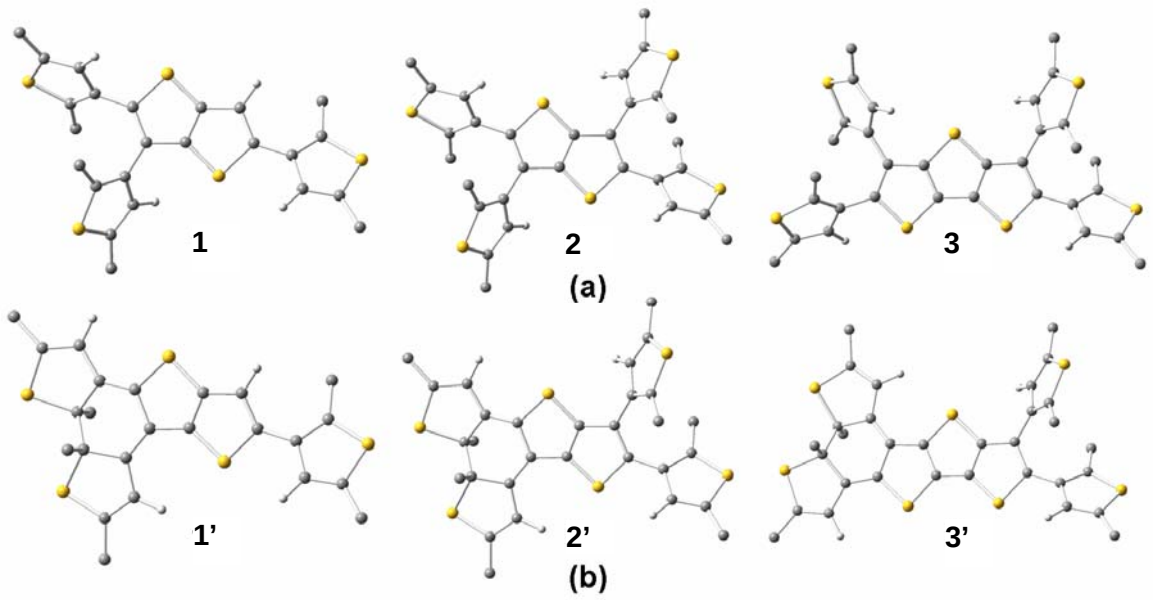

Figure S1. PBE1PBE optimized geometries of the (a) open forms **1**–**3** and (b) closed forms **1'**–**3'** (The open forms **2** and **3** are with C_2 symmetry). Hydrogen atoms on the methyl groups are omitted for clarity.

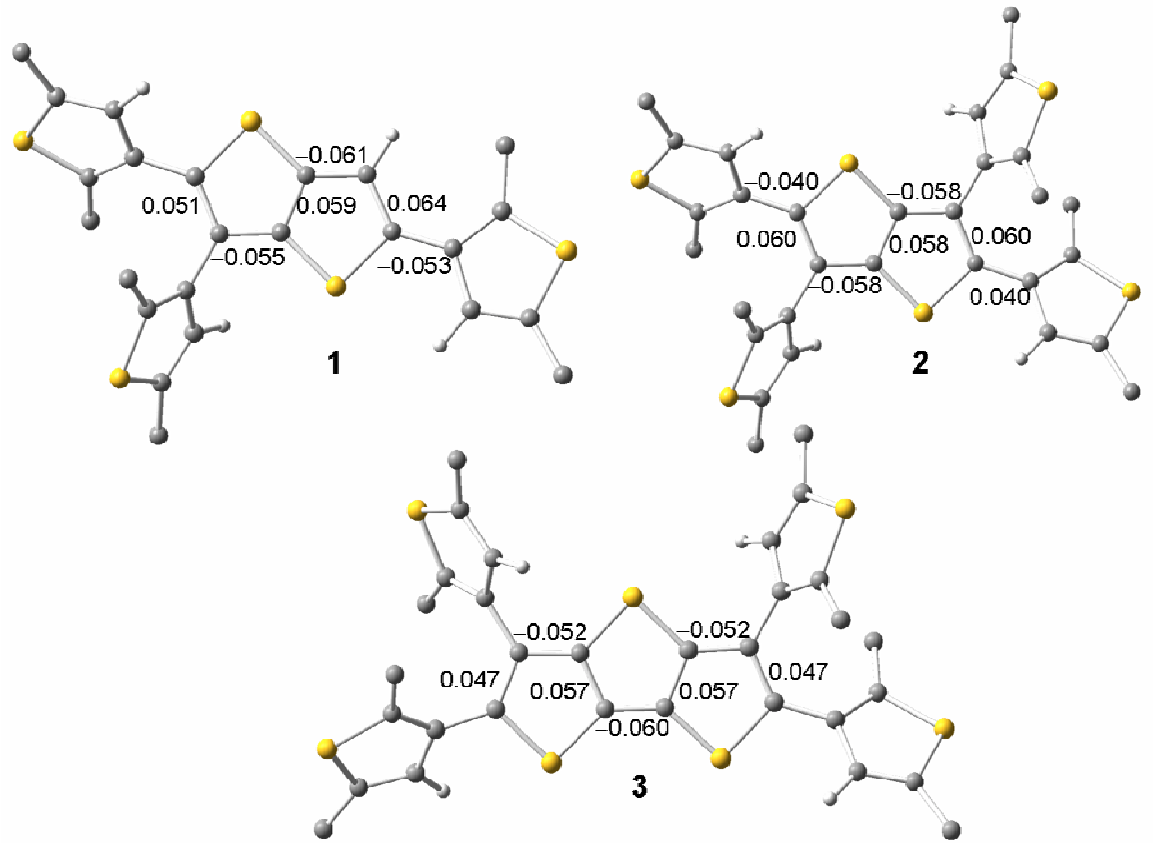

Figure S2. CIS optimized structures of the first singlet states of the open forms **1–3** with the change in bond distances (in Å), relative to their corresponding HF optimized ground states. Only differences in bond distances larger than or equal to 0.04 Å were shown. Hydrogen atoms on the methyl groups are omitted for clarity.

Cartesian coordinates for all optimized structures reported in the paper with the calculated electronic energy (Hartree) in parenthesis

PBE1PBE optimized geometries of the open forms **1**–**3**

1 (-2916.921319)

1	C	6.389153	0.550456	-0.712266
2	S	6.904602	-0.779675	0.274452
3	C	5.283874	-1.308080	0.574254
4	C	4.382415	-0.491036	-0.075706
5	C	5.029957	0.566486	-0.798211
6	C	5.028692	-2.481158	1.460876
7	C	2.934509	-0.655283	-0.033578
8	S	1.908264	0.769335	-0.016427
9	C	0.479029	-0.204035	0.036964
10	C	0.804550	-1.550886	0.042272
11	C	2.196438	-1.814613	-0.003305
12	S	-0.627137	-2.517961	0.048140
13	C	-1.652128	-1.092733	0.035590
14	C	-0.920292	0.081579	0.014905
15	C	-3.099686	-1.297006	0.081660
16	C	-3.954688	-0.674867	0.965031
17	S	-5.583945	-1.196598	0.695438
18	C	-5.129639	-2.272020	-0.587948
19	C	-3.783137	-2.212073	-0.788247
20	C	-1.455171	1.449853	-0.049509
21	C	-2.384176	1.897836	-0.959888
22	S	-2.717875	3.579224	-0.703481
23	C	-1.600072	3.697759	0.617398
24	C	-1.009864	2.488207	0.835184
25	C	-3.058758	1.155230	-2.063849
26	C	-1.387607	4.981418	1.348632
27	C	-3.643203	0.297099	2.052058
28	C	-6.142381	-3.094532	-1.312710
29	H	2.640126	-2.800968	-0.053353
30	C	7.371534	1.477395	-1.346945
31	H	-3.187193	1.785535	-2.948966
32	H	-4.045947	0.785897	-1.762949
33	H	-2.458016	0.286235	-2.344143
34	H	-0.280495	2.323564	1.622233
35	H	-1.025364	5.774083	0.684912
36	H	-0.642611	4.836858	2.135315
37	H	-2.308514	5.342161	1.819731
38	H	-4.287257	0.141266	2.922656
39	H	-3.765031	1.334255	1.719151
40	H	-2.603128	0.177101	2.366298
41	H	-3.274376	-2.791314	-1.552411
42	H	-6.673317	-3.775375	-0.638462
43	H	-5.646313	-3.698714	-2.076673
44	H	-6.893954	-2.472979	-1.811545
45	H	5.038615	-3.427715	0.906401
46	H	5.783555	-2.557255	2.248930
47	H	4.047519	-2.384036	1.934856
48	H	4.487452	1.301800	-1.384022
49	H	8.041823	0.952830	-2.036468
50	H	6.838715	2.243963	-1.915352
51	H	7.995060	1.983630	-0.602047

2 (-3546.950082)

1	S	1.514130	1.417424	-0.042869
2	S	-4.762301	2.900752	0.687120
3	S	-0.263717	6.237862	-0.619828
4	C	-0.001536	2.302001	-0.028346
5	C	-1.102188	1.463422	-0.034208
6	C	-0.684295	0.098176	-0.086094
7	C	-3.057839	2.728114	0.950703
8	C	-2.515951	1.862422	0.028959
9	C	-3.501018	1.332796	-0.870229
10	H	-3.261503	0.635542	-1.667105
11	C	-4.763589	1.798619	-0.652123
12	C	-0.629412	4.571971	-0.921085
13	C	0.065249	3.763205	-0.048299
14	C	0.907508	4.513595	0.839790
15	H	1.527764	4.047514	1.598991
16	C	0.842353	5.863157	0.663250
17	S	-1.514130	-1.417424	-0.042869
18	S	4.762301	-2.900752	0.687120
19	S	0.263717	-6.237862	-0.619828
20	C	0.001536	-2.302001	-0.028346
21	C	1.102188	-1.463422	-0.034208
22	C	0.684295	-0.098176	-0.086094
23	C	3.057839	-2.728114	0.950703
24	C	2.515951	-1.862422	0.028959
25	C	3.501018	-1.332796	-0.870229
26	H	3.261503	-0.635542	-1.667105
27	C	4.763589	-1.798619	-0.652123
28	C	0.629412	-4.571971	-0.921085
29	C	-0.065249	-3.763205	-0.048299
30	C	-0.907508	-4.513595	0.839790
31	H	-1.527764	-4.047514	1.598991
32	C	-0.842353	-5.863157	0.663250
33	C	1.562380	6.935179	1.411425
34	H	2.193953	7.539800	0.751414
35	H	0.870422	7.615979	1.919116
36	H	2.206403	6.484026	2.170668
37	C	-1.562380	4.191055	-2.020114
38	H	-1.345930	3.171762	-2.350335
39	H	-2.608181	4.211802	-1.692656
40	H	-1.461417	4.861328	-2.878957
41	C	-2.391935	3.452625	2.071812
42	H	-1.466956	2.938519	2.345018
43	H	-2.124923	4.478442	1.792882
44	H	-3.035277	3.497916	2.955760
45	C	-6.016146	1.474026	-1.395998
46	H	-6.773755	1.026164	-0.743696
47	H	-6.461894	2.362817	-1.855914
48	H	-5.795178	0.758928	-2.192605
49	C	-1.562380	-6.935179	1.411425
50	H	-2.193953	-7.539800	0.751414
51	H	-0.870422	-7.615979	1.919116
52	H	-2.206403	-6.484026	2.170668
53	C	1.562380	-4.191055	-2.020114
54	H	1.345930	-3.171762	-2.350335
55	H	2.608181	-4.211802	-1.692656
56	H	1.461417	-4.861328	-2.878957
57	C	2.391935	-3.452625	2.071812
58	H	1.466956	-2.938519	2.345018
59	H	2.124923	-4.478442	1.792882
60	H	3.035277	-3.497916	2.955760
61	C	6.016146	-1.474026	-1.395998
62	H	6.773755	-1.026164	-0.743696
63	H	6.461894	-2.362817	-1.855914
64	H	5.795178	-0.758928	-2.192605

3 (-4021.115128)

1	C	-0.556700	3.929758	3.553495
2	C	-0.781800	3.161344	2.449953
3	C	0.130887	3.404769	1.369730
4	C	1.068801	4.362392	1.679151
5	S	0.804831	4.969042	3.280953
6	C	0.064211	2.661210	0.102517
7	C	0.000000	1.235910	0.043925
8	C	-0.001285	0.708393	-1.239118
9	S	0.045550	1.964289	-2.418616
10	C	0.077399	3.200112	-1.172138
11	S	0.000000	0.000000	1.276338
12	C	0.000000	-1.235910	0.043925
13	C	0.001285	-0.708393	-1.239118
14	C	-0.064211	-2.661210	0.102517
15	S	-0.045550	-1.964289	-2.418616
16	C	0.078442	4.597426	-1.603643
17	C	-0.784258	5.565448	-1.137394
18	S	-0.459193	7.082454	-1.906465
19	C	0.819859	6.426457	-2.877847
20	C	0.978131	5.101303	-2.602564
21	H	1.732246	4.485485	-3.082592
22	H	-1.592804	2.442193	2.390206
23	C	-0.077399	-3.200112	-1.172138
24	C	-0.130887	-3.404769	1.369730
25	C	-1.068801	-4.362392	1.679151
26	C	0.781800	-3.161344	2.449953
27	S	-0.804831	-4.969042	3.280953
28	C	0.556700	-3.929758	3.553495
29	H	1.592804	-2.442193	2.390206
30	C	-0.078442	-4.597426	-1.603643
31	C	0.784258	-5.565448	-1.137394
32	C	-0.978131	-5.101303	-2.602564
33	S	0.459193	-7.082454	-1.906465
34	C	-0.819859	-6.426457	-2.877847
35	H	-1.732246	-4.485485	-3.082592
36	C	1.583258	7.274551	-3.839809
37	H	0.932188	7.709315	-4.606030
38	H	2.098356	8.100908	-3.338020
39	H	2.337780	6.667262	-4.346386
40	C	-1.889875	5.443514	-0.144396
41	H	-2.237159	4.407775	-0.104992
42	H	-1.562637	5.715871	0.865585
43	H	-2.737370	6.081837	-0.411292
44	C	2.204211	4.872738	0.857111
45	H	2.470647	4.133849	0.097098
46	H	1.943824	5.799940	0.333681
47	H	3.087368	5.067206	1.473071
48	C	-1.310012	3.950113	4.841786
49	H	-2.119988	3.217102	4.804963
50	H	-0.668544	3.698902	5.693498
51	H	-1.753327	4.931700	5.041989
52	C	1.310012	-3.950113	4.841786
53	H	2.119988	-3.217102	4.804963
54	H	0.668544	-3.698902	5.693498
55	H	1.753327	-4.931700	5.041989
56	C	-2.204211	-4.872738	0.857111
57	H	-2.470647	-4.133849	0.097098
58	H	-1.943824	-5.799940	0.333681
59	H	-3.087368	-5.067206	1.473071
60	C	1.889875	-5.443514	-0.144396
61	H	2.237159	-4.407775	-0.104992
62	H	1.562637	-5.715871	0.865585
63	H	2.737370	-6.081837	-0.411292
64	C	-1.583258	-7.274551	-3.839809
65	H	-0.932188	-7.709315	-4.606030
66	H	-2.098356	-8.100908	-3.338020
67	H	-2.337780	-6.667262	-4.346386

PBE1PBE optimized geometries of the closed forms **1'**–**3'**

1' (-2916.900435)

1	C	3.096886	-0.524510	-0.076802
2	C	2.404436	-1.706333	-0.231086
3	C	1.005895	-1.509882	-0.194479
4	C	0.620367	-0.196719	-0.023771
5	C	-1.484718	-1.264170	-0.150644
6	C	-0.798670	0.027937	-0.051328
7	H	2.890518	-2.658192	-0.403546
8	S	-0.350877	-2.609831	-0.377286
9	S	2.001911	0.827162	0.111533
10	C	4.534590	-0.294236	-0.049205
11	C	5.458508	-1.166751	0.488581
12	C	5.148576	0.892404	-0.573553
13	S	7.058410	-0.528097	0.326883
14	C	6.504564	0.920489	-0.449756
15	H	4.586812	1.688078	-1.052625
16	C	7.457260	1.977808	-0.898613
17	H	8.038100	2.384543	-0.063717
18	H	8.167796	1.598842	-1.641113
19	H	6.903100	2.801988	-1.354926
20	C	5.238674	-2.477062	1.168327
21	H	5.989702	-2.654814	1.943392
22	H	4.251413	-2.493548	1.639382
23	H	5.287689	-3.318940	0.466667
24	C	-2.830227	-1.372768	-0.022912
25	C	-3.609165	-0.123413	0.395446
26	C	-3.683063	-2.517695	-0.141913
27	S	-5.364653	-0.510301	-0.057253
28	C	-5.006734	-2.231989	-0.171273
29	H	-3.305542	-3.531452	-0.236729
30	C	-1.531079	1.183180	-0.041208
31	C	-3.028618	1.092633	-0.336862
32	C	-1.103295	2.535732	0.126874
33	S	-3.713319	2.713549	0.243803
34	C	-2.109273	3.433869	0.281325
35	H	-0.060246	2.834283	0.165298
36	C	-1.980780	4.902848	0.485676
37	H	-2.456696	5.458507	-0.330548
38	H	-2.468639	5.217339	1.415613
39	H	-0.928259	5.192402	0.534373
40	C	-3.205383	1.035418	-1.865194
41	H	-4.260910	1.051076	-2.143410
42	H	-2.708358	1.900265	-2.310887
43	H	-2.749468	0.124172	-2.262935
44	C	-3.536134	-0.013557	1.928199
45	H	-3.896045	-0.946978	2.367374
46	H	-2.501119	0.147070	2.244344
47	H	-4.149039	0.810693	2.297625
48	C	-6.134758	-3.195031	-0.300962
49	H	-6.789766	-3.156342	0.576920
50	H	-6.754212	-2.962914	-1.174997
51	H	-5.757530	-4.215000	-0.407644

2' (-3546.928861)

1	C	2.246629	-0.861607	-0.107537
2	C	1.868631	0.468323	0.005692
3	C	0.449103	0.587174	-0.010755
4	C	-0.236918	-0.602400	-0.101131
5	C	-2.028125	0.932019	0.039086
6	C	-1.667513	-0.487552	-0.015810
7	S	-0.604563	1.982754	0.165124
8	S	0.862177	-1.925979	-0.196719
9	C	3.577532	-1.459955	-0.196427
10	C	4.576500	-1.036788	-1.046347
11	C	3.972321	-2.594626	0.589748
12	S	5.990770	-2.015665	-0.847352
13	C	5.247866	-3.015396	0.360262
14	H	3.319306	-3.063094	1.319439
15	C	5.986019	-4.141829	1.003456
16	H	6.307668	-4.890004	0.270809
17	H	6.879510	-3.795702	1.534333
18	H	5.337201	-4.639887	1.728521
19	C	4.555617	0.063659	-2.052295
20	H	5.135942	-0.198855	-2.941810
21	H	3.525755	0.263553	-2.359273
22	H	4.960520	0.996716	-1.643984
23	C	-3.316135	1.346909	-0.053186
24	C	-4.380826	0.297742	-0.382638
25	C	-3.873978	2.663445	0.033760
26	S	-5.978102	1.103768	0.102453
27	C	-5.225447	2.697173	0.117835
28	H	-3.267439	3.563589	0.066442
29	C	-2.647119	-1.439123	0.057247
30	C	-4.068813	-0.987519	0.393796
31	C	-2.552849	-2.860400	-0.053295
32	S	-5.135364	-2.426615	-0.080410
33	C	-3.745664	-3.503572	-0.129659
34	H	-1.610333	-3.396246	-0.108786
35	C	-3.970966	-4.969224	-0.261304
36	H	-4.529075	-5.361809	0.596519
37	H	-4.556527	-5.200683	-1.158650
38	H	-3.017610	-5.499210	-0.326396
39	C	-4.162703	-0.824282	1.921830
40	H	-5.180094	-0.579592	2.232970
41	H	-3.862677	-1.761606	2.396247
42	H	-3.490519	-0.029287	2.257352
43	C	-4.399148	0.107430	-1.909162
44	H	-4.551084	1.079207	-2.384838
45	H	-3.443594	-0.303900	-2.247900
46	H	-5.201136	-0.566214	-2.216668
47	C	-6.092545	3.901992	0.232968
48	H	-6.774417	3.980894	-0.621481
49	H	-6.712283	3.858257	1.136058
50	H	-5.484575	4.808913	0.276577
51	C	2.767544	1.623108	0.155405
52	C	3.778098	1.725232	1.083243
53	C	2.644403	2.801669	-0.653732
54	S	4.579536	3.254651	0.935802
55	C	3.553320	3.775119	-0.362000
56	H	1.902931	2.905575	-1.439716
57	C	3.721191	5.112696	-1.002567
58	H	3.591443	5.928640	-0.283235
59	H	4.711432	5.228647	-1.456555
60	H	2.973975	5.238690	-1.790317
61	C	4.203882	0.748448	2.127332
62	H	5.052315	0.139501	1.794386
63	H	4.492214	1.254582	3.053540
64	H	3.380440	0.065512	2.351121

3' (-4021.093891)

1	C	1.335609	0.085020	-0.056749
2	C	0.823561	-1.203097	-0.155944
3	C	-0.588063	-1.229822	-0.127855
4	C	-1.136726	0.031317	-0.011559
5	C	-3.081676	-1.313127	-0.080575
6	C	-2.573157	0.061567	-0.043946
7	S	-1.779710	-2.507290	-0.252959
8	S	0.075569	1.277328	0.078486
9	C	2.759199	0.161909	-0.015554
10	C	-4.399841	-1.596161	0.061243
11	C	-5.338795	-0.444552	0.427299
12	C	-5.091118	-2.849400	0.000133
13	S	-7.026657	-1.083394	0.004107
14	C	-6.441188	-2.744779	-0.033941
15	H	-4.581441	-3.806926	-0.050818
16	C	-3.454501	1.107910	-0.080463
17	C	-4.926279	0.803093	-0.363315
18	C	-3.213940	2.511946	0.025304
19	S	-5.824283	2.341341	0.146268
20	C	-4.332349	3.272066	0.144529
21	H	-2.221449	2.951249	0.045183
22	C	-4.403246	4.752570	0.283032
23	H	-4.949061	5.202135	-0.554494
24	H	-4.929860	5.039432	1.200670
25	H	-3.399416	5.183105	0.313618
26	C	-5.092474	0.651967	-1.886478
27	H	-6.140112	0.511000	-2.159245
28	H	-4.717676	1.554998	-2.374001
29	H	-4.516250	-0.205920	-2.244889
30	C	-5.280305	-0.255887	1.953041
31	H	-5.511972	-1.207817	2.436583
32	H	-4.275975	0.055947	2.254796
33	H	-5.997748	0.495194	2.288594
34	C	-7.429878	-3.855170	-0.112652
35	H	-8.083750	-3.864293	0.766849
36	H	-8.075125	-3.748121	-0.992233
37	H	-6.919377	-4.819222	-0.175519
38	S	2.098184	-2.362087	-0.234700
39	C	3.315239	-1.101840	-0.120515
40	C	4.718323	-1.509110	-0.178799
41	C	5.664639	-0.955861	-1.014008
42	C	5.251492	-2.573157	0.624169
43	S	7.197289	-1.726453	-0.780326
44	C	6.577539	-2.812906	0.421934
45	H	4.655715	-3.125062	1.344418
46	C	3.485263	1.430949	0.143898
47	C	4.452062	1.677768	1.090796
48	C	3.212928	2.577534	-0.674689
49	S	5.031567	3.304809	0.949858
50	C	3.968920	3.670901	-0.370945
51	H	2.484320	2.571705	-1.479470
52	C	3.961517	5.015784	-1.018169
53	H	4.934230	5.265099	-1.456019
54	H	3.218570	5.033638	-1.819729
55	H	3.707843	5.809553	-0.307120
56	C	4.990869	0.773570	2.147857
57	H	5.186680	1.317427	3.076814
58	H	4.268407	-0.018852	2.359066
59	H	5.923199	0.290458	1.833687
60	C	5.509841	0.124808	-2.029684
61	H	6.136913	-0.060310	-2.906835
62	H	4.467955	0.177924	-2.356050
63	H	5.774527	1.107517	-1.622850
64	C	7.452578	-3.822523	1.086997
65	H	7.887655	-4.523110	0.366002
66	H	8.279859	-3.353015	1.630238
67	H	6.865729	-4.401500	1.804682

HF optimized geometries of the open forms **1**−**3**

1 (-2909.209905)

1	C	-6.390374	0.360983	0.940894
2	S	-6.900960	-0.645529	-0.380461
3	C	-5.267277	-1.075028	-0.787195
4	C	-4.394089	-0.479962	0.057596
5	C	-5.052977	0.349986	1.043575
6	C	-5.004603	-1.977275	-1.958890
7	C	-2.928226	-0.634495	0.010208
8	S	-1.897546	0.785285	0.039149
9	C	-0.477004	-0.207033	-0.029023
10	C	-0.805175	-1.523771	-0.070685
11	C	-2.213462	-1.778459	-0.043701
12	S	0.613541	-2.511793	-0.107133
13	C	1.646650	-1.091890	-0.058922
14	C	0.938868	0.064740	-0.010928
15	C	3.110797	-1.300995	-0.076776
16	C	3.954373	-0.846127	-1.029610
17	S	5.587210	-1.327007	-0.682564
18	C	5.115349	-2.171373	0.761243
19	C	3.789846	-2.071710	0.943821
20	C	1.484508	1.443560	0.049485
21	C	2.254613	1.945445	1.038546
22	S	2.644559	3.611138	0.728332
23	C	1.737176	3.628260	-0.753475
24	C	1.185144	2.424825	-0.972501
25	C	2.761435	1.278807	2.284229
26	C	1.643619	4.863546	-1.599668
27	C	3.655656	-0.045065	-2.262900
28	C	6.122989	-2.879717	1.617782
29	H	-2.658860	-2.754381	-0.039639
30	C	-7.383338	1.091828	1.795481
31	H	2.665996	1.936847	3.141409
32	H	3.806608	1.003791	2.185636
33	H	2.195273	0.378536	2.482590
34	H	0.579705	2.203513	-1.832677
35	H	1.194846	5.686040	-1.051499
36	H	1.031279	4.665970	-2.471567
37	H	2.622386	5.187280	-1.939967
38	H	4.226885	-0.411189	-3.109240
39	H	3.899251	1.002559	-2.119351
40	H	2.603888	-0.114274	-2.506742
41	H	3.274400	-2.515212	1.776090
42	H	6.638844	-3.656794	1.062394
43	H	5.626452	-3.342308	2.462579
44	H	6.871913	-2.193253	2.000371
45	H	-5.186811	-3.018061	-1.706370
46	H	-5.649725	-1.724288	-2.793326
47	H	-3.976649	-1.883490	-2.283044
48	H	-4.515595	0.894020	1.798413
49	H	-8.060173	0.404364	2.293095
50	H	-6.863350	1.662885	2.555419
51	H	-7.982420	1.779459	1.206721

2 (-3537.431785)

1	S	1.910796	0.799081	-0.028475
2	S	-3.530584	4.303966	0.616619
3	S	2.039290	5.913284	-0.574420
4	C	0.796585	2.155348	-0.018840
5	C	-0.502571	1.763567	-0.024424
6	C	-0.594845	0.325258	-0.057340
7	C	-2.027003	3.508526	0.976274
8	C	-1.701595	2.637617	-0.003069
9	C	-2.692503	2.594589	-1.058198
10	H	-2.602015	1.953287	-1.916099
11	C	-3.725765	3.430611	-0.872786
12	C	1.171361	4.458647	-0.959996
13	C	1.368870	3.519321	-0.008569
14	C	2.255187	3.972416	1.043074
15	H	2.528702	3.354404	1.878705
16	C	2.692503	5.230877	0.884225
17	S	-1.910796	-0.799081	-0.028475
18	S	3.530584	-4.303966	0.616619
19	S	-2.039290	-5.913284	-0.574420
20	C	-0.796585	-2.155348	-0.018840
21	C	0.502571	-1.763567	-0.024424
22	C	0.594845	-0.325258	-0.057340
23	C	2.027003	-3.508526	0.976274
24	C	1.701595	-2.637617	-0.003069
25	C	2.692503	-2.594589	-1.058198
26	H	2.602015	-1.953287	-1.916099
27	C	3.725765	-3.430611	-0.872786
28	C	-1.171361	-4.458647	-0.959996
29	C	-1.368870	-3.519321	-0.008569
30	C	-2.255187	-3.972416	1.043074
31	H	-2.528702	-3.354404	1.878705
32	C	-2.692503	-5.230877	0.884225
33	C	3.606692	6.018691	1.775498
34	H	4.505353	6.325537	1.249503
35	H	3.120912	6.913793	2.151429
36	H	3.902956	5.413746	2.624294
37	C	0.359130	4.383440	-2.219618
38	H	0.168433	3.350646	-2.479260
39	H	-0.597254	4.882074	-2.100762
40	H	0.883260	4.851840	-3.045802
41	C	-1.296673	3.831265	2.247301
42	H	-0.576221	3.055866	2.471050
43	H	-0.762872	4.772640	2.166055
44	H	-1.986360	3.906353	3.081329
45	C	-4.916605	3.649911	-1.758532
46	H	-5.842807	3.421159	-1.240650
47	H	-4.973645	4.678739	-2.100391
48	H	-4.850016	3.007989	-2.628993
49	C	-3.606692	-6.018691	1.775498
50	H	-4.505353	-6.325537	1.249503
51	H	-3.120912	-6.913793	2.151429
52	H	-3.902956	-5.413746	2.624294
53	C	-0.359130	-4.383440	-2.219618
54	H	-0.168433	-3.350646	-2.479260
55	H	0.597254	-4.882074	-2.100762
56	H	-0.883260	-4.851840	-3.045802
57	C	1.296673	-3.831265	2.247301
58	H	0.576221	-3.055866	2.471050
59	H	0.762872	-4.772640	2.166055
60	H	1.986360	-3.906353	3.081329
61	C	4.916605	-3.649911	-1.758532
62	H	5.842807	-3.421159	-1.240650
63	H	4.973645	-4.678739	-2.100391
64	H	4.850016	-3.007989	-2.628993

3 (-4010.673864)

1	C	-0.890025	4.013170	3.452009
2	C	-1.065602	3.283894	2.339159
3	C	0.000511	3.422772	1.369176
4	C	0.977327	4.255094	1.789102
5	S	0.602459	4.898214	3.359991
6	C	-0.007757	2.672896	0.088251
7	C	-0.021988	1.232572	0.036200
8	C	-0.012264	0.714238	-1.221051
9	S	-0.004882	1.963551	-2.411821
10	C	-0.007077	3.198241	-1.162995
11	S	0.000000	0.000000	1.274144
12	C	0.021988	-1.232572	0.036200
13	C	0.012264	-0.714238	-1.221051
14	C	0.007757	-2.672896	0.088251
15	S	0.004882	-1.963551	-2.411821
16	C	-0.009001	4.613553	-1.592371
17	C	-0.977327	5.513946	-1.312628
18	S	-0.602458	7.055449	-2.019711
19	C	0.874751	6.464663	-2.718852
20	C	1.047316	5.169996	-2.411582
21	H	1.896005	4.595372	-2.735010
22	H	-1.923128	2.656570	2.176462
23	C	0.007077	-3.198241	-1.162995
24	C	-0.000511	-3.422772	1.369176
25	C	-0.977327	-4.255094	1.789102
26	C	1.065602	-3.283894	2.339159
27	S	-0.602459	-4.898214	3.359991
28	C	0.890025	-4.013170	3.452009
29	H	1.923128	-2.656570	2.176462
30	C	0.009001	-4.613553	-1.592371
31	C	0.977327	-5.513946	-1.312628
32	C	-1.047316	-5.169996	-2.411582
33	S	0.602458	-7.055449	-2.019711
34	C	-0.874751	-6.464663	-2.718852
35	H	-1.896005	-4.595372	-2.735010
36	C	1.765440	7.355343	-3.533816
37	H	1.246453	7.745740	-4.403648
38	H	2.120743	8.200735	-2.952846
39	H	2.627508	6.796504	-3.878362
40	C	-2.245678	5.336991	-0.530316
41	H	-2.491163	4.286366	-0.450200
42	H	-2.146702	5.736784	0.473566
43	H	-3.072655	5.844306	-1.015373
44	C	2.255543	4.646621	1.106464
45	H	2.483726	3.948746	0.311911
46	H	2.181200	5.638303	0.671995
47	H	3.083795	4.647365	1.807046
48	C	-1.788049	4.115452	4.649450
49	H	-2.658499	3.485247	4.510527
50	H	-1.280224	3.794850	5.553701
51	H	-2.129155	5.134355	4.804529
52	C	1.788049	-4.115452	4.649450
53	H	2.658499	-3.485247	4.510527
54	H	1.280224	-3.794850	5.553701
55	H	2.129155	-5.134355	4.804529
56	C	-2.255543	-4.646621	1.106464
57	H	-2.483726	-3.948746	0.311911
58	H	-2.181200	-5.638303	0.671995
59	H	-3.083795	-4.647365	1.807046
60	C	2.245678	-5.336991	-0.530316
61	H	2.491163	-4.286366	-0.450200
62	H	2.146702	-5.736784	0.473566
63	H	3.072655	-5.844306	-1.015373
64	C	-1.765440	-7.355343	-3.533816
65	H	-1.246453	-7.745740	-4.403648
66	H	-2.120743	-8.200735	-2.952846
67	H	-2.627508	-6.796504	-3.878362

CIS S_1 optimized geometries of the open forms **1**−**3**

1 (-2909.188529)

1	C	-6.319900	0.703486	0.351940
2	S	-6.879152	-0.904701	-0.012695
3	C	-5.277637	-1.510234	-0.221648
4	C	-4.335573	-0.513461	-0.006421
5	C	-4.984529	0.751557	0.312486
6	C	-5.095686	-2.942715	-0.626042
7	C	-2.921000	-0.641751	-0.070930
8	S	-1.887111	0.813861	-0.019167
9	C	-0.446273	-0.175873	-0.121101
10	C	-0.788841	-1.549531	-0.177477
11	C	-2.133246	-1.813106	-0.151115
12	S	0.654097	-2.533561	-0.214501
13	C	1.678598	-1.080813	-0.160369
14	C	0.912580	0.099037	-0.092317
15	C	3.111560	-1.275127	-0.184492
16	C	4.036953	-0.546947	-0.884762
17	S	5.638829	-1.141447	-0.595120
18	C	5.069577	-2.410172	0.452326
19	C	3.736618	-2.360402	0.558956
20	C	1.437055	1.476885	0.073302
21	C	2.214822	1.906359	1.091225
22	S	2.558970	3.602774	0.926403
23	C	1.620062	3.731696	-0.530272
24	C	1.092836	2.539466	-0.848127
25	C	2.756041	1.147438	2.268339
26	C	1.480925	5.035595	-1.259044
27	C	3.839963	0.554438	-1.883024
28	C	6.022464	-3.362116	1.112100
29	H	-2.550853	-2.797116	-0.150452
30	C	-7.283114	1.809674	0.664045
31	H	2.633231	1.717347	3.183259
32	H	3.812726	0.931814	2.145580
33	H	2.233142	0.207519	2.380775
34	H	0.477379	2.380318	-1.714783
35	H	1.024673	5.793841	-0.630302
36	H	0.855672	4.902246	-2.133940
37	H	2.444811	5.412934	-1.586377
38	H	4.541957	0.449702	-2.704079
39	H	3.985812	1.534897	-1.441569
40	H	2.838074	0.516825	-2.289267
41	H	3.174931	-3.040319	1.172648
42	H	6.601122	-3.914410	0.378181
43	H	5.472133	-4.075233	1.714352
44	H	6.720199	-2.839387	1.758993
45	H	-4.693752	-3.546481	0.185258
46	H	-6.043816	-3.381413	-0.913965
47	H	-4.422955	-3.027685	-1.473884
48	H	-4.437586	1.652155	0.520755
49	H	-7.881420	1.577026	1.539376
50	H	-6.739541	2.726274	0.859597
51	H	-7.961620	1.988046	-0.164331

2 (-3537.410318)

1	S	1.933612	0.825405	-0.116902
2	S	-3.594980	4.153994	0.815592
3	S	1.786270	6.008473	-0.490078
4	C	0.773567	2.175007	-0.130000
5	C	-0.566467	1.714957	-0.131401
6	C	-0.623279	0.333408	-0.182079
7	C	-2.035119	3.413395	1.018399
8	C	-1.780978	2.552162	0.007469
9	C	-2.874749	2.470726	-0.938357
10	H	-2.847892	1.833802	-1.803655
11	C	-3.912194	3.269826	-0.646622
12	C	0.827151	4.604238	-0.817110
13	C	1.305979	3.511909	-0.131482
14	C	2.506888	3.844885	0.624727
15	H	3.027949	3.125531	1.229166
16	C	2.874749	5.128256	0.547747
17	S	-1.933612	-0.825405	-0.116902
18	S	3.594980	-4.153994	0.815592
19	S	-1.786270	-6.008473	-0.490078
20	C	-0.773567	-2.175007	-0.130000
21	C	0.566467	-1.714957	-0.131401
22	C	0.623279	-0.333408	-0.182079
23	C	2.035119	-3.413395	1.018399
24	C	1.780978	-2.552162	0.007469
25	C	2.874749	-2.470726	-0.938357
26	H	2.847892	-1.833802	-1.803655
27	C	3.912194	-3.269826	-0.646622
28	C	-0.827151	-4.604238	-0.817110
29	C	-1.305979	-3.511909	-0.131482
30	C	-2.506888	-3.844885	0.624727
31	H	-3.027949	-3.125531	1.229166
32	C	-2.874749	-5.128256	0.547747
33	C	4.020719	5.812404	1.231564
34	H	4.700981	6.257817	0.512268
35	H	3.673600	6.601200	1.891772
36	H	4.576968	5.095544	1.823790
37	C	-0.266290	4.697535	-1.838682
38	H	-0.464115	3.724142	-2.266925
39	H	-1.192867	5.071054	-1.414605
40	H	0.025967	5.366712	-2.641870
41	C	-1.201107	3.755619	2.219379
42	H	-0.415953	3.024048	2.351915
43	H	-0.737396	4.731180	2.112731
44	H	-1.809272	3.769205	3.117706
45	C	-5.193733	3.447054	-1.406062
46	H	-6.053988	3.188629	-0.796506
47	H	-5.319849	4.472607	-1.739160
48	H	-5.194613	2.805621	-2.279373
49	C	-4.020719	-5.812404	1.231564
50	H	-4.700981	-6.257817	0.512268
51	H	-3.673600	-6.601200	1.891772
52	H	-4.576968	-5.095544	1.823790
53	C	0.266290	-4.697535	-1.838682
54	H	0.464115	-3.724142	-2.266925
55	H	1.192867	-5.071054	-1.414605
56	H	-0.025967	-5.366712	-2.641870
57	C	1.201107	-3.755619	2.219379
58	H	0.415953	-3.024048	2.351915
59	H	0.737396	-4.731180	2.112731
60	H	1.809272	-3.769205	3.117706
61	C	5.193733	-3.447054	-1.406062
62	H	6.053988	-3.188629	-0.796506
63	H	5.319849	-4.472607	-1.739160
64	H	5.194613	-2.805621	-2.279373

3 (-4010.654623)

1	C	0.735464	3.941125	3.536730
2	C	0.255533	3.347909	2.432864
3	C	1.243723	3.147773	1.393810
4	C	2.469495	3.587658	1.752789
5	S	2.430798	4.273612	3.349789
6	C	0.909440	2.468892	0.116775
7	C	0.412257	1.172566	0.075673
8	C	0.228699	0.644917	-1.226931
9	S	0.674622	1.818109	-2.433370
10	C	1.100976	2.989064	-1.173428
11	S	0.000000	0.000000	1.330724
12	C	-0.412257	-1.172566	0.075673
13	C	-0.228699	-0.644917	-1.226931
14	C	-0.909440	-2.468892	0.116775
15	S	-0.674622	-1.818109	-2.433370
16	C	1.589073	4.285973	-1.606354
17	C	1.233942	5.507838	-1.108549
18	S	2.075575	6.778704	-1.934054
19	C	2.895961	5.664394	-2.989049
20	C	2.533638	4.406813	-2.706864
21	H	2.931966	3.553889	-3.224907
22	H	-0.772414	3.054234	2.322310
23	C	-1.100976	-2.989064	-1.173428
24	C	-1.243723	-3.147773	1.393810
25	C	-2.469495	-3.587658	1.752789
26	C	-0.255533	-3.347909	2.432864
27	S	-2.430798	-4.273612	3.349789
28	C	-0.735464	-3.941125	3.536730
29	H	0.772414	-3.054234	2.322310
30	C	-1.589073	-4.285973	-1.606354
31	C	-1.233942	-5.507838	-1.108549
32	C	-2.533638	-4.406813	-2.706864
33	S	-2.075575	-6.778704	-1.934054
34	C	-2.895961	-5.664394	-2.989049
35	H	-2.931966	-3.553889	-3.224907
36	C	3.868824	6.143666	-4.025223
37	H	3.393965	6.817329	-4.731715
38	H	4.702057	6.671888	-3.572245
39	H	4.263801	5.299117	-4.577293
40	C	0.209791	5.863464	-0.072319
41	H	-0.512522	5.064645	0.029605
42	H	0.660312	6.034346	0.899768
43	H	-0.321168	6.765404	-0.358845
44	C	3.763671	3.538337	0.993123
45	H	3.688386	2.842041	0.168958
46	H	4.019217	4.512321	0.588031
47	H	4.576269	3.218043	1.636521
48	C	0.000000	4.305748	4.792444
49	H	-1.039121	4.010509	4.708061
50	H	0.423527	3.806415	5.658241
51	H	0.034246	5.375029	4.976932
52	C	0.000000	-4.305748	4.792444
53	H	1.039121	-4.010509	4.708061
54	H	-0.423527	-3.806415	5.658241
55	H	-0.034246	-5.375029	4.976932
56	C	-3.763671	-3.538337	0.993123
57	H	-3.688386	-2.842041	0.168958
58	H	-4.019217	-4.512321	0.588031
59	H	-4.576269	-3.218043	1.636521
60	C	-0.209791	-5.863464	-0.072319
61	H	0.512522	-5.064645	0.029605
62	H	-0.660312	-6.034346	0.899768
63	H	0.321168	-6.765404	-0.358845
64	C	-3.868824	-6.143666	-4.025223
65	H	-3.393965	-6.817329	-4.731715
66	H	-4.702057	-6.671888	-3.572245
67	H	-4.263801	-5.299117	-4.577293