Evaluating Atomic Components in Fluorene Wires

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Supporting Information

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I. General Information

All reactions were performed in oven-dried round bottom flasks, unless otherwise noted. The flasks were fitted with rubber septa and reactions were conducted under a positive pressure of nitrogen, unless otherwise noted. Anhydrous and anaerobic solvents were obtained from a Schlenck manifold with purification columns packed with activated alumina and supported copper catalyst (Glass Contour, Irvine, CA). Automated flash chromatography was performed using a Teledyne Isco Combiflash R_f200 and Redisep R_f Gold Silica columns.

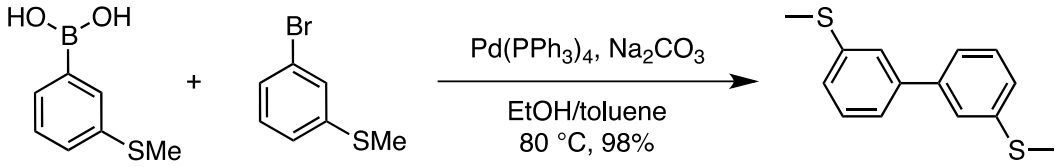
Materials. Commercial reagents were used without further purification. All reagents were purchased from Sigma-Aldrich, with the following exceptions. Tetrakis(triphenylphosphine)palladium was purchased from Strem Chemicals. 3-(Methylthio)phenyl boronic acid was purchased from Alfa Aesar. 4-Iodothioanisole was purchased from Oakwood. 3-Bromothioanisole was purchased from America TCI Fine Chemicals.

Instrumentation. ^{1}H, ^{13}C, and ^{29}Si NMR spectra were recorded on a Bruker DRX300 (300 MHz), Bruker DRX400 (400 MHz) or a Bruker DMX500 (500 MHz) spectrometer. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CHCl_3$: δ 7.26l C_6H_6 δ 7.15). Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$ δ 77.0; C_6D_6 δ 128.5). Chemical shifts for silicon are reported in parts per million downfield from tetramethylsilane and referenced to the silicon resonance of tetramethylsilane (TMS δ 0.0). Data are represented as follows: chemical shift,

multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants in Hertz, and integration. The mass spectroscopic data were obtained at the Columbia University mass spectrometry facility using a JEOL JMSHX110A/110A tandem mass spectrometer.

II. Synthetic Procedures and Characterization of Organic Compounds

*3,3'-Bis(methylthio)-1,1'-biphenyl (**5**)*



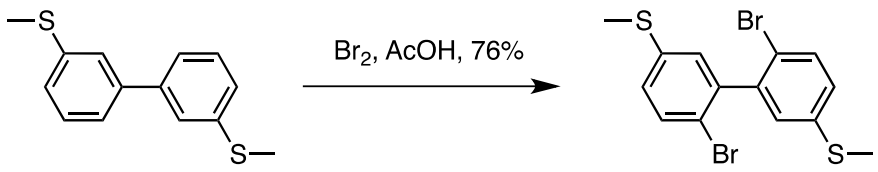
While the multistep synthesis of **5** has been reported,[1] we instead chose to prepare **5** by an adaptation of the Suzuki-Miyaura reaction.[2]

An oven-dried 100 mL Schlenk flask and stir bar were cooled under N_2. The flask was charged with 3-(methylthio)phenylboronic acid (1.26g, 7.50 mmol, 1.50 equiv.), 3-(methylthio)bromobenzene (0.67 mL, 5.00 mmol, 1.00 equiv.) and sodium carbonate (11.25 mL, 2.0 M in water, 4.50 equiv.). The flask was sealed with a rubber septum and toluene (40 mL) and ethanol (12.5 mL) were added by syringe. The suspension was sparged with N_2 gas for 30 minutes. At this time, under a positive pressure of N_2 tetrakistriphenylphospine palladium (58 mg, 0.05 mmol, 1 mol %) was added and the flask sealed with a reflux condenser. The apparatus was heated to 80 °C overnight, during which the color was observed to darken.

The flask was cooled to room temperature. The biphasic mixture was poured into a separatory funnel and diluted with sodium bicarbonate (saturated aqueous, 20 mL). The organic and aqueous layers were separated and the aqueous layer was extracted three times with ethyl acetate (20 ml). The combined organic fractions were dried over magnesium sulfate, filtered, and then concentrated under reduced pressure to yield a black oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 10% EtOAc/hexanes) yielded a white solid (1.21 g, 98% yield). ^{1}H NMR (500

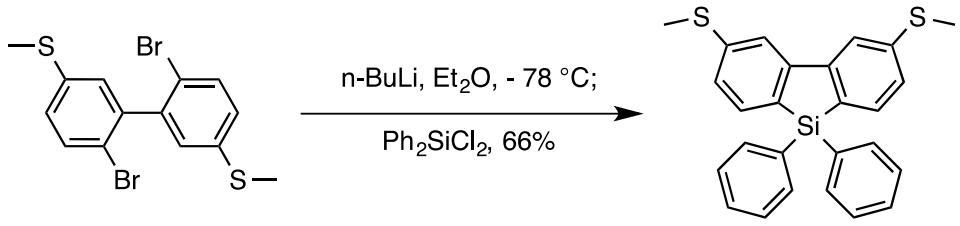
MHz, C_6D_6) δ 7.46 (t, *J* = 1.7 Hz, 2H), 7.15 – 7.12 (m, 2H), 7.11 – 7.03 (m, 4H), 1.99 (s, 6H). ^{13}C NMR (126 MHz, C_6D_6) δ 142.07, 139.95, 129.48, 125.83, 125.73, 124.28, 15.35. HRMS (EI+) predicted for $C_{14}H_{14}S_2$ 246.05, observed 246.0534 (100%).

*(6,6'-Dibromo-[1,1'-biphenyl]-3,3'-diyl)bis(methylsulfane) (**4**)*



The synthesis of **4** has not been reported. The procedure below is adapted from the synthesis of 2,2'-dibromo-5,5'-dimethoxy-1,1'-biphenyl.[3] In a 50 mL round bottom flask equipped with a magnetic stir bar, biphenyl **5** (1.0 g, 4.06 mmol, 1.00 equiv.) was completely dissolved in glacial acetic acid (8 mL). Gentle heating to 40 °C was necessary for complete dissolution, after which the solution was cooled back to room temperature without precipitation. The flask was sealed with a rubber septum and outfitted with a N_2 inlet. Bromine (CAUTION: TOXIC) (0.625 mL, 12.2 mmol, 3.00 equiv.) was added dropwise by syringe. While a solid was immediately observed to precipitate, the mixture was allowed to stir for 90 minutes. The mixture was filtered and the red filtrate quenched with 10% aqueous sodium thiosulfate until the color dissipated. While the purity of the solid was high (90%) by ^1H NMR analysis, analytically pure material was obtained by recrystallization from hot ethanol cooled to –30 °C (1.24 g, 76% yield). ^1H NMR (400 MHz, C_6D_6) δ 7.29 (d, *J* = 8.4 Hz, 2H), 6.98 (d, *J* = 2.4 Hz, 2H), 6.73 (dd, *J* = 8.4, 2.4 Hz, 2H), 1.82 (s, 6H). ^{13}C NMR (101 MHz, C_6D_6) δ 142.63, 138.99, 133.13, 128.67, 127.60, 119.87, 15.11. HRMS (EI+) predicted for $C_{14}H_{12}Br_2S_2$ 401.87, 403.87, 405.87, observed 401.8741 (12.1%), 403.8743 (21.8%), 405.8714 (12.4%).

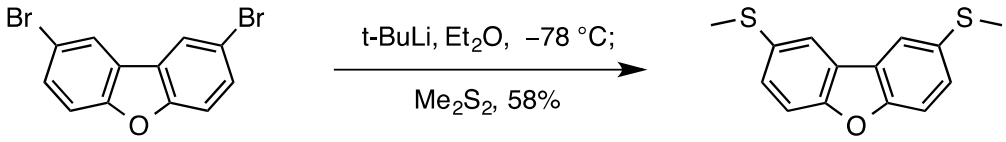
2,8-Bis(methylthio)-5,5-diphenyl-5H-dibenzo[b,d]silole ***(1)***



The synthesis of **1** has not been reported. The procedure below is adapted from the synthesis of dichlorosilafluorene reported by West et al.[4] We note both n-butyllithium and t-butyllithium can be used for the double lithium halogen exchange. Both reagents are pyrophoric and appropriate precautions should be taken. A 10 mL, flame-dried round bottom flask equipped with a stir bar was charged with bromobiphenyl **4** (100 mg, 0.247 mmol) and dissolved in THF (4 mL). The flask was cooled to -78 °C in a dry ice/acetone bath and stirred at that temperature for 5 minutes. A 1.39 M solution of *n*-butyllithium (0.390 mL, 0.544 mmol, 2.20 equiv.) was added dropwise by syringe and the solution was stirred for 90 minutes. Dichlorodiphenylsilane (0.0520 mL, 0.247 mmol) was added dropwise by syringe. The mixture was stirred at -78 °C for 30 minutes, then allowed to warm to room temperature and stir for 3 hours. Over this time, the reaction mixture proceeded from bright yellow, to light yellow, then finally a clear solution. The reaction was quenched with 0.5 mL saturated NH_4Cl solution then 0.5 mL water. The biphasic mixture was poured into a separatory funnel and the organic and aqueous layers were separated. The aqueous layer was extracted with Et_2O (3 x 5 mL) and the combined organic layers were dried over magnesium sulfate, filtered, and concentrated to yield a yellow oil. Purification by column chromatography on silica gel (gradient of 100% hexanes to 30% dichloromethane/hexanes) yielded a white solid (70 mg, 66% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, J = 1.7 Hz, 2H), 7.67 (d, J = 7.6 Hz, 2H), 7.62 (dd, J

= 8.0, 1.4 Hz, 4H), 7.43 – 7.37 (m, 2H), 7.37 – 7.31 (m, 4H), 7.20 (dd, *J* = 7.6, 1.7 Hz, 2H), 2.57 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.86, 142.13, 135.59, 134.32, 132.69, 130.29, 128.27, 125.76, 119.28, 15.70. ^{29}Si NMR (99 MHz, $CDCl_3$) δ -11.81. HRMS (FAB+) predicted for $C_{26}H_{22}S_2Si$ 426.09, observed 426.0942.

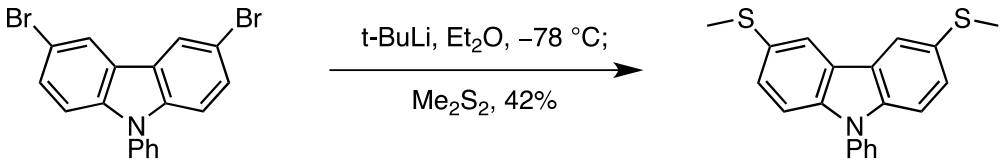
*2,8-Bis(methylthio)dibenzofuran (**2**)*



An oven-dried 50 mL round bottom flask and stir bar were cooled under N_2. The flask was charged with 2,8-dibromodibenzofuran (50 mg, 0.154 mmol), which was dissolved in Et_2O (1.5 mL). The flask was cooled to −78 °C in a dry ice/acetone bath. T-Butyllithium (0.65 mL, 1.18 M, 0.77 mmol) was added dropwise by syringe and the solution was stirred at −78 °C for one hour. Dimethyl disulfide (70 μL, 0.77 mmol) was added dropwise to the chilled reaction and the reaction was allowed to warm to room temperature overnight.

The excess butyllithium was quenched with water. The biphasic mixture was poured into a separatory funnel and the organic and aqueous layers were separated. The aqueous layer was extracted with EtOAc (3 x 5 mL) and the combined organic layers were dried over sodium sulfate, filtered, and concentrated to yield a yellow oil. Purification by preparative thin layer chromatography in hexanes yielded a pale yellow semi-solid (23 mg, 58%). ^{1}H NMR (300 MHz, CD_2Cl_2) δ 7.89 (dd, *J* = 1.9, 0.7 Hz, 2H), 7.49 (dd, *J* = 8.6, 0.7 Hz, 2H), 7.43 (dd, *J* = 8.6, 1.9 Hz, 2H), 2.58 (s, 6H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 155.39, 132.92, 128.15, 124.85, 120.20, 112.47, 17.89. HRMS (FAB+) predicted for $C_{14}H_{12}OS_2$ 260.03, observed 260.0341.

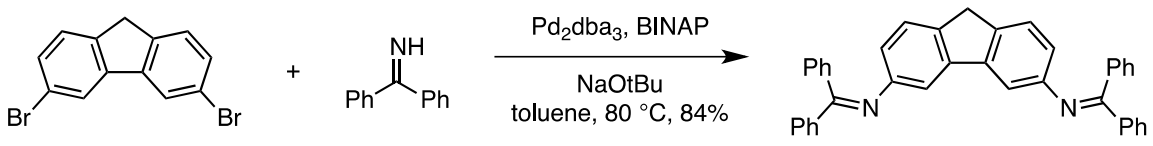
*3,6-Bis(methylthio)-9-phenylcarbazole (**3**)*



An oven-dried 50 mL round bottom flask and stir bar were cooled under N_2. The flask was charged with 3,6-dibromo-9-phenylcarbazole (100 mg, 0.154 mmol), which was dissolved in Et_2O (3 mL). The flask was cooled to −78 °C in a dry ice/acetone bath. T-Butyllithium (0.65 mL, 1.18 M, 0.77 mmol) was added dropwise by syringe and the solution was stirred at −78 °C for one hour. Dimethyl disulfide (70 µL, 0.77 mmol) was added dropwise to the chilled reaction and the reaction was allowed to warm to room temperature overnight.

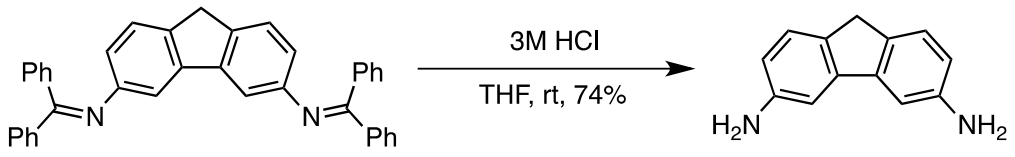
The excess butyllithium was quenched with water. The biphasic mixture was poured into a separatory funnel and the organic and aqueous layers were separated. The aqueous layer was extracted with EtOAc (3 x 5 mL) and the combined organic layers were dried over sodium sulfate, filter, and concentrated to yield a yellow oil. Purification by preparative thin layer chromatography in hexanes yielded a white semi-solid (22 mg, 42% yield). ^{1}H NMR (400 MHz, C_6D_6) δ 8.13 (dd, J = 1.8, 0.5 Hz, 2H), 7.41 (dd, *J* = 8.6, 1.8 Hz, 2H), 7.15 – 7.02 (m, 9H), 2.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.87, 137.37, 130.00, 128.64, 128.00, 127.69, 126.92, 123.52, 121.06, 110.51, 18.84. HRMS (EI+) predicted for $C_{20}H_{17}NS_2$ 335.08, observed 335.0810.

*3,6- N,N'-(9H-fluorene-3,6-diyl)bis(1,1-diphenylmethanimine) (**S1**)*



3,6-dibromofluorene was synthesized according to literature procedures.[5] **S1** was synthesized according to Rotzler *et al.*,[6] which was adapted from the procedures of Wolfe *et al.*[7] A 10 mL Schlenk flask was charged with $Pd_2(dba)_3$ (0.0080 mmol, 7.3 mg, 0.04 equiv.) and racemic BINAP (0.0240 mmol, 149.4 mg, 0.12 equiv.). The Schlenk flask was filled with a nitrogen atmosphere. These solids were stirred in 2 mL toluene for 15 minutes as a purple solution. Under a heavy flow of N_2, the dibromofluorene (0.200 mmol, 65.0 mg, 1.00 equiv.) and sodium *t*-butoxide (0.562 mmol, 54.0 mg, 2.80 equiv.) were added and stirred for two minutes. Benzophenone imine (0.480 mmol, 0.080 mL, 2.40 equiv.) was then added to the solution dropwise from a microsyringe. The reaction mixture was heated at 80˚C for 2 hours, at which point a TLC plate in 100% hexanes revealed the starting material had been completely consumed. The reaction mixture was diluted with 8 mL Et_2O, then filtered over Celite to give a bright orange solution. The solvent was evaporated. Purification by column chromatography on silica gel (gradient of 100% hexanes to 10% ethyl acetate/hexanes) yielded a yellow semi-solid (88 mg, 84% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 - 7.72 (m, 4H), 7.54 - 7.33 (m, 6H), 7.32 - 7.10 (m, 10H), 7.06 (d, J = 1.5 Hz, 2H), 6.61 (d, J = 7.7 Hz, 2H), 3.67 (s, 2H). HRMS (FAB+) predicted for $C_{39}H_{28}N_2$ 524.23, observed 525.2324 (M+1, 100%).

*3,6-diaminofluorene (**6**)*

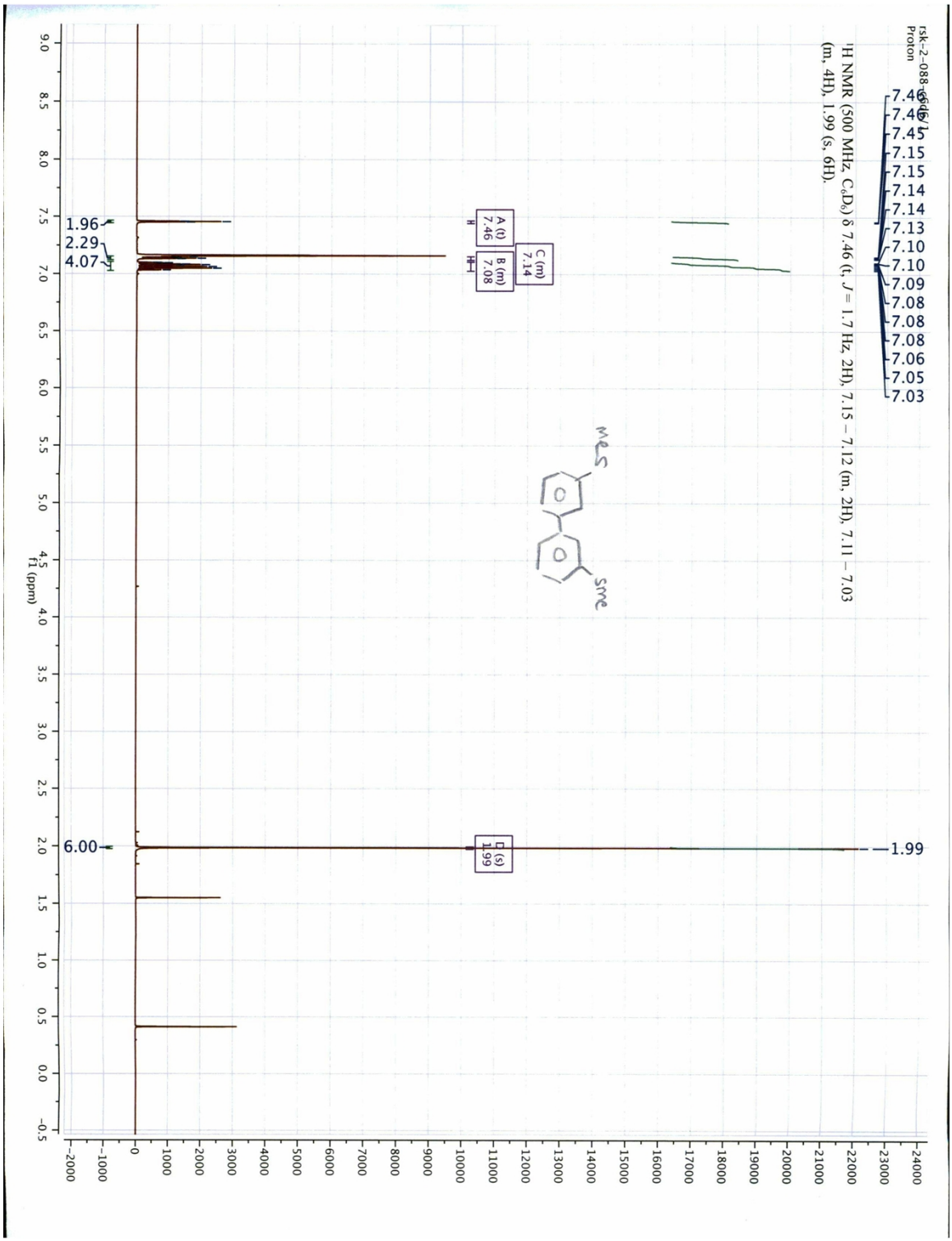


3,6-Diaminofluorene **6** was synthesized according to Rotzler et al.,[6] which was adapted from the procedures of Wolfe et al.[7] **S1** (0.167 mmol, 88.0 mg, 1.00 equiv.) was dissolved in 1.5 mL THF in a 20 mL scintillation vial. 3 M HCl (0.450 mL, 30% volume

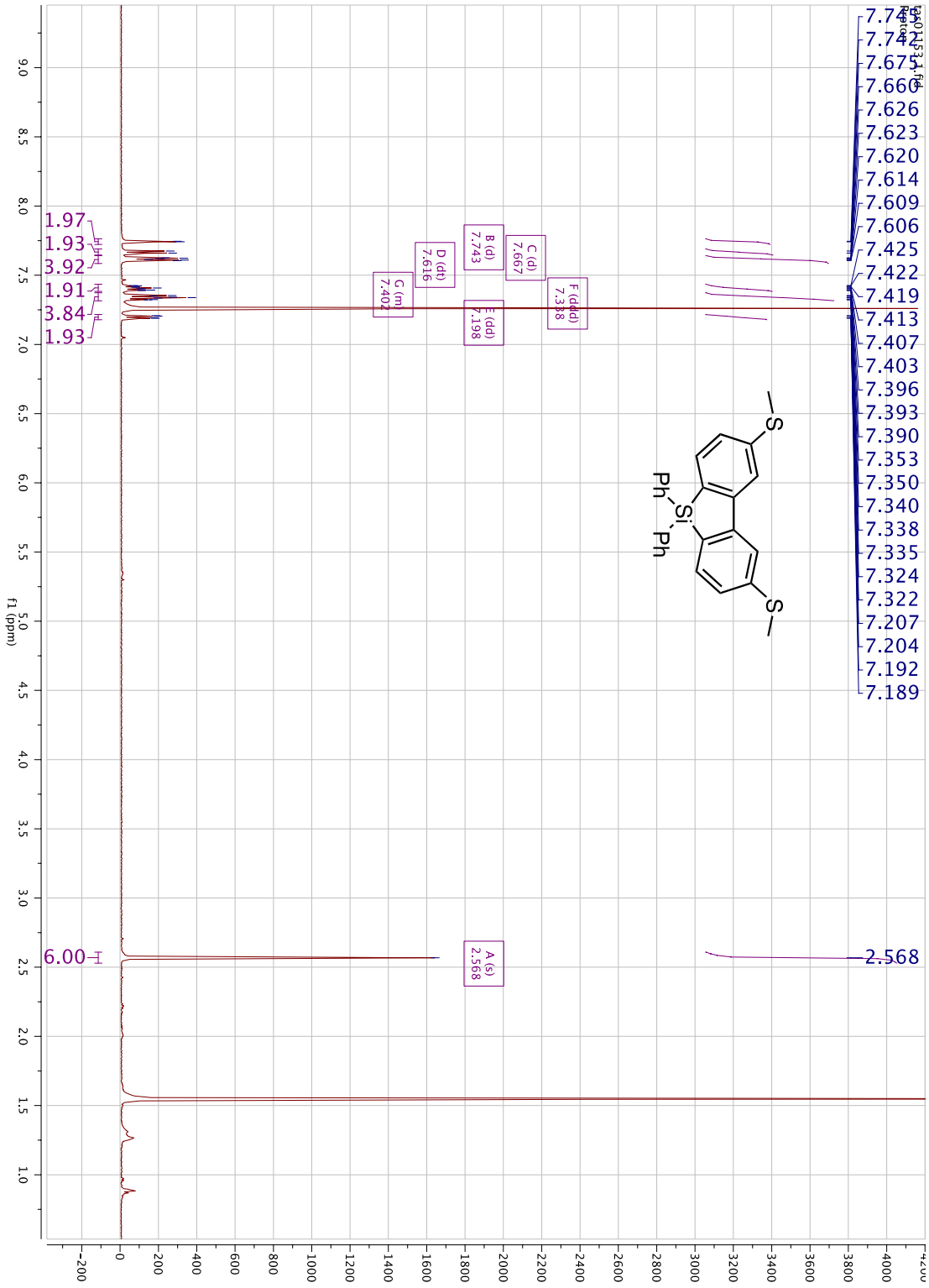
of THF) was added dropwise to the vial. Over 15 seconds, the physical appearance changed from clear yellow to cloudy yellow to clear yellow to cloudy white. At this point, a TLC in 10% ethyl acetate/hexanes revealed complete deprotection. The mixture was partitioned between 0.5 M HCl and a 2:1 solution of hexanes:ethyl acetate (10 mL). The organic layer was extracted 3x8 mL with 0.5 M HCl. The aqueous layers were combined and made alkaline with 1 M NaOH, then extracted 3x15 mL with dichloromethane. The slight yellow DCM solution was dried over sodium sulfate, filtered, and concentrated to yield a yellow (amine) and white (benzophenone) crude solid. Purification by column chromatography on silica gel (gradient of 80/19/1 hexanes/ethyl acetate/triethylamine to 95/5 ethyl acetate/triethylamine) yielded a yellow solid (24.3 mg, 74% yield). ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.13 (d, J = 8.0 Hz, 2H), 6.87 (d, J = 2.1 Hz, 2H), 6.49 (dd, J = 8.0, 2.1 Hz, 2H), 4.96 (s, 4H), 3.52 (s, 2H). ^{13}C NMR (126 MHz, DMSO) δ 147.53, 142.30, 131.37, 125.06, 113.17, 104.78, 34.67. HRMS (FAB+) predicted for $C_{13}H_{12}N_2$ 196.10, observed 196.0992 (M, 99.0%) and 197.1071 (M+1, 100%).

^{1}H NMR Spectra

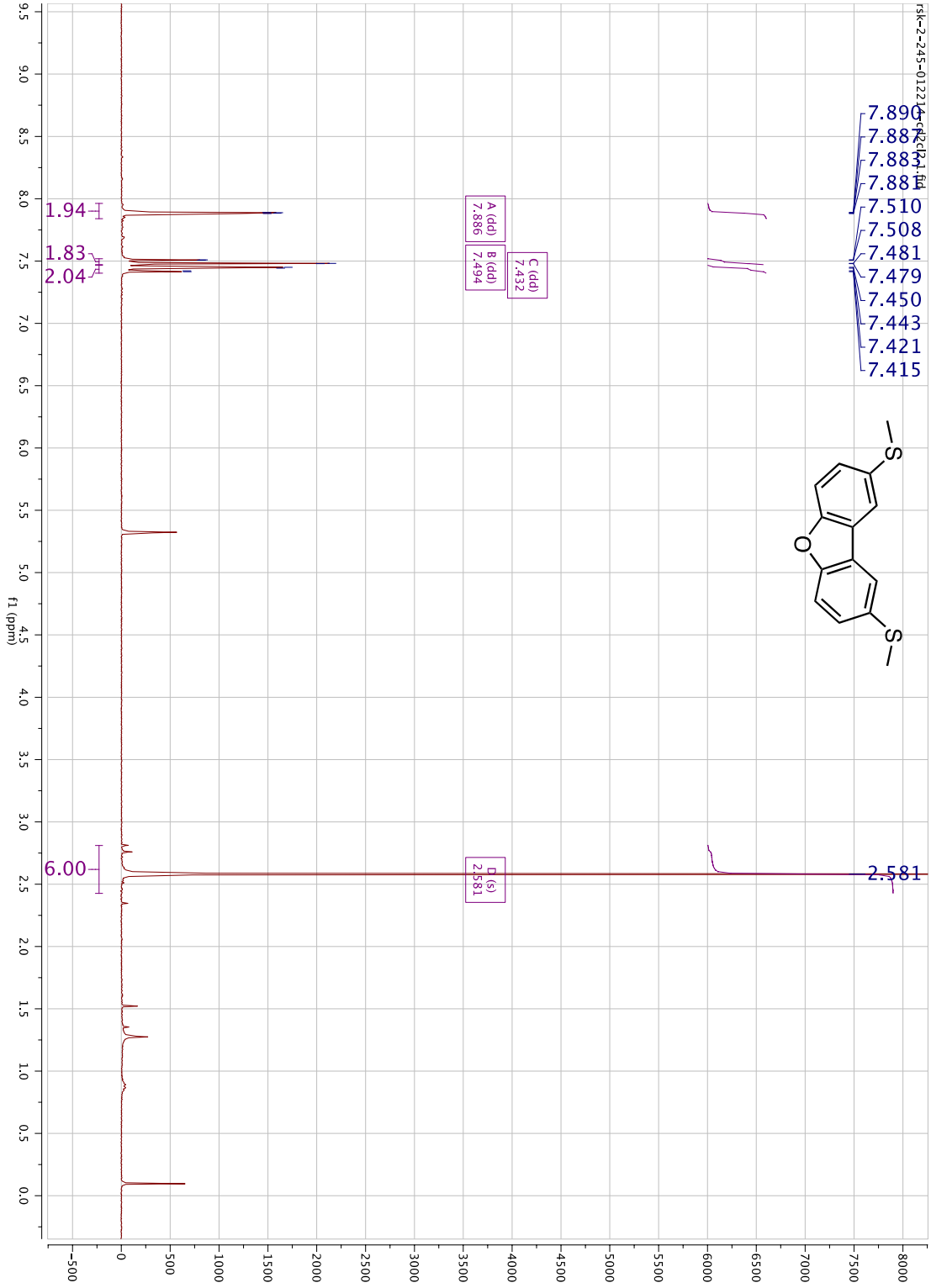
1. 3,3'-bis(methylthio)biphenyl (**5**)



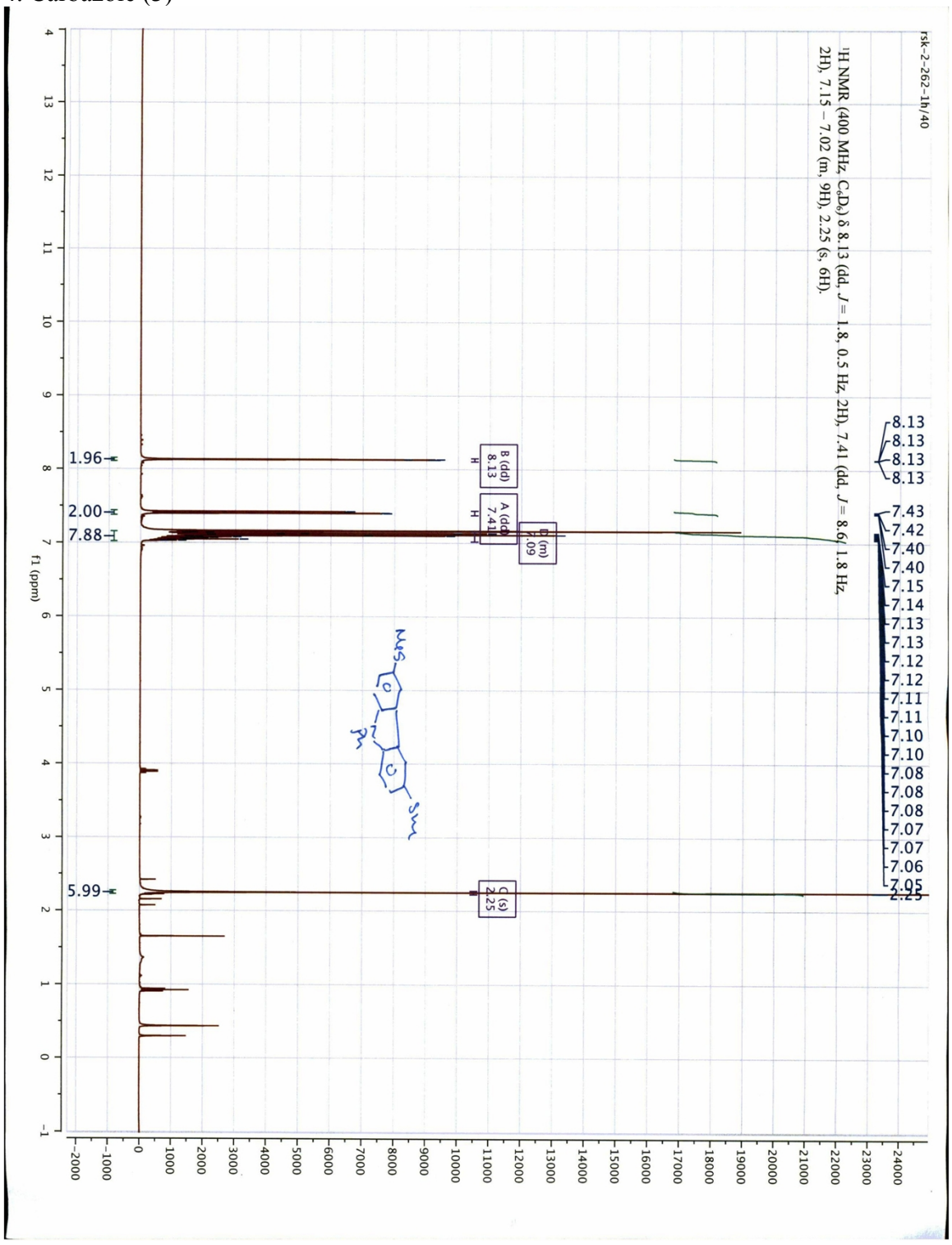
2. Dibenzosilole (**1**)



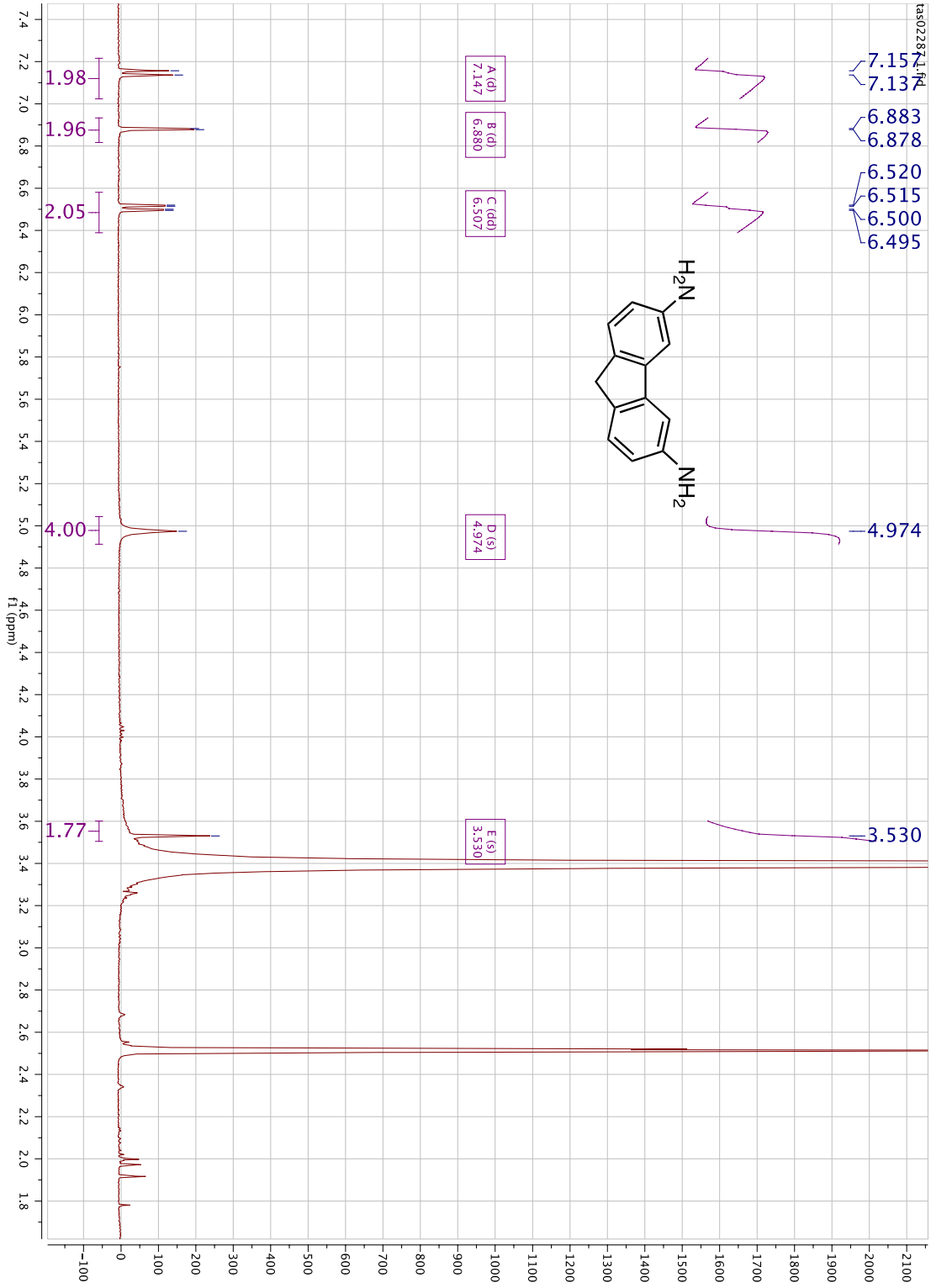
3. Dibenzofuran (**2**)



4. Carbazole (**3**)



5. 3,6-Diaminofluorene (**6**)



III. STM Break Junction Experiments

General Procedure and Instrumentation:

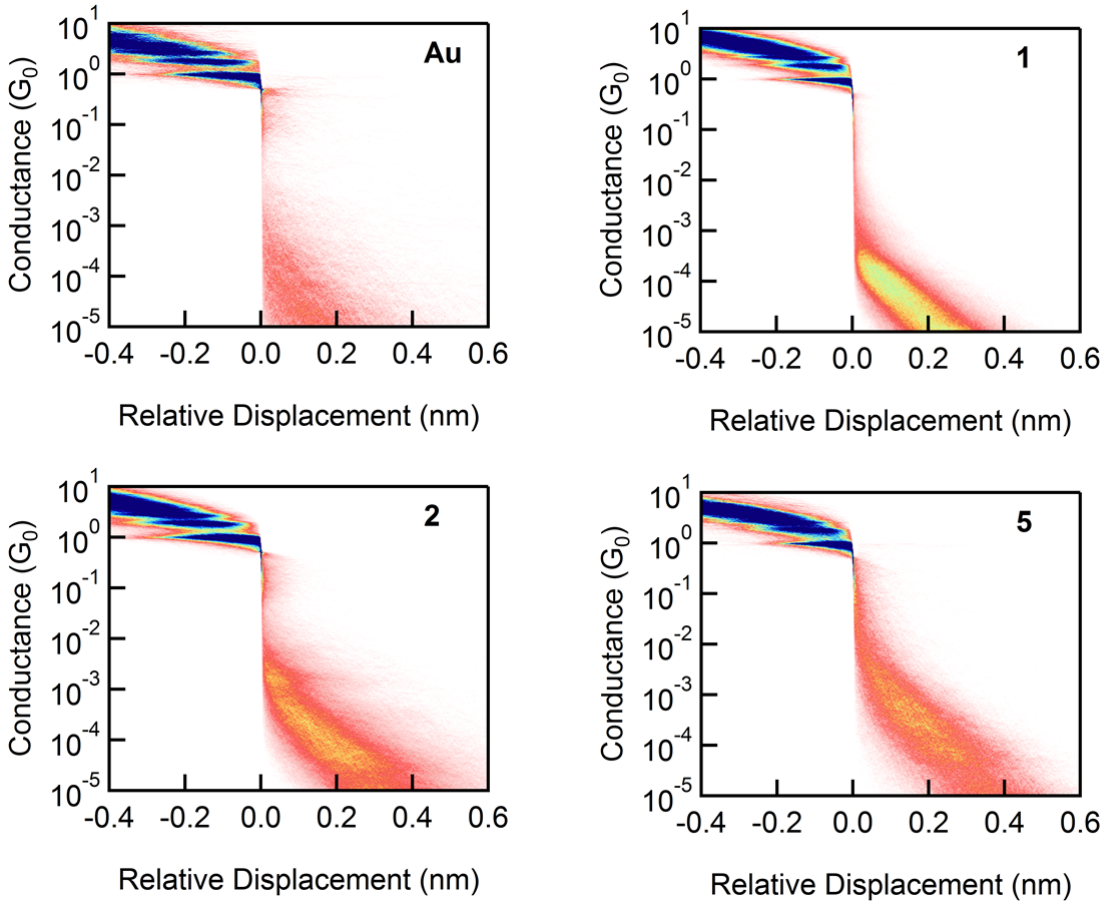
We measure the conductance of single molecules attached to gold electrodes using a home-built modified Scanning Tunneling Microscope (STM). A hand-cut 0.25 mm diameter gold wire (99.998%, Alfa Aesar) is used as the STM tip and a gold-coated (99.999%, Alfa Aesar) mounted mica surface is used as the substrate. A commercially available single-axis piezoelectric positioner (Nano-P15, Mad City Labs) is used to achieve sub-angstrom level control of the tip-substrate distance. The STM is controlled using a custom written program in IgorPro (Wavemetrics, Inc.) and operates in ambient conditions at room temperature. The break junction technique is carried out in 1-10 mM solutions of the molecules in 1,2,4-Trichlorobenzene (Sigma-Aldrich or Alfa Aesar, 99% purity), which is introduced after collection of at least a thousand clean gold breaks to ensure the cleanliness of the system. The substrate is UV/Ozone cleaned for 15 minutes immediately before use.

Measurement of conductance is achieved by repeatedly moving the tip in and out of contact with the substrate, requiring that a gold metal contact with a conductance of at least 5 G_0 is formed before pulling out. The tip is withdrawn from the substrate at a speed of about 16 nm/s for about 4 nm and the measured current is recorded as a function of tip/substrate displacement while holding the applied voltage at 225 or 350 mV. The data is collected at a 40 kHz acquisition rate and plotted as conductance traces. Directly after the gold point contact breaks, a target molecule in the vicinity can bridge the gap so that its conductance (G=I/V) can be measured. Tens of thousands of conductance vs.

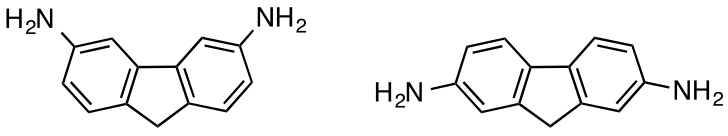
displacement traces were collected for each molecule studied and conductance histograms were constructed without any sort of data selection. The measurements were repeated on multiple days with multiple tip/substrate pairs to ensure reproducibility.

Additional Figures:

Figure S1: Two-dimensional histograms corresponding to molecules 1, 2 and 5. The same data sets are used to create the 1D log-binned histograms included in the manuscript (Figure 1a). These 2D conductance histograms of molecule 1, 2 and 5 do not show clear signatures extending a molecular length, suggesting that minor features observed in the 1D histograms do not correspond to molecular junctions.

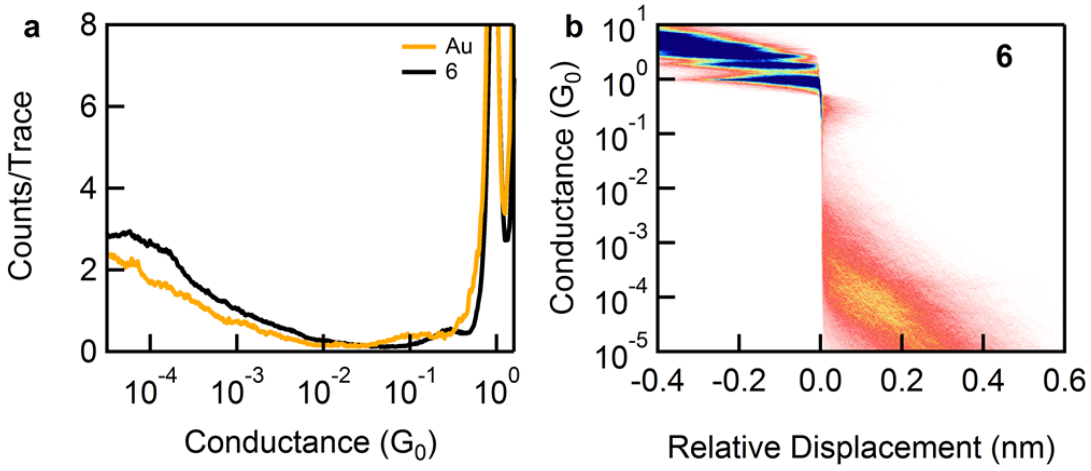


3,6-diaminofluorene (**6**), in which the amine contacts are meta-linked, does not conduct (Figure S2). We note that the isomeric 2,7-diaminofluorene shows a molecular conductance peak at 1.54 x10^{-3} G_0.[8]



3,6-diaminofluorene (**6**) 2,7-diaminofluorene

Figure S2. (a) Logarithmically binned one dimensional conductance histogram of **6** and clean gold (shown as control). (b) Two dimensional conductance histogram of **6**. The same data set of conductance traces of **6** are used to create 1D conductance histogram and 2D conductance histogram shown in Figure S2.



IV. Computational Chemistry

A. General Comments

All quantum chemical calculations were performed using Jaguar, version 7.8, Schrodinger, LLC, New York, NY, 2010. Density functional theory methods with the B3LYP functional were used throughout. The various geometries were optimized using the 6-31G** basis. At the optimized geometries single-point calculations with the larger cc-pVTZ basis set were used to calculate more reliable energy values.

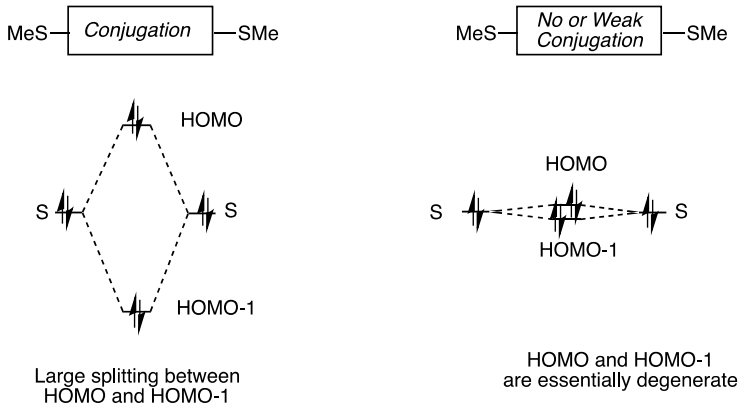
In each of the dithiomethylphenyl-substituted molecules the angle of rotation about the S-aryl bonds is problematic since there is essentially free rotation about these bonds in the free molecules, while the electronic coupling between the two aurophilic sulfur atoms depends strongly on these angles when the molecules are captured between the two electrodes. In order to get a sense of this coupling we restricted our geometry searches by requiring the (aryl)C-(aryl)C-S-(methyl)C array to be planar. This gives two cases, viz., the associated dihedral angle being either 0 or 180 degrees. In each molecule the difference in the total energies of the two rotamers is small (<1 kcal/mol). The difference in the sulfur-to-sulfur couplings between the two different rotamers could be significant (though always < ~0.2 eV). Realizing that in the actual experiment there is likely to be extensive rotation about these bonds, we chose to simply average the values from the two optimized "planar" (i.e., dihedral = 0 and 180 degrees) geometries. This procedure gives a reasonable, albeit necessarily approximate, estimate of the extent of coupling through the pi-space of the molecules.

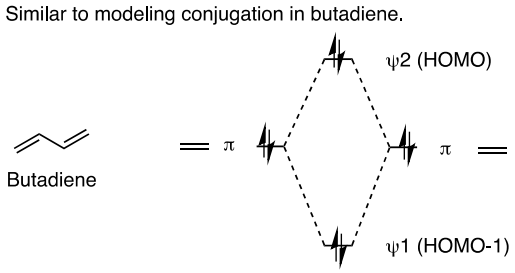
We also chose to restrict the biphenyl backbone of **5** to planarity. While this is inaccurate (the actual inter-ring dihedral rotation is significant), we believe this procedure

gives a more conceptually useful appreciation of the relationship of the fluorenes to their constituent parts.

B. Comments on Orbital Splitting

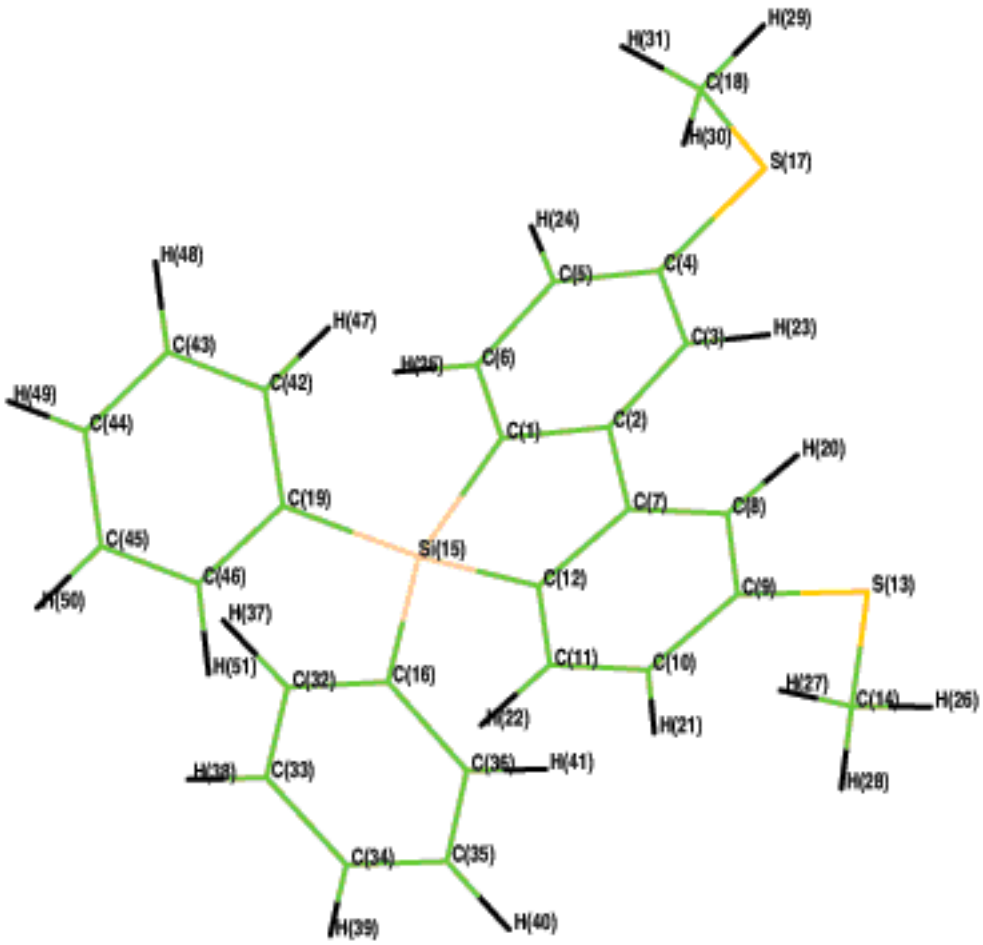
In this section, we elaborate further on the origin of orbital splitting. We use conjugation in butadiene as a model to understand the splitting phenomenon. The combination of two filled orbitals creates two new molecular orbitals displaced above and below the original filled orbitals. For example, the ethylene π orbitals combine to create Ψ1 (HOMO-1) and Ψ2 (HOMO) of butadiene (the combination of ethylene π* orbitals gives the unoccupied orbitals of butadiene). The strength of the orbital overlap determines the degree to which the new molecular orbitals are displaced from the original orbitals, i.e. determines the splitting. In butadiene overlap and conjugation are strong, while in butane it is weak.





The bridging atom X is an opportunity to provide a conductive pathway from terminal to terminal (terminal = thioanisole). X = $SiPh_2$ and O are less effective channels because of weak overlap with the orbitals of the terminals due to geometric and energetic reasons. Therefore, the combination of S lone pair orbitals creates a HOMO and HOMO-1 that are essentially degenerate (small splitting). An effective channel, which combines ideal geometry and energetics, like X = NPh is strongly "conjugating" and as a result the splitting is much larger between the new HOMO and HOMO-1.

*C. Diphenyldibenzosilole (**1**) – Syn Conformer*



Final energy (B3LYP; cc-pVTZ) = -2090.371553 h

Optimized geometry. Optimization done with the 6-31g** basis set.

		angstroms	
atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4195274070

C3	1.2052186429	0.0000000000	2.1196747879
C4	2.4294954212	-0.0020952622	1.4304812595
C5	2.4340460638	-0.0066513833	0.0301101802
C6	1.2228618026	-0.0067206362	-0.6685091896
C7	-1.3529595706	0.0024155195	2.0485582865
C8	-1.5950063761	0.0049146170	3.4209858092
C9	-2.9109103182	0.0062913369	3.9116869182
C10	-3.9837939610	0.0066784196	3.0128061340
C11	-3.7374073562	0.0042465462	1.6368733475
C12	-2.4379478882	-0.0003295779	1.1338078060
S13	-3.0843598188	0.0083175687	5.6870950770
C14	-4.8873919317	-0.0079510379	5.9462643517
Si15	-1.7760298427	0.0028064701	-0.6278465767
C16	-2.2821114595	-1.5333412420	-1.5984397821
S17	3.8980290113	0.0019690226	2.4422330528
C18	5.2566750884	0.0240602511	1.2291004321
C19	-2.2014215745	1.5515491160	-1.6179114822
H20	-0.7702090104	0.0045939755	4.1274046851
H21	-5.0078136225	0.0100916567	3.3680436983
H22	-4.5866786390	0.0061325373	0.9575344122
H23	1.2123237974	0.0026630440	3.2060412726
H24	3.3653892654	-0.0112034498	-0.5238947201
H25	1.2510587081	-0.0117009329	-1.7556745152
H26	-5.0270975467	-0.0123137705	7.0292636547
H27	-5.3611010769	0.8849040125	5.5323972956
H28	-5.3449403493	-0.9069081163	5.5273666509
H29	6.1754129063	0.0355418412	1.8191494202
H30	5.2500252930	-0.8705324065	0.6022387126
H31	5.2244226424	0.9215378182	0.6071516179
C32	-2.1467125249	-1.5905585723	-2.9976628916
C33	-2.4694981289	-2.7471764656	-3.7068728849
C34	-2.9412547865	-3.8723438408	-3.0301520718
C35	-3.0880232383	-3.8354040372	-1.6434710033
C36	-2.7608594827	-2.6784399445	-0.9368695720
H37	-1.7943745106	-0.7184164755	-3.5429854972
H38	-2.3571941241	-2.7690209103	-4.7875375943
H39	-3.1964996911	-4.7729759016	-3.5818023580
H40	-3.4588504423	-4.7076821661	-1.1120137149
H41	-2.8836080107	-2.6629563067	0.1428577306
C42	-1.3851286066	2.6949062851	-1.5549375953
C43	-1.7296885634	3.8652696410	-2.2308881444
C44	-2.9024280421	3.9178889069	-2.9842395731
C45	-3.7260139448	2.7944510609	-3.0623670520
C46	-3.3764582311	1.6244825269	-2.3885680274
H47	-0.4682238725	2.6685892219	-0.9721477070
H48	-1.0827175113	4.7362078014	-2.1699888239
H49	-3.1721646544	4.8291166118	-3.5110844121
H50	-4.6392210521	2.8286938643	-3.6504558097
H51	-4.0243119788	0.7552018266	-2.4708261461

principal moments of inertia:

amu*angstrom^2:	4166.87045	4730.56749	6256.82273
g*cm^2:	6.91925031E-37	7.85529114E-37	1.03896973E-36

```
 rotational constants:
              cm^(-1):     0.00404563     0.00356355     0.00269428
                  GHz:     0.12128503     0.10683264     0.08077247

 Z-matrix: (angstroms and degrees)
C1
C2      C1    cc2
C3      C2    cc3      C1    ccc3
C4      C3    cc4      C2    ccc4      C1    dih4
C5      C4    cc5      C3    ccc5      C2    dih5
C6      C5    cc6      C4    ccc6      C3    dih6
C7      C2    cc7      C3    ccc7      C4    dih7
C8      C7    cc8      C2    ccc8      C3    dih8
C9      C8    cc9      C7    ccc9      C2    dih9
C10     C9    cc10     C8    ccc10     C7    dih10
C11     C10   cc11     C9    ccc11     C8    dih11
C12     C11   cc12     C10   ccc12     C9    dih12
S13     C9    sc13     C8    scc13     C7    dih13
C14     S13   cs14     C9    csc14     C8    dih14
Si15    C12   sic15    C7    sicc15    C8    dih15
C16     Si15  csi16    C12   csic16    C7    dih16
S17     C4    sc17     C3    scc17     C2    dih17
C18     S17   cs18     C4    csc18     C3    dih18
C19     Si15  csi19    C12   csic19    C7    dih19
H20     C8    hc20     C7    hcc20     C12   dih20
H21     C10   hc21     C9    hcc21     C8    dih21
H22     C11   hc22     C10   hcc22     C9    dih22
H23     C3    hc23     C2    hcc23     C7    dih23
H24     C5    hc24     C4    hcc24     C3    dih24
H25     C6    hc25     C5    hcc25     C4    dih25
H26     C14   hc26     S13   hcs26     C9    dih26
H27     C14   hc27     S13   hcs27     C9    dih27
H28     C14   hc28     S13   hcs28     C9    dih28
H29     C18   hc29     S17   hcs29     C4    dih29
H30     C18   hc30     S17   hcs30     C4    dih30
H31     C18   hc31     S17   hcs31     C4    dih31
C32     C16   cc32     Si15  ccsi32    C12   dih32
C33     C32   cc33     C16   ccc33     Si15  dih33
C34     C33   cc34     C32   ccc34     C16   dih34
C35     C34   cc35     C33   ccc35     C32   dih35
C36     C35   cc36     C34   ccc36     C33   dih36
H37     C32   hc37     C16   hcc37     C33   dih37
H38     C33   hc38     C32   hcc38     C34   dih38
H39     C34   hc39     C33   hcc39     C35   dih39
H40     C35   hc40     C34   hcc40     C33   dih40
H41     C36   hc41     C35   hcc41     C34   dih41
C42     C19   cc42     Si15  ccsi42    C12   dih42
C43     C42   cc43     C19   ccc43     Si15  dih43
C44     C43   cc44     C42   ccc44     C19   dih44
C45     C44   cc45     C43   ccc45     C42   dih45
C46     C45   cc46     C44   ccc46     C43   dih46
H47     C42   hc47     C19   hcc47     C43   dih47
H48     C43   hc48     C42   hcc48     C44   dih48
H49     C44   hc49     C43   hcc49     C45   dih49
```

```
H50     C45   hc50     C44   hcc50     C43   dih50
H51     C46   hc51     C45   hcc51     C44   dih51

 Z-variables: (angstroms and degrees)
 cc2 =     1.419527407
 cc3 =     1.3938286595
 ccc3 =   120.1535790164
 cc4 =     1.4049362048
 ccc4 =   120.4695127188
 dih4 =    -0.0991398345
 cc5 =     1.4003858848
 ccc5 =   119.5631698226
 dih5 =    -0.115570788
 cc6 =     1.3982261417
 ccc6 =   119.7902918954
 dih6 =     0.1109465815
 cc7 =     1.4920406435
 ccc7 =   124.9112600497
 dih7 =  -179.9860253891
 cc8 =     1.3936104931
 ccc8 =   124.9372516227
 dih8 =    -0.0042013771
 cc9 =     1.4044189754
 ccc9 =   120.4526091384
 dih9 =  -179.9633718761
 cc10 =     1.3996664335
 ccc10 =   119.5926281542
 dih10 =    -0.0724917516
 cc11 =     1.3978209134
 ccc11 =   119.8044996875
 dih11 =     0.0683600398
 cc12 =     1.3934456534
 ccc12 =   121.3155649778
 dih12 =     0.084244814
 sc13 =     1.7838618123
 scc13 =   116.0303814795
 dih13 =   179.9588301641
 cs14 =     1.8216361274
 csc14 =   103.7583826699
 dih14 =  -179.4265237724
 sic15 =     1.8819063467
 sicc15 =   109.5408402251
 dih15 =   179.8048789568
 csi16 =     1.8862448321
 csic16 =   112.7032047838
 dih16 =   118.0845779955
 sc17 =     1.783325297
 scc17 =   116.0577618785
 dih17 =   179.8631336559
 cs18 =     1.8215646957
 csc18 =   103.6739136302
 dih18 =  -179.1576523241
 csi19 =     1.8867406885
 csic19 =   114.411295466
```

```
dih19 =  -115.5998484711
hc20 =     1.0859642837
hcc20 =   120.5771024788
dih20 =   179.8511334528
hc21 =     1.083891897
hcc21 =   120.9111024934
dih21 =  -179.8547822679
hc22 =     1.087550761
hcc22 =   118.5040203111
dih22 =  -179.9081615529
hc23 =     1.0863929833
hcc23 =   120.5282033185
dih23 =    -0.0499353318
hc24 =     1.0836707572
hcc24 =   120.9327045007
dih24 =  -179.8236246194
hc25 =     1.0875423275
hcc25 =   118.4906311092
dih25 =  -179.9161759602
hc26 =     1.0919817685
hcs26 =   105.5315670713
dih26 =   179.7123175981
hc27 =     1.0921888277
hcs27 =   111.5973943134
dih27 =   -62.172982266
hc28 =     1.0922223524
hcs28 =   111.5566943309
dih28 =    61.6265175659
hc29 =     1.0919564155
hcs29 =   105.5337771439
dih29 =   179.5331521539
hc30 =     1.092380821
hcs30 =   111.5739640471
dih30 =   -62.3468850105
hc31 =     1.0923948605
hcs31 =   111.5378869268
dih31 =    61.4295899449
cc32 =     1.406922885
ccsi32 =   121.2683565085
dih32 =   165.8015602566
cc33 =     1.3946090176
ccc33 =   121.1451266107
dih33 =   177.3091947454
cc34 =     1.3951727582
ccc34 =   120.0295035939
dih34 =     0.2719942532
cc35 =     1.3949157369
ccc35 =   119.7622252896
dih35 =    -0.0163722122
cc36 =     1.3945922764
ccc36 =   120.0640321552
dih36 =    -0.1598593806
hc37 =     1.0872675188
hcc37 =   119.826363259
```

```
 dih37 =   179.3775417319
 hc38 =     1.0867039999
 hcc38 =   119.8983447166
 dih38 =   179.7265379018
 hc39 =     1.0865569974
 hcc39 =   120.1089354117
 dih39 =   179.7972821736
 hc40 =     1.0866594678
 hcc40 =   120.0552945567
 dih40 =   179.753403932
 hc41 =     1.0867925249
 hcc41 =   119.2552768487
 dih41 =   179.7859503258
 cc42 =     1.4062594128
 ccsi42 =   120.8653211921
 dih42 =    86.4483738373
 cc43 =     1.39476919
 ccc43 =   121.1403320789
 dih43 =  -176.7351636498
 cc44 =     1.3948566404
 ccc44 =   120.0727834218
 dih44 =     0.1179861813
 cc45 =     1.3951739088
 ccc45 =   119.7474166395
 dih45 =    -0.2221279815
 cc46 =     1.3946399869
 ccc46 =   120.0330855574
 dih46 =     0.0263644329
 hc47 =     1.0867616726
 hcc47 =   119.6085233925
 dih47 =  -179.8629658347
 hc48 =     1.0866524508
 hcc48 =   119.8871892586
 dih48 =  -179.978100546
 hc49 =     1.0865814533
 hcc49 =   120.1470203229
 dih49 =  -179.7953833297
 hc50 =     1.0867235975
 hcc50 =   120.0653238615
 dih50 =  -179.8001450382
 hc51 =     1.0872579328
 hcc51 =   119.0005025642
 dih51 =  -179.2634842362

 Molecular weight:     426.09 amu

 Stoichiometry: SiC26H22S2
 Molecular Point Group: C1
 Point Group used: C1


 bond lengths (angstroms):

C1      -C2      :   1.419527      C1      -C6      :   1.393679
```

C1	-Si15	:	1.883741	C2	-C3	:	1.393829
C2	-C7	:	1.492041	C3	-C4	:	1.404936
C3	-H23	:	1.086393	C4	-C5	:	1.400386
C4	-S17	:	1.783325	C5	-C6	:	1.398226
C5	-H24	:	1.083671	C6	-H25	:	1.087542
C7	-C8	:	1.393610	C7	-C12	:	1.419146
C8	-C9	:	1.404419	C8	-H20	:	1.085964
C9	-C10	:	1.399666	C9	-S13	:	1.783862
C10	-C11	:	1.397821	C10	-H21	:	1.083892
C11	-C12	:	1.393446	C11	-H22	:	1.087551
C12	-Si15	:	1.881906	S13	-C14	:	1.821636
C14	-H26	:	1.091982	C14	-H27	:	1.092189
C14	-H28	:	1.092222	Si15	-C16	:	1.886245
Si15	-C19	:	1.886741	C16	-C32	:	1.406923
C16	-C36	:	1.406459	S17	-C18	:	1.821565
C18	-H29	:	1.091956	C18	-H30	:	1.092381
C18	-H31	:	1.092395	C19	-C42	:	1.406259
C19	-C46	:	1.407104	C32	-C33	:	1.394609
C32	-H37	:	1.087268	C33	-C34	:	1.395173
C33	-H38	:	1.086704	C34	-C35	:	1.394916
C34	-H39	:	1.086557	C35	-C36	:	1.394592
C35	-H40	:	1.086659	C36	-H41	:	1.086793
C42	-C43	:	1.394769	C42	-H47	:	1.086762
C43	-C44	:	1.394857	C43	-H48	:	1.086652
C44	-C45	:	1.395174	C44	-H49	:	1.086581
C45	-C46	:	1.394640	C45	-H50	:	1.086724
C46	-H51	:	1.087258				

bond angles:

C6	-C1	-C2	: 118.664004	Si15	-C1	-C2	: 109.469053
Si15	-C1	-C6	: 131.866454	C3	-C2	-C1	: 120.153579
C7	-C2	-C1	: 114.935074	C7	-C2	-C3	: 124.911260
C4	-C3	-C2	: 120.469513	H23	-C3	-C2	: 120.528203
H23	-C3	-C4	: 119.002254	C5	-C4	-C3	: 119.563170
S17	-C4	-C3	: 116.057762	S17	-C4	-C5	: 124.379065
C6	-C5	-C4	: 119.790292	H24	-C5	-C4	: 120.932705
H24	-C5	-C6	: 119.276972	C5	-C6	-C1	: 121.358567
H25	-C6	-C1	: 120.150796	H25	-C6	-C5	: 118.490631
C8	-C7	-C2	: 124.937252	C12	-C7	-C2	: 114.930469
C12	-C7	-C8	: 120.132197	C9	-C8	-C7	: 120.452609
H20	-C8	-C7	: 120.577102	H20	-C8	-C9	: 118.970246

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 C10     -C9     -C8     : 119.592628  S13     -C9     -C8     :
116.030381
 S13     -C9     -C10    : 124.376982  C11     -C10    -C9     :
119.804500
 H21     -C10    -C9     : 120.911102  H21     -C10    -C11    :
119.284354
 C12     -C11    -C10    : 121.315565  H22     -C11    -C10    :
118.504020
 H22     -C11    -C12    : 120.180414  C11     -C12    -C7     :
118.702079
 Si15    -C12    -C7     : 109.540840  Si15    -C12    -C11    :
131.755408
 C14     -S13    -C9     : 103.758383  H26     -C14    -S13    :
105.531567
 H27     -C14    -S13    : 111.597394  H27     -C14    -H26    :
108.880349
 H28     -C14    -S13    : 111.556694  H28     -C14    -H26    :
108.874099
 H28     -C14    -H27    : 110.231468  C12     -Si15   -C1     :
91.123817
 C16     -Si15   -C1     : 115.039905  C16     -Si15   -C12    :
112.703205
 C19     -Si15   -C1     : 112.873160  C19     -Si15   -C12    :
114.411295
 C19     -Si15   -C16    : 109.754579  C32     -C16    -Si15   :
121.268357
 C36     -C16    -Si15   : 120.820099  C36     -C16    -C32    :
117.869115
 C18     -S17    -C4     : 103.673914  H29     -C18    -S17    :
105.533777
 H30     -C18    -S17    : 111.573964  H30     -C18    -H29    :
108.893946
 H31     -C18    -S17    : 111.537887  H31     -C18    -H29    :
108.896103
 H31     -C18    -H30    : 110.237775  C42     -C19    -Si15   :
120.865321
 C46     -C19    -Si15   : 121.213294  C46     -C19    -C42    :
117.847550
 C33     -C32    -C16    : 121.145127  H37     -C32    -C16    :
119.826363
 H37     -C32    -C33    : 119.025639  C34     -C33    -C32    :
120.029504
 H38     -C33    -C32    : 119.898345  H38     -C33    -C34    :
120.071586
 C35     -C34    -C33    : 119.762225  H39     -C34    -C33    :
120.108935
 H39     -C34    -C35    : 120.128528  C36     -C35    -C34    :
120.064032
 H40     -C35    -C34    : 120.055295  H40     -C35    -C36    :
119.880617
 C35     -C36    -C16    : 121.129117  H41     -C36    -C16    :
119.614935
 H41     -C36    -C35    : 119.255277  C43     -C42    -C19    :
121.140332
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 H47     -C42     -C19     : 119.608523  H47     -C42     -C43     :
119.251005
 C44     -C43     -C42     : 120.072783  H48     -C43     -C42     :
119.887189
 H48     -C43     -C44     : 120.040024  C45     -C44     -C43     :
119.747417
 H49     -C44     -C43     : 120.147020  H49     -C44     -C45     :
120.105246
 C46     -C45     -C44     : 120.033086  H50     -C45     -C44     :
120.065324
 H50     -C45     -C46     : 119.901364  C45     -C46     -C19     :
121.157688
 H51     -C46     -C19     : 119.840231  H51     -C46     -C45     :
119.000503

  torsional angles:

 C1      -C2      -C3      -C4      :  -0.099140
 C1      -C2      -C3      -H23     : 179.836950
 C1      -C2      -C7      -C8      :-179.896339
 C1      -C2      -C7      -C12     :   0.208461
 C1      -C6      -C5      -C4      :   0.112115
 C1      -C6      -C5      -H24     :-179.952226
 C1      -Si15    -C12     -C7      :   0.238741
 C1      -Si15    -C12     -C11     : 179.749785
 C1      -Si15    -C16     -C32     : -91.553297
 C1      -Si15    -C16     -C36     :  86.026964
 C1      -Si15    -C19     -C42     : -15.957959
 C1      -Si15    -C19     -C46     : 167.234163
 C2      -C1      -C6      -C5      :  -0.322744
 C2      -C1      -C6      -H25     : 179.706012
 C2      -C1      -Si15    -C12     :  -0.127348
 C2      -C1      -Si15    -C16     :-115.928020
 C2      -C1      -Si15    -C19     : 117.060988
 C2      -C3      -C4      -C5      :  -0.115571
 C2      -C3      -C4      -S17     : 179.863134
 C2      -C7      -C8      -C9      :-179.963372
 C2      -C7      -C8      -H20     :  -0.038984
 C2      -C7      -C12     -C11     :-179.878603
 C2      -C7      -C12     -Si15    :  -0.294457
 C3      -C2      -C1      -C6      :   0.314884
 C3      -C2      -C1      -Si15    :-179.909462
 C3      -C2      -C7      -C8      :  -0.004201
 C3      -C2      -C7      -C12     :-179.899402
 C3      -C4      -C5      -C6      :   0.110947
 C3      -C4      -C5      -H24     :-179.823625
 C3      -C4      -S17     -C18     :-179.157652
 C4      -C3      -C2      -C7      :-179.986025
 C4      -C5      -C6      -H25     :-179.916176
 C4      -S17     -C18     -H29     : 179.533152
 C4      -S17     -C18     -H30     : -62.346885
 C4      -S17     -C18     -H31     :  61.429590
 C5      -C4      -C3      -H23     : 179.947373
 C5      -C4      -S17     -C18     :   0.819904
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C5      -C6      -C1      -Si15    : 179.961287
C6      -C1      -C2      -C7      :-179.787409
C6      -C1      -Si15    -C12     : 179.608315
C6      -C1      -Si15    -C16     :  63.807643
C6      -C1      -Si15    -C19     : -63.203349
C6      -C5      -C4      -S17     :-179.865873
C7      -C2      -C1      -Si15    :  -0.011755
C7      -C2      -C3      -H23     :  -0.049935
C7      -C8      -C9      -C10     :  -0.072492
C7      -C8      -C9      -S13     : 179.958830
C7      -C12     -C11     -C10     :  -0.227175
C7      -C12     -C11     -H22     : 179.765105
C7      -C12     -Si15    -C16     : 118.084578
C7      -C12     -Si15    -C19     :-115.599848
C8      -C7      -C12     -C11     :   0.220733
C8      -C7      -C12     -Si15    : 179.804879
C8      -C9      -C10     -C11     :   0.068360
C8      -C9      -C10     -H21     :-179.854782
C8      -C9      -S13     -C14     :-179.426524
C9      -C8      -C7      -C12     :  -0.073255
C9      -C10     -C11     -C12     :   0.084245
C9      -C10     -C11     -H22     :-179.908162
C9      -S13     -C14     -H26     : 179.712318
C9      -S13     -C14     -H27     : -62.172982
C9      -S13     -C14     -H28     :  61.626518
C10     -C9      -C8      -H20     :-179.998084
C10     -C9      -S13     -C14     :   0.606476
C10     -C11     -C12     -Si15    :-179.701831
C11     -C10     -C9      -S13     :-179.965741
C11     -C12     -Si15    -C16     : -62.404378
C11     -C12     -Si15    -C19     :  63.911196
C12     -C7      -C8      -H20     : 179.851133
C12     -C11     -C10     -H21     :-179.991358
C12     -Si15    -C16     -C32     : 165.801560
C12     -Si15    -C16     -C36     : -16.618178
C12     -Si15    -C19     -C42     :  86.448374
C12     -Si15    -C19     -C46     : -90.359504
S13     -C9      -C8      -H20     :   0.033238
S13     -C9      -C10     -H21     :   0.111117
Si15    -C1      -C6      -H25     :  -0.009957
Si15    -C12     -C11     -H22     :   0.290449
Si15    -C16     -C32     -C33     : 177.309195
Si15    -C16     -C32     -H37     :  -3.313264
Si15    -C16     -C36     -C35     :-177.498746
Si15    -C16     -C36     -H41     :   2.801411
Si15    -C19     -C42     -C43     :-176.735164
Si15    -C19     -C42     -H47     :   3.401871
Si15    -C19     -C46     -C45     : 176.525563
Si15    -C19     -C46     -H51     :  -3.936101
C16     -Si15    -C19     -C42     :-145.719859
C16     -Si15    -C19     -C46     :  37.472263
C16     -C32     -C33     -C34     :   0.271994
C16     -C32     -C33     -H38     : 179.998532
C16     -C36     -C35     -C34     :   0.085047
```

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C16     -C36     -C35     -H40     :-179.828369
S17     -C4      -C3      -H23     :  -0.073923
S17     -C4      -C5      -H24     :   0.199555
C19     -Si15    -C16     -C32     :  37.026863
C19     -Si15    -C16     -C36     :-145.392876
C19     -C42     -C43     -C44     :   0.117986
C19     -C42     -C43     -H48     :-179.860114
C19     -C46     -C45     -C44     :   0.278651
C19     -C46     -C45     -H50     :-179.894553
H21     -C10     -C11     -H22     :   0.016235
H24     -C5      -C6      -H25     :   0.019482
C32     -C16     -C36     -C35     :   0.161684
C32     -C16     -C36     -H41     :-179.538158
C32     -C33     -C34     -C35     :  -0.016372
C32     -C33     -C34     -H39     : 179.780910
C33     -C32     -C16     -C36     :  -0.340186
C33     -C34     -C35     -C36     :  -0.159859
C33     -C34     -C35     -H40     : 179.753404
C34     -C33     -C32     -H37     :-179.110435
C34     -C35     -C36     -H41     : 179.785950
C35     -C34     -C33     -H38     :-179.742433
C36     -C16     -C32     -H37     : 179.037355
C36     -C35     -C34     -H39     :-179.957101
H37     -C32     -C33     -H38     :   0.616103
H38     -C33     -C34     -H39     :   0.054850
H39     -C34     -C35     -H40     :  -0.043838
H40     -C35     -C36     -H41     :  -0.127465
C42     -C19     -C46     -C45     :  -0.375615
C42     -C19     -C46     -H51     : 179.162720
C42     -C43     -C44     -C45     :  -0.222128
C42     -C43     -C44     -H49     : 179.982489
C43     -C42     -C19     -C46     :   0.177331
C43     -C44     -C45     -C46     :   0.026364
C43     -C44     -C45     -H50     :-179.800145
C44     -C43     -C42     -H47     : 179.981434
C44     -C45     -C46     -H51     :-179.263484
C45     -C44     -C43     -H48     : 179.755939
C46     -C19     -C42     -H47     :-179.685635
C46     -C45     -C44     -H49     : 179.821834
H47     -C42     -C43     -H48     :   0.003333
H48     -C43     -C44     -H49     :  -0.039444
H49     -C44     -C45     -H50     :  -0.004675
H50     -C45     -C46     -H51     :   0.563311
```
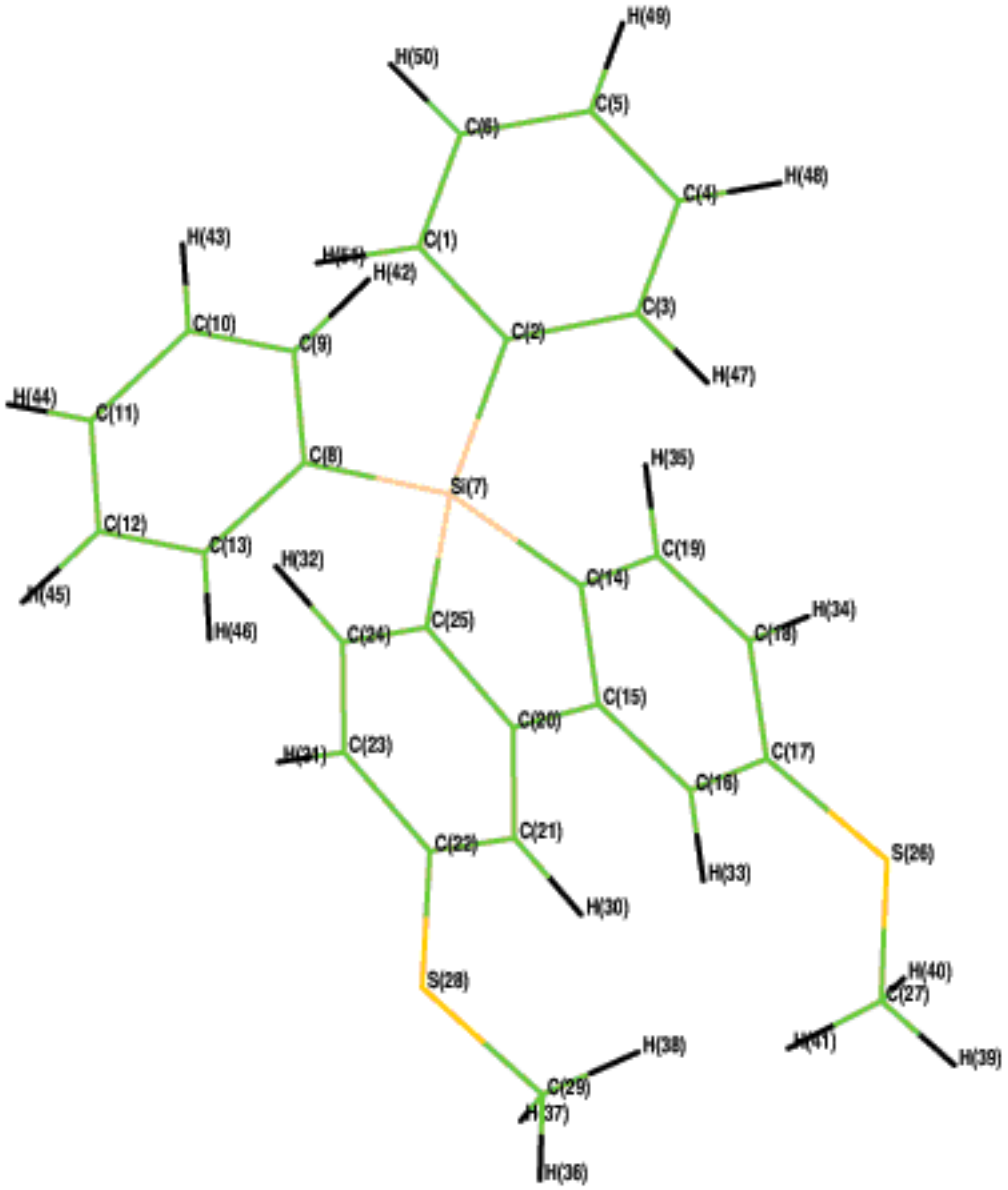

*Diphenyldibenzosilole (**1**) – Anti Conformer*



Final energy (B3LYP; cc-pVTZ) = -2090.371296 h

Optimized geometry (Optimization done with the 6-31g** basis set):

		angstroms	
atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4074125585

C3	1.2436030592	0.0000000000	2.0640755726
C4	2.4387033977	0.0025659141	1.3446272989
C5	2.4154495959	0.0081910524	-0.0499516299
C6	1.1928976486	0.0074310261	-0.7219526468
Si7	-1.6174880000	0.0617044784	2.3770070195
C8	-2.9112606586	-0.9932357337	1.4968848594
C9	-2.5584273942	-2.2057204340	0.8757220260
C10	-3.5202524129	-3.0125904927	0.2687597140
C11	-4.8588753528	-2.6199129871	0.2639578428
C12	-5.2299723295	-1.4192252450	0.8690728626
C13	-4.2661748698	-0.6166186186	1.4795528186
C14	-1.3923902344	-0.3212102388	4.2083417940
C15	-1.7752888037	0.8043735275	4.9757480827
C16	-1.7027845878	0.7696356795	6.3726463415
C17	-1.2503562516	-0.3841645330	7.0223335903
C18	-0.8721891241	-1.5039968148	6.2643859110
C19	-0.9459814597	-1.4658354456	4.8746197061
C20	-2.2409220354	1.9787032764	4.1837291419
C21	-2.6621021327	3.1914350457	4.7393182319
C22	-3.0820061391	4.2357211358	3.9084663278
C23	-3.0751158988	4.0589557137	2.5155053215
C24	-2.6549524969	2.8507263090	1.9657662725
C25	-2.2364880064	1.7950931790	2.7807256272
S26	-1.1106062371	-0.5507593517	8.7926783948
C27	-1.6864007136	1.0566503464	9.4263296582
S28	-3.6435620266	5.8227080801	4.4981729795
C29	-3.5397099499	5.6721545535	6.3103134437
H30	-2.6628351166	3.3192090504	5.8149706245
H31	-3.3988810527	4.8683222879	1.8671069708
H32	-2.6578866578	2.7394585034	0.8840978999
H33	-1.9968368287	1.6379403296	6.9495100702
H34	-0.5221841876	-2.4018531633	6.7661047958
H35	-0.6489496392	-2.3469086443	4.3108276206
H36	-3.8876888225	6.6293329107	6.7040137157
H37	-4.1902541088	4.8783813295	6.6850116850
H38	-2.5118615400	5.5070427870	6.6419576894
H39	-1.6115742720	0.9864459781	10.5134162350
H40	-1.0513881057	1.8758559115	9.0807976701
H41	-2.7279462146	1.2450691703	9.1556309311
H42	-1.5179033361	-2.5202944808	0.8552471182
H43	-3.2243934134	-3.9448737272	-0.2047201054
H44	-5.6087115280	-3.2454418655	-0.2125026464
H45	-6.2705764147	-1.1063916708	0.8637771271
H46	-4.5702336266	0.3176193999	1.9443622262
H47	1.2777538004	-0.0070511232	3.1503597649
H48	3.3883924567	-0.0017532714	1.8726680276
H49	3.3458261930	0.0095783432	-0.6111863098
H50	1.1685968121	0.0076920404	-1.8083555305
H51	-0.9429650568	-0.0167322195	-0.5409948155

principal moments of inertia:

amu*angstrom^2:	3540.67517	5160.34028	6093.01953
g*cm^2:	5.87942871E-37	8.56894557E-37	1.01176957E-36

```
 rotational constants:
              cm^(-1):     0.00476113     0.00326677     0.00276671
                  GHz:     0.14273521     0.09793521     0.08294393

 Z-matrix: (angstroms and degrees)
C1
C2     C1   cc2
C3     C2   cc3      C1   ccc3
C4     C3   cc4      C2   ccc4      C1   dih4
C5     C4   cc5      C3   ccc5      C2   dih5
C6     C5   cc6      C4   ccc6      C3   dih6
Si7    C2   sic7     C3   sicc7     C4   dih7
C8     Si7  csi8     C2   csic8     C3   dih8
C9     C8   cc9      Si7  ccsi9     C2   dih9
C10    C9   cc10     C8   ccc10     Si7  dih10
C11    C10  cc11     C9   ccc11     C8   dih11
C12    C11  cc12     C10  ccc12     C9   dih12
C13    C12  cc13     C11  ccc13     C10  dih13
C14    Si7  csi14    C8   csic14    C9   dih14
C15    C14  cc15     Si7  ccsi15    C8   dih15
C16    C15  cc16     C14  ccc16     Si7  dih16
C17    C16  cc17     C15  ccc17     C14  dih17
C18    C17  cc18     C16  ccc18     C15  dih18
C19    C18  cc19     C17  ccc19     C16  dih19
C20    C15  cc20     C14  ccc20     C19  dih20
C21    C20  cc21     C15  ccc21     C14  dih21
C22    C21  cc22     C20  ccc22     C15  dih22
C23    C22  cc23     C21  ccc23     C20  dih23
C24    C23  cc24     C22  ccc24     C21  dih24
C25    C24  cc25     C23  ccc25     C22  dih25
S26    C17  sc26     C16  scc26     C15  dih26
C27    S26  cs27     C17  csc27     C16  dih27
S28    C22  sc28     C21  scc28     C20  dih28
C29    S28  cs29     C22  csc29     C21  dih29
H30    C21  hc30     C20  hcc30     C15  dih30
H31    C23  hc31     C22  hcc31     C21  dih31
H32    C24  hc32     C23  hcc32     C22  dih32
H33    C16  hc33     C15  hcc33     C14  dih33
H34    C18  hc34     C17  hcc34     C16  dih34
H35    C19  hc35     C14  hcc35     C15  dih35
H36    C29  hc36     S28  hcs36     C22  dih36
H37    C29  hc37     S28  hcs37     C22  dih37
H38    C29  hc38     S28  hcs38     C22  dih38
H39    C27  hc39     S26  hcs39     C17  dih39
H40    C27  hc40     S26  hcs40     C17  dih40
H41    C27  hc41     S26  hcs41     C17  dih41
H42    C9   hc42     C8   hcc42     Si7  dih42
H43    C10  hc43     C9   hcc43     C8   dih43
H44    C11  hc44     C10  hcc44     C9   dih44
H45    C12  hc45     C11  hcc45     C10  dih45
H46    C13  hc46     C8   hcc46     Si7  dih46
H47    C3   hc47     C2   hcc47     Si7  dih47
H48    C4   hc48     C3   hcc48     C2   dih48
H49    C5   hc49     C4   hcc49     C3   dih49
```

```
H50    C6   hc50     C5   hcc50     C4   dih50
H51    C1   hc51     C2   hcc51     Si7  dih51

 Z-variables: (angstroms and degrees)
 cc2 =     1.4074125585
 cc3 =     1.4063267341
 ccc3 =   117.8355166269
 cc4 =     1.3949470317
 ccc4 =   121.1165591276
 dih4 =     0.1231044776
 cc5 =     1.3947841303
 ccc5 =   120.0927451443
 dih5 =     0.14237684
 cc6 =     1.3950696069
 ccc6 =   119.7511767417
 dih6 =    -0.1801296122
 sic7 =     1.8868461229
 sicc7 =   121.2055552988
 dih7 =  -177.6856900223
 csi8 =     1.8871570046
 csic8 =   109.254286153
 dih8 =  -143.9875788599
 cc9 =     1.4072859434
 ccsi9 =   121.0374988527
 dih9 =    37.7089907979
 cc10 =     1.3944711925
 ccc10 =   121.1791726309
 dih10 =   177.5285038958
 cc11 =     1.3950376542
 ccc11 =   120.031496048
 dih11 =     0.323392088
 cc12 =     1.3948219267
 ccc12 =   119.7426674561
 dih12 =    -0.0563265357
 cc13 =     1.3949081392
 ccc13 =   120.0885846953
 dih13 =    -0.1718787937
 csi14 =     1.8844308799
 csic14 =   114.9315651132
 dih14 =   -90.4859861353
 cc15 =     1.4150839343
 ccsi15 =   109.4554889748
 dih15 =  -115.7643563114
 cc16 =     1.3992098931
 ccc16 =   120.5067411367
 dih16 =   179.8352290261
 cc17 =     1.3992997717
 ccc17 =   120.0498013037
 dih17 =    -0.063352477
 cc18 =     1.4041080444
 ccc18 =   119.6082541942
 dih18 =    -0.06959609
 cc19 =     1.3922469979
 ccc19 =   120.1794415354
```

```
dih19 =     0.0547074014
cc20 =     1.4910260454
ccc20 =   115.0180628353
dih20 =  -179.8661721101
cc21 =     1.398853193
ccc21 =   124.4619039383
dih21 =  -179.8774917499
cc22 =     1.3989880982
ccc22 =   120.1079837682
dih22 =  -179.9850757164
cc23 =     1.4041488009
ccc23 =   119.5853816032
dih23 =    -0.1251187243
cc24 =     1.3923248905
ccc24 =   120.1597754508
dih24 =     0.1079716307
cc25 =     1.3977240732
ccc25 =   121.0325352193
dih25 =     0.1120023555
sc26 =     1.7836492443
scc26 =   124.2758920627
dih26 =   179.8997249251
cs27 =     1.8212136449
csc27 =   103.7759217651
dih27 =     0.4194244767
sc28 =     1.7837114428
scc28 =   124.2136378094
dih28 =   179.8398964574
cs29 =     1.8213469412
csc29 =   103.7355162911
dih29 =    -0.8086835946
hc30 =     1.083215031
hcc30 =   119.79306651
dih30 =    -0.0315354587
hc31 =     1.0864246626
hcc31 =   119.7896154409
dih31 =  -179.8937593178
hc32 =     1.0873801553
hcc32 =   118.7339897987
dih32 =  -179.9297009298
hc33 =     1.083139625
hcc33 =   119.8502500099
dih33 =   179.887256079
hc34 =     1.0864489484
hcc34 =   119.7741449209
dih34 =  -179.8920961452
hc35 =     1.0873727049
hcc35 =   120.2432489612
dih35 =   179.762836279
hc36 =     1.0919155679
hcs36 =   105.5515215431
dih36 =  -179.4724428562
hc37 =     1.0925577357
hcs37 =   111.55076897
```

```
 dih37 =   -61.379617957
 hc38 =     1.0925759263
 hcs38 =   111.6010912439
 dih38 =    62.4539365909
 hc39 =     1.0919179801
 hcs39 =   105.5438806587
 dih39 =  -179.9459644907
 hc40 =     1.0925800313
 hcs40 =   111.5911191816
 dih40 =   -61.8533255409
 hc41 =     1.0925184139
 hcs41 =   111.5564274173
 dih41 =    61.9894691856
 hc42 =     1.0872287561
 hcc42 =   119.8377692851
 dih42 =    -3.1461289603
 hc43 =     1.0866773745
 hcc43 =   119.8857250083
 dih43 =  -179.9915915514
 hc44 =     1.0865336005
 hcc44 =   120.11036152
 dih44 =   179.7247490851
 hc45 =     1.0866230957
 hcc45 =   120.032878095
 dih45 =   179.6958731307
 hc46 =     1.0868763445
 hcc46 =   119.6319766258
 dih46 =     2.5604978451
 hc47 =     1.0868437505
 hcc47 =   119.6355095759
 dih47 =     2.618870606
 hc48 =     1.0866254991
 hcc48 =   119.8766487558
 dih48 =  -179.7404211413
 hc49 =     1.0865481595
 hcc49 =   120.1445607162
 dih49 =  -179.9625054272
 hc50 =     1.0866746636
 hcc50 =   120.0776803829
 dih50 =  -179.7499841605
 hc51 =     1.0872619077
 hcc51 =   119.8397212227
 dih51 =    -3.2012440409

 Molecular weight:     426.09 amu

 Stoichiometry: SiC26H22S2
 Molecular Point Group: C1
 Point Group used: C1


 bond lengths (angstroms):

C1      -C2      :   1.407413      C1      -C6      :   1.394373
```

C1	-H51	:	1.087262	C2	-C3	:	1.406327
C2	-Si7	:	1.886846	C3	-C4	:	1.394947
C3	-H47	:	1.086844	C4	-C5	:	1.394784
C4	-H48	:	1.086625	C5	-C6	:	1.395070
C5	-H49	:	1.086548	C6	-H50	:	1.086675
Si7	-C8	:	1.887157	Si7	-C14	:	1.884431
Si7	-C25	:	1.884353	C8	-C9	:	1.407286
C8	-C13	:	1.406390	C9	-C10	:	1.394471
C9	-H42	:	1.087229	C10	-C11	:	1.395038
C10	-H43	:	1.086677	C11	-C12	:	1.394822
C11	-H44	:	1.086534	C12	-C13	:	1.394908
C12	-H45	:	1.086623	C13	-H46	:	1.086876
C14	-C15	:	1.415084	C14	-C19	:	1.397632
C15	-C16	:	1.399210	C15	-C20	:	1.491026
C16	-C17	:	1.399300	C16	-H33	:	1.083140
C17	-C18	:	1.404108	C17	-S26	:	1.783649
C18	-C19	:	1.392247	C18	-H34	:	1.086449
C19	-H35	:	1.087373	C20	-C21	:	1.398853
C20	-C25	:	1.414974	C21	-C22	:	1.398988
C21	-H30	:	1.083215	C22	-C23	:	1.404149
C22	-S28	:	1.783711	C23	-C24	:	1.392325
C23	-H31	:	1.086425	C24	-C25	:	1.397724
C24	-H32	:	1.087380	S26	-C27	:	1.821214
C27	-H39	:	1.091918	C27	-H40	:	1.092580
C27	-H41	:	1.092518	S28	-C29	:	1.821347
C29	-H36	:	1.091916	C29	-H37	:	1.092558
C29	-H38	:	1.092576				

bond angles:

C6	-C1	-C2	: 121.182220	H51	-C1	-C2	: 119.839721
H51	-C1	-C6	: 118.974838	C3	-C2	-C1	: 117.835517
Si7	-C2	-C1	: 120.921984	Si7	-C2	-C3	: 121.205555
C4	-C3	-C2	: 121.116559	H47	-C3	-C2	: 119.635510
H47	-C3	-C4	: 119.247241	C5	-C4	-C3	: 120.092745
H48	-C4	-C3	: 119.876649	H48	-C4	-C5	: 120.030502
C6	-C5	-C4	: 119.751177	H49	-C5	-C4	: 120.144561
H49	-C5	-C6	: 120.103904	C5	-C6	-C1	: 120.020697
H50	-C6	-C1	: 119.900941	H50	-C6	-C5	: 120.077680
C8	-Si7	-C2	: 109.254286	C14	-Si7	-C2	: 112.976121
C14	-Si7	-C8	: 114.931565	C25	-Si7	-C2	: 114.946914
C25	-Si7	-C8	: 112.888560	C25	-Si7	-C14	: 91.028392

```
 C9      -C8      -Si7     : 121.037499  C13     -C8      -Si7     :
121.099406
 C13     -C8      -C9      : 117.828346  C10     -C9      -C8      :
121.179173
 H42     -C9      -C8      : 119.837769  H42     -C9      -C10     :
118.979689
 C11     -C10     -C9      : 120.031496  H43     -C10     -C9      :
119.885725
 H43     -C10     -C11     : 120.082028  C12     -C11     -C10     :
119.742667
 H44     -C11     -C10     : 120.110362  H44     -C11     -C12     :
120.146608
 C13     -C12     -C11     : 120.088585  H45     -C12     -C11     :
120.032878
 H45     -C12     -C13     : 119.878405  C12     -C13     -C8      :
121.128688
 H46     -C13     -C8      : 119.631977  H46     -C13     -C12     :
119.238579
 C15     -C14     -Si7     : 109.455489  C19     -C14     -Si7     :
131.901755
 C19     -C14     -C15     : 118.641402  C16     -C15     -C14     :
120.506741
 C20     -C15     -C14     : 115.018063  C20     -C15     -C16     :
124.475150
 C17     -C16     -C15     : 120.049801  H33     -C16     -C15     :
119.850250
 H33     -C16     -C17     : 120.099930  C18     -C17     -C16     :
119.608254
 S26     -C17     -C16     : 124.275892  S26     -C17     -C18     :
116.115847
 C19     -C18     -C17     : 120.179442  H34     -C18     -C17     :
119.774145
 H34     -C18     -C19     : 120.046392  C18     -C19     -C14     :
121.013967
 H35     -C19     -C14     : 120.243249  H35     -C19     -C18     :
118.742783
 C21     -C20     -C15     : 124.461904  C25     -C20     -C15     :
115.056874
 C25     -C20     -C21     : 120.481168  C22     -C21     -C20     :
120.107984
 H30     -C21     -C20     : 119.793067  H30     -C21     -C22     :
120.098933
 C23     -C22     -C21     : 119.585382  S28     -C22     -C21     :
124.213638
 S28     -C22     -C23     : 116.200972  C24     -C23     -C22     :
120.159775
 H31     -C23     -C22     : 119.789615  H31     -C23     -C24     :
120.050609
 C25     -C24     -C23     : 121.032535  H32     -C24     -C23     :
118.733990
 H32     -C24     -C25     : 120.233462  C20     -C25     -Si7     :
109.440701
 C24     -C25     -Si7     : 131.926215  C24     -C25     -C20     :
118.632372
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 C27     -S26     -C17     : 103.775922  H39     -C27     -S26     :
105.543881
 H40     -C27     -S26     : 111.591119  H40     -C27     -H39     :
108.858545
 H41     -C27     -S26     : 111.556427  H41     -C27     -H39     :
108.850344
 H41     -C27     -H40     : 110.268333  C29     -S28     -C22     :
103.735516
 H36     -C29     -S28     : 105.551522  H37     -C29     -S28     :
111.550769
 H37     -C29     -H36     : 108.872634  H38     -C29     -S28     :
111.601091
 H38     -C29     -H36     : 108.834468  H38     -C29     -H37     :
110.258812

  torsional angles:

 C1      -C2      -C3      -C4      :   0.123104
 C1      -C2      -C3      -H47     :-179.572335
 C1      -C2      -Si7     -C8      :  38.271154
 C1      -C2      -Si7     -C14     : 167.549146
 C1      -C2      -Si7     -C25     : -89.816468
 C1      -C6      -C5      -C4      :  -0.050625
 C1      -C6      -C5      -H49     : 179.731841
 C2      -C1      -C6      -C5      :   0.325188
 C2      -C1      -C6      -H50     :-179.974918
 C2      -C3      -C4      -C5      :   0.142377
 C2      -C3      -C4      -H48     :-179.740421
 C2      -Si7     -C8      -C9      :  37.708991
 C2      -Si7     -C8      -C13     :-144.481812
 C2      -Si7     -C14     -C15     : 117.931291
 C2      -Si7     -C14     -C19     : -62.509198
 C2      -Si7     -C25     -C20     :-116.094177
 C2      -Si7     -C25     -C24     :  63.586338
 C3      -C2      -C1      -C6      :  -0.356913
 C3      -C2      -C1      -H51     : 178.983435
 C3      -C2      -Si7     -C8      :-143.987579
 C3      -C2      -Si7     -C14     : -14.709587
 C3      -C2      -Si7     -C25     :  87.924799
 C3      -C4      -C5      -C6      :  -0.180130
 C3      -C4      -C5      -H49     :-179.962505
 C4      -C3      -C2      -Si7     :-177.685690
 C4      -C5      -C6      -H50     :-179.749984
 C5      -C4      -C3      -H47     : 179.838979
 C5      -C6      -C1      -H51     :-179.020750
 C6      -C1      -C2      -Si7     : 177.458407
 C6      -C5      -C4      -H48     : 179.702487
 Si7     -C2      -C1      -H51     :  -3.201244
 Si7     -C2      -C3      -H47     :   2.618871
 Si7     -C8      -C9      -C10     : 177.528504
 Si7     -C8      -C9      -H42     :  -3.146129
 Si7     -C8      -C13     -C12     :-177.758330
 Si7     -C8      -C13     -H46     :   2.560498
 Si7     -C14     -C15     -C16     : 179.835229
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Si7     -C14     -C15     -C20     :  -0.239734
Si7     -C14     -C19     -C18     :-179.751782
Si7     -C14     -C19     -H35     :   0.236082
Si7     -C25     -C20     -C15     :  -0.064170
Si7     -C25     -C20     -C21     :-179.982868
Si7     -C25     -C24     -C23     :-179.963751
Si7     -C25     -C24     -H32     :   0.078574
C8      -Si7     -C14     -C15     :-115.764356
C8      -Si7     -C14     -C19     :  63.795154
C8      -Si7     -C25     -C20     : 117.665867
C8      -Si7     -C25     -C24     : -62.653617
C8      -C9      -C10     -C11     :   0.323392
C8      -C9      -C10     -H43     :-179.991592
C8      -C13     -C12     -C11     :   0.139065
C8      -C13     -C12     -H45     :-179.728892
C9      -C8      -Si7     -C14     : -90.485986
C9      -C8      -Si7     -C25     : 166.937885
C9      -C8      -C13     -C12     :   0.119074
C9      -C8      -C13     -H46     :-179.562098
C9      -C10     -C11     -C12     :  -0.056327
C9      -C10     -C11     -H44     : 179.724749
C10     -C9      -C8      -C13     :  -0.350282
C10     -C11     -C12     -C13     :  -0.171879
C10     -C11     -C12     -H45     : 179.695873
C11     -C10     -C9      -H42     :-179.007647
C11     -C12     -C13     -H46     : 179.821470
C12     -C11     -C10     -H43     :-179.740720
C13     -C8      -Si7     -C14     :  87.323211
C13     -C8      -Si7     -C25     : -15.252918
C13     -C8      -C9      -H42     : 178.975085
C13     -C12     -C11     -H44     :-179.952874
C14     -Si7     -C25     -C20     :  -0.058251
C14     -Si7     -C25     -C24     : 179.622265
C14     -C15     -C16     -C17     :  -0.063352
C14     -C15     -C16     -H33     : 179.887256
C14     -C15     -C20     -C21     :-179.877492
C14     -C15     -C20     -C25     :   0.207488
C14     -C19     -C18     -C17     :   0.095550
C14     -C19     -C18     -H34     :-179.957792
C15     -C14     -Si7     -C25     :   0.168834
C15     -C14     -C19     -C18     :  -0.225028
C15     -C14     -C19     -H35     : 179.762836
C15     -C16     -C17     -C18     :  -0.069596
C15     -C16     -C17     -S26     : 179.899725
C15     -C20     -C21     -C22     :-179.985076
C15     -C20     -C21     -H30     :  -0.031535
C15     -C20     -C25     -C24     :-179.793355
C16     -C15     -C14     -C19     :   0.208790
C16     -C15     -C20     -C21     :   0.044163
C16     -C15     -C20     -C25     :-179.870857
C16     -C17     -C18     -C19     :   0.054707
C16     -C17     -C18     -H34     :-179.892096
C16     -C17     -S26     -C27     :   0.419424
C17     -C16     -C15     -C20     :-179.980951
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C17     -C18     -C19     -H35     :-179.892492
C17     -S26     -C27     -H39     :-179.945964
C17     -S26     -C27     -H40     : -61.853326
C17     -S26     -C27     -H41     :  61.989469
C18     -C17     -C16     -H33     : 179.979920
C18     -C17     -S26     -C27     :-179.610281
C19     -C14     -Si7     -C25     : 179.728345
C19     -C14     -C15     -C20     :-179.866172
C19     -C18     -C17     -S26     :-179.917059
C20     -C15     -C16     -H33     :  -0.030343
C20     -C21     -C22     -C23     :  -0.125119
C20     -C21     -C22     -S28     : 179.839896
C20     -C25     -C24     -C23     :  -0.306995
C20     -C25     -C24     -H32     : 179.735330
C21     -C20     -C25     -C24     :   0.287948
C21     -C22     -C23     -C24     :   0.107972
C21     -C22     -C23     -H31     :-179.893759
C21     -C22     -S28     -C29     :  -0.808684
C22     -C21     -C20     -C25     :  -0.074403
C22     -C23     -C24     -C25     :   0.112002
C22     -C23     -C24     -H32     :-179.929701
C22     -S28     -C29     -H36     :-179.472443
C22     -S28     -C29     -H37     : -61.379618
C22     -S28     -C29     -H38     :  62.453937
C23     -C22     -C21     -H30     : 179.921484
C23     -C22     -S28     -C29     : 179.157409
C24     -C23     -C22     -S28     :-179.859785
C25     -C20     -C21     -H30     : 179.879137
C25     -C24     -C23     -H31     :-179.886262
S26     -C17     -C16     -H33     :  -0.050759
S26     -C17     -C18     -H34     :   0.136137
S28     -C22     -C21     -H30     :  -0.113501
S28     -C22     -C23     -H31     :   0.138484
H31     -C23     -C24     -H32     :   0.072035
H34     -C18     -C19     -H35     :   0.054166
H42     -C9      -C10     -H43     :   0.677370
H43     -C10     -C11     -H44     :   0.040356
H44     -C11     -C12     -H45     :  -0.085122
H45     -C12     -C13     -H46     :  -0.046487
H47     -C3      -C4      -H48     :  -0.043819
H48     -C4      -C5      -H49     :  -0.079889
H49     -C5      -C6      -H50     :   0.032481
H50     -C6      -C1      -H51     :   0.679145
```
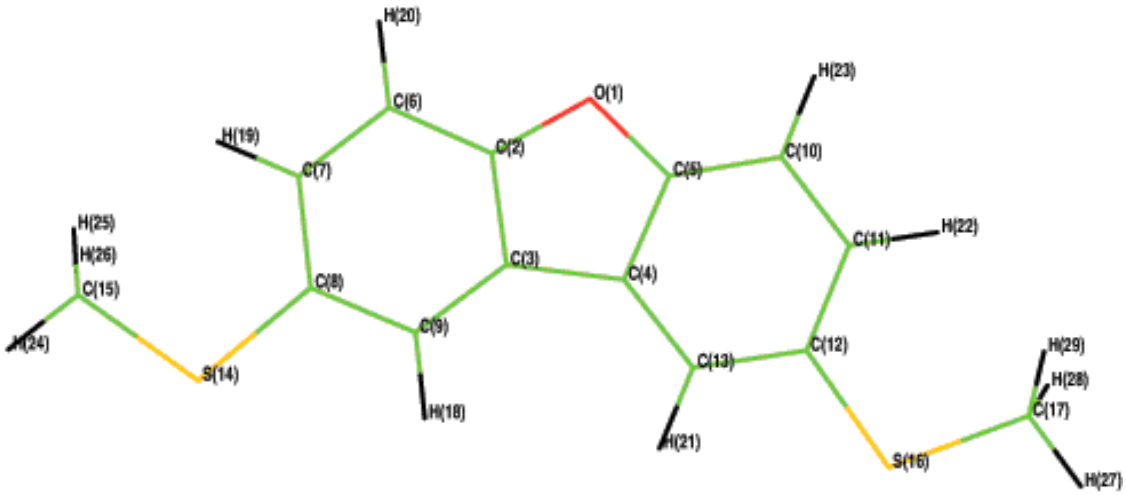

*D. Dibenzofuran (**2**) – Syn Conformer*



Final energy (B3LYP; cc-pVTZ) = -1412.6088146 h

Optimized geometry (Optimization done with the 6-31g** basis set):

		angstroms	
atom	x	y	z
O1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.3778685155
C3	1.3060819737	0.0000000000	1.9021790956
C4	2.1843097425	-0.0003525589	0.7440175123
C5	1.3269563390	-0.0000734290	-0.3719596298
C6	-1.1250111297	0.0007839053	2.1848313541
C7	-0.9235122096	0.0016491642	3.5673502609
C8	0.3705289464	0.0033183733	4.1221244070
C9	1.4936171866	0.0028530902	3.2842804373
C10	1.7989209678	0.0004305883	-1.6732773001
C11	3.1841932619	0.0004968266	-1.8529881695
C12	4.0683637877	-0.0013058549	-0.7571109216
C13	3.5658448750	-0.0015978037	0.5511318733
S14	0.7022710493	0.0032244537	5.8812378350

```
 C15          -0.9539822493      0.0576552337      6.6365047880
 S16           5.8516062614     -0.0001994171     -0.9160805321
 C17           6.1276861302     -0.0318429941     -2.7160634477
 H18           2.4935127241      0.0056504380      3.7074612511
 H19          -1.7934088457      0.0007414592      4.2130759015
 H20          -2.1231491341      0.0006993795      1.7611071660
 H21           4.2436011822     -0.0034722435      1.3997337278
 H22           3.5701254624      0.0018924999     -2.8651144043
 H23           1.1205989890      0.0012690954     -2.5192713702
 H24          -0.7807886419      0.0744493133      7.7145745154
 H25          -1.4967308019      0.9623128712      6.3525834492
 H26          -1.5413151123     -0.8296318124      6.3888522595
 H27           7.2121646882     -0.0418749656     -2.8435484694
 H28           5.7111444612     -0.9331097560     -3.1720565764
 H29           5.7246242727      0.8594704421     -3.2026791892

 principal moments of inertia:
       amu*angstrom^2:      528.75772     3038.45899     3560.65584
              g*cm^2: 8.78022735E-38 5.04547922E-37 5.91260739E-37

 rotational constants:
              cm^(-1):     0.03188158     0.00554809     0.00473442
                  GHz:     0.95578559     0.16632741     0.14193425

 Z-matrix: (angstroms and degrees)
O1
C2     O1    co2
C3     C2    cc3      O1    cco3
C4     C3    cc4      C2    ccc4      O1    dih4
C5     C4    cc5      C3    ccc5      C2    dih5
C6     C2    cc6      C3    ccc6      C4    dih6
C7     C6    cc7      C2    ccc7      C3    dih7
C8     C7    cc8      C6    ccc8      C2    dih8
C9     C8    cc9      C7    ccc9      C6    dih9
C10    C5    cc10     C4    ccc10     C3    dih10
C11    C10   cc11     C5    ccc11     C4    dih11
C12    C11   cc12     C10   ccc12     C5    dih12
C13    C12   cc13     C11   ccc13     C10   dih13
S14    C8    sc14     C9    scc14     C3    dih14
C15    S14   cs15     C8    csc15     C9    dih15
S16    C12   sc16     C13   scc16     C4    dih16
C17    S16   cs17     C12   csc17     C13   dih17
H18    C9    hc18     C3    hcc18     C2    dih18
H19    C7    hc19     C8    hcc19     C9    dih19
H20    C6    hc20     C7    hcc20     C8    dih20
H21    C13   hc21     C4    hcc21     C3    dih21
H22    C11   hc22     C12   hcc22     C13   dih22
H23    C10   hc23     C11   hcc23     C12   dih23
H24    C15   hc24     S14   hcs24     C8    dih24
H25    C15   hc25     S14   hcs25     C8    dih25
H26    C15   hc26     S14   hcs26     C8    dih26
H27    C17   hc27     S16   hcs27     C12   dih27
H28    C17   hc28     S16   hcs28     C12   dih28
H29    C17   hc29     S16   hcs29     C12   dih29
```

```
Z-variables: (angstroms and degrees)
co2 =     1.3778685155
cc3 =     1.4073918098
cco3 =   111.8723878351
cc4 =     1.4534862886
ccc4 =   105.3004604849
dih4 =    -0.0144084177
cc5 =     1.4072881433
ccc5 =   105.2937483158
dih5 =     0.0193840794
cc6 =     1.3844997939
ccc6 =   122.4759892789
dih6 =  -179.9759538173
cc7 =     1.3971260112
ccc7 =   117.3592898181
dih7 =     0.0025185156
cc8 =     1.4079487394
ccc8 =   121.4978705871
dih8 =     0.0760883259
cc9 =     1.401181619
ccc9 =   120.0708367499
dih9 =    -0.0613220147
cc10 =     1.38426101
ccc10 =   122.5318004729
dih10 =   179.9649889523
cc11 =     1.396880571
ccc11 =   117.3264794202
dih11 =     0.007548842
cc12 =     1.4080865424
ccc12 =   121.5054090013
dih12 =     0.0656212797
cc13 =     1.4014366034
ccc13 =   120.0902147264
dih13 =    -0.0768554269
sc14 =     1.7901209134
scc14 =   116.0439075463
dih14 =   179.8639022451
cs15 =     1.82114411
csc15 =   103.8273439949
dih15 =   178.2580488496
sc16 =     1.790314576
scc16 =   116.1069020712
dih16 =   179.9013536158
cs17 =     1.8213071971
csc17 =   103.8115046382
dih17 =   178.9701967982
hc18 =     1.085762825
hcc18 =   120.6666490738
dih18 =  -179.8313011383
hc19 =     1.0833663205
hcc19 =   120.2079604739
dih19 =   179.9226834862
hc20 =     1.0843531116
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```
hcc20 =   121.2942688443
dih20 =  -179.9257340846
hc21 =     1.0860397013
hcc21 =   120.6654132601
dih21 =     0.0529708668
hc22 =     1.0832105642
hcc22 =   120.2306666634
dih22 =   179.9285923246
hc23 =     1.0843557427
hcc23 =   121.3311096131
dih23 =  -179.9658235664
hc24 =     1.0920221627
hcs24 =   105.4051615935
dih24 =  -179.1328946438
hc25 =     1.0925167088
hcs25 =   111.6403347148
dih25 =   -61.1420447228
hc26 =     1.0925062787
hcs26 =   111.7551841603
dih26 =    62.8939016492
hc27 =     1.0919921309
hcs27 =   105.4310457873
dih27 =  -179.4474537191
hc28 =     1.0925742408
hcs28 =   111.6546505472
dih28 =   -61.45478478
hc29 =     1.092562759
hcs29 =   111.7205209729
dih29 =    62.5578659706

Molecular weight:     260.03 amu

Stoichiometry: C14H12S2O
Molecular Point Group: C1
Point Group used: C1


bond lengths (angstroms):

O1      -C2      :   1.377869      O1      -C5      :   1.378103
C2      -C3      :   1.407392      C2      -C6      :   1.384500
C3      -C4      :   1.453486      C3      -C9      :   1.394769
C4      -C5      :   1.407288      C4      -C13     :   1.394936
C5      -C10     :   1.384261      C6      -C7      :   1.397126
C6      -H20     :   1.084353      C7      -C8      :   1.407949
C7      -H19     :   1.083366      C8      -C9      :   1.401182
C8      -S14     :   1.790121      C9      -H18     :   1.085763
C10     -C11     :   1.396881      C10     -H23     :   1.084356
C11     -C12     :   1.408087      C11     -H22     :   1.083211
C12     -C13     :   1.401437      C12     -S16     :   1.790315
C13     -H21     :   1.086040      S14     -C15     :   1.821144
C15     -H24     :   1.092022      C15     -H25     :   1.092517
C15     -H26     :   1.092506      S16     -C17     :   1.821307
C17     -H27     :   1.091992      C17     -H28     :   1.092574
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 C17     -H29     :   1.092563

  bond angles:

 C5      -O1      -C2      : 105.658735  C3      -C2      -O1      :
111.872388
 C6      -C2      -O1      : 125.651610  C6      -C2      -C3      :
122.475989
 C4      -C3      -C2      : 105.300460  C9      -C3      -C2      :
119.599504
 C9      -C3      -C4      : 135.099885  C5      -C4      -C3      :
105.293748
 C13     -C4      -C3      : 135.120922  C13     -C4      -C5      :
119.585317
 C4      -C5      -O1      : 111.874664  C10     -C5      -O1      :
125.593533
 C10     -C5      -C4      : 122.531800  C7      -C6      -C2      :
117.359290
 H20     -C6      -C2      : 121.346441  H20     -C6      -C7      :
121.294269
 C8      -C7      -C6      : 121.497871  H19     -C7      -C6      :
118.294167
 H19     -C7      -C8      : 120.207960  C9      -C8      -C7      :
120.070837
 S14     -C8      -C7      : 123.885170  S14     -C8      -C9      :
116.043908
 C8      -C9      -C3      : 118.996391  H18     -C9      -C3      :
120.666649
 H18     -C9      -C8      : 120.336934  C11     -C10     -C5      :
117.326479
 H23     -C10     -C5      : 121.342403  H23     -C10     -C11     :
121.331110
 C12     -C11     -C10     : 121.505409  H22     -C11     -C10     :
118.263924
 H22     -C11     -C12     : 120.230667  C13     -C12     -C11     :
120.090215
 S16     -C12     -C11     : 123.802782  S16     -C12     -C13     :
116.106902
 C12     -C13     -C4      : 118.960710  H21     -C13     -C4      :
120.665413
 H21     -C13     -C12     : 120.373863  C15     -S14     -C8      :
103.827344
 H24     -C15     -S14     : 105.405162  H25     -C15     -S14     :
111.640335
 H25     -C15     -H24     : 108.821045  H26     -C15     -S14     :
111.755184
 H26     -C15     -H24     : 108.756070  H26     -C15     -H25     :
110.274778
 C17     -S16     -C12     : 103.811505  H27     -C17     -S16     :
105.431046
 H28     -C17     -S16     : 111.654651  H28     -C17     -H27     :
108.803408
 H29     -C17     -S16     : 111.720521  H29     -C17     -H27     :
108.776252
```

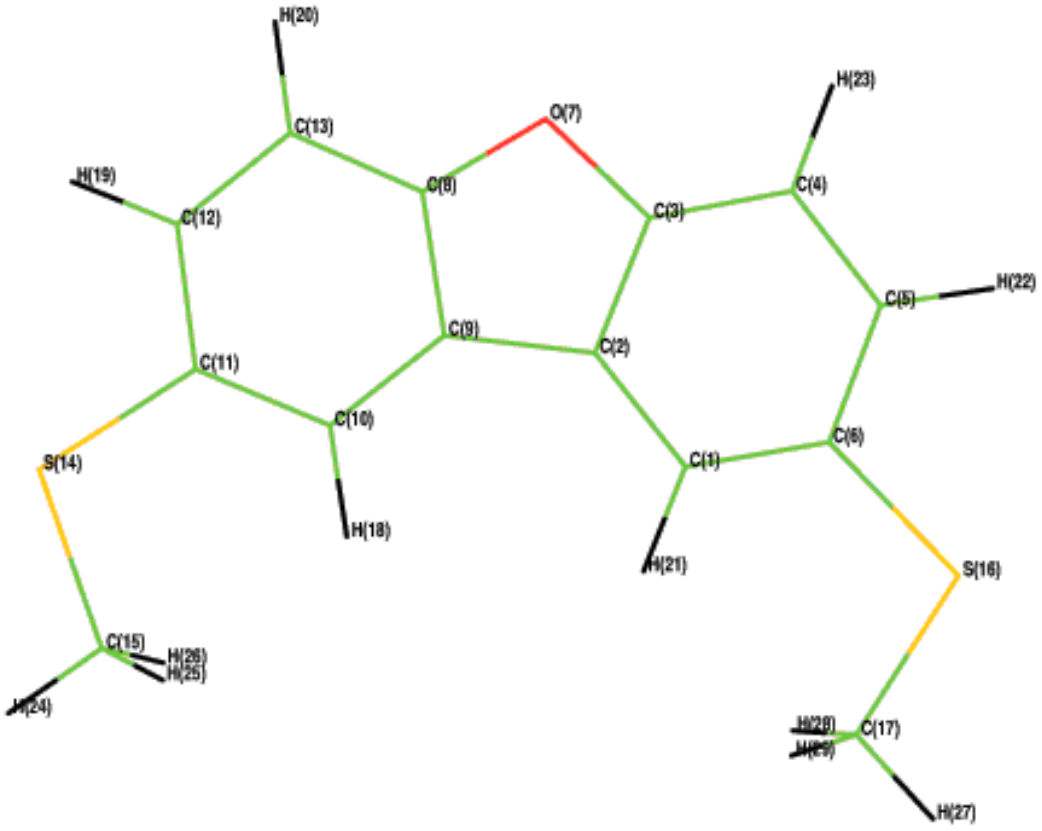
```
H29     -C17     -H28     : 110.268608

 torsional angles:

O1      -C2      -C3      -C4      :  -0.014408
O1      -C2      -C3      -C9      : 179.865207
O1      -C2      -C6      -C7      :-179.953564
O1      -C2      -C6      -H20     :   0.048260
O1      -C5      -C4      -C3      :  -0.018788
O1      -C5      -C4      -C13     : 179.946363
O1      -C5      -C10     -C11     : 179.989035
O1      -C5      -C10     -H23     :   0.020484
C2      -O1      -C5      -C4      :   0.010165
C2      -O1      -C5      -C10     :-179.973016
C2      -C3      -C4      -C5      :   0.019384
C2      -C3      -C4      -C13     :-179.937668
C2      -C3      -C9      -C8      :   0.109783
C2      -C3      -C9      -H18     :-179.831301
C2      -C6      -C7      -C8      :   0.076088
C2      -C6      -C7      -H19     :-179.908214
C3      -C2      -O1      -C5      :   0.003171
C3      -C2      -C6      -C7      :   0.002519
C3      -C2      -C6      -H20     :-179.995658
C3      -C4      -C5      -C10     : 179.964989
C3      -C4      -C13     -C12     :-179.989720
C3      -C4      -C13     -H21     :   0.052971
C3      -C9      -C8      -C7      :  -0.033946
C3      -C9      -C8      -S14     : 179.863902
C4      -C3      -C2      -C6      :-179.975954
C4      -C3      -C9      -C8      : 179.945281
C4      -C3      -C9      -H18     :   0.004197
C4      -C5      -C10     -C11     :   0.007549
C4      -C5      -C10     -H23     :-179.961003
C4      -C13     -C12     -C11     :   0.012798
C4      -C13     -C12     -S16     : 179.901354
C5      -O1      -C2      -C6      : 179.963247
C5      -C4      -C3      -C9      :-179.832325
C5      -C4      -C13     -C12     :   0.057918
C5      -C4      -C13     -H21     :-179.899391
C5      -C10     -C11     -C12     :   0.065621
C5      -C10     -C11     -H22     :-179.939723
C6      -C2      -C3      -C9      :  -0.096338
C6      -C7      -C8      -C9      :  -0.061322
C6      -C7      -C8      -S14     :-179.950766
C7      -C8      -C9      -H18     : 179.907337
C7      -C8      -S14     -C15     :  -1.848440
C8      -C7      -C6      -H20     :-179.925734
C8      -S14     -C15     -H24     :-179.132895
C8      -S14     -C15     -H25     : -61.142045
C8      -S14     -C15     -H26     :  62.893902
C9      -C3      -C4      -C13     :   0.210622
C9      -C8      -C7      -H19     : 179.922683
C9      -C8      -S14     -C15     : 178.258049
C10     -C5      -C4      -C13     :  -0.069859
```

```
C10     -C11     -C12     -C13     :  -0.076855
C10     -C11     -C12     -S16     :-179.956423
C11     -C12     -C13     -H21     : 179.970234
C11     -C12     -S16     -C17     :  -1.145845
C12     -C11     -C10     -H23     :-179.965824
C12     -S16     -C17     -H27     :-179.447454
C12     -S16     -C17     -H28     : -61.454785
C12     -S16     -C17     -H29     :  62.557866
C13     -C12     -C11     -H22     : 179.928592
C13     -C12     -S16     -C17     : 178.970197
S14     -C8      -C7      -H19     :   0.033240
S14     -C8      -C9      -H18     :  -0.194814
S16     -C12     -C11     -H22     :   0.049024
S16     -C12     -C13     -H21     :  -0.141210
H19     -C7      -C6      -H20     :   0.089964
H22     -C11     -C10     -H23     :   0.028832
```

*Dibenzofuran (**2**) – Anti Conformer*



Final energy (B3LYP; cc-pVTZ) = -1412.609762 h

Optimized geometry (Optimization done with the 6-31g** basis set):

		angstroms	
atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4013045275
C3	1.2186026994	0.0000000000	2.0992445999
C4	2.4484448092	0.0003248506	1.4548276684
C5	2.4344070362	-0.0001872229	0.0640689900
C6	1.2256666352	-0.0006096040	-0.6685741263
O7	1.0292411191	-0.0007939544	3.4627818224
C8	-0.3352496210	-0.0011555057	3.6472224171
C9	-1.0284120359	-0.0001937130	2.4262402607
C10	-2.4294702307	-0.0009361625	2.4216847355
C11	-3.1023294075	-0.0018035788	3.6449294978
C12	-2.3740308286	-0.0029028933	4.8563028300
C13	-0.9833615369	-0.0031665139	4.8748998879
S14	-4.8829284473	-0.0039256252	3.8149208338
C15	-5.4733381047	0.0408487052	2.0937649272
S16	1.4032530564	-0.0013202615	-2.4484283947
C17	-0.3154482972	-0.0302699826	-3.0473406445
H18	-2.9669898206	-0.0016840585	1.4812510774
H19	-2.9147894417	-0.0022884975	5.7980703422
H20	-0.4282673401	-0.0035068381	5.8063009404
H21	-0.9387698456	0.0005193762	-0.5410199922
H22	3.3780513700	-0.0015198048	-0.4735003989
H23	3.3783450633	-0.0003712456	2.0124598177
H24	-6.5633043479	0.0535057132	2.1573141623
H25	-5.1390847699	0.9445696703	1.5786733341
H26	-5.1627703180	-0.8473291336	1.5383627900
H27	-0.2462699870	-0.0382276487	-4.1370565182
H28	-0.8399351107	-0.9313357711	-2.7202185908
H29	-0.8648820571	0.8611578969	-2.7355613646

principal moments of inertia:

amu*angstrom^2:	765.82962	2469.50103	3228.77943
g*cm^2:	1.27168984E-37	4.10070243E-37	5.36151371E-37

rotational constants:

cm^(-1):	0.02201224	0.00682633	0.00522105
GHz:	0.65991050	0.20464823	0.15652324

Z-matrix: (angstroms and degrees)

```
C1
C2     C1   cc2
C3     C2   cc3     C1   ccc3
```

```
C4     C3   cc4     C2   ccc4     C1   dih4
C5     C4   cc5     C3   ccc5     C2   dih5
C6     C5   cc6     C4   ccc6     C3   dih6
O7     C3   oc7     C2   occ7     C1   dih7
C8     O7   co8     C3   coc8     C2   dih8
C9     C8   cc9     O7   cco9     C3   dih9
C10    C9   cc10    C8   ccc10    O7   dih10
C11    C10  cc11    C9   ccc11    C8   dih11
C12    C11  cc12    C10  ccc12    C9   dih12
C13    C12  cc13    C11  ccc13    C10  dih13
S14    C11  sc14    C12  scc14    C13  dih14
C15    S14  cs15    C11  csc15    C12  dih15
S16    C6   sc16    C5   scc16    C4   dih16
C17    S16  cs17    C6   csc17    C5   dih17
H18    C10  hc18    C9   hcc18    C8   dih18
H19    C12  hc19    C13  hcc19    C8   dih19
H20    C13  hc20    C8   hcc20    O7   dih20
H21    C1   hc21    C2   hcc21    C9   dih21
H22    C5   hc22    C4   hcc22    C3   dih22
H23    C4   hc23    C3   hcc23    O7   dih23
H24    C15  hc24    S14  hcs24    C11  dih24
H25    C15  hc25    S14  hcs25    C11  dih25
H26    C15  hc26    S14  hcs26    C11  dih26
H27    C17  hc27    S16  hcs27    C6   dih27
H28    C17  hc28    S16  hcs28    C6   dih28
H29    C17  hc29    S16  hcs29    C6   dih29

 Z-variables: (angstroms and degrees)
 cc2 =     1.4013045275
 cc3 =     1.4043193667
 ccc3 =   119.8014064849
 cc4 =     1.3884469389
 ccc4 =   122.5447972852
 dih4 =     0.0159024597
 cc5 =     1.3908296167
 ccc5 =   117.075485398
 dih5 =    -0.0390989567
 cc6 =     1.4134424188
 ccc6 =   121.7992444641
 dih6 =     0.018772223
 oc7 =     1.3766234763
 occ7 =   111.8950063017
 dih7 =  -179.9643863492
 co8 =     1.3768999396
 coc8 =   105.604513848
 dih8 =    -0.0068889697
 cc9 =     1.4040201155
 cco9 =   111.8858332932
 dih9 =    -0.018233867
 cc10 =     1.4010657976
 ccc10 =   119.770221975
 dih10 =   179.9745507427
 cc11 =     1.3960902452
 ccc11 =   118.6271899657
```

```
dih11 =     0.0386001849
cc12 =     1.4134515833
ccc12 =   120.171528632
dih12 =    -0.0460090528
cc13 =     1.390793658
ccc13 =   121.7811664695
dih13 =    -0.0004379201
sc14 =     1.7886963123
scc14 =   115.561504667
dih14 =   179.9181711394
cs15 =     1.8201554767
csc15 =   103.4742458375
dih15 =   178.6161384872
sc16 =     1.7886918848
scc16 =   115.5230681713
dih16 =  -179.9971544864
cs17 =     1.8202934686
csc17 =   103.5125599964
dih17 =   179.0763666082
hc18 =     1.083209737
hcc18 =   119.9371099808
dih18 =  -179.9092502835
hc19 =     1.0859771186
hcc19 =   119.0980915982
dih19 =  -179.8701937424
hc20 =     1.0842682342
hcc20 =   121.3756565955
dih20 =     0.0703276104
hc21 =     1.0835089869
hcc21 =   119.9551612034
dih21 =     0.0424913058
hc22 =     1.0860235966
hcc22 =   119.090730563
dih22 =  -179.9054455366
hc23 =     1.0842825191
hcc23 =   121.3963861534
dih23 =     0.0202370627
hc24 =     1.0918906156
hcs24 =   105.6078135703
dih24 =  -179.2963166603
hc25 =     1.0925915174
hcs25 =   111.5252088757
dih25 =   -61.1998656311
hc26 =     1.0926041175
hcs26 =   111.6220372383
dih26 =    62.5913249535
hc27 =     1.091938482
hcs27 =   105.5838281648
dih27 =  -179.6250409487
hc28 =     1.0927098475
hcs28 =   111.5809570117
dih28 =   -61.519338358
hc29 =     1.0925783451
hcs29 =   111.5890487873
```

dih29 = 62.3065003661

Molecular weight: 260.03 amu

Stoichiometry: C14H12S2O
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

C1	-C2	:	1.401305	C1	-C6	:	1.396156
C1	-H21	:	1.083509	C2	-C3	:	1.404319
C2	-C9	:	1.451938	C3	-C4	:	1.388447
C3	-O7	:	1.376623	C4	-C5	:	1.390830
C4	-H23	:	1.084283	C5	-C6	:	1.413442
C5	-H22	:	1.086024	C6	-S16	:	1.788692
O7	-C8	:	1.376900	C8	-C9	:	1.404020
C8	-C13	:	1.388253	C9	-C10	:	1.401066
C10	-C11	:	1.396090	C10	-H18	:	1.083210
C11	-C12	:	1.413452	C11	-S14	:	1.788696
C12	-C13	:	1.390794	C12	-H19	:	1.085977
C13	-H20	:	1.084268	S14	-C15	:	1.820155
C15	-H24	:	1.091891	C15	-H25	:	1.092592
C15	-H26	:	1.092604	S16	-C17	:	1.820293
C17	-H27	:	1.091938	C17	-H28	:	1.092710
C17	-H29	:	1.092578				

bond angles:

C6	-C1	-C2	: 118.611490	H21	-C1	-C2	:	119.955161
H21	-C1	-C6	: 121.433348	C3	-C2	-C1	:	119.801406
C9	-C2	-C1	: 134.902998	C9	-C2	-C3	:	105.295595
C4	-C3	-C2	: 122.544797	O7	-C3	-C2	:	111.895006
O7	-C3	-C4	: 125.560193	C5	-C4	-C3	:	117.075485
H23	-C4	-C3	: 121.396386	H23	-C4	-C5	:	121.528076
C6	-C5	-C4	: 121.799244	H22	-C5	-C4	:	119.090731
H22	-C5	-C6	: 119.109982	C5	-C6	-C1	:	120.167554
S16	-C6	-C1	: 124.309374	S16	-C6	-C5	:	115.523068
C8	-O7	-C3	: 105.604514	C9	-C8	-O7	:	111.885833
C13	-C8	-O7	: 125.528433	C13	-C8	-C9	:	122.585719
C8	-C9	-C2	: 105.319038	C10	-C9	-C2	:	134.910702

```
 C10     -C9      -C8      : 119.770222  C11     -C10     -C9      :
118.627190
 H18     -C10     -C9      : 119.937110  H18     -C10     -C11     :
121.435679
 C12     -C11     -C10     : 120.171529  S14     -C11     -C10     :
124.266912
 S14     -C11     -C12     : 115.561505  C13     -C12     -C11     :
121.781166
 H19     -C12     -C11     : 119.120698  H19     -C12     -C13     :
119.098092
 C12     -C13     -C8      : 117.064134  H20     -C13     -C8      :
121.375657
 H20     -C13     -C12     : 121.560154  C15     -S14     -C11     :
103.474246
 H24     -C15     -S14     : 105.607814  H25     -C15     -S14     :
111.525209
 H25     -C15     -H24     : 108.858873  H26     -C15     -S14     :
111.622037
 H26     -C15     -H24     : 108.829485  H26     -C15     -H25     :
110.229001
 C17     -S16     -C6      : 103.512560  H27     -C17     -S16     :
105.583828
 H28     -C17     -S16     : 111.580957  H28     -C17     -H27     :
108.854004
 H29     -C17     -S16     : 111.589049  H29     -C17     -H27     :
108.819346
 H29     -C17     -H28     : 110.242602

  torsional angles:

 C1      -C2      -C3      -C4      :   0.015902
 C1      -C2      -C3      -O7      :-179.964386
 C1      -C2      -C9      -C8      : 179.953780
 C1      -C2      -C9      -C10     :   0.027633
 C1      -C6      -C5      -C4      :   0.024683
 C1      -C6      -C5      -H22     : 179.948887
 C1      -C6      -S16     -C17     :  -0.946490
 C2      -C1      -C6      -C5      :  -0.047992
 C2      -C1      -C6      -S16     : 179.975866
 C2      -C3      -C4      -C5      :  -0.039099
 C2      -C3      -C4      -H23     :-179.957281
 C2      -C3      -O7      -C8      :  -0.006889
 C2      -C9      -C8      -O7      :   0.034806
 C2      -C9      -C8      -C13     :-179.923758
 C2      -C9      -C10     -C11     : 179.956542
 C2      -C9      -C10     -H18     :   0.008692
 C3      -C2      -C1      -C6      :   0.028497
 C3      -C2      -C1      -H21     :-179.968301
 C3      -C2      -C9      -C8      :  -0.036511
 C3      -C2      -C9      -C10     :-179.962658
 C3      -C4      -C5      -C6      :   0.018772
 C3      -C4      -C5      -H22     :-179.905446
 C3      -O7      -C8      -C9      :  -0.018234
 C3      -O7      -C8      -C13     : 179.938865
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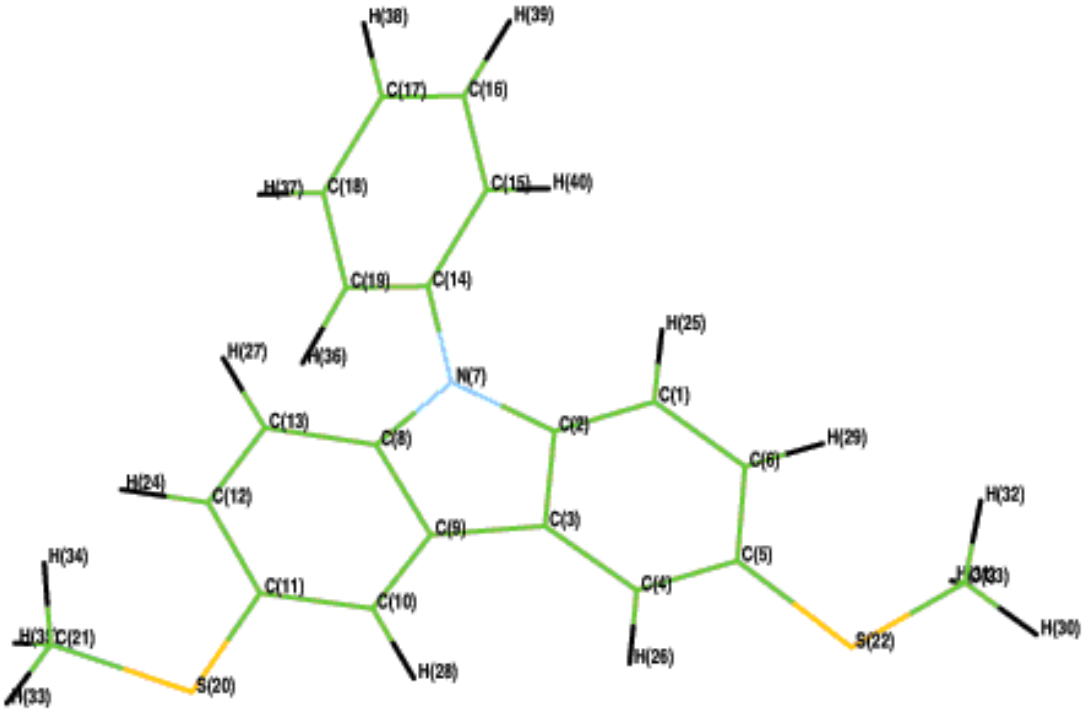
```
C4      -C3      -C2      -C9      :-179.992022
C4      -C3      -O7      -C8      :-179.986464
C4      -C5      -C6      -S16     :-179.997154
C5      -C4      -C3      -O7      : 179.938419
C5      -C6      -C1      -H21     : 179.948757
C5      -C6      -S16     -C17     : 179.076367
C6      -C1      -C2      -C9      :-179.960711
C6      -C5      -C4      -H23     : 179.936839
C6      -S16     -C17     -H27     :-179.625041
C6      -S16     -C17     -H28     : -61.519338
C6      -S16     -C17     -H29     :  62.306500
O7      -C3      -C2      -C9      :   0.027689
O7      -C3      -C4      -H23     :   0.020237
O7      -C8      -C9      -C10     : 179.974551
O7      -C8      -C13     -C12     : 179.986175
O7      -C8      -C13     -H20     :   0.070328
C8      -C9      -C10     -C11     :   0.038600
C8      -C9      -C10     -H18     :-179.909250
C8      -C13     -C12     -C11     :   0.053060
C8      -C13     -C12     -H19     :-179.870194
C9      -C2      -C1      -H21     :   0.042491
C9      -C8      -C13     -C12     :  -0.061071
C9      -C8      -C13     -H20     :-179.976918
C9      -C10     -C11     -C12     :  -0.046009
C9      -C10     -C11     -S14     :-179.957163
C10     -C9      -C8      -C13     :   0.015987
C10     -C11     -C12     -C13     :  -0.000438
C10     -C11     -C12     -H19     : 179.922799
C10     -C11     -S14     -C15     :  -1.469005
C11     -C12     -C13     -H20     : 179.968741
C11     -S14     -C15     -H24     :-179.296317
C11     -S14     -C15     -H25     : -61.199866
C11     -S14     -C15     -H26     :  62.591325
C12     -C11     -C10     -H18     : 179.901026
C12     -C11     -S14     -C15     : 178.616138
C13     -C12     -C11     -S14     : 179.918171
S14     -C11     -C10     -H18     :  -0.010128
S14     -C11     -C12     -H19     :  -0.158592
S16     -C6      -C1      -H21     :  -0.027385
S16     -C6      -C5      -H22     :  -0.072951
H19     -C12     -C13     -H20     :   0.045488
H22     -C5      -C4      -H23     :   0.012621
```

*E. Carbazole (**3**) – Syn Conformer*



Final energy (B3LYP; cc-pVTZ) = -1623.86822 h

Optimized geometry - subject to the constraint that the thiomethyl groups are coplanar with the fluorene ring. Optimization done with the 6-31g** basis set.

atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.3938222089
C3	1.2144805328	0.0000000000	2.1236025983
C4	2.4345262039	0.0204697084	1.4450101912
C5	2.4438863921	0.0347226112	0.0462016020
C6	1.2261241827	0.0201030348	-0.6611352559
N7	-1.0745977592	-0.0397993859	2.2890292879
C8	-0.5580207358	-0.0678673974	3.5889910681
C9	0.8573771402	-0.0411752586	3.5286084265
C10	1.6047056160	-0.0433410995	4.7078577260
C11	0.9447829201	-0.0673239631	5.9408217775

C12	-0.4629655709	-0.0795920398	5.9801196415
C13	-1.2242407004	-0.0771353371	4.8133646952
C14	-2.4488125376	-0.0668881426	1.9379616603
C15	-2.9796563680	0.9211837792	1.0993452715
C16	-4.3277574053	0.8848899221	0.7472133693
C17	-5.1594008299	-0.1201096389	1.2422369457
C18	-4.6322790537	-1.0984367630	2.0860866425
C19	-3.2808691914	-1.0817909278	2.4268820871
S20	1.9795574880	-0.0728175123	7.4031503752
C21	0.7820024437	-0.0962838048	8.7755716466
S22	4.0510714235	0.0661891237	-0.7444467083
C23	3.6530929012	0.0783117757	-2.5220381269
H24	-0.9832779634	-0.0882186804	6.9303756864
H25	-0.9254451905	-0.0203999761	-0.5647907987
H26	3.3690728983	0.0206507302	1.9988307546
H27	-2.3073343740	-0.0776958320	4.8669111904
H28	2.6900854387	-0.0225606823	4.6681682353
H29	1.2232966297	0.0209035549	-1.7445790139
H30	4.6158736590	0.0900876205	-3.0371005360
H31	3.1055939630	-0.8192067034	-2.8199599583
H32	3.0918625949	0.9724814541	-2.8041226251
H33	1.3825528358	-0.1007774861	9.6875641328
H34	0.1494826699	0.7947341942	8.7751442992
H35	0.1635066634	-0.9969438429	8.7567785504
H36	-2.8607865023	-1.8564420063	3.0599799846
H37	-5.2713860050	-1.8881569357	2.4700813859
H38	-6.2109577478	-0.1409122213	0.9722933190
H39	-4.7316508097	1.6540167812	0.0953946026
H40	-2.3354576767	1.7166531173	0.7393667651

Z-matrix: (angstroms and degrees)

C1						
C2	C1	cc2				
C3	C2	cc3	C1	ccc3		
C4	C3	cc4	C2	ccc4	C1	dih4
C5	C4	cc5	C3	ccc5	C2	dih5
C6	C5	cc6	C4	ccc6	C3	dih6
N7	C2	nc7	C3	ncc7	C4	dih7
C8	N7	cn8	C2	cnc8	C3	dih8
C9	C8	cc9	N7	ccn9	C2	dih9
C10	C9	cc10	C8	ccc10	N7	dih10
C11	C10	cc11	C9	ccc11	C8	dih11
C12	C11	cc12	C10	ccc12	C9	dih12
C13	C12	cc13	C11	ccc13	C10	dih13
C14	N7	cn14	C8	cnc14	C9	dih14
C15	C14	cc15	N7	ccn15	C8	dih15
C16	C15	cc16	C14	ccc16	N7	dih16
C17	C16	cc17	C15	ccc17	C14	dih17
C18	C17	cc18	C16	ccc18	C15	dih18
C19	C18	cc19	C17	ccc19	C16	dih19
S20	C11	sc20	C12	scc20	C13	dih20
C21	S20	cs21	C11	csc21	C12	dih21
S22	C5	sc22	C4	scc22	C3	dih22
C23	S22	cs23	C5	csc23	C4	dih23

```
H24    C12  hc24    C13  hcc24    C8   dih24
H25    C1   hc25    C2   hcc25    N7   dih25
H26    C4   hc26    C3   hcc26    C9   dih26
H27    C13  hc27    C8   hcc27    N7   dih27
H28    C10  hc28    C9   hcc28    C8   dih28
H29    C6   hc29    C5   hcc29    C4   dih29
H30    C23  hc30    S22  hcs30    C5   dih30
H31    C23  hc31    S22  hcs31    C5   dih31
H32    C23  hc32    S22  hcs32    C5   dih32
H33    C21  hc33    S20  hcs33    C11  dih33
H34    C21  hc34    S20  hcs34    C11  dih34
H35    C21  hc35    S20  hcs35    C11  dih35
H36    C19  hc36    C14  hcc36    C15  dih36
H37    C18  hc37    C19  hcc37    C14  dih37
H38    C17  hc38    C18  hcc38    C19  dih38
H39    C16  hc39    C15  hcc39    C14  dih39
H40    C15  hc40    C14  hcc40    C19  dih40

 Z-variables: (angstroms and degrees)
 cc2 =     1.3938222089
 cc3 =     1.4168776875
 ccc3 =   121.00162443
 cc4 =     1.3962156364
 ccc4 =   119.9119128376
 dih4 =     0.9691412101
 cc5 =     1.398912516
 ccc5 =   119.47098191
 dih5 =    -0.2874594186
 cc6 =     1.4083621555
 ccc6 =   119.7563124585
 dih6 =    -0.3839230815
 nc7 =     1.399192642
 ncc7 =   109.1938901307
 dih7 =   179.2432002447
 cn8 =     1.3991212472
 cnc8 =   108.1476381849
 dih8 =    -0.1081090288
 cc9 =     1.4169367245
 ccn9 =   109.1984901285
 dih9 =     0.2049204919
 cc10 =     1.3961136959
 ccc10 =   119.9131083434
 dih10 =   179.1302364717
 cc11 =     1.398668472
 ccc11 =   119.4760442594
 dih11 =    -0.2181224719
 cc12 =     1.4083503263
 ccc12 =   119.7599656838
 dih12 =    -0.4400825204
 cc13 =     1.3931485789
 ccc13 =   121.5218897185
 dih13 =     0.4217342298
 cn14 =     1.4186079575
 cnc14 =   125.9594443152
```

```
dih14 =   179.3571350416
cc15 =     1.4004851811
ccn15 =   120.1255943113
dih15 =   126.4299157432
cc16 =     1.3938043361
ccc16 =   119.9685725692
dih16 =   179.4475751986
cc17 =     1.3952430772
ccc17 =   120.3733363565
dih17 =     0.9924251831
cc18 =     1.3953722225
ccc18 =   119.6311176111
dih18 =    -0.4950639785
cc19 =     1.3938175041
ccc19 =   120.3819156621
dih19 =    -0.5002380394
sc20 =     1.7914222041
scc20 =   123.6815431421
dih20 =  -179.8808552533
cs21 =     1.8216006415
csc21 =   103.6095997813
dih21 =     0.0000012074#
sc22 =     1.7914124643
scc22 =   116.5836440275
dih22 =   179.8016715181
cs23 =     1.8216380306
csc23 =   103.5795078025
dih23 =  -179.9999945332#
hc24 =     1.0834140278
hcc24 =   118.1736675606
dih24 =  -179.9148841809
hc25 =     1.084367837
hcc25 =   121.3891495994
dih25 =     0.8582777499
hc26 =     1.0863216712
hcc26 =   120.2622947984
dih26 =    -0.9652521658
hc27 =     1.0844166391
hcc27 =   121.3817584571
dih27 =     0.9808645262
hc28 =     1.0863040279
hcc28 =   120.2614083896
dih28 =  -179.9755385615
hc29 =     1.0834477434
hcc29 =   120.2973578561
dih29 =  -179.384015751
hc30 =     1.0919591308
hcs30 =   105.5289621407
dih30 =  -179.5920481793
hc31 =     1.0927268301
hcs31 =   111.718445628
dih31 =   -61.5289764125
hc32 =     1.0927444965
hcs32 =   111.6881038701
```

```
 dih32 =    62.3442990289
 hc33 =     1.091975852
 hcs33 =   105.5291639971
 dih33 =   179.9624607784
 hc34 =     1.0927005635
 hcs34 =   111.7004408245
 dih34 =   -61.9829314115
 hc35 =     1.0927390883
 hcs35 =   111.7009998331
 dih35 =    61.8916006628
 hc36 =     1.0850653008
 hcc36 =   119.408895558
 dih36 =   178.7687043385
 hc37 =     1.086079007
 hcc37 =   119.5238574685
 dih37 =  -179.9328156791
 hc38 =     1.0858518595
 hcc38 =   120.1815895318
 dih38 =   179.4949160786
 hc39 =     1.0860726091
 hcc39 =   119.5297225264
 dih39 =  -179.9205423477
 hc40 =     1.085056656
 hcc40 =   119.3963524503
 dih40 =   178.7712846859


 bond lengths (angstroms):

C1      -C2      :   1.393822      C1      -C6      :   1.393156
C1      -H25     :   1.084368      C2      -C3      :   1.416878
C2      -N7      :   1.399193      C3      -C4      :   1.396216
C3      -C9      :   1.450262      C4      -C5      :   1.398913
C4      -H26     :   1.086322      C5      -C6      :   1.408362
C5      -S22     :   1.791412      C6      -H29     :   1.083448
N7      -C8      :   1.399121      N7      -C14     :   1.418608
C8      -C9      :   1.416937      C8      -C13     :   1.393925
C9      -C10     :   1.396114      C10     -C11     :   1.398668
C10     -H28     :   1.086304      C11     -C12     :   1.408350
C11     -S20     :   1.791422      C12     -C13     :   1.393149
C12     -H24     :   1.083414      C13     -H27     :   1.084417
C14     -C15     :   1.400485      C14     -C19     :   1.400496
C15     -C16     :   1.393804      C15     -H40     :   1.085057
C16     -C17     :   1.395243      C16     -H39     :   1.086073
C17     -C18     :   1.395372      C17     -H38     :   1.085852
C18     -C19     :   1.393818      C18     -H37     :   1.086079
C19     -H36     :   1.085065      S20     -C21     :   1.821601
C21     -H33     :   1.091976      C21     -H34     :   1.092701
C21     -H35     :   1.092739      S22     -C23     :   1.821638
C23     -H30     :   1.091959      C23     -H31     :   1.092727
C23     -H32     :   1.092744

 bond angles:
```

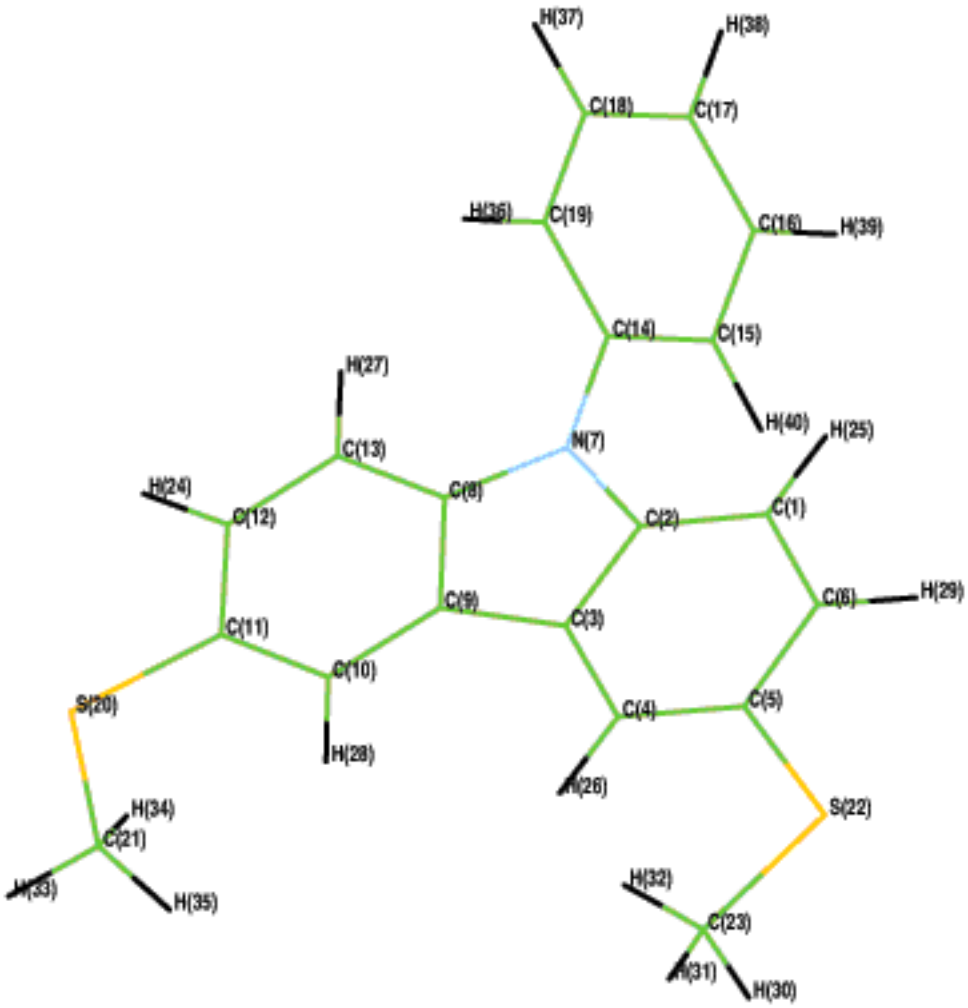
```
 C6      -C1      -C2      : 118.330659  H25     -C1      -C2      :
121.389150
 H25     -C1      -C6      : 120.279397  C3      -C2      -C1      :
121.001624
 N7      -C2      -C1      : 129.777101  N7      -C2      -C3      :
109.193890
 C4      -C3      -C2      : 119.911913  C9      -C3      -C2      :
106.734052
 C9      -C3      -C4      : 133.348730  C5      -C4      -C3      :
119.470982
 H26     -C4      -C3      : 120.262295  H26     -C4      -C5      :
120.266114
 C6      -C5      -C4      : 119.756312  S22     -C5      -C4      :
116.583644
 S22     -C5      -C6      : 123.659763  C5      -C6      -C1      :
121.520491
 H29     -C6      -C1      : 118.181834  H29     -C6      -C5      :
120.297358
 C8      -N7      -C2      : 108.147638  C14     -N7      -C2      :
125.886963
 C14     -N7      -C8      : 125.959444  C9      -C8      -N7      :
109.198490
 C13     -C8      -N7      : 129.775482  C13     -C8      -C9      :
120.996325
 C8      -C9      -C3      : 106.725468  C10     -C9      -C3      :
133.357202
 C10     -C9      -C8      : 119.913108  C11     -C10     -C9      :
119.476044
 H28     -C10     -C9      : 120.261408  H28     -C10     -C11     :
120.262100
 C12     -C11     -C10     : 119.759966  S20     -C11     -C10     :
116.557846
 S20     -C11     -C12     : 123.681543  C13     -C12     -C11     :
121.521890
 H24     -C12     -C11     : 120.304185  H24     -C12     -C13     :
118.173668
 C12     -C13     -C8      : 118.324709  H27     -C13     -C8      :
121.381758
 H27     -C13     -C12     : 120.292901  C15     -C14     -N7      :
120.125594
 C19     -C14     -N7      : 120.196516  C19     -C14     -C15     :
119.677866
 C16     -C15     -C14     : 119.968573  H40     -C15     -C14     :
119.396352
 H40     -C15     -C16     : 120.630968  C17     -C16     -C15     :
120.373336
 H39     -C16     -C15     : 119.529723  H39     -C16     -C17     :
120.090630
 C18     -C17     -C16     : 119.631118  H38     -C17     -C16     :
120.187293
 H38     -C17     -C18     : 120.181590  C19     -C18     -C17     :
120.381916
 H37     -C18     -C17     : 120.087747  H37     -C18     -C19     :
119.523857
```

```
 C18     -C19     -C14     : 119.956074  H36     -C19     -C14     :
119.408896
 H36     -C19     -C18     : 120.630835  C21     -S20     -C11     :
103.609600
 H33     -C21     -S20     : 105.529164  H34     -C21     -S20     :
111.700441
 H34     -C21     -H33     : 108.786072  H35     -C21     -S20     :
111.701000
 H35     -C21     -H33     : 108.799388  H35     -C21     -H34     :
110.148202
 C23     -S22     -C5      : 103.579508  H30     -C23     -S22     :
105.528962
 H31     -C23     -S22     : 111.718446  H31     -C23     -H30     :
108.785317
 H32     -C23     -S22     : 111.688104  H32     -C23     -H30     :
108.799146
 H32     -C23     -H31     : 110.144333

  torsional angles:

 C1      -C2      -C3      -C4      :   0.969141
 C1      -C2      -C3      -C9      :-178.301097
 C1      -C2      -N7      -C8      : 177.966876
 C1      -C2      -N7      -C14     :  -1.186115
 C1      -C6      -C5      -C4      :   0.407402
 C1      -C6      -C5      -S22     :-179.792004
 C2      -C1      -C6      -C5      :   0.255117
 C2      -C1      -C6      -H29     :-179.949198
 C2      -C3      -C4      -C5      :  -0.287459
 C2      -C3      -C4      -H26     : 179.995807
 C2      -C3      -C9      -C8      :   0.149159
 C2      -C3      -C9      -C10     :-179.074819
 C2      -N7      -C8      -C9      :   0.204920
 C2      -N7      -C8      -C13     : 178.200033
 C2      -N7      -C14     -C15     : -54.564468
 C2      -N7      -C14     -C19     : 125.379053
 C3      -C2      -C1      -C6      :  -0.939314
 C3      -C2      -C1      -H25     : 178.737210
 C3      -C2      -N7      -C8      :  -0.108109
 C3      -C2      -N7      -C14     :-179.261100
 C3      -C4      -C5      -C6      :  -0.383923
 C3      -C4      -C5      -S22     : 179.801672
 C3      -C9      -C8      -N7      :  -0.218815
 C3      -C9      -C8      -C13     :-178.421324
 C3      -C9      -C10     -C11     : 178.924457
 C3      -C9      -C10     -H28     :  -0.832959
 C4      -C3      -C2      -N7      : 179.243200
 C4      -C3      -C9      -C8      :-178.980971
 C4      -C3      -C9      -C10     :   1.795051
 C4      -C5      -C6      -H29     :-179.384016
 C4      -C5      -S22     -C23     :-179.999995
 C5      -C4      -C3      -C9      : 178.751482
 C5      -C6      -C1      -H25     :-179.425126
 C5      -S22     -C23     -H30     :-179.592048
```

```
C5      -S22     -C23     -H31     : -61.528976
C5      -S22     -C23     -H32     :  62.344299
C6      -C1      -C2      -N7      :-178.818246
C6      -C5      -C4      -H26     : 179.332800
C6      -C5      -S22     -C23     :   0.193583
N7      -C2      -C1      -H25     :   0.858278
N7      -C2      -C3      -C9      :  -0.027038
N7      -C8      -C9      -C10     : 179.130236
N7      -C8      -C13     -C12     :-178.730898
N7      -C8      -C13     -H27     :   0.980865
N7      -C14     -C15     -C16     : 179.447575
N7      -C14     -C15     -H40     :  -1.284901
N7      -C14     -C19     -C18     : 179.565250
N7      -C14     -C19     -H36     :  -1.175070
C8      -N7      -C14     -C15     : 126.429916
C8      -N7      -C14     -C19     : -53.626563
C8      -C9      -C10     -C11     :  -0.218122
C8      -C9      -C10     -H28     :-179.975539
C8      -C13     -C12     -C11     :   0.269173
C8      -C13     -C12     -H24     :-179.914884
C9      -C3      -C4      -H26     :  -0.965252
C9      -C8      -N7      -C14     : 179.357135
C9      -C8      -C13     -C12     :  -0.939797
C9      -C8      -C13     -H27     : 178.771966
C9      -C10     -C11     -C12     :  -0.440083
C9      -C10     -C11     -S20     : 179.841415
C10     -C9      -C8      -C13     :   0.927727
C10     -C11     -C12     -C13     :   0.421734
C10     -C11     -C12     -H24     :-179.390337
C10     -C11     -S20     -C21     : 179.706332
C11     -C12     -C13     -H27     :-179.445842
C11     -S20     -C21     -H33     : 179.962461
C11     -S20     -C21     -H34     : -61.982931
C11     -S20     -C21     -H35     :  61.891601
C12     -C11     -C10     -H28     : 179.317332
C12     -C11     -S20     -C21     :   0.000001
C13     -C8      -N7      -C14     :  -2.647753
C13     -C12     -C11     -S20     :-179.880855
C14     -C15     -C16     -C17     :   0.992425
C14     -C15     -C16     -H39     :-179.920542
C14     -C19     -C18     -C17     :   0.992353
C14     -C19     -C18     -H37     :-179.932816
C15     -C14     -C19     -C18     :  -0.490975
C15     -C14     -C19     -H36     : 178.768704
C15     -C16     -C17     -C18     :  -0.495064
C15     -C16     -C17     -H38     : 179.509782
C16     -C15     -C14     -C19     :  -0.496239
C16     -C17     -C18     -C19     :  -0.500238
C16     -C17     -C18     -H37     :-179.569838
C17     -C16     -C15     -H40     :-178.265923
C17     -C18     -C19     -H36     :-178.258146
C18     -C17     -C16     -H39     :-179.576961
C19     -C14     -C15     -H40     : 178.771285
C19     -C18     -C17     -H38     : 179.494916
```

```
S20     -C11    -C10    -H28    :  -0.401171
S20     -C11    -C12    -H24    :   0.307074
S22     -C5     -C4     -H26    :  -0.481606
S22     -C5     -C6     -H29    :   0.416579
H24     -C12    -C13    -H27    :   0.370101
H25     -C1     -C6     -H29    :   0.370559
H36     -C19    -C18    -H37    :   0.816685
H37     -C18    -C17    -H38    :   0.425316
H38     -C17    -C16    -H39    :   0.427885
H39     -C16    -C15    -H40    :   0.821109
```

*Carbazole (**3**) – Anti Conformer*




```
Final energy (B3LYP; cc-pVTZ) =  -1623.86960 h
```

Optimized geometry - subject to the constraint that the thiomethyl groups are coplanar with the fluorene ring. Optimization done with the 6-31g** basis set.

		angstroms	
atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.3985215876
C3	1.2125446593	0.0000000000	2.1250546760
C4	2.4403122838	0.0207808481	1.4486418987
C5	2.4469672099	0.0356309544	0.0557354771
C6	1.2238243982	0.0205494163	-0.6533072746
N7	-1.0725059901	-0.0403215463	2.2954678360
C8	-0.5515438891	-0.0694217323	3.5932416064
C9	0.8601721956	-0.0418353782	3.5270553284
C10	1.6218056938	-0.0435479467	4.7040966597
C11	0.9686557404	-0.0673747027	5.9341471791
C12	-0.4444433982	-0.0810527538	5.9800544054
C13	-1.2134744899	-0.0789312463	4.8253926175
C14	-2.4485426086	-0.0696931443	1.9477875254
C15	-2.9841333329	0.9188012317	1.1129539476
C16	-4.3332029203	0.8793830932	0.7643796304
C17	-5.1606618526	-0.1289823632	1.2595184503
C18	-4.6285974992	-1.1077609334	2.0998323523
C19	-3.2762530815	-1.0880259841	2.4368648444
S20	1.7968617865	-0.0777909808	7.5202241811
C21	3.5599628200	-0.0562368269	7.0701847308
S22	3.9271268946	0.0662348791	-0.9500427162
C23	5.2685636840	0.0712826354	0.2794514968
H24	-0.9424463540	-0.0899927766	6.9453184992
H25	-0.9251883887	-0.0201877220	-0.5652311733
H26	3.3631589912	0.0202666609	2.0165944926
H27	-2.2961954797	-0.0802176516	4.8852709013
H28	2.7033787064	-0.0207804125	4.6407119531
H29	1.2416863044	0.0216418650	-1.7393598340
H30	6.1974657397	0.0838723623	-0.2942700822
H31	5.2299348363	0.9630005749	0.9100642353
H32	5.2471954493	-0.8286758757	0.8990066515
H33	4.1078628320	-0.0632908904	8.0145303490
H34	3.8361544734	-0.9420005380	6.4929790031
H35	3.8209503300	0.8497041436	6.5171647326
H36	-2.8525797505	-1.8628631291	3.0673115726
H37	-5.2646180209	-1.8998700434	2.4840304631
H38	-6.2129606101	-0.1520760641	0.9923923400
H39	-4.7411524657	1.6485438283	0.1151391961
H40	-2.3435376048	1.7170422521	0.7526845463

principal moments of inertia:

amu*angstrom^2:	2497.50900	2774.69846	5148.55948
g*cm^2:	4.14721074E-37	4.60749462E-37	8.54938309E-37

rotational constants:

```
             cm^(-1):     0.00674978     0.00607548     0.00327424
                 GHz:     0.20235323     0.18213835     0.09815930

 Z-matrix: (angstroms and degrees)
C1
C2     C1   cc2
C3     C2   cc3     C1   ccc3
C4     C3   cc4     C2   ccc4     C1   dih4
C5     C4   cc5     C3   ccc5     C2   dih5
C6     C5   cc6     C4   ccc6     C3   dih6
N7     C2   nc7     C3   ncc7     C4   dih7
C8     N7   cn8     C2   cnc8     C3   dih8
C9     C8   cc9     N7   ccn9     C2   dih9
C10    C9   cc10    C8   ccc10    N7   dih10
C11    C10  cc11    C9   ccc11    C8   dih11
C12    C11  cc12    C10  ccc12    C9   dih12
C13    C12  cc13    C11  ccc13    C10  dih13
C14    N7   cn14    C8   cnc14    C9   dih14
C15    C14  cc15    N7   ccn15    C8   dih15
C16    C15  cc16    C14  ccc16    N7   dih16
C17    C16  cc17    C15  ccc17    C14  dih17
C18    C17  cc18    C16  ccc18    C15  dih18
C19    C18  cc19    C17  ccc19    C16  dih19
S20    C11  sc20    C12  scc20    C13  dih20
C21    S20  cs21    C11  csc21    C12  dih21
S22    C5   sc22    C4   scc22    C3   dih22
C23    S22  cs23    C5   csc23    C4   dih23
H24    C12  hc24    C13  hcc24    C8   dih24
H25    C1   hc25    C2   hcc25    N7   dih25
H26    C4   hc26    C3   hcc26    C9   dih26
H27    C13  hc27    C8   hcc27    N7   dih27
H28    C10  hc28    C9   hcc28    C8   dih28
H29    C6   hc29    C5   hcc29    C4   dih29
H30    C23  hc30    S22  hcs30    C5   dih30
H31    C23  hc31    S22  hcs31    C5   dih31
H32    C23  hc32    S22  hcs32    C5   dih32
H33    C21  hc33    S20  hcs33    C11  dih33
H34    C21  hc34    S20  hcs34    C11  dih34
H35    C21  hc35    S20  hcs35    C11  dih35
H36    C19  hc36    C14  hcc36    C15  dih36
H37    C18  hc37    C19  hcc37    C14  dih37
H38    C17  hc38    C18  hcc38    C19  dih38
H39    C16  hc39    C15  hcc39    C14  dih39
H40    C15  hc40    C14  hcc40    C19  dih40

 Z-variables: (angstroms and degrees)
 cc2 =     1.3985215876
 cc3 =     1.4135469144
 ccc3 =   120.9292181954
 cc4 =     1.4019199081
 ccc4 =   120.2154721453
 dih4 =     0.9828798353
 cc5 =     1.3930014763
 ccc5 =   119.1304279984
```

```
dih5 =    -0.2687079695
cc6 =      1.4138767324
ccc6 =   119.8154225613
dih6 =    -0.4226117299
nc7 =      1.3987163753
ncc7 =   109.1564684703
dih7 =   179.2340896428
cn8 =      1.3987369626
cnc8 =   108.0585051946
dih8 =    -0.1415364185
cc9 =      1.4135359684
ccn9 =   109.1548789618
dih9 =     0.2492827962
cc10 =     1.401968193
ccc10 =  120.2136518817
dih10 =  179.0814754001
cc11 =     1.3929094932
ccc11 =  119.1227450313
dih11 =   -0.2518371285
cc12 =     1.4139107957
ccc12 =  119.833346493
dih12 =   -0.389071413
cc13 =     1.387320138
ccc13 =  121.8011107078
dih13 =    0.3652165928
cn14 =     1.4195848212
cnc14 =  126.0034618415
dih14 =  179.2656268655
cc15 =     1.4003305531
ccn15 =  120.1422127498
dih15 =  126.3943737344
cc16 =     1.3939320628
ccc16 =  119.9526706848
dih16 =  179.4251770964
cc17 =     1.3952245802
ccc17 =  120.3759568865
dih17 =    1.0040106526
cc18 =     1.3954309082
ccc18 =  119.6373115854
dih18 =   -0.5010002107
cc19 =     1.393849272
ccc19 =  120.3721768662
dih19 =   -0.5013148177
sc20 =     1.7893222208
scc20 =  115.7062846597
dih20 = -179.8097510312
cs21 =     1.8197596937
csc21 =  103.2478569387
dih21 =  179.9999954023#
sc22 =     1.7898041978
scc22 =  124.4747890524
dih22 =  179.8628513569
cs23 =     1.8196522083
csc23 =  103.2975743149
```

```
dih23 =    -0.0000019091#
hc24 =      1.0861959486
hcc24 =   119.0448921888
dih24 =  -179.9040221719
hc25 =      1.0843741872
hcc25 =   121.4162062842
dih25 =     0.9030548856
hc26 =      1.0836126885
hcc26 =   119.5347074525
dih26 =    -0.9617645477
hc27 =      1.0843762287
hcc27 =   121.4105225773
dih27 =     1.0697772879
hc28 =      1.0836679211
hcc28 =   119.5430573788
dih28 =  -179.9113533278
hc29 =      1.0861999829
hcc29 =   119.1556326678
dih29 =  -179.3526167542
hc30 =      1.0918671991
hcs30 =   105.7930509564
dih30 =   179.6724461647
hc31 =      1.0928520017
hcs31 =   111.4749043017
dih31 =   -62.1016112817
hc32 =      1.0928085436
hcs32 =   111.4917424307
dih32 =    61.4256878332
hc33 =      1.0918025598
hcs33 =   105.7966096347
dih33 =  -179.9257154438
hc34 =      1.0927147997
hcs34 =   111.4643127623
dih34 =   -61.6346393814
hc35 =      1.0930117295
hcs35 =   111.4869094942
dih35 =    61.8914318125
hc36 =      1.085050584
hcc36 =   119.4318169973
dih36 =   178.7877325213
hc37 =      1.0860787883
hcc37 =   119.5355850096
dih37 =  -179.914926954
hc38 =      1.0859200491
hcc38 =   120.178889929
dih38 =   179.494271813
hc39 =      1.0860682343
hcc39 =   119.5373736868
dih39 =  -179.8981269628
hc40 =      1.0850556
hcc40 =   119.435824438
dih40 =   178.771293711

Molecular weight:     335.08 amu
```

Stoichiometry: C20NH17S2
Molecular Point Group: C1
Point Group used: C1

bond lengths (angstroms):

C1	-C2	:	1.398522	C1	-C6	:	1.387436
C1	-H25	:	1.084374	C2	-C3	:	1.413547
C2	-N7	:	1.398716	C3	-C4	:	1.401920
C3	-C9	:	1.446210	C4	-C5	:	1.393001
C4	-H26	:	1.083613	C5	-C6	:	1.413877
C5	-S22	:	1.789804	C6	-H29	:	1.086200
N7	-C8	:	1.398737	N7	-C14	:	1.419585
C8	-C9	:	1.413536	C8	-C13	:	1.398728
C9	-C10	:	1.401968	C10	-C11	:	1.392909
C10	-H28	:	1.083668	C11	-C12	:	1.413911
C11	-S20	:	1.789322	C12	-C13	:	1.387320
C12	-H24	:	1.086196	C13	-H27	:	1.084376
C14	-C15	:	1.400331	C14	-C19	:	1.400465
C15	-C16	:	1.393932	C15	-H40	:	1.085056
C16	-C17	:	1.395225	C16	-H39	:	1.086068
C17	-C18	:	1.395431	C17	-H38	:	1.085920
C18	-C19	:	1.393849	C18	-H37	:	1.086079
C19	-H36	:	1.085051	S20	-C21	:	1.819760
C21	-H33	:	1.091803	C21	-H34	:	1.092715
C21	-H35	:	1.093012	S22	-C23	:	1.819652
C23	-H30	:	1.091867	C23	-H31	:	1.092852
C23	-H32	:	1.092809				

bond angles:

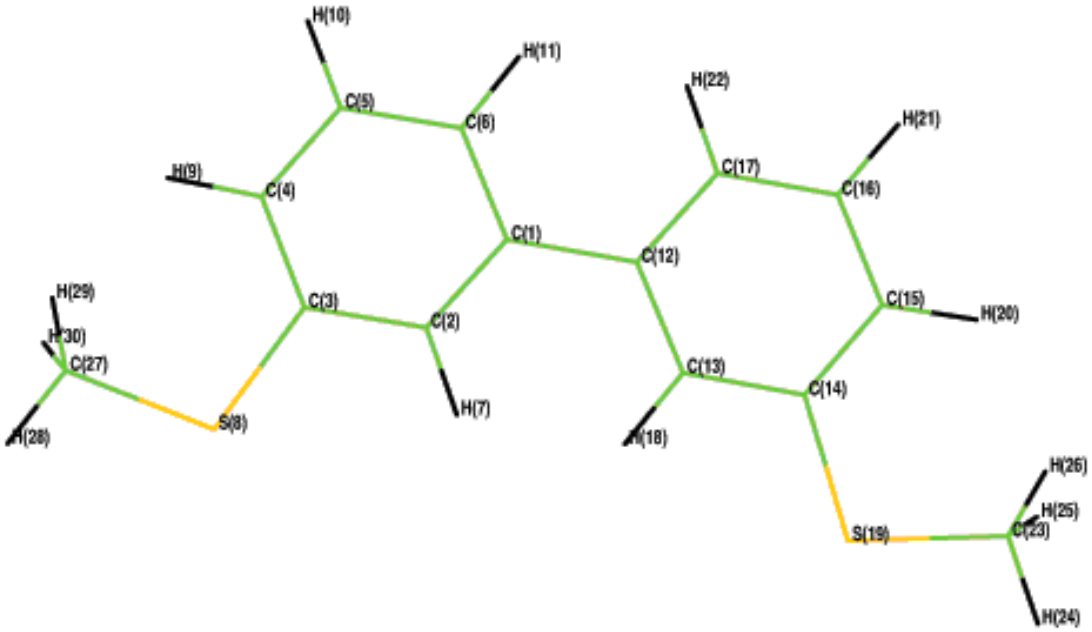
C6	-C1	-C2	: 118.091031	H25	-C1	-C2	: 121.416206
H25	-C1	-C6	: 120.492130	C3	-C2	-C1	: 120.929218
N7	-C2	-C1	: 129.886126	N7	-C2	-C3	: 109.156468
C4	-C3	-C2	: 120.215472	C9	-C3	-C2	: 106.813734
C9	-C3	-C4	: 132.965262	C5	-C4	-C3	: 119.130428
H26	-C4	-C3	: 119.534707	H26	-C4	-C5	: 121.334227
C6	-C5	-C4	: 119.815423	S22	-C5	-C4	: 124.474789
S22	-C5	-C6	: 115.709224	C5	-C6	-C1	: 121.809938
H29	-C6	-C1	: 119.034095	H29	-C6	-C5	: 119.155633
C8	-N7	-C2	: 108.058505	C14	-N7	-C2	: 125.930012

```
 C14     -N7     -C8     : 126.003462  C9      -C8      -N7      :
109.154879
 C13     -C8     -N7     : 129.881828  C13     -C8      -C9      :
120.931176
 C8      -C9     -C3     : 106.815761  C10     -C9      -C3      :
132.966269
 C10     -C9     -C8     : 120.213652  C11     -C10     -C9      :
119.122745
 H28     -C10    -C9     : 119.543057  H28     -C10     -C11     :
121.333297
 C12     -C11    -C10    : 119.833346  S20     -C11     -C10     :
124.460116
 S20     -C11    -C12    : 115.706285  C13     -C12     -C11     :
121.801111
 H24     -C12    -C11    : 119.153651  H24     -C12     -C13     :
119.044892
 C12     -C13    -C8     : 118.090032  H27     -C13     -C8      :
121.410523
 H27     -C13    -C12    : 120.498903  C15     -C14     -N7      :
120.142213
 C19     -C14    -N7     : 120.159457  C19     -C14     -C15     :
119.698295
 C16     -C15    -C14    : 119.952671  H40     -C15     -C14     :
119.435824
 H40     -C15    -C16    : 120.607515  C17     -C16     -C15     :
120.375957
 H39     -C16    -C15    : 119.537374  H39     -C16     -C17     :
120.080509
 C18     -C17    -C16    : 119.637312  H38     -C17     -C16     :
120.183798
 H38     -C17    -C18    : 120.178890  C19     -C18     -C17     :
120.372177
 H37     -C18    -C17    : 120.085976  H37     -C18     -C19     :
119.535585
 C18     -C19    -C14    : 119.952314  H36     -C19     -C14     :
119.431817
 H36     -C19    -C18    : 120.611850  C21     -S20     -C11     :
103.247857
 H33     -C21    -S20    : 105.796610  H34     -C21     -S20     :
111.464313
 H34     -C21    -H33    : 108.954083  H35     -C21     -S20     :
111.486909
 H35     -C21    -H33    : 108.853810  H35     -C21     -H34     :
110.136313
 C23     -S22    -C5     : 103.297574  H30     -C23     -S22     :
105.793051
 H31     -C23    -S22    : 111.474904  H31     -C23     -H30     :
108.896846
 H32     -C23    -S22    : 111.491742  H32     -C23     -H30     :
108.906727
 H32     -C23    -H31    : 110.128567

  torsional angles:
```

```
C1      -C2     -C3     -C4     :   0.982880
C1      -C2     -C3     -C9     :-178.268288
C1      -C2     -N7     -C8     : 177.903380
C1      -C2     -N7     -C14    :  -1.113879
C1      -C6     -C5     -C4     :   0.434778
C1      -C6     -C5     -S22    :-179.826406
C2      -C1     -C6     -C5     :   0.260161
C2      -C1     -C6     -H29    :-179.952193
C2      -C3     -C4     -C5     :  -0.268708
C2      -C3     -C4     -H26    :-179.982171
C2      -C3     -C9     -C8     :   0.166457
C2      -C3     -C9     -C10    :-179.052188
C2      -N7     -C8     -C9     :   0.249283
C2      -N7     -C8     -C13    : 178.162442
C2      -N7     -C14    -C15    : -54.760596
C2      -N7     -C14    -C19    : 125.170834
C3      -C2     -C1     -C6     :  -0.961971
C3      -C2     -C1     -H25    : 178.749998
C3      -C2     -N7     -C8     :  -0.141536
C3      -C2     -N7     -C14    :-179.158795
C3      -C4     -C5     -C6     :  -0.422612
C3      -C4     -C5     -S22    : 179.862851
C3      -C9     -C8     -N7     :  -0.256889
C3      -C9     -C8     -C13    :-178.390099
C3      -C9     -C10    -C11    : 178.882636
C3      -C9     -C10    -H28    :  -0.776881
C4      -C3     -C2     -N7     : 179.234090
C4      -C3     -C9     -C8     :-178.949242
C4      -C3     -C9     -C10    :   1.832114
C4      -C5     -C6     -H29    :-179.352617
C4      -C5     -S22    -C23    :  -0.000002
C5      -C4     -C3     -C9     : 178.751698
C5      -C6     -C1     -H25    :-179.454581
C5      -S22    -C23    -H30    : 179.672446
C5      -S22    -C23    -H31    : -62.101611
C5      -S22    -C23    -H32    :  61.425688
C6      -C1     -C2     -N7     :-178.808914
C6      -C5     -C4     -H26    : 179.285514
C6      -C5     -S22    -C23    :-179.725113
N7      -C2     -C1     -H25    :   0.903055
N7      -C2     -C3     -C9     :  -0.017078
N7      -C8     -C9     -C10    : 179.081475
N7      -C8     -C13    -C12    :-178.663396
N7      -C8     -C13    -H27    :   1.069777
N7      -C14    -C15    -C16    : 179.425177
N7      -C14    -C15    -H40    :  -1.296959
N7      -C14    -C19    -C18    : 179.580718
N7      -C14    -C19    -H36    :  -1.144003
C8      -N7     -C14    -C15    : 126.394374
C8      -N7     -C14    -C19    : -53.674196
C8      -C9     -C10    -C11    :  -0.251837
C8      -C9     -C10    -H28    :-179.911353
C8      -C13    -C12    -C11    :   0.311738
C8      -C13    -C12    -H24    :-179.904022
```

```
C9      -C3     -C4     -H26    :  -0.961765
C9      -C8     -N7     -C14    : 179.265627
C9      -C8     -C13    -C12    :  -0.961635
C9      -C8     -C13    -H27    : 178.771538
C9      -C10    -C11    -C12    :  -0.389071
C9      -C10    -C11    -S20    : 179.802132
C10     -C9     -C8     -C13    :   0.948266
C10     -C11    -C12    -C13    :   0.365217
C10     -C11    -C12    -H24    :-179.418796
C10     -C11    -S20    -C21    :  -0.184088
C11     -C12    -C13    -H27    :-179.423970
C11     -S20    -C21    -H33    :-179.925715
C11     -S20    -C21    -H34    : -61.634639
C11     -S20    -C21    -H35    :  61.891432
C12     -C11    -C10    -H28    : 179.264135
C12     -C11    -S20    -C21    : 179.999995
C13     -C8     -N7     -C14    :  -2.821214
C13     -C12    -C11    -S20    :-179.809751
C14     -C15    -C16    -C17    :   1.004011
C14     -C15    -C16    -H39    :-179.898127
C14     -C19    -C18    -C17    :   0.994582
C14     -C19    -C18    -H37    :-179.914927
C15     -C14    -C19    -C18    :  -0.487546
C15     -C14    -C19    -H36    : 178.787733
C15     -C16    -C17    -C18    :  -0.501000
C15     -C16    -C17    -H38    : 179.503413
C16     -C15    -C14    -C19    :  -0.506571
C16     -C17    -C18    -C19    :  -0.501315
C16     -C17    -C18    -H37    :-179.586786
C17     -C16    -C15    -H40    :-178.265269
C17     -C18    -C19    -H36    :-178.272020
C18     -C17    -C16    -H39    :-179.593949
C19     -C14    -C15    -H40    : 178.771294
C19     -C18    -C17    -H38    : 179.494272
S20     -C11    -C10    -H28    :  -0.544662
S20     -C11    -C12    -H24    :   0.406237
S22     -C5     -C4     -H26    :  -0.429023
S22     -C5     -C6     -H29    :   0.386199
H24     -C12    -C13    -H27    :   0.360270
H25     -C1     -C6     -H29    :   0.333065
H36     -C19    -C18    -H37    :   0.818472
H37     -C18    -C17    -H38    :   0.408801
H38     -C17    -C16    -H39    :   0.410464
H39     -C16    -C15    -H40    :   0.832594
```

*F. Biphenyl (**5**) – Syn Conformer*



Final energy (B3LYP; cc-pVTZ) = -1338.562974 h

Optimized geometry - subject to the constraint that the heavy atoms (C and S) are all coplanar. Optimization done with the 6-31g** basis set.

		angstroms	
atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4023936291
C3	1.1876943685	0.0000000000	2.1460688685
C4	2.4176666971	0.0000000079	1.4816898305
C5	2.4320217148	0.0000000222	0.0870685240
C6	1.2517777827	0.0000000422	-0.6458688675
H7	-0.9365163778	0.0000000000	1.9484593374
S8	1.0038638894	0.0000000136	3.9232116999
H9	3.3535830020	0.0000000104	2.0275972858
H10	3.3849943055	0.0000000424	-0.4347977908
H11	1.3179417324	0.0000000610	-1.7264795293
C12	-1.2753362055	0.0000000280	-0.7822679205
C13	-2.5254152760	-0.0000000282	-0.1466499469
C14	-3.7266277636	0.0000000107	-0.8682865134
C15	-3.6918773126	0.0000001223	-2.2657928073
C16	-2.4552326478	0.0000001690	-2.9106839828
C17	-1.2669685862	0.0000000963	-2.1908218578
H18	-2.5877078228	-0.0000001208	0.9356486821
S19	-5.2274354246	-0.0000001112	0.1010465836
H20	-4.6026862916	0.0000001641	-2.8526328906

```
 H21          -2.4219697681      0.0000002428     -3.9966834258
 H22          -0.3337115114      0.0000001327     -2.7395734436
 C23          -6.5458295792     -0.0000000092     -1.1560069302
 H24          -7.4836896943     -0.0000000924     -0.5968145971
 H25          -6.5071975459      0.8960806565     -1.7798391136
 H26          -6.5071975015     -0.8960805394     -1.7798393055
 C27           2.7219345217     -0.0000000117      4.5286701922
 H28           2.6485500711      0.0000000088      5.6181160987
 H29           3.2605025851     -0.8960806265      4.2114895503
 H30           3.2605026225      0.8960805694      4.2114895190

 principal moments of inertia:
       amu*angstrom^2:      606.63113     2664.69070     3264.84788
                g*cm^2: 1.00733456E-37 4.42482247E-37 5.42140678E-37

 rotational constants:
              cm^(-1):     0.02778893     0.00632630     0.00516337
                  GHz:     0.83309112     0.18965766     0.15479404

 Z-matrix: (angstroms and degrees)
C1
C2     C1   cc2
C3     C2   cc3     C1   ccc3
C4     C3   cc4     C2   ccc4     C1   dih4
C5     C4   cc5     C3   ccc5     C2   dih5
C6     C5   cc6     C4   ccc6     C3   dih6
H7     C2   hc7     C1   hcc7     C3   dih7
S8     C3   sc8     C2   scc8     C4   dih8
H9     C4   hc9     C3   hcc9     C5   dih9
H10    C5   hc10    C4   hcc10    C3   dih10
H11    C6   hc11    C5   hcc11    C4   dih11
C12    C1   cc12    C6   ccc12    C5   dih12
C13    C12  cc13    C1   ccc13    C6   dih13
C14    C13  cc14    C12  ccc14    C1   dih14
C15    C14  cc15    C13  ccc15    C12  dih15
C16    C15  cc16    C14  ccc16    C13  dih16
C17    C16  cc17    C15  ccc17    C14  dih17
H18    C13  hc18    C12  hcc18    C14  dih18
S19    C14  sc19    C13  scc19    C15  dih19
H20    C15  hc20    C14  hcc20    C16  dih20
H21    C16  hc21    C15  hcc21    C14  dih21
H22    C17  hc22    C16  hcc22    C15  dih22
C23    S19  cs23    C14  csc23    C13  dih23
H24    C23  hc24    S19  hcs24    C14  dih24
H25    C23  hc25    S19  hcs25    H24  dih25
H26    C23  hc26    S19  hcs26    H24  dih26
C27    S8   cs27    C3   csc27    C2   dih27
H28    C27  hc28    S8   hcs28    C3   dih28
H29    C27  hc29    S8   hcs29    H28  dih29
H30    C27  hc30    S8   hcs30    H28  dih30

 Z-variables: (angstroms and degrees)
 cc2 =     1.4023936291
 cc3 =     1.4013103777
```

```
ccc3 =   122.052754628
cc4 =     1.3979382802
ccc4 =   119.5712034168
dih4 =     0.0
cc5 =     1.3946951836
ccc5 =   118.9657740055
dih5 =     0.0000012074
cc6 =     1.3893066469
ccc6 =   121.2507560087
dih6 =     0.0
hc7 =     1.084089795
hcc7 =   120.2456855634
dih7 =   180.0
sc8 =     1.7866253911
scc8 =   116.1469925627
dih8 =   180.0
hc9 =     1.0834917072
hcc9 =   121.369518009
dih9 =   180.0
hc10 =     1.0865087249
hcc10 =   119.2957018079
dih10 =   179.9999987926
hc11 =     1.0826343199
hcc11 =   118.3367391329
dih11 =   179.9999991462
cc12 =     1.4961368709
ccc12 =   121.1838260722
dih12 =   180.0
cc13 =     1.4023936291
ccc13 =   121.5241919018
dih13 =   180.0
cc14 =     1.4013103777
ccc14 =   122.052754628
dih14 =   180.0
cc15 =     1.3979382802
ccc15 =   119.5712034168
dih15 =     0.0
cc16 =     1.3946951836
ccc16 =   118.9657740055
dih16 =     0.0000012074
cc17 =     1.3893066469
ccc17 =   121.2507560087
dih17 =     0.0
hc18 =     1.084089795
hcc18 =   120.2456855634
dih18 =   180.0
sc19 =     1.7866253911
scc19 =   116.1469925627
dih19 =   179.9999991462
hc20 =     1.0834917072
hcc20 =   121.369518009
dih20 =   180.0
hc21 =     1.0865087249
hcc21 =   119.2957018079
```

```
  dih21 =   179.9999991462
  hc22 =     1.0826343199
  hcc22 =   118.3367391329
  dih22 =   180.0
  cs23 =     1.8216329717
  csc23 =   103.507004147
  dih23 =   180.0
  hc24 =     1.0919146765
  hcs24 =   105.5591766584
  dih24 =   180.0
  hc25 =     1.0925289866
  hcs25 =   111.6192496884
  dih25 =   118.084602889
  hc26 =     1.0925289866
  hcs26 =   111.6192496884
  dih26 =  -118.084602889
  cs27 =     1.8216329717
  csc27 =   103.507004147
  dih27 =   179.9999985212
  hc28 =     1.0919146765
  hcs28 =   105.5591766584
  dih28 =   179.9999987926
  hc29 =     1.0925289866
  hcs29 =   111.6192496884
  dih29 =   118.084602889
  hc30 =     1.0925289866
  hcs30 =   111.6192496884
  dih30 =  -118.084602889

  Molecular weight:     246.05 amu

  Stoichiometry: C14H14S2
  Molecular Point Group: C2v
      Molecule translated to center of mass
      Molecule reoriented along symmetry axes
  Point Group used: C2v


Number of optimization coordinates:    97
Number of independent coordinates:     97
Number of non-redundant coordinates:   84
Number of constrained coordinates:      0

Number of geometric degrees of freedom:    84
Maximum geometric degrees of freedom:      84
 " " " " " excluding dummy atoms:          84


 Symmetrized geometry:
                                    angstroms
  atom               x                   y                   z
  C1           0.0000000000      0.7480684354      1.0113806557
  C2           0.0000000000      1.4813219026     -0.1840469848
  C3           0.0000000000      2.8825726525     -0.1969741137
```

C4	0.0000000000	3.5836487735	1.0124570368
C5	0.0000000000	2.8666956281	2.2087650416
C6	0.0000000000	1.4774101506	2.2164345441
H7	0.0000000000	0.9685322157	-1.1391896028
S8	0.0000000000	3.6550662551	-1.8079626059
H9	0.0000000000	4.6668744264	1.0364667111
H10	0.0000000000	3.4061657707	3.1518838965
H11	0.0000000000	0.9688030911	3.1721625020
C12	0.0000000000	-0.7480684354	1.0113806557
C13	0.0000000000	-1.4813219026	-0.1840469848
C14	0.0000000000	-2.8825726525	-0.1969741137
C15	0.0000000000	-3.5836487735	1.0124570368
C16	0.0000000000	-2.8666956281	2.2087650416
C17	0.0000000000	-1.4774101506	2.2164345441
H18	0.0000000000	-0.9685322157	-1.1391896028
S19	0.0000000000	-3.6550662551	-1.8079626059
H20	0.0000000000	-4.6668744264	1.0364667111
H21	0.0000000000	-3.4061657707	3.1518838965
H22	0.0000000000	-0.9688030911	3.1721625020
C23	0.0000000000	-5.4361522563	-1.4257593358
H24	0.0000000000	-5.9432240034	-2.3927939288
H25	0.8960805980	-5.7293975665	-0.8737934523
H26	-0.8960805980	-5.7293975665	-0.8737934523
C27	0.0000000000	5.4361522563	-1.4257593358
H28	0.0000000000	5.9432240034	-2.3927939288
H29	-0.8960805980	5.7293975665	-0.8737934523
H30	0.8960805980	5.7293975665	-0.8737934523

Z-matrix: (angstroms and degrees)

C1						
C2	C1	cc2				
C3	C2	cc3	C1	ccc3		
C4	C3	cc4	C2	ccc4	C1	dih4
C5	C4	cc5	C3	ccc5	C2	dih5
C6	C5	cc6	C4	ccc6	C3	dih6
H7	C2	hc7	C1	hcc7	C3	dih7
S8	C3	sc8	C2	scc8	C4	dih8
H9	C4	hc9	C3	hcc9	C5	dih9
H10	C5	hc10	C4	hcc10	C3	dih10
H11	C6	hc11	C5	hcc11	C4	dih11
C12	C1	cc12	C6	ccc12	C5	dih12
C13	C12	cc13	C1	ccc13	C6	dih13
C14	C13	cc14	C12	ccc14	C1	dih14
C15	C14	cc15	C13	ccc15	C12	dih15
C16	C15	cc16	C14	ccc16	C13	dih16
C17	C16	cc17	C15	ccc17	C14	dih17
H18	C13	hc18	C12	hcc18	C14	dih18
S19	C14	sc19	C13	scc19	C15	dih19
H20	C15	hc20	C14	hcc20	C16	dih20
H21	C16	hc21	C15	hcc21	C14	dih21
H22	C17	hc22	C16	hcc22	C15	dih22
C23	S19	cs23	C14	csc23	C13	dih23
H24	C23	hc24	S19	hcs24	C14	dih24
H25	C23	hc25	S19	hcs25	H24	dih25

```
H26    C23  hc26    S19  hcs26    H24  dih26
C27    S8   cs27    C3   csc27    C2   dih27
H28    C27  hc28    S8   hcs28    C3   dih28
H29    C27  hc29    S8   hcs29    H28  dih29
H30    C27  hc30    S8   hcs30    H28  dih30

 Z-variables: (angstroms and degrees)
 cc2 =     1.4023936291
 cc3 =     1.4013103777
 ccc3 =   122.052754628
 cc4 =     1.3979382802
 ccc4 =   119.5712034168
 dih4 =     0.0
 cc5 =     1.3946951836
 ccc5 =   118.9657740055
 dih5 =     0.0
 cc6 =     1.3893066469
 ccc6 =   121.2507560087
 dih6 =     0.0
 hc7 =     1.084089795
 hcc7 =   120.2456855634
 dih7 =   180.0
 sc8 =     1.7866253911
 scc8 =   116.1469925627
 dih8 =   180.0
 hc9 =     1.0834917072
 hcc9 =   121.369518009
 dih9 =   180.0
 hc10 =     1.0865087249
 hcc10 =   119.2957018079
 dih10 =   180.0
 hc11 =     1.0826343199
 hcc11 =   118.3367391329
 dih11 =   179.9999991462
 cc12 =     1.4961368709
 ccc12 =   121.1838260728
 dih12 =   180.0
 cc13 =     1.4023936291
 ccc13 =   121.5241919024
 dih13 =   180.0
 cc14 =     1.4013103777
 ccc14 =   122.052754628
 dih14 =   180.0
 cc15 =     1.3979382802
 ccc15 =   119.5712034168
 dih15 =     0.0
 cc16 =     1.3946951836
 ccc16 =   118.9657740055
 dih16 =     0.0
 cc17 =     1.3893066469
 ccc17 =   121.2507560087
 dih17 =     0.0
 hc18 =     1.084089795
 hcc18 =   120.2456855634
```

```
 dih18 =   180.0
 sc19 =     1.7866253911
 scc19 =   116.1469925627
 dih19 =   180.0
 hc20 =     1.0834917072
 hcc20 =   121.369518009
 dih20 =   180.0
 hc21 =     1.0865087249
 hcc21 =   119.2957018079
 dih21 =   180.0
 hc22 =     1.0826343199
 hcc22 =   118.3367391329
 dih22 =   179.9999991462
 cs23 =     1.8216329717
 csc23 =   103.507004147
 dih23 =   180.0
 hc24 =     1.0919146765
 hcs24 =   105.5591766584
 dih24 =   180.0
 hc25 =     1.0925289866
 hcs25 =   111.6192496884
 dih25 =   118.084602889
 hc26 =     1.0925289866
 hcs26 =   111.6192496884
 dih26 =  -118.084602889
 cs27 =     1.8216329717
 csc27 =   103.507004147
 dih27 =   180.0
 hc28 =     1.0919146765
 hcs28 =   105.5591766584
 dih28 =   180.0
 hc29 =     1.0925289866
 hcs29 =   111.6192496884
 dih29 =   118.084602889
 hc30 =     1.0925289866
 hcs30 =   111.6192496884
 dih30 =  -118.084602889


 bond lengths (angstroms):

C1      -C2      :   1.402394      C1      -C6      :   1.408579
C1      -C12     :   1.496137      C2      -C3      :   1.401310
C2      -H7      :   1.084090      C3      -C4      :   1.397938
C3      -S8      :   1.786625      C4      -C5      :   1.394695
C4      -H9      :   1.083492      C5      -C6      :   1.389307
C5      -H10     :   1.086509      C6      -H11     :   1.082634
S8      -C27     :   1.821633      C12     -C13     :   1.402394
C12     -C17     :   1.408579      C13     -C14     :   1.401310
C13     -H18     :   1.084090      C14     -C15     :   1.397938
C14     -S19     :   1.786625      C15     -C16     :   1.394695
C15     -H20     :   1.083492      C16     -C17     :   1.389307
C16     -H21     :   1.086509      C17     -H22     :   1.082634
S19     -C23     :   1.821633      C23     -H24     :   1.091915
```

```
 C23     -H25     :   1.092529      C23     -H26     :   1.092529
 C27     -H28     :   1.091915      C27     -H29     :   1.092529
 C27     -H30     :   1.092529

  bond angles:

 C6      -C1      -C2      : 117.291982  C12     -C1      -C2      :
121.524192
 C12     -C1      -C6      : 121.183826  C3      -C2      -C1      :
122.052755
 H7      -C2      -C1      : 120.245686  H7      -C2      -C3      :
117.701560
 C4      -C3      -C2      : 119.571203  S8      -C3      -C2      :
116.146993
 S8      -C3      -C4      : 124.281804  C5      -C4      -C3      :
118.965774
 H9      -C4      -C3      : 121.369518  H9      -C4      -C5      :
119.664708
 C6      -C5      -C4      : 121.250756  H10     -C5      -C4      :
119.295702
 H10     -C5      -C6      : 119.453542  C5      -C6      -C1      :
120.867530
 H11     -C6      -C1      : 120.795731  H11     -C6      -C5      :
118.336739
 C27     -S8      -C3      : 103.507004  C13     -C12     -C1      :
121.524192
 C17     -C12     -C1      : 121.183826  C17     -C12     -C13     :
117.291982
 C14     -C13     -C12     : 122.052755  H18     -C13     -C12     :
120.245686
 H18     -C13     -C14     : 117.701560  C15     -C14     -C13     :
119.571203
 S19     -C14     -C13     : 116.146993  S19     -C14     -C15     :
124.281804
 C16     -C15     -C14     : 118.965774  H20     -C15     -C14     :
121.369518
 H20     -C15     -C16     : 119.664708  C17     -C16     -C15     :
121.250756
 H21     -C16     -C15     : 119.295702  H21     -C16     -C17     :
119.453542
 C16     -C17     -C12     : 120.867530  H22     -C17     -C12     :
120.795731
 H22     -C17     -C16     : 118.336739  C23     -S19     -C14     :
103.507004
 H24     -C23     -S19     : 105.559177  H25     -C23     -S19     :
111.619250
 H25     -C23     -H24     : 108.831831  H26     -C23     -S19     :
111.619250
 H26     -C23     -H24     : 108.831831  H26     -C23     -H25     :
110.207498
 H28     -C27     -S8      : 105.559177  H29     -C27     -S8      :
111.619250
 H29     -C27     -H28     : 108.831831  H30     -C27     -S8      :
111.619250
```

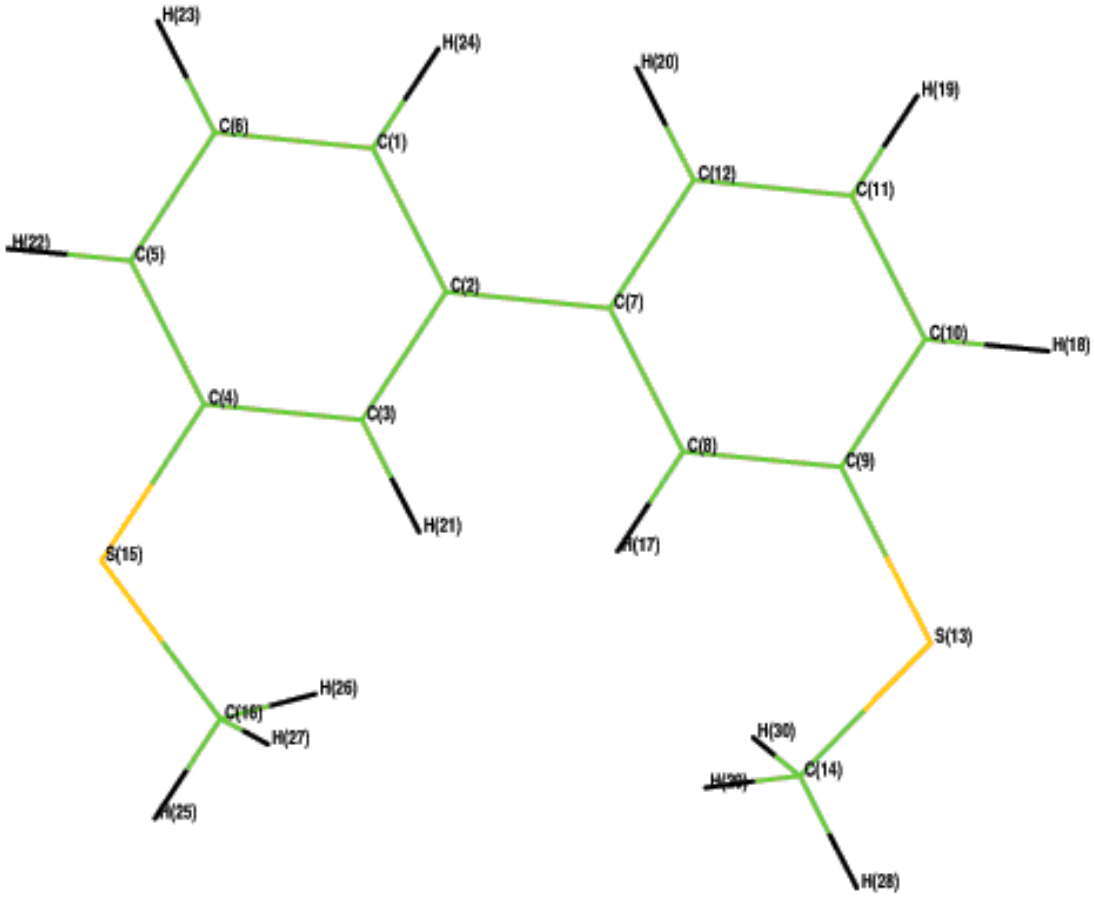
H30 -C27 -H28 : 108.831831 H30 -C27 -H29 : 110.207498

torsional angles:

C1	-C2	-C3	-C4	: 0.000000
C1	-C2	-C3	-S8	: 180.000000
C1	-C6	-C5	-C4	: 0.000000
C1	-C6	-C5	-H10	: 180.000000
C1	-C12	-C13	-C14	: 180.000000
C1	-C12	-C13	-H18	: 0.000000
C1	-C12	-C17	-C16	: 180.000000
C1	-C12	-C17	-H22	: 0.000000
C2	-C1	-C6	-C5	: 0.000000
C2	-C1	-C6	-H11	: 180.000000
C2	-C1	-C12	-C13	: 0.000000
C2	-C1	-C12	-C17	: 180.000000
C2	-C3	-C4	-C5	: 0.000000
C2	-C3	-C4	-H9	: 180.000000
C2	-C3	-S8	-C27	: 180.000000
C3	-C2	-C1	-C6	: 0.000000
C3	-C2	-C1	-C12	: 180.000000
C3	-C4	-C5	-C6	: 0.000000
C3	-C4	-C5	-H10	: 180.000000
C3	-S8	-C27	-H28	: 180.000000
C3	-S8	-C27	-H29	: -61.915397
C3	-S8	-C27	-H30	: 61.915397
C4	-C3	-C2	-H7	: 180.000000
C4	-C3	-S8	-C27	: 0.000000
C4	-C5	-C6	-H11	: 179.999999
C5	-C4	-C3	-S8	: 180.000000
C5	-C6	-C1	-C12	: 180.000000
C6	-C1	-C2	-H7	: 180.000000
C6	-C1	-C12	-C13	: 180.000000
C6	-C1	-C12	-C17	: 0.000000
C6	-C5	-C4	-H9	: 180.000000
H7	-C2	-C1	-C12	: 0.000000
H7	-C2	-C3	-S8	: 0.000000
S8	-C3	-C4	-H9	: 0.000000
H9	-C4	-C5	-H10	: 0.000001
H10	-C5	-C6	-H11	: 0.000000
H11	-C6	-C1	-C12	: 0.000000
C12	-C13	-C14	-C15	: 0.000000
C12	-C13	-C14	-S19	: 180.000000
C12	-C17	-C16	-C15	: 0.000000
C12	-C17	-C16	-H21	: 180.000000
C13	-C12	-C17	-C16	: 0.000000
C13	-C12	-C17	-H22	: 180.000000
C13	-C14	-C15	-C16	: 0.000000
C13	-C14	-C15	-H20	: 180.000000
C13	-C14	-S19	-C23	: 180.000000
C14	-C13	-C12	-C17	: 0.000000
C14	-C15	-C16	-C17	: 0.000000
C14	-C15	-C16	-H21	: 180.000000

```
C14     -S19     -C23     -H24     : 180.000000
C14     -S19     -C23     -H25     : -61.915397
C14     -S19     -C23     -H26     :  61.915397
C15     -C14     -C13     -H18     : 180.000000
C15     -C14     -S19     -C23     :   0.000000
C15     -C16     -C17     -H22     : 179.999999
C16     -C15     -C14     -S19     : 180.000000
C17     -C12     -C13     -H18     : 180.000000
C17     -C16     -C15     -H20     : 180.000000
H18     -C13     -C14     -S19     :   0.000000
S19     -C14     -C15     -H20     :   0.000000
H20     -C15     -C16     -H21     :   0.000001
H21     -C16     -C17     -H22     :   0.000000
```

*Biphenyl (**5**) – Anti Conformer*



Final energy (B3LYP; cc-pVTZ) = -1338.562527 h

Optimized geometry - subject to the constraint that the heavy atoms (C and S) are all coplanar. Optimization done with the 6-31g** basis set.

		angstroms	
atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4040055496
C3	1.2498216316	0.0000000000	2.0539192212
C4	2.4503709477	0.0000000000	1.3412750861
C5	2.4218477138	0.0000000000	-0.0607629408
C6	1.1962757248	0.0000000000	-0.7149110674
C7	-1.2766550691	0.0000000000	2.1834701825
C8	-1.2695949368	0.0000000000	3.5921546915
C9	-2.4520390807	0.0000000000	4.3344525901
C10	-3.6861419832	0.0000000000	3.6684839500
C11	-3.7080484896	0.0000000000	2.2794351471
C12	-2.5255404940	0.0000000000	1.5419744469
S13	-2.5173241543	0.0000000000	6.1202237598
C14	-0.7666312241	0.0000000000	6.6219289731
S15	4.0686720171	0.0000000000	2.0991289376
C16	3.7150482578	0.0000000000	3.8856294536
H17	-0.3266107000	-0.0000000140	4.1200163370
H18	-4.6135837525	0.0000000000	4.2336497432
H19	-4.6619063283	0.0000000000	1.7597590398
H20	-2.5936830572	0.0000000000	0.4613488065
H21	1.2885097613	0.0000000000	3.1339008953
H22	3.3483235828	0.0000000000	-0.6275107446
H23	1.1698369545	0.0000000000	-1.8008249795
H24	-0.9300992069	0.0000000000	-0.5543560667
H25	4.6904280401	0.0000000000	4.3765981301
H26	3.1688421937	0.8966931307	4.1883507612
H27	3.1688421937	-0.8966931307	4.1883507612
H28	-0.7755616352	0.0000000000	7.7138704591
H29	-0.2477920430	-0.8966931307	6.2743845033
H30	-0.2477920430	0.8966931307	6.2743845033

principal moments of inertia:

amu*angstrom^2:	798.93297	2050.07329	2842.52346
g*cm^2:	1.32665925E-37	3.40422636E-37	4.72012066E-37

rotational constants:

cm^(-1):	0.02110018	0.00822294	0.00593052
GHz:	0.63256747	0.24651753	0.17779238

Z-matrix: (angstroms and degrees)

C1						
C2	C1	cc2				
C3	C2	cc3	C1	ccc3		
C4	C3	cc4	C2	ccc4	C1	dih4
C5	C4	cc5	C3	ccc5	C2	dih5
C6	C5	cc6	C4	ccc6	C3	dih6
C7	C2	cc7	C3	ccc7	C4	dih7
C8	C7	cc8	C2	ccc8	C3	dih8
C9	C8	cc9	C7	ccc9	C2	dih9
C10	C9	cc10	C8	ccc10	C7	dih10
C11	C10	cc11	C9	ccc11	C8	dih11
C12	C11	cc12	C10	ccc12	C9	dih12

```
S13    C9   sc13    C8   scc13    C7   dih13
C14    S13  cs14    C9   csc14    C8   dih14
S15    C4   sc15    C3   scc15    C2   dih15
C16    S15  cs16    C4   csc16    C3   dih16
H17    C8   hc17    C7   hcc17    C12  dih17
H18    C10  hc18    C9   hcc18    C8   dih18
H19    C11  hc19    C10  hcc19    C9   dih19
H20    C12  hc20    C7   hcc20    C8   dih20
H21    C3   hc21    C2   hcc21    C7   dih21
H22    C5   hc22    C4   hcc22    C3   dih22
H23    C6   hc23    C5   hcc23    C4   dih23
H24    C1   hc24    C2   hcc24    C7   dih24
H25    C16  hc25    S15  hcs25    C4   dih25
H26    C16  hc26    S15  hcs26    C4   dih26
H27    C16  hc27    S15  hcs27    C4   dih27
H28    C14  hc28    S13  hcs28    C9   dih28
H29    C14  hc29    S13  hcs29    C9   dih29
H30    C14  hc30    S13  hcs30    C9   dih30

 Z-variables: (angstroms and degrees)
 cc2 =     1.4040055496
 cc3 =     1.4087022011
 ccc3 =   117.4746634081
 cc4 =     1.3961304823
 ccc4 =   121.8320371304
 dih4 =     0.0
 cc5 =     1.4023281369
 ccc5 =   119.5278278546
 dih5 =     0.0
 cc6 =     1.3892215345
 ccc6 =   119.2565081969
 dih6 =     0.0
 cc7 =     1.4957985424
 ccc7 =   121.1190902298
 dih7 =   180.0
 cc8 =     1.4087022011
 ccc8 =   121.1190902298
 dih8 =     0.0000012074
 cc9 =     1.3961304823
 ccc9 =   121.8320371304
 dih9 =   180.0
 cc10 =     1.4023281369
 ccc10 =   119.5278278546
 dih10 =     0.0
 cc11 =     1.3892215345
 ccc11 =   119.2565081969
 dih11 =     0.0
 cc12 =     1.3936188303
 ccc12 =   121.0458349795
 dih12 =     0.0
 sc13 =     1.7869641327
 scc13 =   124.2129072452
 dih13 =   180.0
 cs14 =     1.821162776
```

```
csc14 =   103.8972766317
dih14 =     0.0
sc15 =     1.7869641327
scc15 =   124.2129072452
dih15 =   180.0
cs16 =     1.821162776
csc16 =   103.8972766317
dih16 =     0.0
hc17 =     1.0806744134
hcc17 =   119.5262899534
dih17 =   179.9999991462
hc18 =     1.0860757842
hcc18 =   120.2896671727
dih18 =   180.0
hc19 =     1.0862357171
hcc19 =   119.4857426734
dih19 =   179.9999991462
hc20 =     1.0827719905
hcc20 =   120.7957120922
dih20 =   180.0
hc21 =     1.0806744134
hcc21 =   119.5262899534
dih21 =     0.0
hc22 =     1.0860757842
hcc22 =   120.2896671727
dih22 =   180.0
hc23 =     1.0862357171
hcc23 =   119.4857426734
dih23 =   180.0
hc24 =     1.0827719905
hcc24 =   120.7957120922
dih24 =     0.0
hc25 =     1.0919780039
hcs25 =   105.5224092253
dih25 =   180.0
hc26 =     1.0927212934
hcs26 =   111.6429488841
dih26 =   -61.9875935654
hc27 =     1.0927212934
hcs27 =   111.6429488841
dih27 =    61.9875935654
hc28 =     1.0919780039
hcs28 =   105.5224092253
dih28 =   180.0
hc29 =     1.0927212934
hcs29 =   111.6429488841
dih29 =   -61.9875935654
hc30 =     1.0927212934
hcs30 =   111.6429488841
dih30 =    61.9875935654

Molecular weight:     246.05 amu

Stoichiometry: C14H14S2
```

```
 Molecular Point Group: C2v
    Molecule translated to center of mass
    Molecule reoriented along symmetry axes
 Point Group used: C2v


Symmetrized geometry:
                                    angstroms
 atom              x                   y                   z
 C1           0.0000000000      1.4795303293      2.3939501820
 C2           0.0000000000      0.7478992712      1.1956398807
 C3           0.0000000000      1.4759427672     -0.0103429381
 C4           0.0000000000      2.8719651659     -0.0277149195
 C5           0.0000000000      3.5782265339      1.1837796466
 C6           0.0000000000      2.8730865481      2.3807399936
 C7           0.0000000000     -0.7478992712      1.1956398807
 C8           0.0000000000     -1.4759427672     -0.0103429381
 C9           0.0000000000     -2.8719651659     -0.0277149195
 C10          0.0000000000     -3.5782265339      1.1837796466
 C11          0.0000000000     -2.8730865481      2.3807399936
 C12          0.0000000000     -1.4795303293      2.3939501820
 S13          0.0000000000     -3.8582557309     -1.5178396569
 C14          0.0000000000     -2.6254897657     -2.8583328243
 S15          0.0000000000      3.8582557309     -1.5178396569
 C16          0.0000000000      2.6254897657     -2.8583328243
 H17          0.0000000000     -0.9461815059     -0.9522612965
 H18          0.0000000000     -4.6643019227      1.1847064315
 H19          0.0000000000     -3.4163938691      3.3213383075
 H20          0.0000000000     -0.9745726777      3.3517669460
 H21          0.0000000000      0.9461815059     -0.9522612965
 H22          0.0000000000      4.6643019227      1.1847064315
 H23          0.0000000000      3.4163938691      3.3213383075
 H24          0.0000000000      0.9745726777      3.3517669460
 H25          0.0000000000      3.2021254554     -3.7856446610
 H26          0.8966931307      2.0015572862     -2.8320741964
 H27         -0.8966931307      2.0015572862     -2.8320741964
 H28          0.0000000000     -3.2021254554     -3.7856446610
 H29         -0.8966931307     -2.0015572862     -2.8320741964
 H30          0.8966931307     -2.0015572862     -2.8320741964

 Z-matrix: (angstroms and degrees)
C1
C2     C1    cc2
C3     C2    cc3      C1    ccc3
C4     C3    cc4      C2    ccc4      C1    dih4
C5     C4    cc5      C3    ccc5      C2    dih5
C6     C5    cc6      C4    ccc6      C3    dih6
C7     C2    cc7      C3    ccc7      C4    dih7
C8     C7    cc8      C2    ccc8      C3    dih8
C9     C8    cc9      C7    ccc9      C2    dih9
C10    C9    cc10     C8    ccc10     C7    dih10
C11    C10   cc11     C9    ccc11     C8    dih11
C12    C11   cc12     C10   ccc12     C9    dih12
S13    C9    sc13     C8    scc13     C7    dih13
```

```
C14    S13  cs14    C9   csc14    C8   dih14
S15    C4   sc15    C3   scc15    C2   dih15
C16    S15  cs16    C4   csc16    C3   dih16
H17    C8   hc17    C7   hcc17    C12  dih17
H18    C10  hc18    C9   hcc18    C8   dih18
H19    C11  hc19    C10  hcc19    C9   dih19
H20    C12  hc20    C7   hcc20    C8   dih20
H21    C3   hc21    C2   hcc21    C7   dih21
H22    C5   hc22    C4   hcc22    C3   dih22
H23    C6   hc23    C5   hcc23    C4   dih23
H24    C1   hc24    C2   hcc24    C7   dih24
H25    C16  hc25    S15  hcs25    C4   dih25
H26    C16  hc26    S15  hcs26    C4   dih26
H27    C16  hc27    S15  hcs27    C4   dih27
H28    C14  hc28    S13  hcs28    C9   dih28
H29    C14  hc29    S13  hcs29    C9   dih29
H30    C14  hc30    S13  hcs30    C9   dih30

 Z-variables: (angstroms and degrees)
 cc2 =     1.4040055496
 cc3 =     1.4087022011
 ccc3 =   117.4746634094
 cc4 =     1.3961304823
 ccc4 =   121.8320371304
 dih4 =     0.0
 cc5 =     1.4023281369
 ccc5 =   119.5278278546
 dih5 =     0.0
 cc6 =     1.3892215345
 ccc6 =   119.2565081969
 dih6 =     0.0
 cc7 =     1.4957985424
 ccc7 =   121.1190902298
 dih7 =   180.0
 cc8 =     1.4087022011
 ccc8 =   121.1190902298
 dih8 =     0.0
 cc9 =     1.3961304823
 ccc9 =   121.8320371304
 dih9 =   180.0
 cc10 =     1.4023281369
 ccc10 =   119.5278278546
 dih10 =     0.0
 cc11 =     1.3892215345
 ccc11 =   119.2565081969
 dih11 =     0.0
 cc12 =     1.3936188303
 ccc12 =   121.0458349788
 dih12 =     0.0
 sc13 =     1.7869641327
 scc13 =   124.2129072452
 dih13 =   180.0
 cs14 =     1.821162776
 csc14 =   103.8972766317
```

```
 dih14 =     0.0000012074
 sc15 =     1.7869641327
 scc15 =   124.2129072452
 dih15 =   180.0
 cs16 =     1.821162776
 csc16 =   103.8972766317
 dih16 =     0.0000012074
 hc17 =     1.0806744134
 hcc17 =   119.5262899534
 dih17 =   180.0
 hc18 =     1.0860757842
 hcc18 =   120.2896671727
 dih18 =   180.0
 hc19 =     1.0862357171
 hcc19 =   119.4857426734
 dih19 =   180.0
 hc20 =     1.0827719905
 hcc20 =   120.7957120922
 dih20 =   180.0
 hc21 =     1.0806744134
 hcc21 =   119.5262899534
 dih21 =     0.0
 hc22 =     1.0860757842
 hcc22 =   120.2896671727
 dih22 =   180.0
 hc23 =     1.0862357171
 hcc23 =   119.4857426734
 dih23 =   180.0
 hc24 =     1.0827719905
 hcc24 =   120.7957120922
 dih24 =     0.0
 hc25 =     1.0919780039
 hcs25 =   105.5224092253
 dih25 =   180.0
 hc26 =     1.0927212934
 hcs26 =   111.6429488841
 dih26 =   -61.9875935654
 hc27 =     1.0927212934
 hcs27 =   111.6429488841
 dih27 =    61.9875935654
 hc28 =     1.0919780039
 hcs28 =   105.5224092253
 dih28 =   180.0
 hc29 =     1.0927212934
 hcs29 =   111.6429488841
 dih29 =   -61.9875935654
 hc30 =     1.0927212934
 hcs30 =   111.6429488841
 dih30 =    61.9875935654


 bond lengths (angstroms):

C1      -C2      :   1.404006      C1      -C6      :   1.393619
```

C1	-H24	:	1.082772	C2	-C3	:	1.408702
C2	-C7	:	1.495799	C3	-C4	:	1.396130
C3	-H21	:	1.080674	C4	-C5	:	1.402328
C4	-S15	:	1.786964	C5	-C6	:	1.389222
C5	-H22	:	1.086076	C6	-H23	:	1.086236
C7	-C8	:	1.408702	C7	-C12	:	1.404006
C8	-C9	:	1.396130	C8	-H17	:	1.080674
C9	-C10	:	1.402328	C9	-S13	:	1.786964
C10	-C11	:	1.389222	C10	-H18	:	1.086076
C11	-C12	:	1.393619	C11	-H19	:	1.086236
C12	-H20	:	1.082772	S13	-C14	:	1.821163
C14	-H28	:	1.091978	C14	-H29	:	1.092721
C14	-H30	:	1.092721	S15	-C16	:	1.821163
C16	-H25	:	1.091978	C16	-H26	:	1.092721
C16	-H27	:	1.092721				

bond angles:

C6	-C1	-C2	: 120.863128	H24	-C1	-C2	: 120.795712
H24	-C1	-C6	: 118.341159	C3	-C2	-C1	: 117.474663
C7	-C2	-C1	: 121.406246	C7	-C2	-C3	: 121.119090
C4	-C3	-C2	: 121.832037	H21	-C3	-C2	: 119.526290
H21	-C3	-C4	: 118.641673	C5	-C4	-C3	: 119.527828
S15	-C4	-C3	: 124.212907	S15	-C4	-C5	: 116.259265
C6	-C5	-C4	: 119.256508	H22	-C5	-C4	: 120.289667
H22	-C5	-C6	: 120.453825	C5	-C6	-C1	: 121.045835
H23	-C6	-C1	: 119.468422	H23	-C6	-C5	: 119.485743
C8	-C7	-C2	: 121.119090	C12	-C7	-C2	: 121.406246
C12	-C7	-C8	: 117.474663	C9	-C8	-C7	: 121.832037
H17	-C8	-C7	: 119.526290	H17	-C8	-C9	: 118.641673
C10	-C9	-C8	: 119.527828	S13	-C9	-C8	: 124.212907
S13	-C9	-C10	: 116.259265	C11	-C10	-C9	: 119.256508
H18	-C10	-C9	: 120.289667	H18	-C10	-C11	: 120.453825
C12	-C11	-C10	: 121.045835	H19	-C11	-C10	: 119.485743
H19	-C11	-C12	: 119.468422	C11	-C12	-C7	: 120.863128
H20	-C12	-C7	: 120.795712	H20	-C12	-C11	: 118.341159

```
 C14     -S13     -C9      : 103.897277  H28     -C14     -S13     :
105.522409
 H29     -C14     -S13     : 111.642949  H29     -C14     -H28     :
108.779476
 H30     -C14     -S13     : 111.642949  H30     -C14     -H28     :
108.779476
 H30     -C14     -H29     : 110.290910  C16     -S15     -C4      :
103.897277
 H25     -C16     -S15     : 105.522409  H26     -C16     -S15     :
111.642949
 H26     -C16     -H25     : 108.779476  H27     -C16     -S15     :
111.642949
 H27     -C16     -H25     : 108.779476  H27     -C16     -H26     :
110.290910

  torsional angles:

 C1      -C2      -C3      -C4      :   0.000000
 C1      -C2      -C3      -H21     : 180.000000
 C1      -C2      -C7      -C8      : 180.000000
 C1      -C2      -C7      -C12     :   0.000000
 C1      -C6      -C5      -C4      :   0.000000
 C1      -C6      -C5      -H22     : 180.000000
 C2      -C1      -C6      -C5      :   0.000000
 C2      -C1      -C6      -H23     : 180.000000
 C2      -C3      -C4      -C5      :   0.000000
 C2      -C3      -C4      -S15     : 180.000000
 C2      -C7      -C8      -C9      : 180.000000
 C2      -C7      -C8      -H17     :   0.000000
 C2      -C7      -C12     -C11     : 180.000000
 C2      -C7      -C12     -H20     :   0.000000
 C3      -C2      -C1      -C6      :   0.000000
 C3      -C2      -C1      -H24     : 180.000000
 C3      -C2      -C7      -C8      :   0.000000
 C3      -C2      -C7      -C12     : 180.000000
 C3      -C4      -C5      -C6      :   0.000000
 C3      -C4      -C5      -H22     : 180.000000
 C3      -C4      -S15     -C16     :   0.000001
 C4      -C3      -C2      -C7      : 180.000000
 C4      -C5      -C6      -H23     : 180.000000
 C4      -S15     -C16     -H25     : 180.000000
 C4      -S15     -C16     -H26     : -61.987594
 C4      -S15     -C16     -H27     :  61.987594
 C5      -C4      -C3      -H21     : 180.000000
 C5      -C4      -S15     -C16     : 180.000000
 C5      -C6      -C1      -H24     : 180.000000
 C6      -C1      -C2      -C7      : 180.000000
 C6      -C5      -C4      -S15     : 180.000000
 C7      -C2      -C1      -H24     :   0.000000
 C7      -C2      -C3      -H21     :   0.000000
 C7      -C8      -C9      -C10     :   0.000000
 C7      -C8      -C9      -S13     : 180.000000
 C7      -C12     -C11     -C10     :   0.000000
 C7      -C12     -C11     -H19     : 180.000000
```

C8	-C7	-C12	-C11	:	0.000000
C8	-C7	-C12	-H20	:	180.000000
C8	-C9	-C10	-C11	:	0.000000
C8	-C9	-C10	-H18	:	180.000000
C8	-C9	-S13	-C14	:	0.000001
C9	-C8	-C7	-C12	:	0.000000
C9	-C10	-C11	-C12	:	0.000000
C9	-C10	-C11	-H19	:	180.000000
C9	-S13	-C14	-H28	:	180.000000
C9	-S13	-C14	-H29	:	-61.987594
C9	-S13	-C14	-H30	:	61.987594
C10	-C9	-C8	-H17	:	180.000000
C10	-C9	-S13	-C14	:	180.000000
C10	-C11	-C12	-H20	:	180.000000
C11	-C10	-C9	-S13	:	180.000000
C12	-C7	-C8	-H17	:	180.000000
C12	-C11	-C10	-H18	:	180.000000
S13	-C9	-C8	-H17	:	0.000001
S13	-C9	-C10	-H18	:	0.000000
S15	-C4	-C3	-H21	:	0.000001
S15	-C4	-C5	-H22	:	0.000000
H18	-C10	-C11	-H19	:	0.000000
H19	-C11	-C12	-H20	:	0.000000
H22	-C5	-C6	-H23	:	0.000000
H23	-C6	-C1	-H24	:	0.000000

V. References

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