

Supporting information for:

**Photodeoxygenation of dinaphthothiophene, benzophenanthrothiophene,
and benzonaphthothiophene S-oxides**

X. Zheng,^a S. M. Baumann, S. M. Chintala, K. D. Galloway, J. B. Slaughter, and R. D. McCulla^c

Saint Louis University, Saint Louis, Missouri, 63103 USA

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Supporting Figures and Tables.

Table S1. Comparison of toluene oxidation product yields by **DBTO** and thiophene *S*-oxides **1-5** with including error associated with the ratio of methyl to ring oxidation.^a

Sulfoxide	PhCHO	BnOH	o-cresol	m- & p-cresol ^b	Total %yield oxidized toluene	Oxidation CH ₃ :Ring ^c
DBTO ^d	14 ± 3	10 ± 1	25 ± 3	24 ± 6	73 ± 7	1 : 2.0 ± 0.4
DBTO ^e	17 ± 3	13 ± 4	26 ± 5	22 ± 5	78 ± 9	1 : 1.6 ± 0.3
DBTO ^f	3±1	5±1	20±1	18±1	46 ± 2	1 : 4.8 ± 0.9
1 ^f	2.4±0.5	5.1±0.8	9.8±0.8	5.6±0.3	22.9 ± 1.3	1 : 2.0 ± 0.3
2 ^f	1.7±0.4	3.4±0.6	5.5±0.3	2.7±0.2	13.3 ± 0.8	1 : 1.6 ± 0.2
3 ^f	2.1±0.5	4±1	3.8±0.9	2.4±0.6	12.3 ± 1.6	1 : 1.0 ± 0.3
4 ^f	8.3±1.1	11.8±1.8	2.8±0.4	1.3±0.2	24.2 ± 2.2	4.9 ± 0.7 : 1
5 ^f	1.6±0.2	2.2±0.5	3.3±0.0	2.4±0.1	9.5 ± 0.5	1 : 1.5 ± 0.2

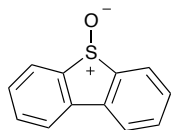
^a Yields of toluene oxidation products relative to the formation of the corresponding sulfide of **DBTO** and thiophene *S*-oxides **1-5**. The oxidation products are benzaldehyde (PhCHO), benzyl alcohol (BnOH), and all three cresol isomers. ^b Measured as a single peak by GC-FID. ^c Ratio of PhCHO plus BnOH yields to combined cresol yields. ^d Values from reference 5. ^e Values from reference 24. ^f This work.

Table S2. TD-B3LYP and B3LYP/6-31G(d,p) excited state energies relative to *S*₀.

Sulfoxide	<i>S</i> ₁ ^a	<i>T</i> ₁ ^a	<i>T</i> ₂ (<i>S</i> ₀) ^b	<i>T</i> ₂ (<i>T</i> ₁) ^c	<i>T</i> ₂ (<i>S</i> ₁) ^d	<i>S</i> ₁ - <i>T</i> ₂ (<i>S</i> ₀) ^e	<i>S</i> ₁ - <i>T</i> ₂ (<i>S</i> ₁) ^f	<i>S</i> ₁ - <i>T</i> ₂ (<i>T</i> ₁) ^g	<i>T</i> ₁ - <i>T</i> ₂ (<i>S</i> ₀) ^h	<i>T</i> ₁ - <i>T</i> ₂ (<i>S</i> ₁) ⁱ	<i>T</i> ₁ - <i>T</i> ₂ (<i>T</i> ₁) ^j
DBTO	70.0	63.0	80.5	79.2	76.2	-10.5	-9.2	-6.2	-17.5	-16.2	-13.2
1	65.0	49.4	73.3	72.9	68.8	-8.3	-7.9	-3.8	-23.9	-23.5	-19.4
2	65.8	52.3	76.0	74.5	73.0	-10.2	-8.7	-7.2	-23.7	-22.2	-20.7
3	64.8	48.0	73.4	74.8	67.9	-8.6	-10	-3.1	-25.4	-26.8	-19.9
4	62.3	42.2	66.9	68.5	60.2	-4.6	-6.2	2.1	-24.7	-26.3	-18
5	62.7	49.0	59.6	68.5	57.4	3.1	-5.8	5.3	-10.6	-19.5	-8.4

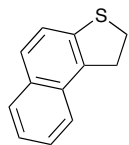
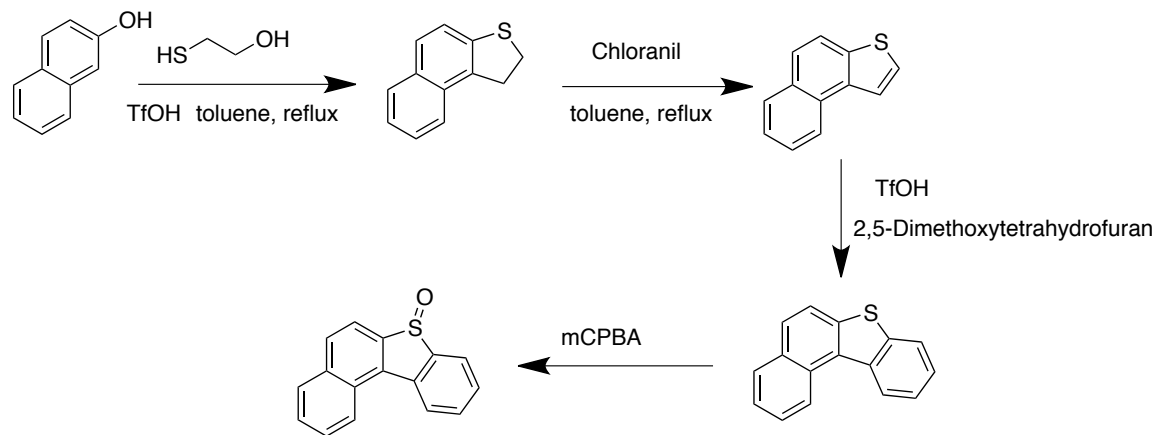
^a *S*₁ and *T*₁ energies in kcal mol⁻¹ determined from the difference between the excited and ground (*S*₀) state energies (H at 0 K) at B3LYP/6-31G(d,p) level of theory. ^b *T*₂ excited state energies at *S*₀ B3LYP/6-31G(d,p) optimized geometry (*E*_{el}(*T*₂)-*E*_{el}(*S*₀)) in kcal mol⁻¹. ^c *T*₂ excited state energy at *T*₁ B3LYP/6-31G(d,p) optimized geometry (*E*_{el}(*T*₂)-*E*_{el}(*S*₀)) in kcal mol⁻¹. ^d *T*₂ excited state energies at *S*₁ TD-B3LYP/6-31G(d,p) optimized geometry (*E*_{el}(*T*₂)- *E*_{el} (*S*₀)) in kcal mol⁻¹. ^e Difference between *S*₁ energy and *T*₂ energy at the *S*₀ geometry in kcal mol⁻¹. ^f Difference between *S*₁ energy and *T*₂ energy at the *S*₁ geometry in kcal mol⁻¹. ^g Difference between *S*₁ energy and *T*₂ energy at the *T*₁ geometry in kcal mol⁻¹. ^h Difference between *T*₁ energy and *T*₂ energy at the *S*₀ geometry in kcal mol⁻¹. ⁱ Difference between *T*₁ energy and *T*₂ energy at the *S*₁ geometry in kcal mol⁻¹. ^j Difference between *T*₁ energy and *T*₂ energy at the *T*₁ geometry in kcal mol⁻¹.

Synthesis Methods.

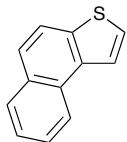


Preparation of Dibenzothiophene S-oxide (DBTO). This compound was prepared by slight modification of a previously reported method.¹ A 250 mL round-bottom flask was charged with 1.84g (10mmol) of dibenzothiophene which was then dissolved in 100ml dichloromethane at -30°C. Then 2.48g 77% mCPBA (11.1 mmol) was dissolved in another 100ml dichloromethane and added into the reaction mixture dropwise. The reaction was monitored by TLC. Once completed the reaction mixture was warmed to room temperature, and the reaction mixture was quenched with saturated sodium bicarbonate solution. The organic layer was separated and then the aqueous layer was extracted with CH₂Cl₂ (3 times), and the combined organic extracts were dried over Na₂SO₄ and removed under reduced pressure. The crude product was subjected to column chromatography (SiO₂, dichloromethane as eluent) to yield dibenzothiophene S-oxide (1108mg, 0.504mmol, 55.4% yield). ¹H NMR (400 MHz, CDCl₃): δ 7.99-7.96 (m, 4H), 7.68 (td, J₁= 7.7 Hz, J₂=1.0 H), 7.56 (td, J₁= 7.6 Hz, J₂=1.1 H) The spectra of this compound were consistent with literature reports.¹

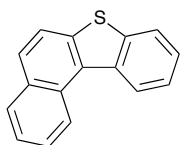
Scheme 1. Synthesis of Benzo[b]naphtho[1,2-d]thiophene S-oxide (**1**)



Preparation of 1,2-dihydro-naphtho[2,1-b]thiophene. This compound was prepared by slight modification of a previously reported method.² 2-naphthol (0.50 g, 3.47 mmol) was dissolved in chlorobenzene (15 ml) and 2-mercaptoethanol (1.46 ml, 20.80 mmol) was added to the solution. Trifluoromethanesulfonic acid (0.77 mL, 8.67 mmol) was added slowly into the reaction mixture at room temperature and the reaction was heated to reflux for 3 hours. Solid started to form in the solution initially, which gradually dissolved during heating. The reaction was cooled to room temperature and quenched with 5% NaOH solution, followed by extraction with CH₂Cl₂. The combined organic extract was dried using anhydrous Na₂SO₄, filtered and concentrated. The crude product was purified by column chromatography with hexanes as eluent which yielded 1,2-dihydro-naphtho[2,1-b]thiophene (0.34 g, 52%) as pale yellow powder. GCMS (EI) *m/z* 186, 185, 184, 152, 139. This spectrum was consistent with the previous literature.²

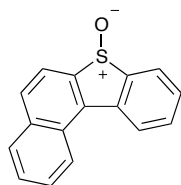


Preparation of naphtho[2,1-b]thiophene. This compound was prepared by slight modification of a previously reported method.² Tetrachloro-p-benzoquinone (0.74 g, 3.03 mmol) and 1,2-dihydro-naphtho[2,1-b]thiophene (0.28 g, 1.51 mmol) were refluxed in toluene (15 mL) for 24 hours. The reaction was monitored by TLC with hexane as eluent. After the completion of the reaction, the reaction mixture was concentrated under reduced pressure. The crude product was purified by column chromatography with hexane as eluent to afford naphtho[2,1-b]thiophene (0.24 g, 86% yield). ¹H NMR (400 MHz, CDCl₃): 8.36 (d, J₁= 8.2 Hz, 1H), 7.91(dd, J₁= 4.7 Hz, J₂= 0.6 Hz, 1H), 7.95-7.97 (m, 1H), 7.91 (dd, J₁= 8.8 Hz, J₂= 0.64 Hz, 1H), 7.76(d, J=8.8 Hz, 1H), 7.60-7.65(m,2H),7.52-7.57(m,1H). The spectra of this compound are consistent with literature report.²



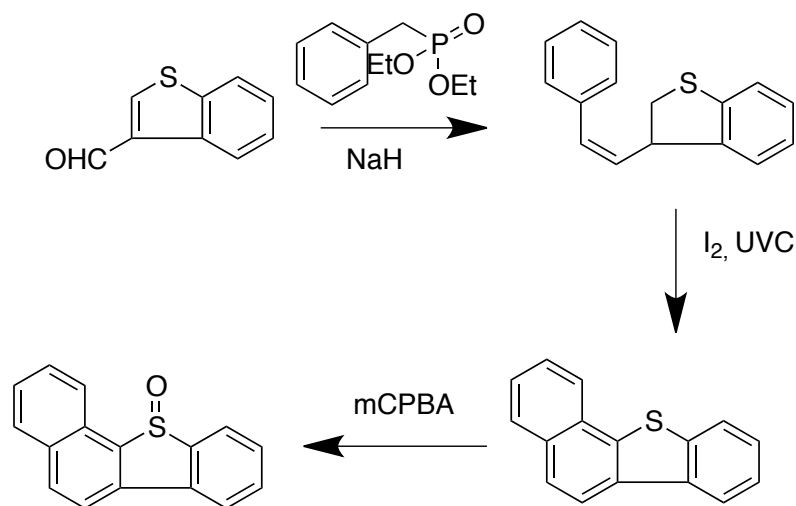
Preparation of benzo[b]naphtho[1,2-d]thiophene. This compound was prepared by slight modification of a previously reported method.³ To a solution of naphtho[2,1-b]thiophene (460mg, 2.5mmol) and 2,5-dimethoxytetrahydrofuran (DMTHF) 4 (0.7.mL 7.7mmol) in dry CH₂Cl₂ (10 mL) at 0 °C, triflic acid (0.22 mL, 2.5 mmol) was added and allowed to stir for 1hr. After consumption (monitored by TLC), the reaction mass was poured over ice water (20 mL), extracted with DCM (2 x 15 mL) and dried with Na₂SO₄. The solvent was then evaporated under reduced pressure and the crude product was purified using column chromatography (silica gel;

hexane) to yield benzo[b] naphtho[1,2-d]thiophene as colorless needles (351 mg, 60% yield). ¹H NMR (400 MHz, CDCl₃): δ 9.03 (d, J= 8.5 Hz, 1H), 8.88 (d, J= 8.3 Hz, 1H), 8.01- 8.06 (m, 2H), 7.89- 7.95 (m, 2H), 7.74-7.78 (m, 1H), 7.58- 7.64 (m, 2H), 7.50-7.54 (m, 1H). The spectra of this compound are consistent with literature report.³



Preparation of benzo[b]naphtho[1,2-d]thiophene S-oxide (1). In the reaction flask, 250.0mg (1.06mmol) benzo[b]naphtho[1,2-d]thiophene was dissolved in 100 mL of dichloromethane at -30°C. Then 355mg 77% mCPBA (1.59mmol) was dissolved in another 100 mL dichloromethane and added into the reaction mixture dropwise. After the reaction mixture warmed to room temperature, the reaction mixture was quenched with saturated sodium bicarbonate solution. After the organic layer was collected, the aqueous layer was then extracted with CH₂Cl₂ (3 times), and the combined organic extracts were dried over Na₂SO₄ and then evaporated to dryness. The crude product was subjected to column chromatography (SiO₂, dichloromethane as eluent) to Benzo[b]naphtho[1,2-d]thiophene S-oxide (83.3mg, 0.331mmol, 31.2% yield). ¹H NMR (400 MHz, CDCl₃): δ 8.16 (d, J=8.4 Hz, 1H), 8.47 (d, J= 7.9 Hz, 1H) 7.98-8.09 (m, 4H), 7.63-7.74 (m, 3H), 7.52- 7.56 (m, 1H). ¹³C NMR (400 MHz, CDCl₃): δ 145.97, 144.09, 138.07, 136.06, 132.58, 132.55, 130.74, 129.77, 129.55, 128.94, 128.66, 128.24, 127.80, 125.39, 124.45, 122.45. HRMS m/z calcd for C₁₆H₁₀OS(Na) 273.035 found 273.035.

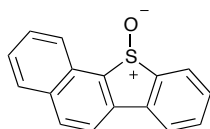
Scheme 2. Synthesis of benzo[b]naphtho[2,1-d]thiophene S-oxide (2)



Preparation of 3-styrylbenzo[b]thiophene. This compound was prepared by slight modification of a previously reported method. Sodium hydride (1.3 g, 54.18 mmol) was added to a mixture of 3-carbaldehydebenzo[b]thiophene (4.27 g, 26.3 mmol), diethyl benzylphosphonate (5.76 g, 25.2 mmol) in 50 mL of 1,2-dimethoxyethane at 0° C and stirred for 15 minutes at 0° C. The solution is gradually warmed to room temperature and stirred for 3 hr. The reaction mixture was poured into water ice and filtered. The filtered solid was recrystallized using ethanol to yield yellow solid of 3-styrylbenzo[b]thiophene (4.5 g, 76%). GCMS (EI) *m/z* 236, 235, 234, 221, 202. The spectra of this compound are consistent with literature report.⁴

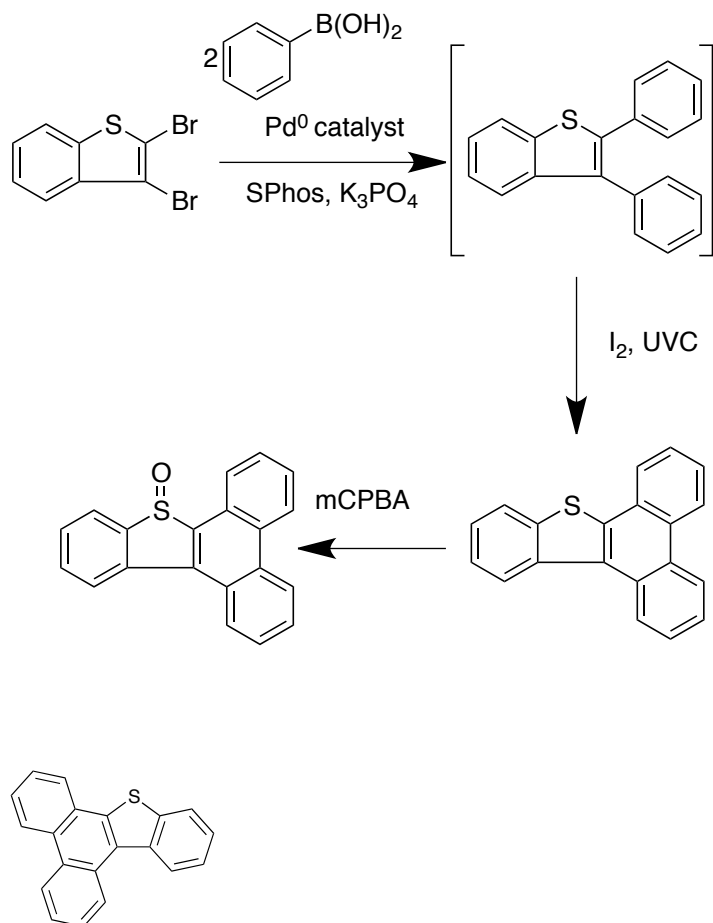
Preparation of benzo[b]naphtho[2,1-d]thiophene. This compound was prepared by slight modification of a previously reported method.⁴ In a 500 mL quartz flask, 3-styrylbenzo[b]thiophene (1.38 g, 5.8 mmol) and iodine (0.013 g, 0.3 mmol) were dissolved in toluene (500 mL). The solution was stirred and irradiated with UVC light (12 Luzchem 8 watts UVC light bulbs) overnight. The crude product was concentrated and recrystallized using hexane

which yielded benzo[b]naphtho[2,1-d]thiophene (920.0 mg, 67%). ¹H NMR (400 MHz, CDCl₃): δ 8.22- 8.24 (m, 1H), 8.19 (d, J= 8.6 Hz, 1H), 8.16 (d, J= 8.0 Hz, 1H), 7.97- 8.01 (m, 2H), 7.88 (d, J=8.6 Hz, 1H), 7.56-7.66 (m, 2H), 7.48-7.55 (m, 2H) The spectra of this compound are consistent with literature report.⁴



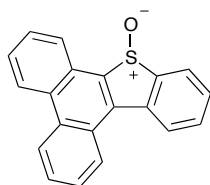
Preparation of benzo[b]naphtho[2,1-d]thiophene S-oxide (2). Benzo[b]naphtho[2,1-d]thiophene (250.0 mg, 1.06 mmol) was dissolved in 100 mL dichloromethane at -30°C. To this solution, 355mg of 77%-pure mCPBA (1.59mmol) was dissolved in another 100 mL dichloromethane and added dropwise. After the reaction mixture warm up to room temperature, the reaction mixture was quenched with saturated sodium bicarbonate solution. After the organic layer was separated, the aqueous layer was then extracted with CH₂Cl₂ (3 times), and the combined organic extracts were dried over Na₂SO₄ and then concentrated. The crude product was subjected to column chromatography (SiO₂, dichloromethane as eluent) to benzo[b]naphtho[1,2-d]thiophene S-oxide (126.1mg, 0.504mmol, 47.2% yield). ¹H NMR (400 MHz, CDCl₃): δ 8.54 (d, J= 8.3 Hz, 1H), 8.08 (dd, J₁= 8.4 Hz, J₂= 7.2 Hz, J₃= 3.6 Hz, 2H), 7.95 (d, J=8.2 Hz, 1H), 7.88 (dd, J₁= 5.5, J₂= 4.7 Hz, J₃= 2.9 Hz, 2H), 7.68-7.72 (m, 1H), 7.58-7.65 (m, 2H), 7.53 (td, J₁= 7.6 Hz, J₂=1.1 Hz, 1H). The spectrum of this compound was consistent with reported literature.⁵

Scheme 3. Synthesis of benzo[b]phenanthro[9,10-d]thiophene S-oxide(3)



Preparation of benzo[b]phenanthro[9,10-d]thiophene. This compound was prepared by slight modification of a previously reported method.⁶ 2,3-dibromobenzo[b]thiophene (3.054g, 10.45mmol), phenyl boronic acid (3.12 g, 25.69mmol), SPhos (197.7mg, 0.478mmol), Tetrakis(triphenylphosphine)palladium(0) (150mg, 0.130mmol) and K_3PO_4 (7.4 g , 32.21mmol) were dissolved in toluene (100.0 ml) and water (5.0 ml) in a 250 ml 3-neck round bottle flask. The mixture was degassed with Argon for 20 min and refluxed for 5 hours. Upon completion, the reaction mixture was cooled to room temperature and washed with water. The product was extracted from aqueous layer with toluene (20.0 ml) twice. The organic layer was dried with anhydrous MgSO_4 . The dried organic layer was diluted to 400 ml of toluene and added to a 500 ml quartz flask. Iodine (800.0 mg, 6.30 mmoles) was added to the quartz flask and the solution

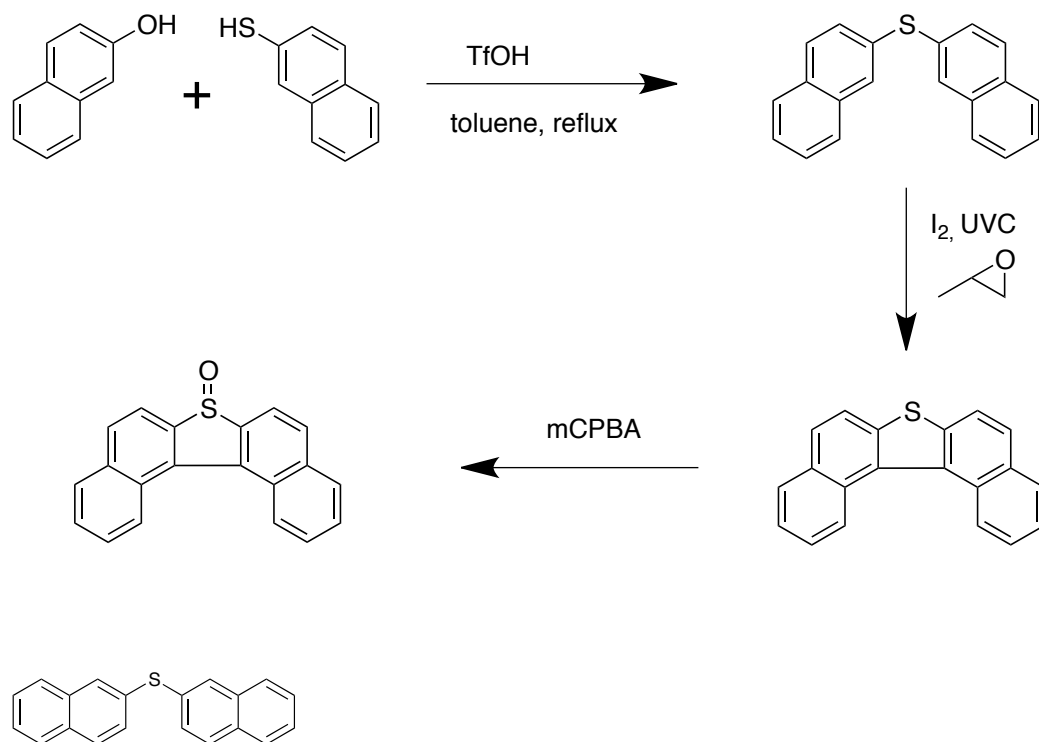
was irradiated with UV-C light (12 Luzchem 8 watts UVC light bulbs) overnight. Upon completion of the reaction, the excess iodine was quenched with saturated sodium bisulfate solution (50mL). The organic layer was separated and dried with anhydrous MgSO_4 and the aqueous layer was washed twice with dichloromethane. The combined organic layer was concentrated under reduced pressure. The crude product was recrystallized in hexanes which afforded white crystals of pure of Benzo[b]phenanthro[9,10-d]thiophene (1.324g, 45.21%). ^1H NMR (400 MHz, CDCl_3): δ 9.02 (dd, $J_1 = 7.1$ Hz, $J_2 = 1.1$ Hz, 1H), 8.78- 8.83 (m, 2H), 8.70- 8.72(m, 1H), 8.17-8.19 (m, 1H), 8.03 (dq, $J_1 = 7.9$ Hz, $J_2 = 0.6$ Hz, 1H), 7.75-7.79 (m, 1H), 7.65- 7.71 (m, 3H), 7.57-7.61 (m, 1H), 7.48-7.52 (m, 1H). The spectra of this compound are consistent with literature report.⁶



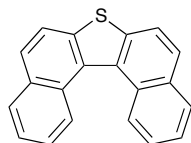
Preparation of benzo[b]phenanthro[9,10-d]thiophene S-oxide (3). The title compound was prepared by dissolving 517.3mg (1.82mmol) of benzo[b]phenanthro[9,10-d]thiophene in 100 mL dichloromethane at -30 °C. Then 600 mg of 77% mCPBA (2.68mmol) was dissolved in another 100 mL dichloromethane and added into the reaction mixture dropwise. After the reaction mixture was warmed to room temperature, the reaction mixture was quenched with saturated sodium bicarbonate solution. After the organic layer was separated, the aqueous layer was then extracted with CH_2Cl_2 (3 times), and the combined organic extracts were dried over Na_2SO_4 and then concentrated. The crude product was subjected to column chromatography (SiO_2 , dichloromethane as eluent) to yield benzo[b]phenanthro[9,10-d]thiophene S-oxide (160.0 mg,

0.533mmol, 29.3% yield). ^1H NMR (400 MHz, CDCl_3): δ 8.81- 8.89 (m, 2H), 8.68- 8.75 (m, 2H), 8.51 (d, J = 7.9 Hz, 1H), 8.14 (dd, J_1 = 7.2 Hz, J_2 = 0.8 Hz, 1H), 7.75-7.82(m, 4H), 7.71 (td, J_1 = 7.5 Hz J_2 = 1.3 Hz, 1H), 7.58 (td, J_1 = 7.5 Hz, J_2 = 0.9 Hz, 1H). ^{13}C NMR (400 MHz, CDCl_3): δ 145.41, 141.72, 138.03, 133.13, 132.39, 132.26, 130.76, 128.71, 128.53, 128.32, 128.29, 127.91, 127.73, 127.59, 125.49, 125.15, 124.08, 123.33. HRMS m/z calcd for $\text{C}_{20}\text{H}_{12}\text{OS}(\text{Na})$ 323.051 found 323.051.

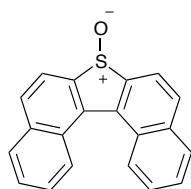
Scheme 4. Synthesis of dinaphtho[2,1-b:1',2'-d]thiophene *S*-oxide (**4**)



Preparation of 2,2'-thiobis-naphthalene. This compound was prepared by slight modification of a previously reported method.⁷ A solution of 2-naphthol (1663.8 mg, 11.59 mmol) and 2-naphthalenethiol (1396.4 mg, 8.73 mmol) in the presence of trifluoromethanesulfonic acid (0.5ml, 5.64 mmol) was refluxed in toluene for 4 h. After the reaction was cooled, the reaction was quenched with saturated NaOH solution. The mixture was then extracted with CH₂Cl₂ (3 times), and the combined organic extracts were washed with H₂O, dried over Na₂SO₄ and then evaporated to dryness. The crude product was stirred in hot hexane (150 mL) and toluene (20 mL) until the solid was dissolved. The hot solution was placed into the freezer at -30 °C overnight to allow crystal formation. This resulted in 2054.8mg (7.18mmol) of a white powder, which was obtained through vacuum filtration (82.3% yield). GCMS (EI) *m/z* 286, 252. The spectra of this compound are consistent with literature report.⁷

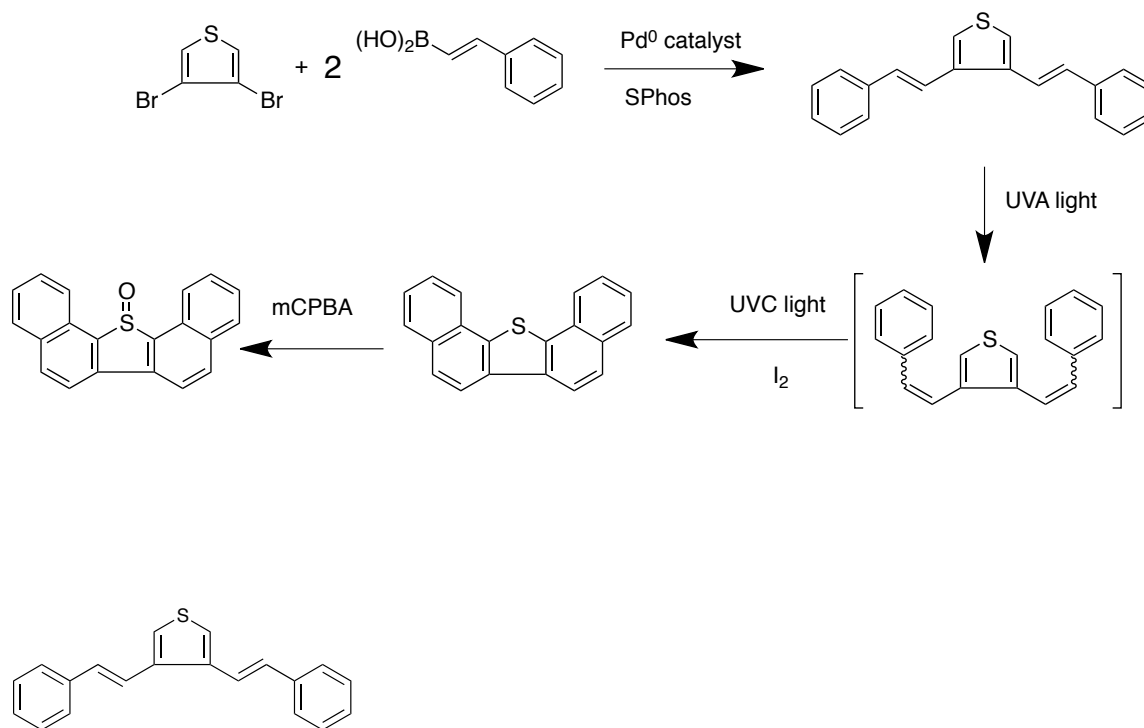


Preparation of dinaphtho[2,1-b:1',2'-d]thiophene. This compound was prepared by slight modification of a previously reported method.⁷ A solution of 2,2'-thiobis-naphthalene (300 mg, 1.05 mmol), I₂ (320 mg, 1.26 mmol) and propylene oxide (366 mg, 0.44 mL, 6.30 mmol in 500 mL dichloromethane was charged in a 500 mL quartz flask. The mixture was irradiated with UVC light (12 Luzchem 8 watts UVC light bulbs) overnight. Upon completion, the solution was evaporated to dryness, and the crude product was subjected to column chromatography (SiO₂, hexane as eluent) to yield dinaphtho[2,1-b:1',2'-d]thiophene (228 mg, 85% yield). ¹H NMR (400 MHz, CDCl₃): δ 8.88- 8.90 (m, 2H), 8.04-8.06 (m, 2H), 7.93-7.99 (m, 4H), 7.58- 7.60 (m, 4H). The spectra of this compound are consistent with literature report.⁷



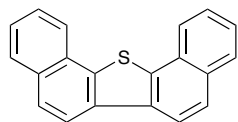
Preparation of dinaphtho[2,1-b:1',2'-d]thiophene *S*-oxide (4). A solution containing 120.0mg (0.42mmol) of dinaphtho[2,1-b:1',2'-d]thiophene in 100 mL dichloromethane at -30°C was prepared. Then 127mg 77% mCPBA (0.56mmol) was dissolved in another 100 mL dichloromethane and added into the reaction mixture dropwise. After the reaction mixture was warmed to room temperature, the reaction mixture was quenched with saturated sodium bicarbonate solution. After the organic layer was separated, the aqueous layer was then extracted with CH₂Cl₂ (3 times), and the combined organic extracts were dried over Na₂SO₄ and then evaporated to dryness. The crude product was subjected to column chromatography (SiO₂, dichloromethane as eluent) to yield dinaphtho[2,1-b:1',2'-d]thiophene *S*-oxide (31.2 mg, 0.110mmol, 26.1% yield). ¹H NMR (400 MHz, CDCl₃): δ 8.44 (d, J= 8.4 Hz, 2H), 8.09-8.15(m, 2H), 8.03 (d, J= 8.7 Hz, 2H), 7.60- 7.69 (m, 4H). ¹³C NMR (400 MHz, DMSO): δ 144.51, 136.90, 135.19, 130.93, 129.30, 129.26, 128.27, 127.96, 126.64, 122.70. C₂₀H₁₂OS(Na) 323.051 found 323.050.

Scheme 5. Synthesis of Dinaphtho[1,2-b:2',1'-d]thiophene S-oxide (**5**)

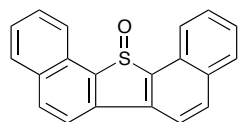


Preparation of 3,4-Distyrylthiophene. 3,4-dibromothiophene (1300.0 mg, 5.37 mmol), *trans*-2-Phenylvinylboronic acid (2000.0 mg, 13.52 mmol), 2-Dicyclohexylphosphino-2',6'-dimethoxybiphenyl (88.0 mg, 0.21 mmol), K₃PO₄ (3439 mg, 16.20 mmol) were dissolved in a solvent mixture of toluene (100.0 ml), water (5.0 mL) and methanol (15.0 mL). Argon gas was purged through the solution for 30 min. Pd₂(dba)₃ (124.4 mg, 0.14 mmol) was then added the solution. The reaction mixture was refluxed overnight at 78⁰C temperature. The crude product was purified using flash chromatography using hexanes as the eluent. This afforded pure 3,4-distyrylthiophene (1098.5 mg, 71.0%) as a white solid. ¹H NMR (400 MHz, DMSO): δ 7.82 (s,2H), 7.67 (d, J=7.6 Hz, 4H), 7.45 (d, J=16.2, 2H), 7.39 (dd, J₁= 7.44 Hz, J₂= 7.4 Hz, 2H), 7.28 (dd, J₁=7.12, J₂=6.96, 2H), 7.13 (d, J=16.2, 2H). ¹³C NMR (400 MHz, DMSO): δ 138.07,

137.09, 130.02, 128.56, 127.49, 126.49, 121.33, 121.08. HRMS m/z calcd for $C_{20}H_{16}S$ 288.097 found 288.097.



Preparation of Dinaphtho[1,2-*b*:2',1'-*d*]thiophene. (300.0 mg, 1.04 mmol) was dissolved in a mixture of hexanes (400.0 ml) and dichloromethane (20.0 ml) in a 500 ml quartz flask. Propylene oxide (1.0 ml, 14.29 mmol) was added to the solution and Argon gas was purged through the solution for 30 min. The solution was irradiated with UV-A light for 2 hours. The color of the solution changed to yellow from colorless. Iodine (150.0 mg, 0.59 mmol) was dissolved in dichloromethane (10.0 ml) and added to the solution. The solution was then irradiated with UV-C light for 2 hours. This afforded dinaphtho[1,2-*b*:2',1'-*d*]thiophene. (21.3mg, 7.2%) as a white solid. 1H NMR (400 MHz, $CDCl_3$): δ 8.27 (d, J = 8.6 Hz, 2H), 8.25 (d, J =8.8 Hz, 2H), 8.02 (d, J = 8.0 Hz, 2H), 7.93 (d, J = 8.6 Hz, 2H), 7.67 (dd, J_1 = 7.7 Hz, J_2 = 7.3 Hz, 2H), 7.59 (dd, J_1 = 7.9 Hz, J_2 = 7.04 Hz, 2H). ^{13}C NMR (400 MHz, $CDCl_3$): δ 136.98, 134.03, 132.34, 129.35, 129.21, 127.08, 126.37, 125.91, 124.52, 120.01. HRMS m/z calcd for $C_{20}H_{12}S$ 284.066 found 284.066.

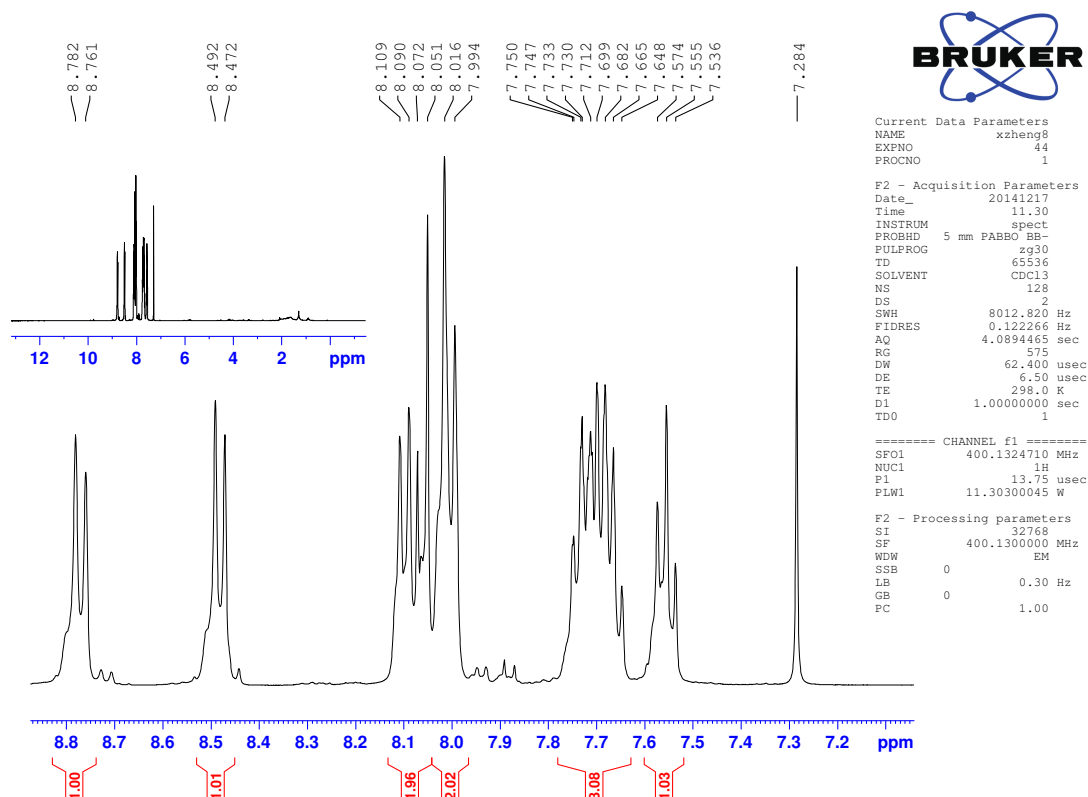


Preparation dinaphtho[1,2-*b*:2',1'-*d*]thiophene *S*-oxide (5). Dinaphtho[1,2-*b*:2',1'-*d*]thiophene (20.0 mg, 0.07 mmol) was dissolved in dichloromethane (20.0 ml) at 0°C. To this solution, 77% mCPBA(19.0 mg, 0.08 mmol) was dissolved in dichloromethane (3.0 mL) and was added

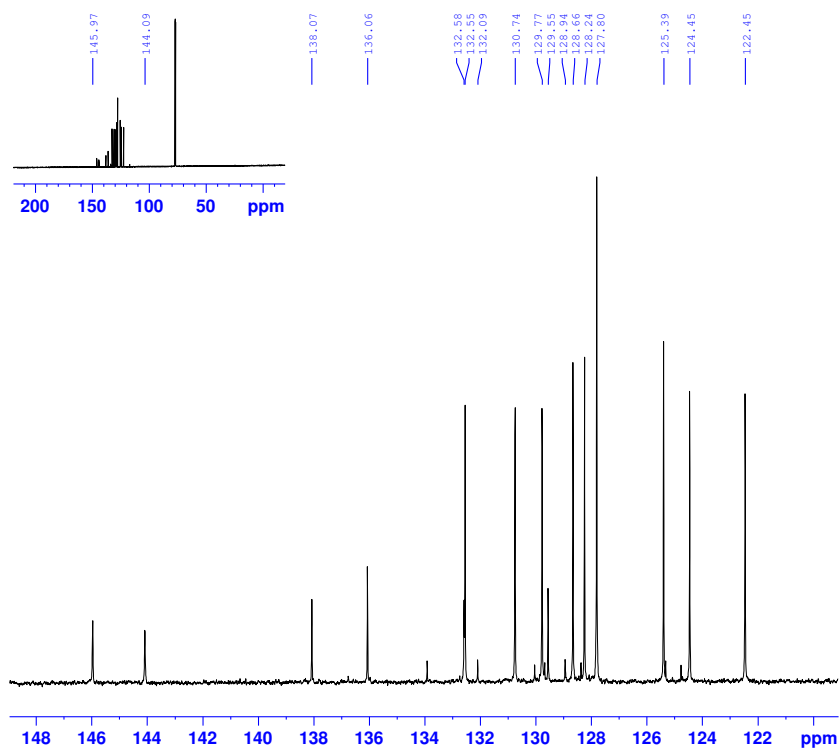
dropwise the solution containing dinaphtho[1,2-*b*:2',1'-*d*]thiophene. The reaction was monitored using TLC with CH₂Cl₂ as eluent. The reaction mixture was stirred for 4 hours and the excess mCPBA was quenched with saturated sodium bicarbonate solution. The product was extracted with CH₂Cl₂ and the organic layer was dried using anhydrous Na₂SO₄. The dried organic layer was concentrated under reduced pressure the crude product was purified using column chromatography with CH₂Cl₂ as eluent. This afforded pure Dinaphtho[1,2-*b*:2',1'-*d*]thiophene *S*-oxide (7.8 mg, 38.1%). ¹H NMR (400 MHz, CDCl₃): δ 8.61 (d, J=8.4 Hz, 2H), 8.12 (d, J=8.4 Hz, 2H), 7.97 (d, J=8.5 Hz, 4H), 7.73 (t, J=7.6 Hz, 2H), 7.61 (t, J=7.6 Hz, 2H). ¹³C NMR (400 MHz, CDCl₃): δ 140.77, 135.98, 134.18, 133.81, 130.96, 129.29, 129.11, 127.47, 124.13, 119.19. HRMS m/z calcd for C₂₀H₁₂OS 300.061 found 300.061.

Supporting Spectra benzo[*b*]naphtho[1,2-*d*]thiophene *S*-oxide (1)

¹H-NMR of compound 1 in CDCl₃



C13 NMR of Compound **1** in CDCl₃



BRUKER

Current Data Parameters
 NAME xzheng8
 EXPNO 45
 PROCNO 1

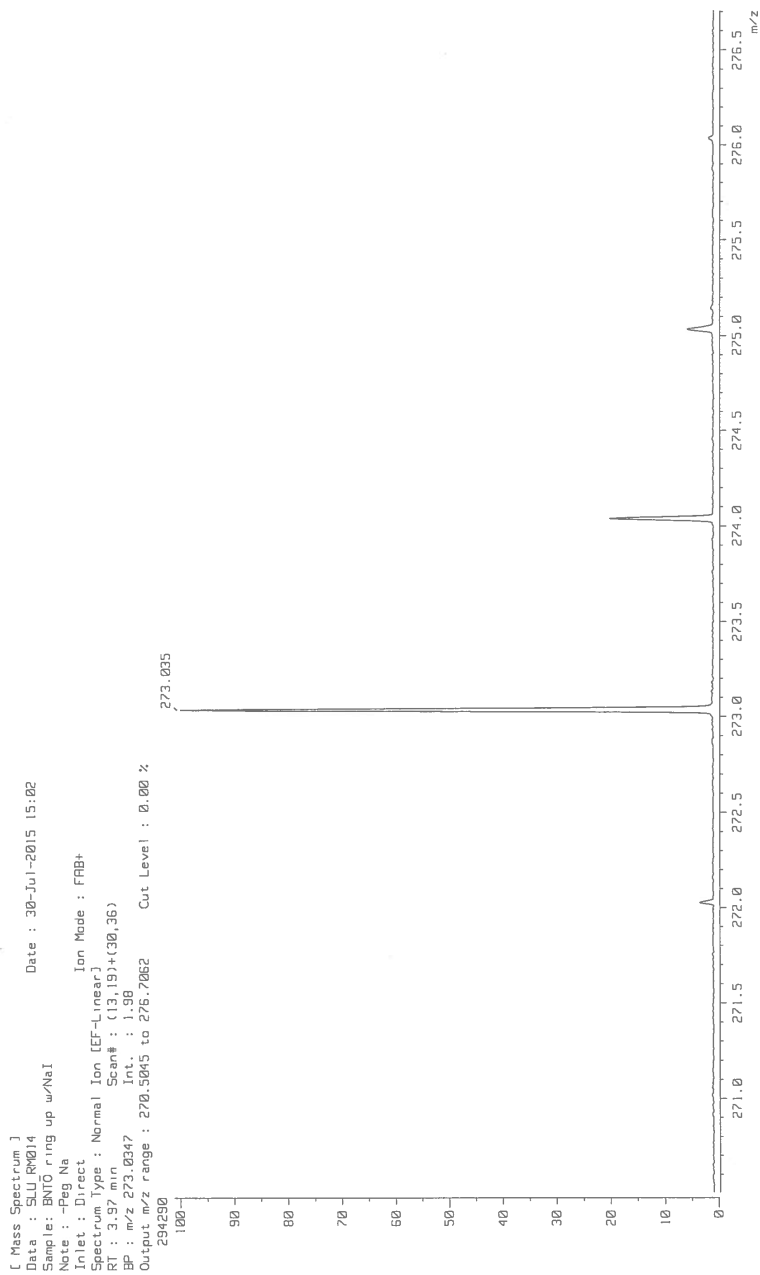
F2 - Acquisition Parameters
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 Time 2.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 10240
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 1150
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 =====
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 P1 8.50 usec
 PLW1 61.42300034 W

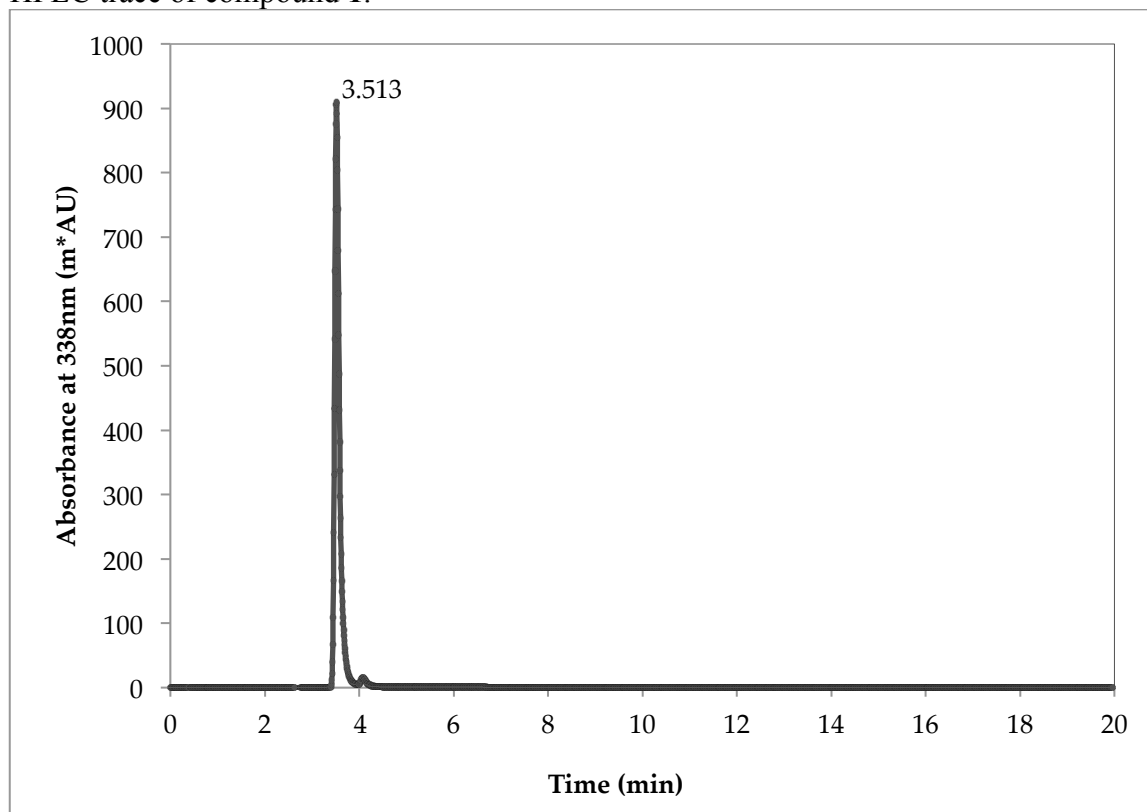
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 NUC2 1H
 CPMRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 11.30300045 W
 PLW12 0.27351999 W
 PLW13 0.22155000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

HRMS of compound 1 with NaI as cosolute

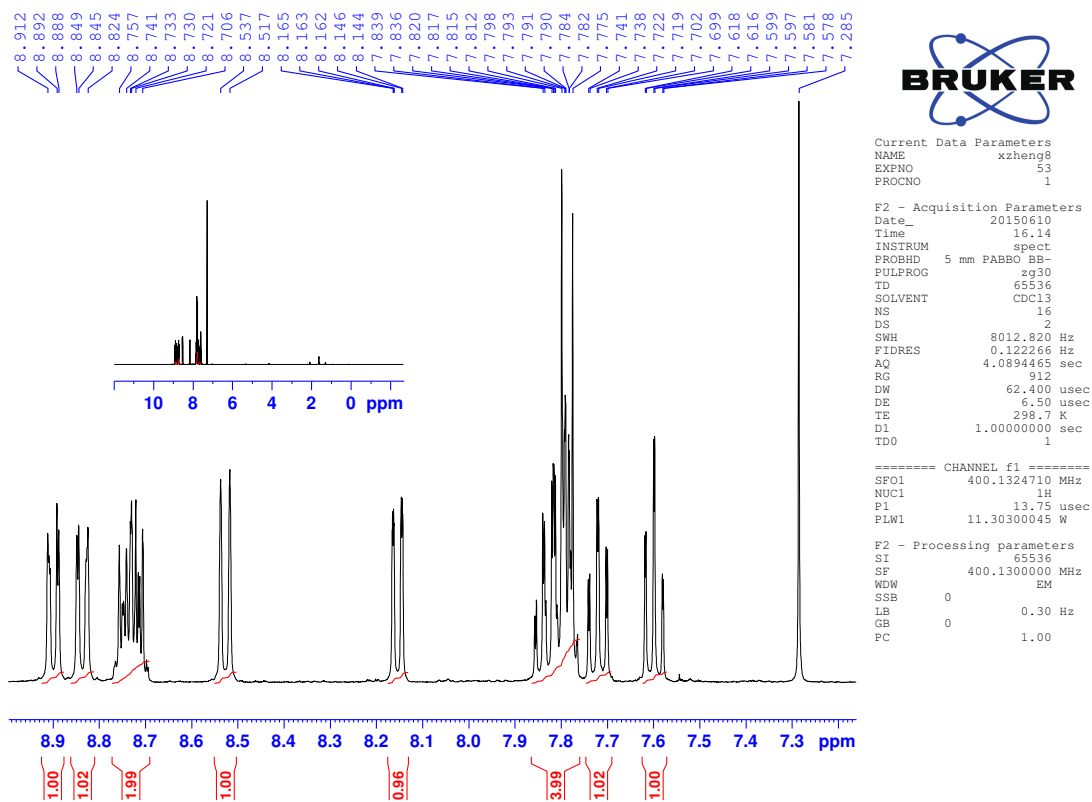


HPLC trace of compound 1.



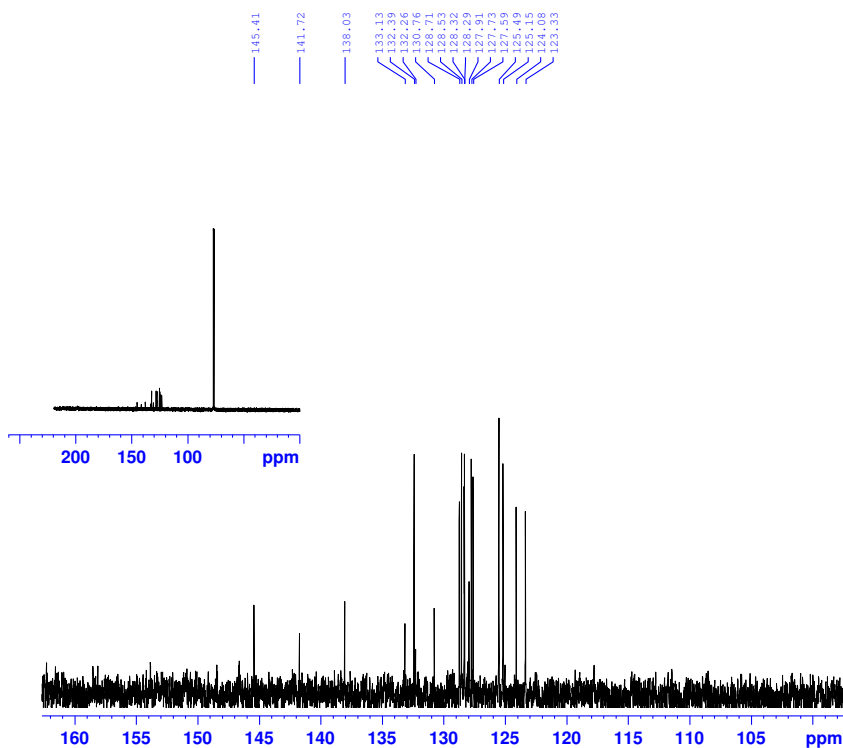
benzo[b]phenanthro[9,10-d]thiophene S-oxide (3)

¹H-NMR of compound 3 in CDCl₃



¹³C-NMR of compound **3** in CDCl₃

BPTO C13 NMR



Current Data Parameters
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EXPNO 56
PROCNO 1

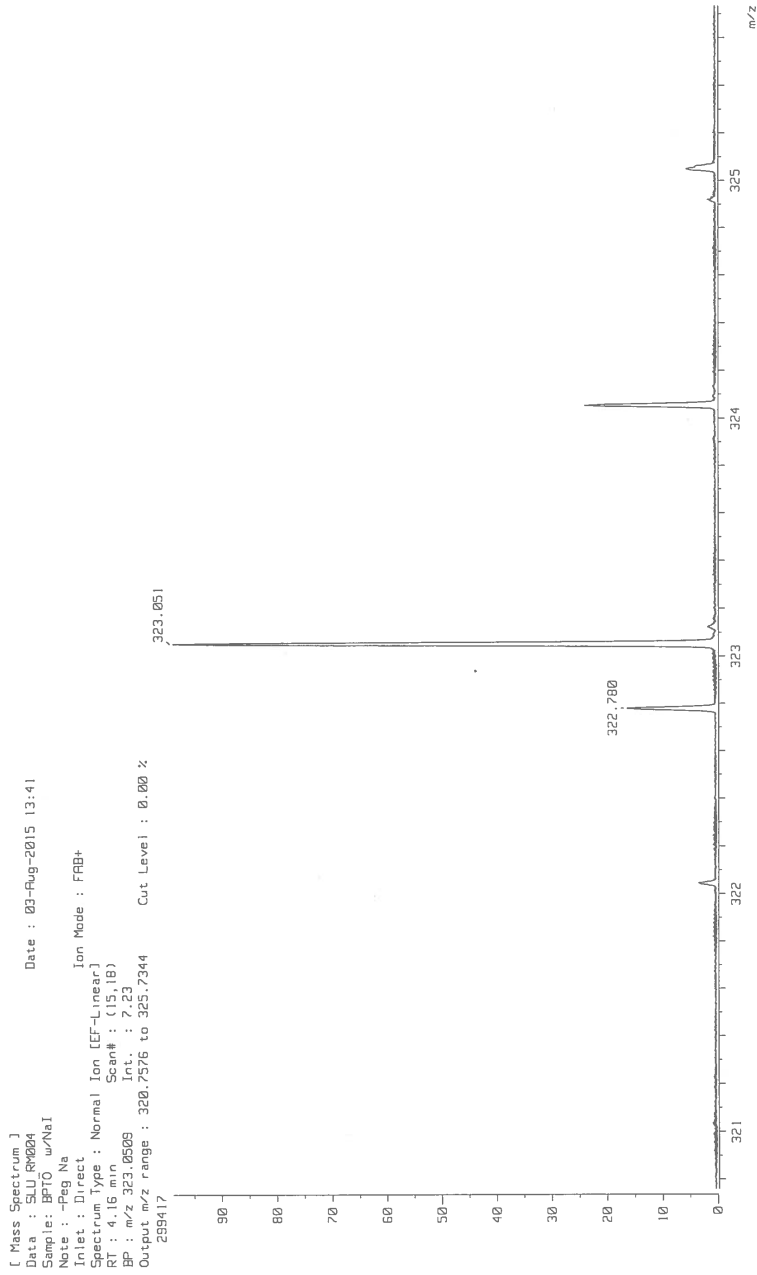
F2 - Acquisition Parameters
Date_ 20150611
Time 5.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 12000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
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NUC1 13C
P1 8.50 usec
PLW1 61.42300034 W

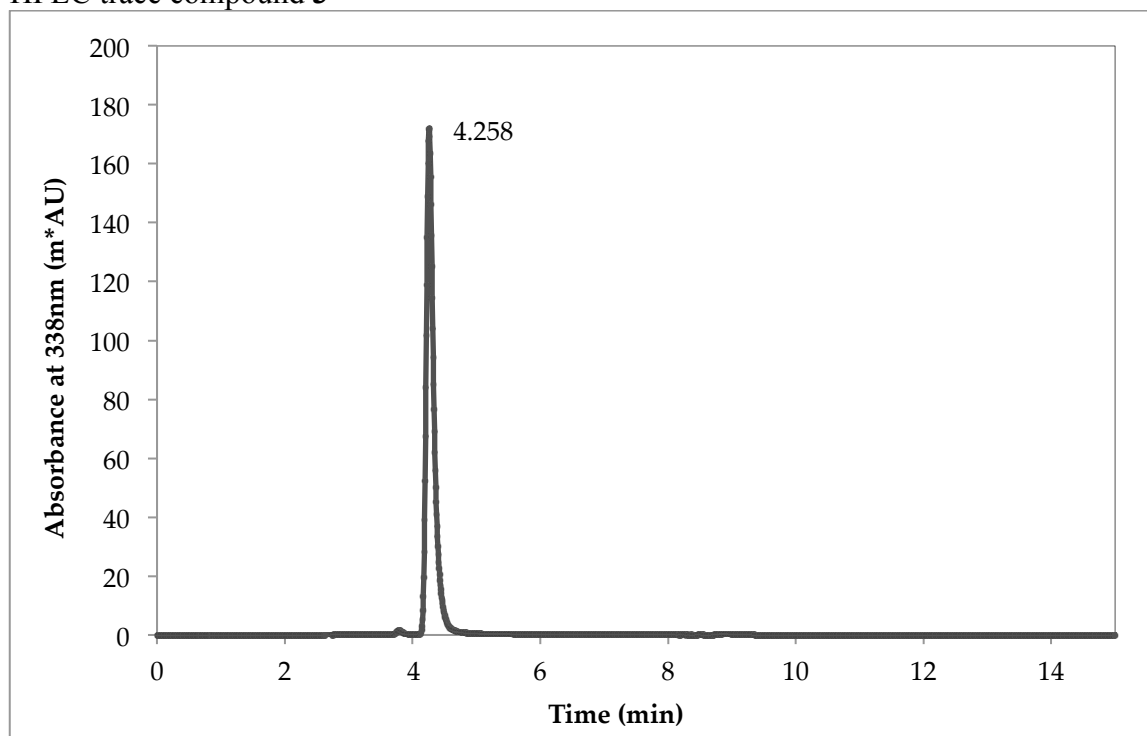
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NUC2 1H
PCPDG[2] waltz16
PCPD2 90.00 usec
PLW2 11.30300045 W
PLW12 0.27351999 W
PLW13 0.22155000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS of compound **3** with NaI as cosolute

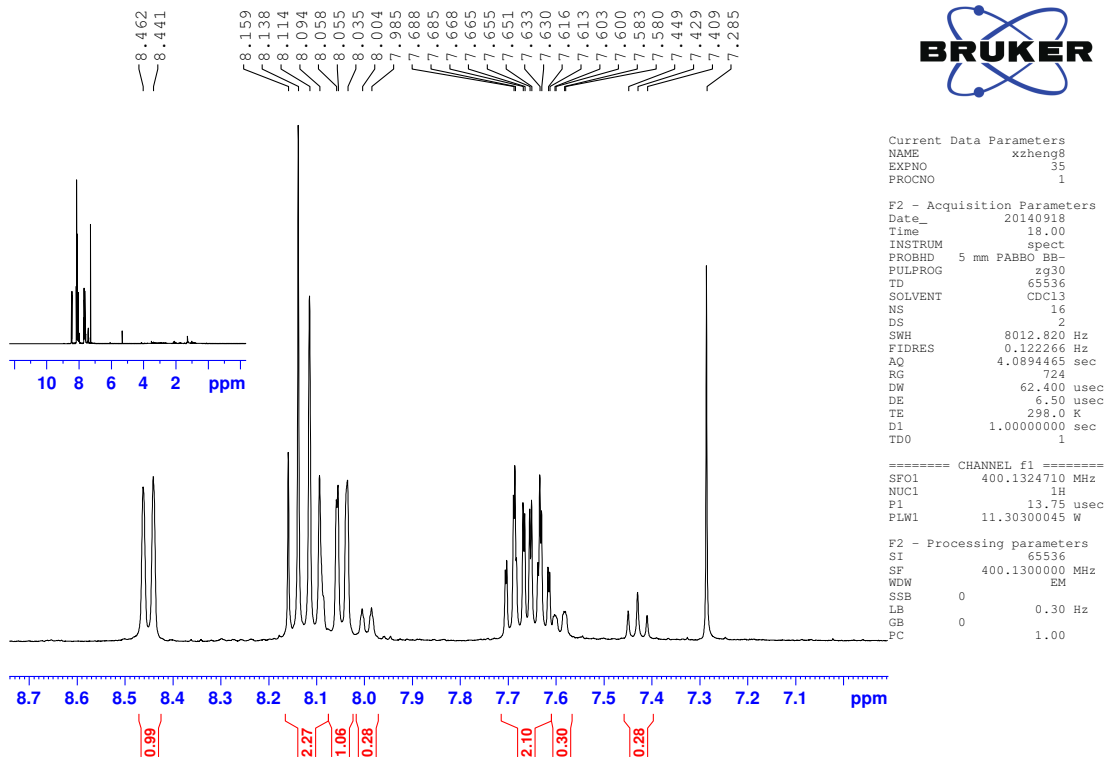


HPLC trace compound 3

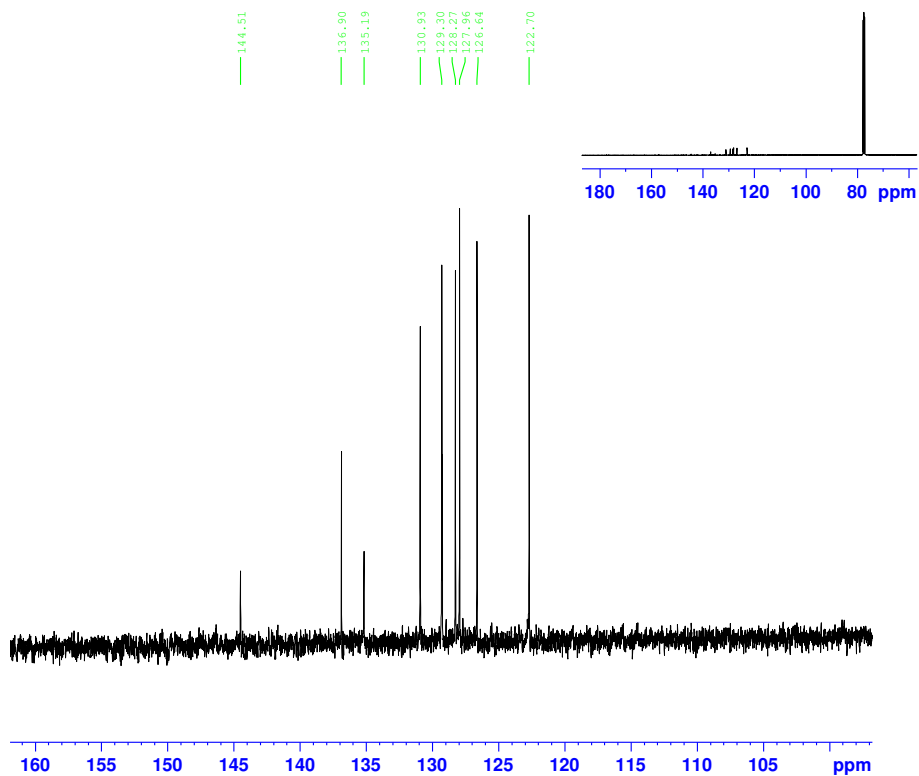


dinaphtho[2,1-*b*:2',1'-*d*]thiophene *S*-oxide (4).

¹H-NMR of Compound 4 in CDCl₃



¹³C-NMR of Compound 4 in CDCl₃



Current Data Parameters
NAME xzheng8
EXPNO 22
PROCNO 22

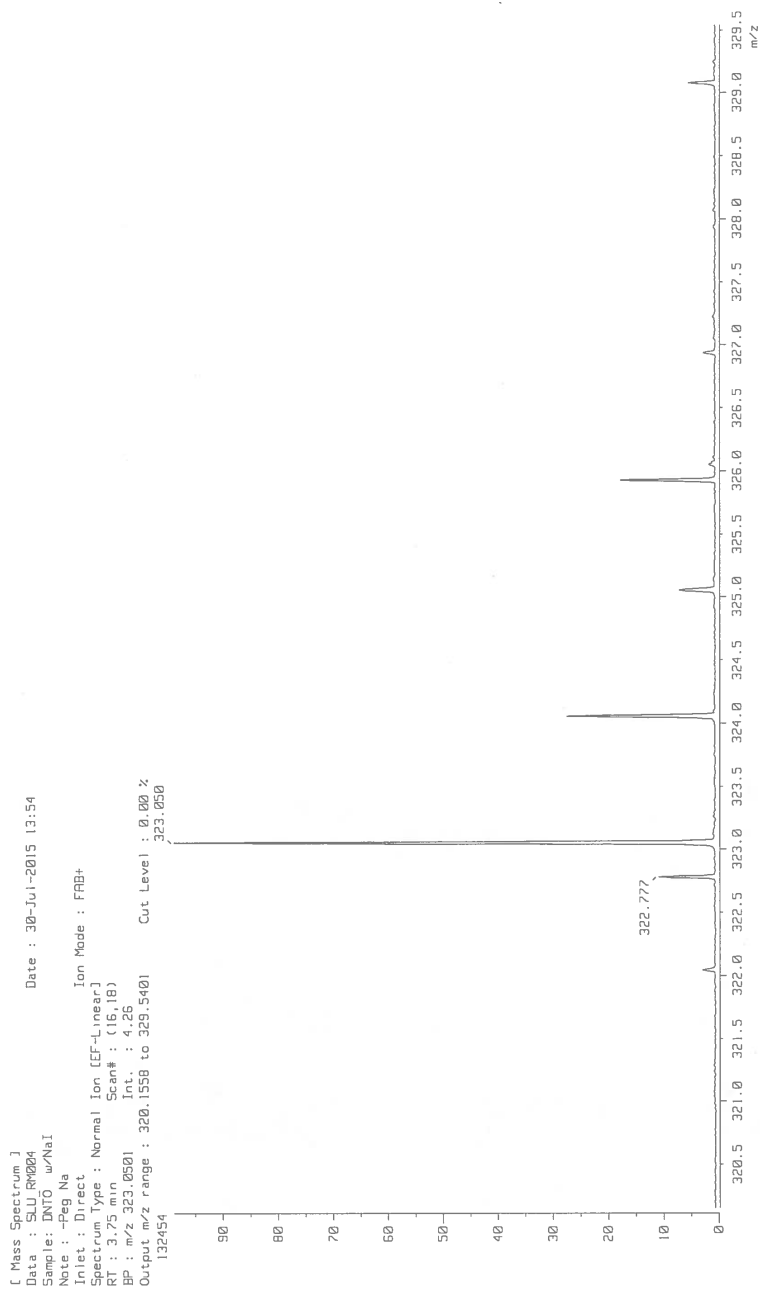
F2 - Acquisition Parameters
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Time 17.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 812
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 8.50 usec
PLW1 61.42300034 W

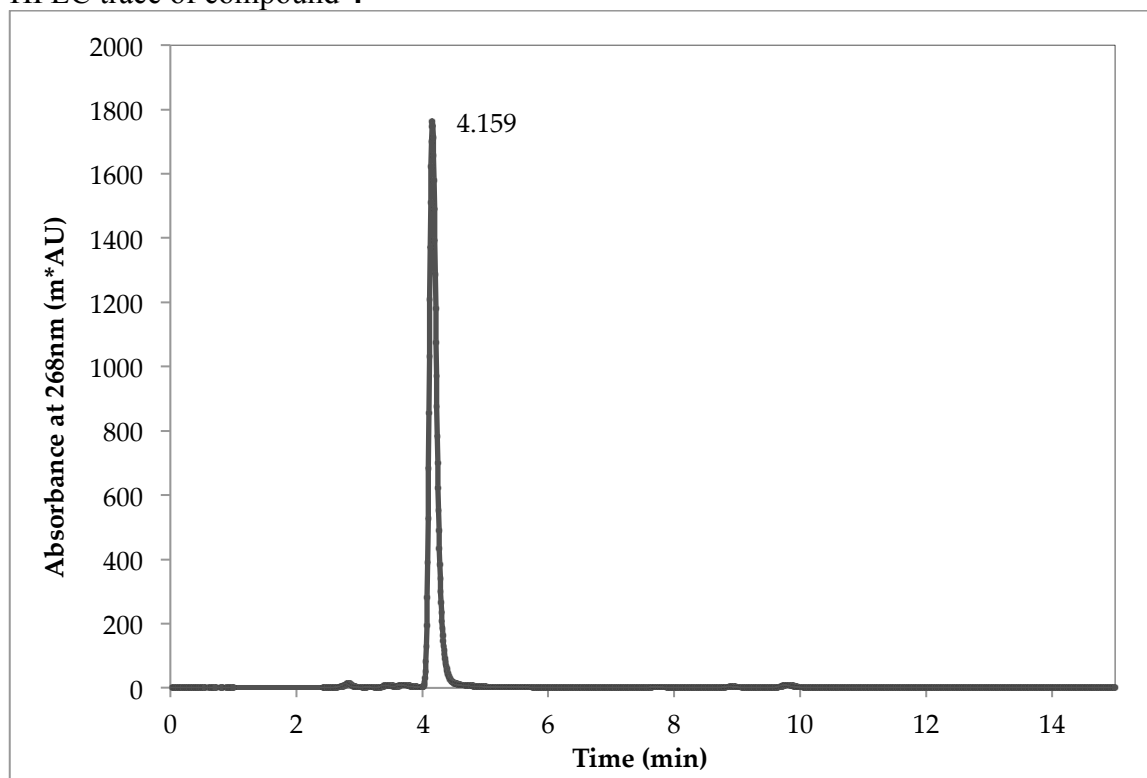
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NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 11.30300045 W
PLW12 0.27351999 W
PLW13 0.22155000 W

F2 - Processing parameters
SI 32768
SF 100.6127378 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

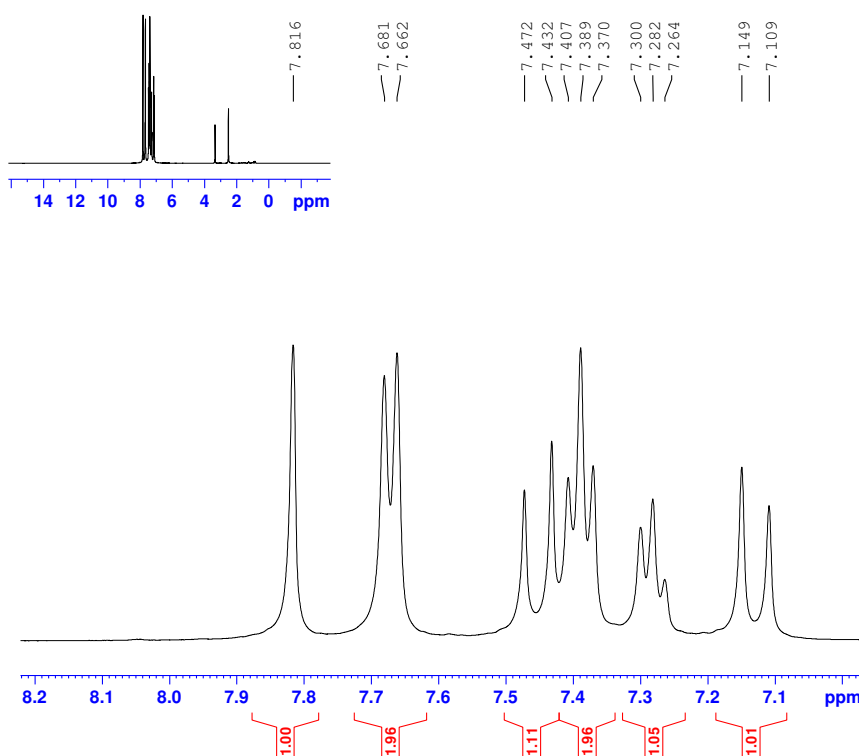
HRMS of compound 4 with NaI as cosolute



HPLC trace of compound 4



¹H-NMR of 3,4-bis[(1E)-2-phenylethenyl]-thiophene in DMSO-d₆



```

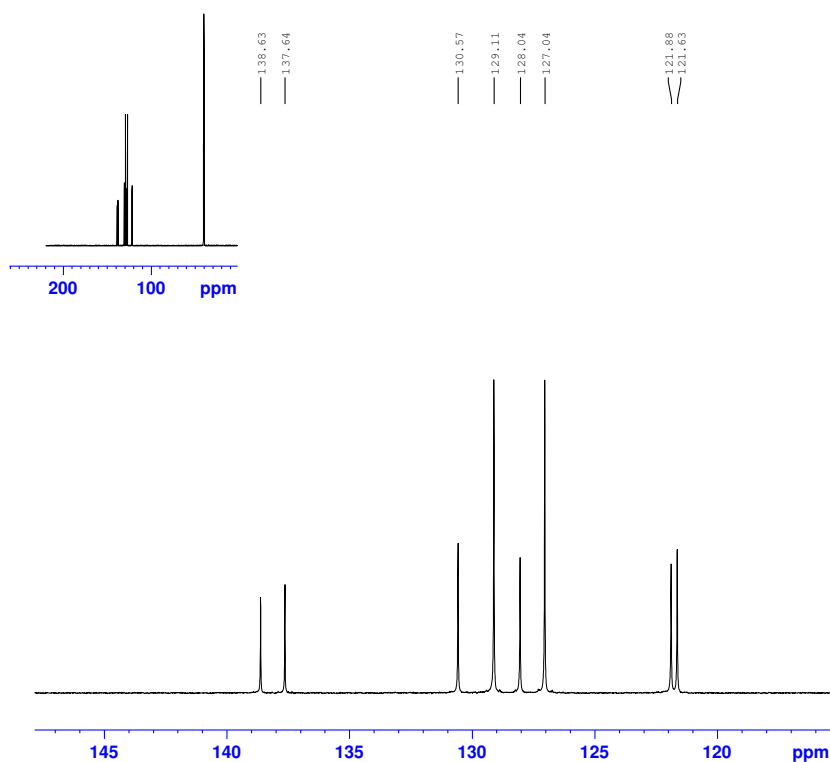
Current Data Parameters
NAME          xzheng8
EXPNO         75
PROCNO        1

F2 - Acquisition Parameters
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Time          21.53
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PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            406
DW            62.400 usec
DE            6.50 usec
TE            298.2 K
D1            1.00000000 sec
TDO           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1           1H
P1            13.75 usec
PLW1          11.30300045 W

F2 - Processing parameters
SI            65536
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
    
```

¹³C-NMR of 3,4-bis[(1E)-2-phenylethenyl]-thiophene in DMSO-d₆



```

Current Data Parameters
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EXPNO         76
PROCNO        1

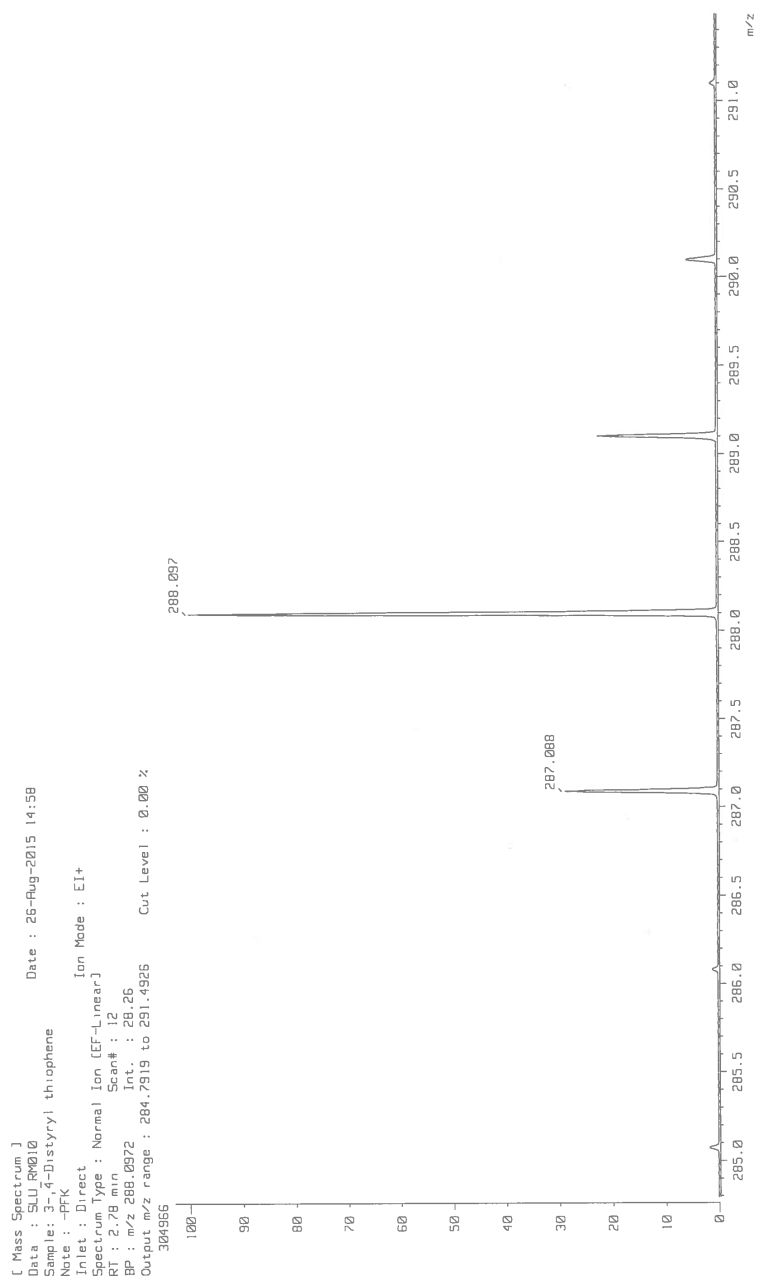
F2 - Acquisition Parameters
Date_         20150823
Time          11.24
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            14000
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            1440
DW            20.800 usec
DE            6.50 usec
TE            298.4 K
D1            2.0000000 sec
D11           0.0300000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          100.6228298 MHz
NUC1           13C
P1             8.50 usec
PLW1          61.42300034 W

===== CHANNEL f2 =====
SFO2          400.1316005 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         90.00 usec
PLW2          11.30300045 W
PLW12         0.27351999 W
PLW13         0.22155000 W

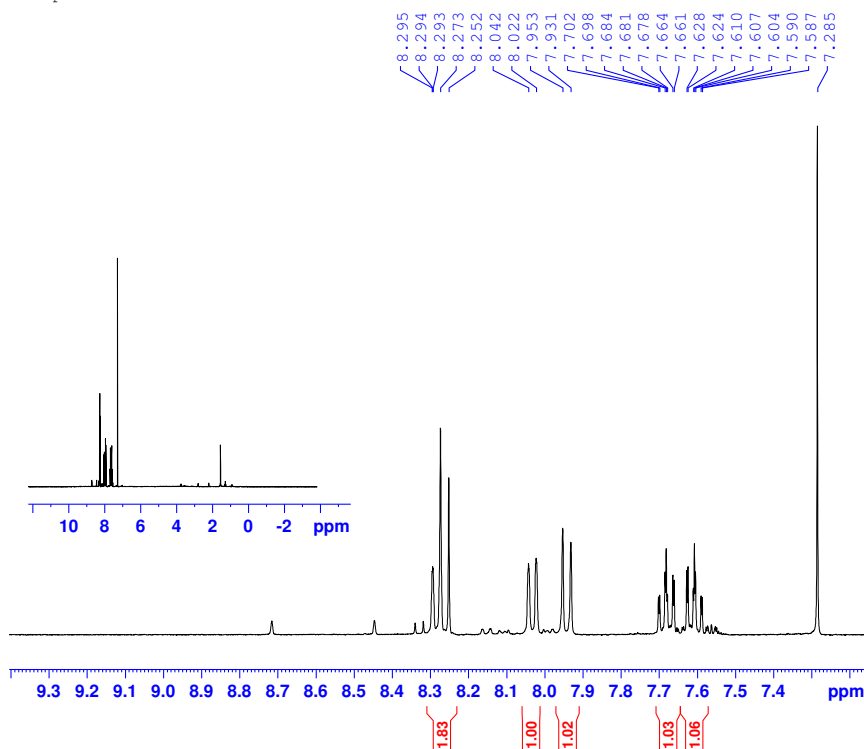
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WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

HRMS of 3,4-bis[(1E)-2-phenylethenyl]-thiophene



¹H-NMR of dinaphtho[1,2-b:2',1'-d]thiophene in CDCl₃

DNT up



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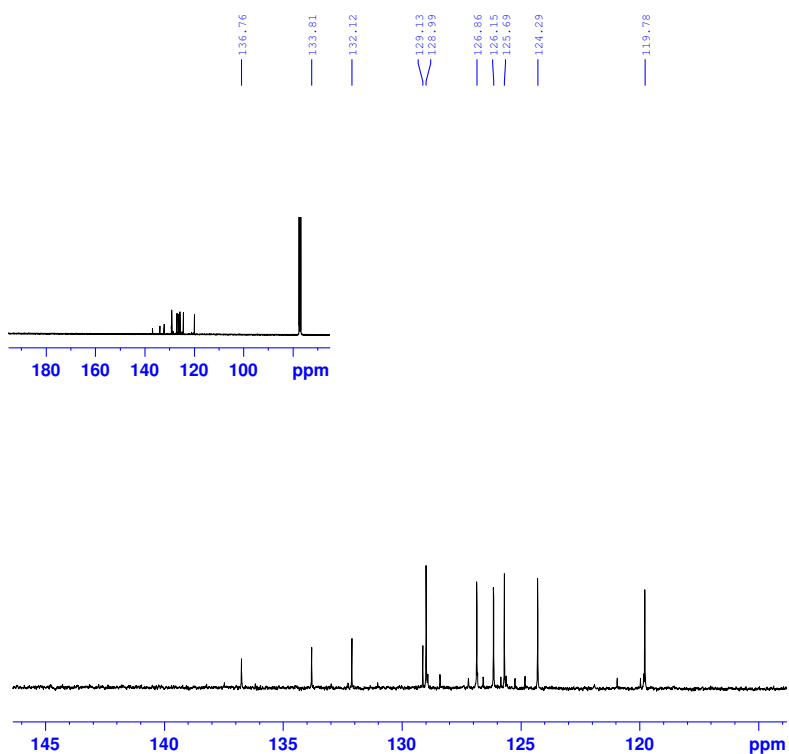
Current Data Parameters
NAME          xzheng8
EXPNO         71
PROCNO        1

F2 - Acquisition Parameters
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Time          19.17
INSTRUM       spect
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PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            16
DS            2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG            1030
DW            62.400 usec
DE            6.50 usec
TE            298.1 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          400.1324710 MHz
NUC1           1H
P1            13.75 usec
PLW1          11.30300045 W

F2 - Processing parameters
SI            65536
SF            400.1300000 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
FC            1.00
    
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¹³C NMR of **dinaphtho[1,2-b:2',1'-d]thiophene** in CDCl₃



Current Data Parameters
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EXPNO 72
PROCNO 1

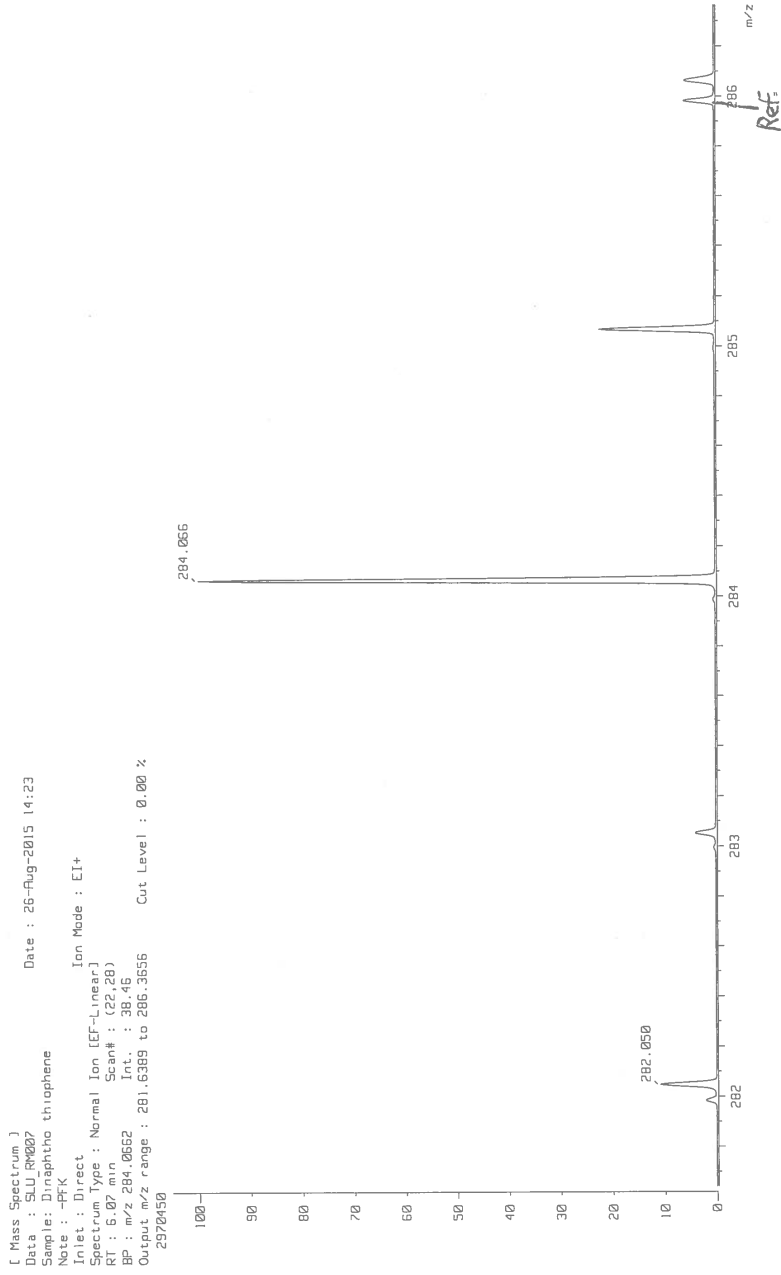
F2 - Acquisition Parameters
Date_ 20150806
Time 7.44
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 1620
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228298 MHz
NUC1 13C
P1 8.50 usec
PLW1 61.4230034 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
PCPDG[2] waltz16
PCPD2 90.00 usec
PLW2 11.3030045 W
PLW12 0.27351999 W
PLW13 0.22155000 W

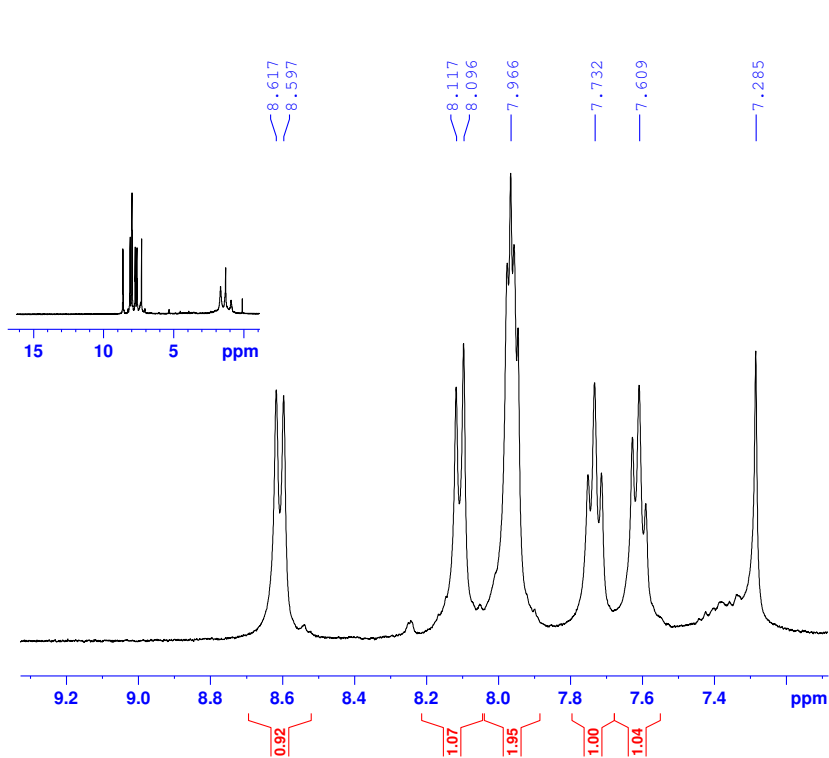
F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS of dinaphtho[1,2-b:2',1'-d]thiophene



dinaphtho[1,2-*b*:2',1'-*d*]thiophene *S*-oxide (5).

¹H-NMR of compound **5** in CDCl₃



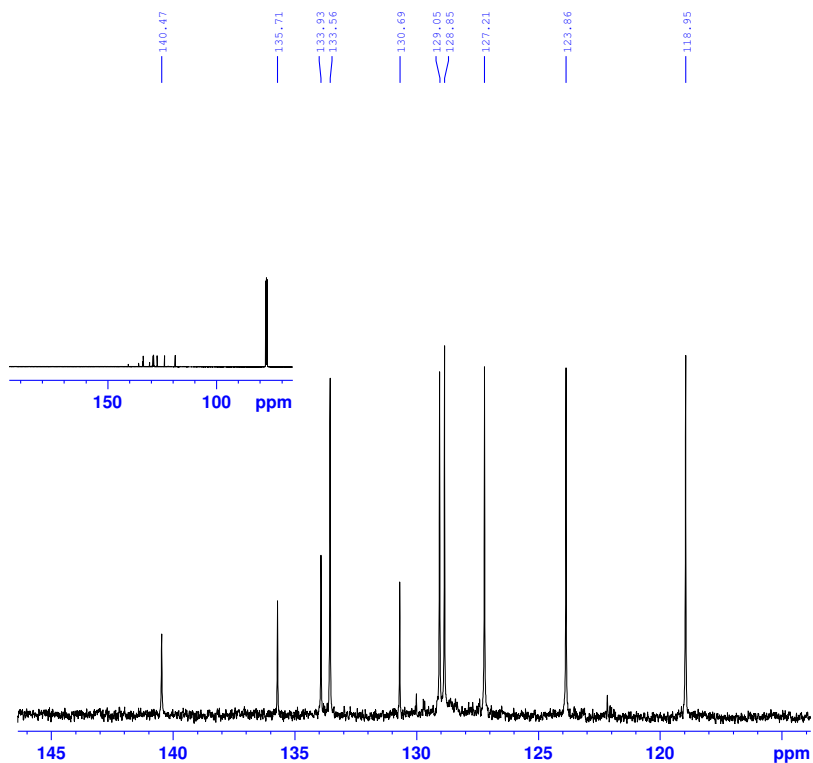
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Current:
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EXPNO     73
PROCNO    1

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PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894465 sec
RG        724
DW        62.400 usec
DE        6.50 usec
TE        298.1 K
D1        1.00000000 sec
TDO       1

===== CHANNEL f1 =====
SF01      400.1324710 MHz
NUC1      1H
P1        13.75 usec
PLW1      11.30300045 W

F2 - Processing parameters
SI        65536
SF        400.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
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^{13}C -NMR of compound **5** in CDCl_3



Current Data Parameters
NAME xzheng8
EXPNO 74
PROCNO 1

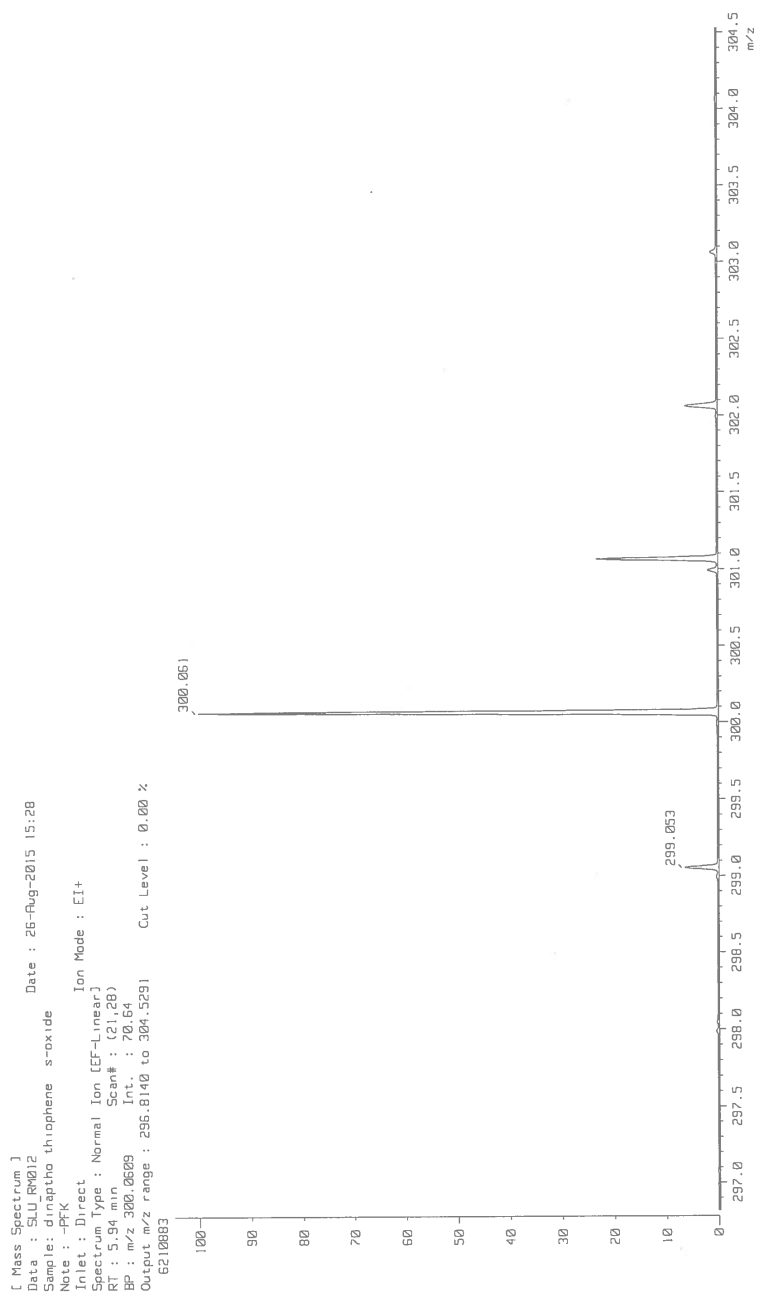
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Time 16.43
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 1820
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
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NUC1 13C
P1 8.50 usec
PLW1 61.42300034 W

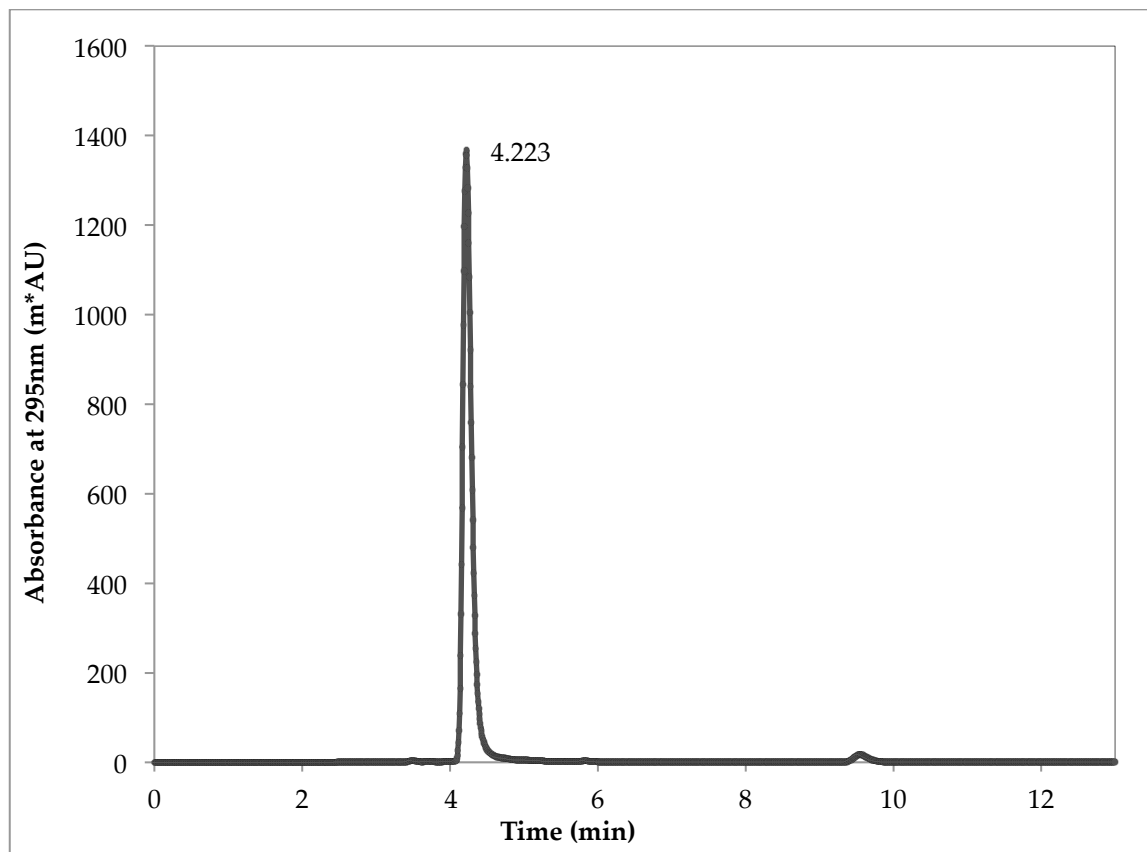
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NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 11.30300045 W
PLW12 0.27351999 W
PLW13 0.22155000 W

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS of compound 5



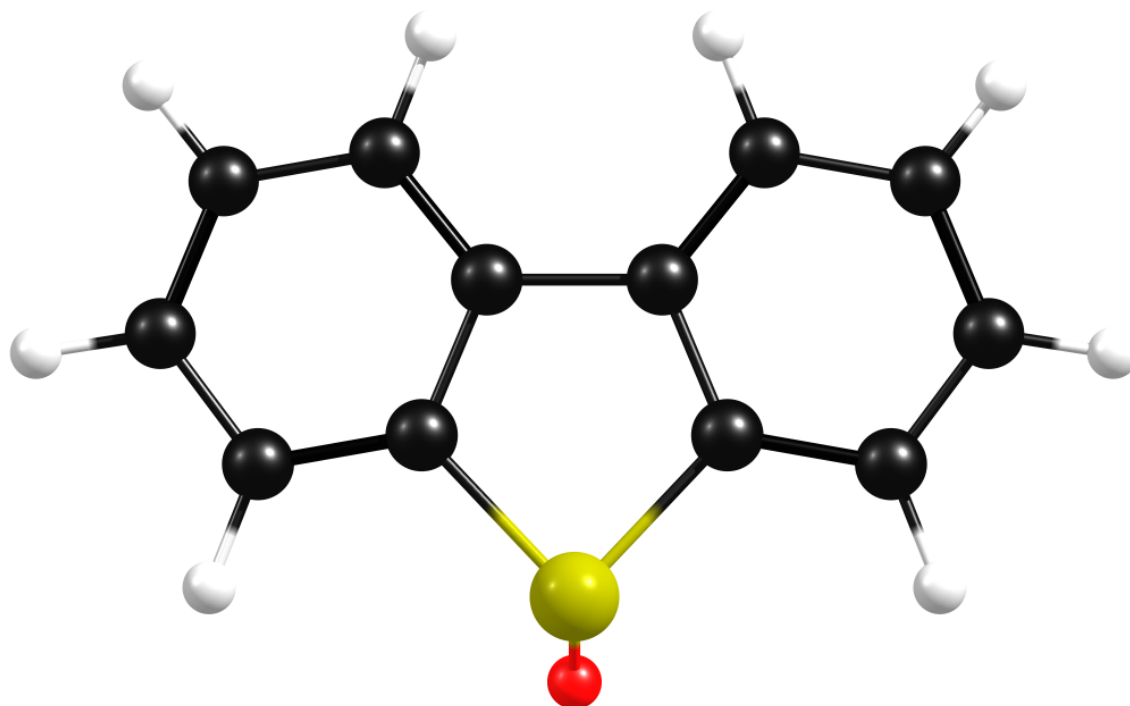
HPLC trace for compound 5



Computational Results

Calculations for Excited State Energies

Dibenzothiophene *S*-oxide (**DBTO**) S_0 state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	0.000013	1.765873	-0.408312
C	1.611913	-1.891700	0.067006
C	0.735551	-0.807517	-0.040894
C	2.988848	-1.658283	0.098599
H	3.670962	-2.498441	0.192409
C	1.267361	0.489072	-0.142909
C	3.500025	-0.358118	0.017258
H	4.573136	-0.193863	0.056554
C	2.634117	0.732203	-0.116150
H	3.018982	1.745792	-0.184679
H	1.229158	-2.906176	0.136812
C	-2.988899	-1.658220	0.098570
C	-3.500048	-0.358044	0.017222
C	-1.611968	-1.891666	0.066991
H	-4.573155	-0.193766	0.056507

H	-1.229238	-2.906151	0.136801
C	-2.634115	0.732258	-0.116177
C	-0.735582	-0.807502	-0.040902
H	-3.018958	1.745856	-0.184710
C	-1.267364	0.489098	-0.142921
H	-3.671030	-2.498364	0.192373
O	0.000017	2.818084	0.678590

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	81.47	cm** ⁻¹
7:	116.59	cm** ⁻¹
8:	123.39	cm** ⁻¹
9:	174.02	cm** ⁻¹
10:	197.60	cm** ⁻¹
11:	283.20	cm** ⁻¹
12:	347.20	cm** ⁻¹
13:	397.84	cm** ⁻¹
14:	405.74	cm** ⁻¹
15:	421.98	cm** ⁻¹
16:	443.89	cm** ⁻¹
17:	487.47	cm** ⁻¹
18:	498.86	cm** ⁻¹
19:	565.63	cm** ⁻¹
20:	568.03	cm** ⁻¹
21:	628.01	cm** ⁻¹
22:	697.52	cm** ⁻¹
23:	699.18	cm** ⁻¹
24:	730.90	cm** ⁻¹
25:	746.38	cm** ⁻¹
26:	768.45	cm** ⁻¹
27:	774.36	cm** ⁻¹
28:	788.44	cm** ⁻¹
29:	880.79	cm** ⁻¹
30:	881.27	cm** ⁻¹
31:	949.49	cm** ⁻¹
32:	949.77	cm** ⁻¹
33:	989.65	cm** ⁻¹
34:	991.78	cm** ⁻¹
35:	1016.92	cm** ⁻¹
36:	1046.26	cm** ⁻¹
37:	1050.35	cm** ⁻¹

38: 1058.02 cm**⁻¹
 39: 1083.54 cm**⁻¹
 40: 1087.38 cm**⁻¹
 41: 1143.25 cm**⁻¹
 42: 1152.10 cm**⁻¹
 43: 1187.64 cm**⁻¹
 44: 1188.43 cm**⁻¹
 45: 1249.12 cm**⁻¹
 46: 1297.32 cm**⁻¹
 47: 1325.00 cm**⁻¹
 48: 1345.55 cm**⁻¹
 49: 1382.94 cm**⁻¹
 50: 1468.54 cm**⁻¹
 51: 1483.25 cm**⁻¹
 52: 1503.25 cm**⁻¹
 53: 1514.91 cm**⁻¹
 54: 1623.95 cm**⁻¹
 55: 1632.39 cm**⁻¹
 56: 1642.14 cm**⁻¹
 57: 1642.87 cm**⁻¹
 58: 3180.84 cm**⁻¹
 59: 3183.08 cm**⁻¹
 60: 3188.87 cm**⁻¹
 61: 3191.16 cm**⁻¹
 62: 3199.35 cm**⁻¹
 63: 3200.02 cm**⁻¹
 64: 3208.09 cm**⁻¹
 65: 3208.67 cm**⁻¹

Electronic energy	-935.07271882 hartree
Total thermal correction	0.01040464 hartree
Non-thermal (ZPE) correction	0.16465251 hartree
Total thermal energy	-934.89766167 hartree
Total Enthalpy	-934.89671746 hartree
Final Gibbs free enthalpy	-934.94341453 hartree

Energy Calculations at this geometry

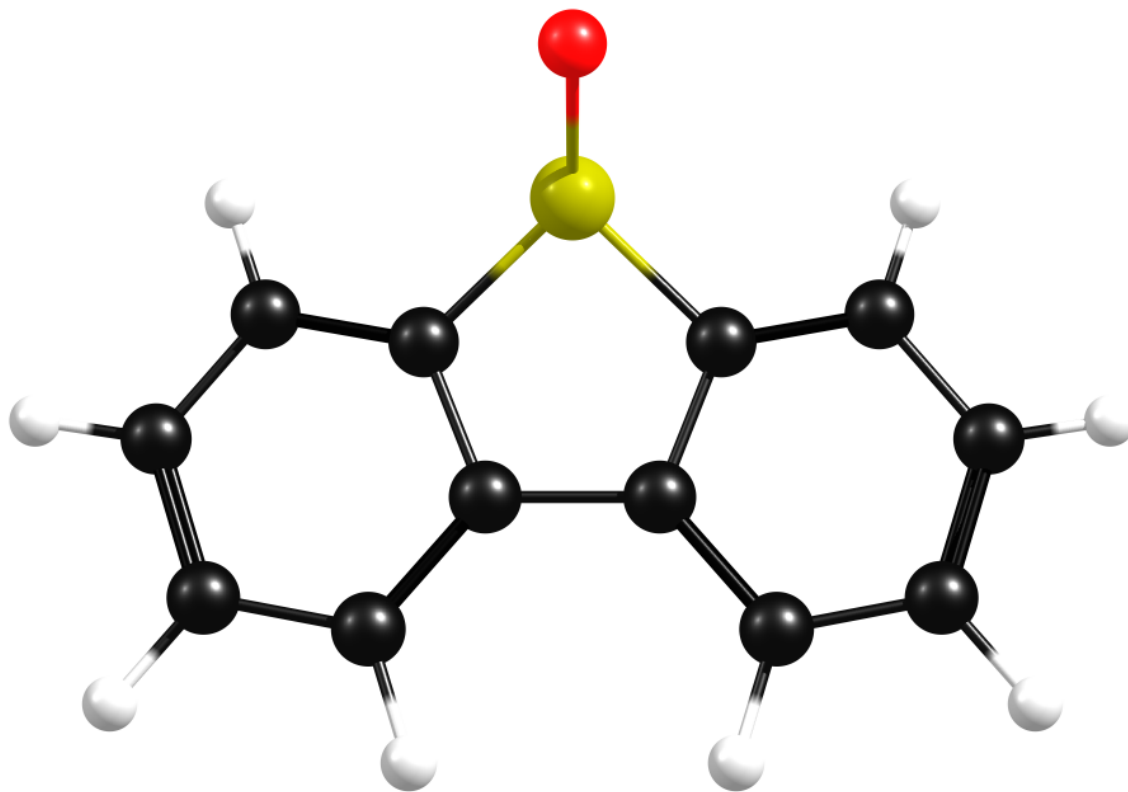
S₀

HF/aug-cc-pV(T+d)Z	-931.62849918 hartree
M06-2X/aug-cc-pV(T+d)Z	-935.46314647 hartree
B3LYP/aug-cc-pV(T+d)Z	-935.32243398 hartree

T₂

TD-B3LYP/6-31G(d,p)	-934.94440827 hartree
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Dibenzothiophene *S*-oxide (**DBTO**) S_1 state



TD-B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

C	-3.510140	-0.328369	-0.190588
C	-3.001928	-1.615991	0.114753
C	-2.638877	0.739866	-0.359299
H	-3.695602	-2.438028	0.265901
H	-3.014499	1.738287	-0.564480
C	-1.638253	-1.848885	0.228926
C	-1.265688	0.494017	-0.262576
H	-1.275700	-2.845178	0.467980
C	-0.717773	-0.803278	0.025218
H	-4.580087	-0.174920	-0.288417
C	0.717773	-0.803277	0.025218
C	1.638255	-1.848884	0.228926
C	1.265688	0.494018	-0.262576
H	1.275702	-2.845177	0.467980
C	3.001929	-1.615989	0.114753
C	2.638876	0.739867	-0.359299
H	3.695604	-2.438026	0.265901
H	3.014498	1.738289	-0.564480
C	3.510141	-0.328367	-0.190588

H	4.580087	-0.174917	-0.288417
S	-0.000001	1.714318	-0.225780
O	-0.000001	2.551487	1.106285

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	90.78	cm** ⁻¹
7:	125.73	cm** ⁻¹
8:	143.56	cm** ⁻¹
9:	145.56	cm** ⁻¹
10:	210.58	cm** ⁻¹
11:	260.43	cm** ⁻¹
12:	261.36	cm** ⁻¹
13:	395.63	cm** ⁻¹
14:	405.17	cm** ⁻¹
15:	412.96	cm** ⁻¹
16:	420.26	cm** ⁻¹
17:	447.78	cm** ⁻¹
18:	487.17	cm** ⁻¹
19:	514.77	cm** ⁻¹
20:	546.58	cm** ⁻¹
21:	612.62	cm** ⁻¹
22:	667.85	cm** ⁻¹
23:	691.49	cm** ⁻¹
24:	703.67	cm** ⁻¹
25:	710.51	cm** ⁻¹
26:	728.36	cm** ⁻¹
27:	738.13	cm** ⁻¹
28:	742.60	cm** ⁻¹
29:	784.63	cm** ⁻¹
30:	842.89	cm** ⁻¹
31:	843.79	cm** ⁻¹
32:	931.39	cm** ⁻¹
33:	931.55	cm** ⁻¹
34:	959.23	cm** ⁻¹
35:	962.77	cm** ⁻¹
36:	999.45	cm** ⁻¹
37:	1008.47	cm** ⁻¹
38:	1031.10	cm** ⁻¹
39:	1038.06	cm** ⁻¹
40:	1071.05	cm** ⁻¹
41:	1150.03	cm** ⁻¹

42: 1159.08 cm**⁻¹
 43: 1184.72 cm**⁻¹
 44: 1186.80 cm**⁻¹
 45: 1221.54 cm**⁻¹
 46: 1288.81 cm**⁻¹
 47: 1354.33 cm**⁻¹
 48: 1359.93 cm**⁻¹
 49: 1385.42 cm**⁻¹
 50: 1462.38 cm**⁻¹
 51: 1467.37 cm**⁻¹
 52: 1479.72 cm**⁻¹
 53: 1522.63 cm**⁻¹
 54: 1556.76 cm**⁻¹
 55: 1556.80 cm**⁻¹
 56: 1581.78 cm**⁻¹
 57: 1605.15 cm**⁻¹
 58: 3178.70 cm**⁻¹
 59: 3181.67 cm**⁻¹
 60: 3189.63 cm**⁻¹
 61: 3190.41 cm**⁻¹
 62: 3198.48 cm**⁻¹
 63: 3199.38 cm**⁻¹
 64: 3212.66 cm**⁻¹
 65: 3213.02 cm**⁻¹

Electronic energy	-934.95814213 hartree
Total thermal correction	0.01081340 hartree
Non-thermal (ZPE) correction	0.16164766 hartree
Total thermal energy	-934.78568554 hartree
Total Enthalpy	-934.78474133 hartree
Final Gibbs free enthalpy	-934.83196261 hartree

Energy Calculations at above geometry

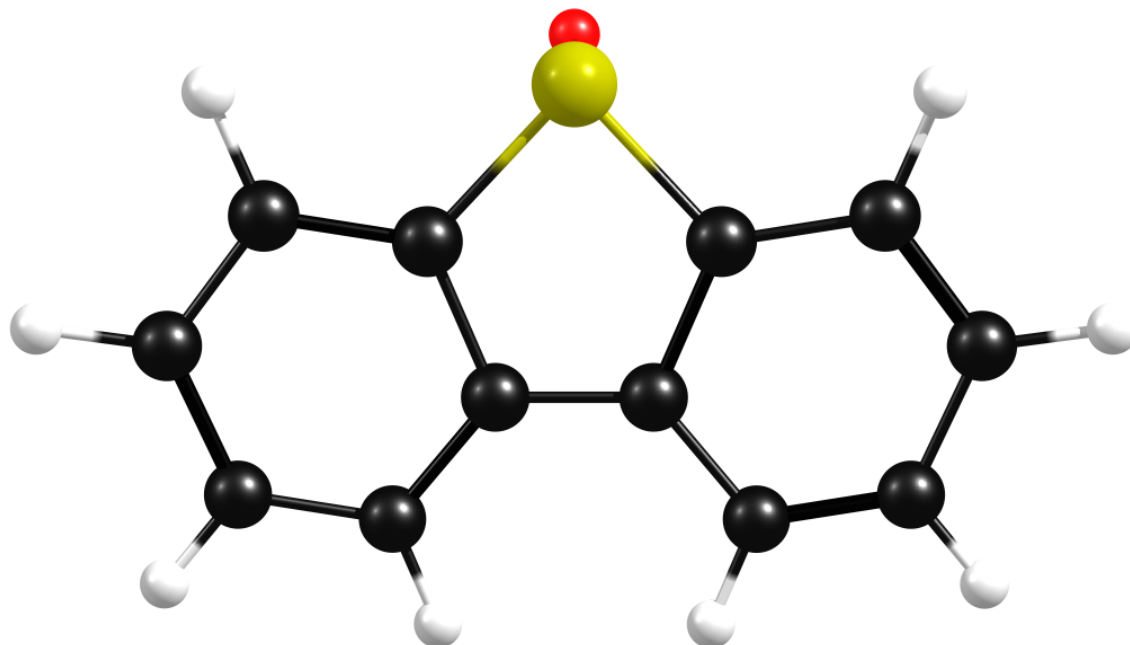
S₁

CIS/aug-cc-pV(T+d)Z	-931.44678615 hartree
M06-2X/aug-cc-pV(T+d)Z	-935.32784267 hartree
TD-B3LYP/aug-cc-pV(T+d)Z	-935.20429725 hartree

T₂

TD-B3LYP/6-31G(d,p)	-934.95133824 hartree
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Dibenzothiophene *S*-oxide (**DBTO**) T_1 state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

C	-4.152854	1.239011	0.063778
C	-4.426955	-0.159325	-0.118826
C	-3.373907	-1.088853	-0.199480
C	-2.872963	1.709905	0.145968
C	-2.073956	-0.641376	-0.123555
C	-1.764159	0.784965	0.044320
H	-4.988460	1.928792	0.140034
H	-5.455576	-0.497989	-0.189275
H	-3.588847	-2.147951	-0.315816
H	-2.679175	2.768603	0.292302
S	-0.617128	-1.718204	-0.114763
C	0.379579	-0.205335	-0.119931
C	-0.403222	1.026774	0.045451
C	1.682297	2.276419	0.066958
C	1.754367	-0.177821	-0.191027
C	2.422413	1.057865	-0.110440
C	0.318526	2.277421	0.146222
H	-0.228567	3.204717	0.288087
H	2.228550	3.212470	0.141353
H	3.505116	1.094988	-0.178665
H	2.321031	-1.098368	-0.302831
O	-0.492516	-2.431055	1.218788

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	64.73	cm** ⁻¹
7:	117.02	cm** ⁻¹
8:	125.29	cm** ⁻¹
9:	151.14	cm** ⁻¹
10:	205.10	cm** ⁻¹
11:	269.47	cm** ⁻¹
12:	300.56	cm** ⁻¹
13:	374.04	cm** ⁻¹
14:	396.16	cm** ⁻¹
15:	402.07	cm** ⁻¹
16:	437.18	cm** ⁻¹
17:	455.25	cm** ⁻¹
18:	482.56	cm** ⁻¹
19:	490.98	cm** ⁻¹
20:	522.40	cm** ⁻¹
21:	578.47	cm** ⁻¹
22:	651.04	cm** ⁻¹
23:	670.34	cm** ⁻¹
24:	673.37	cm** ⁻¹
25:	689.29	cm** ⁻¹
26:	717.72	cm** ⁻¹
27:	748.50	cm** ⁻¹
28:	754.67	cm** ⁻¹
29:	813.41	cm** ⁻¹
30:	815.15	cm** ⁻¹
31:	907.68	cm** ⁻¹
32:	929.87	cm** ⁻¹
33:	930.66	cm** ⁻¹
34:	968.89	cm** ⁻¹
35:	972.62	cm** ⁻¹
36:	989.39	cm** ⁻¹
37:	989.98	cm** ⁻¹
38:	1018.18	cm** ⁻¹
39:	1037.61	cm** ⁻¹
40:	1056.62	cm** ⁻¹
41:	1099.65	cm** ⁻¹
42:	1132.93	cm** ⁻¹
43:	1135.12	cm** ⁻¹
44:	1168.25	cm** ⁻¹
45:	1220.45	cm** ⁻¹

46: 1273.74 cm**⁻¹
 47: 1349.60 cm**⁻¹
 48: 1368.46 cm**⁻¹
 49: 1378.28 cm**⁻¹
 50: 1384.13 cm**⁻¹
 51: 1408.49 cm**⁻¹
 52: 1441.86 cm**⁻¹
 53: 1495.87 cm**⁻¹
 54: 1542.88 cm**⁻¹
 55: 1558.07 cm**⁻¹
 56: 1563.58 cm**⁻¹
 57: 1653.40 cm**⁻¹
 58: 3184.30 cm**⁻¹
 59: 3185.75 cm**⁻¹
 60: 3189.40 cm**⁻¹
 61: 3190.55 cm**⁻¹
 62: 3199.89 cm**⁻¹
 63: 3202.63 cm**⁻¹
 64: 3211.95 cm**⁻¹
 65: 3214.19 cm**⁻¹

Electronic energy	-934.96804621 hartree
Total thermal correction	0.01096646 hartree
Non-thermal (ZPE) correction	0.16052162 hartree
Total thermal energy	-934.79655813 hartree
Total Enthalpy	-934.79561392 hartree
Final Gibbs free enthalpy	-934.84442766 hartree

Energy Calculations at above geometry

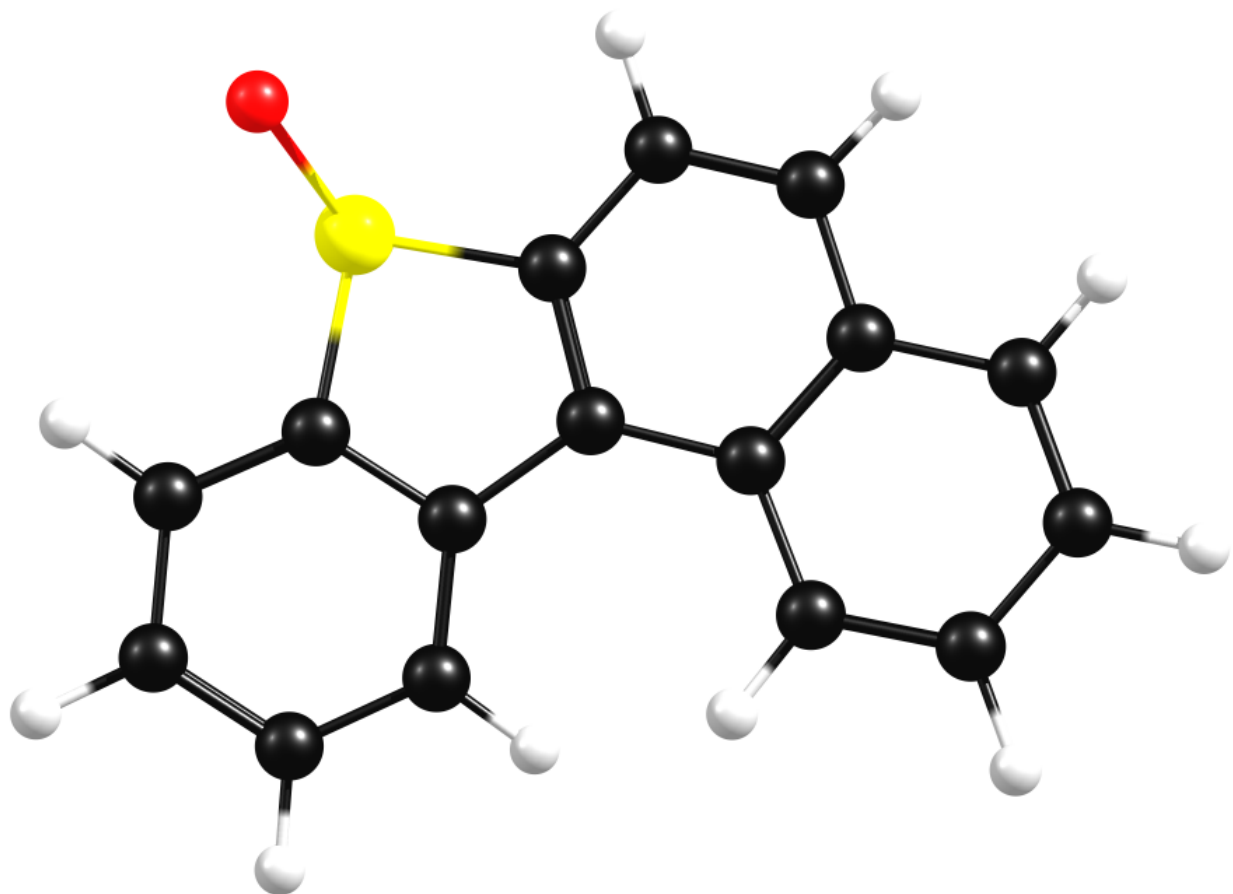
T₁

HF/aug-cc-pV(T+d)Z	-931.49761692 hartree
M06-2X/aug-cc-pV(T+d)Z	-935.34749847 hartree
B3LYP/aug-cc-pV(T+d)Z	-935.21953858 hartree

T₂

TD-B3LYP/6-31G(d,p)	-934.94651594 hartree
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Benzo[b]naphtho[1,2,d]thiophene S-oxide (1) S₀ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	1.858197	-1.730979	-0.440421
C	1.224008	2.207909	-0.113907
C	1.038428	0.816619	-0.128366
C	2.512250	2.745346	-0.038679
H	2.631291	3.825249	-0.013751
C	2.201719	0.016936	-0.145961
C	3.640522	1.924221	0.001598
H	4.632624	2.359305	0.077197
C	3.485480	0.537813	-0.079110
H	4.347130	-0.123775	-0.082778
H	0.388599	2.890790	-0.180166
O	2.374036	-2.642565	0.651903
C	-0.198486	-0.005366	-0.144788
C	0.098660	-1.361048	-0.252461

C	-0.869101	-2.378759	-0.286931
C	-2.194485	-2.022521	-0.214241
C	-2.577512	-0.658612	-0.092907
C	-1.580060	0.381285	-0.038675
C	-2.037003	1.715655	0.149317
C	-3.379815	2.013474	0.239953
C	-4.353064	0.993733	0.149613
C	-3.953209	-0.313083	-0.006147
H	-0.565086	-3.418790	-0.360893
H	-2.971357	-2.782112	-0.237069
H	-4.689282	-1.111442	-0.057790
H	-5.408396	1.242138	0.217610
H	-3.691133	3.043263	0.391407
H	-1.324750	2.519740	0.259663

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	31.55	cm** ⁻¹
7:	77.85	cm** ⁻¹
8:	95.65	cm** ⁻¹
9:	147.32	cm** ⁻¹
10:	174.23	cm** ⁻¹
11:	178.43	cm** ⁻¹
12:	213.10	cm** ⁻¹
13:	281.16	cm** ⁻¹
14:	301.54	cm** ⁻¹
15:	350.41	cm** ⁻¹
16:	380.76	cm** ⁻¹
17:	408.07	cm** ⁻¹
18:	419.65	cm** ⁻¹
19:	436.94	cm** ⁻¹
20:	473.80	cm** ⁻¹
21:	502.36	cm** ⁻¹
22:	533.11	cm** ⁻¹
23:	541.53	cm** ⁻¹
24:	554.39	cm** ⁻¹
25:	584.12	cm** ⁻¹
26:	620.52	cm** ⁻¹
27:	643.06	cm** ⁻¹
28:	678.17	cm** ⁻¹
29:	699.91	cm** ⁻¹
30:	719.88	cm** ⁻¹

31: 741.58 cm**-1
32: 749.95 cm**-1
33: 764.00 cm**-1
34: 797.93 cm**-1
35: 822.27 cm**-1
36: 834.30 cm**-1
37: 865.39 cm**-1
38: 876.57 cm**-1
39: 880.55 cm**-1
40: 941.85 cm**-1
41: 950.55 cm**-1
42: 965.23 cm**-1
43: 975.02 cm**-1
44: 987.08 cm**-1
45: 991.89 cm**-1
46: 1050.71 cm**-1
47: 1056.04 cm**-1
48: 1065.43 cm**-1
49: 1082.54 cm**-1
50: 1134.87 cm**-1
51: 1152.28 cm**-1
52: 1170.47 cm**-1
53: 1177.72 cm**-1
54: 1188.63 cm**-1
55: 1193.77 cm**-1
56: 1228.76 cm**-1
57: 1244.23 cm**-1
58: 1275.96 cm**-1
59: 1317.04 cm**-1
60: 1357.78 cm**-1
61: 1374.82 cm**-1
62: 1399.57 cm**-1
63: 1405.11 cm**-1
64: 1467.44 cm**-1
65: 1477.43 cm**-1
66: 1494.13 cm**-1
67: 1500.43 cm**-1
68: 1559.20 cm**-1
69: 1607.17 cm**-1
70: 1620.74 cm**-1
71: 1631.62 cm**-1
72: 1642.20 cm**-1
73: 1671.31 cm**-1
74: 3176.76 cm**-1
75: 3184.38 cm**-1
76: 3184.78 cm**-1
77: 3188.43 cm**-1
78: 3194.66 cm**-1

79: 3203.20 cm**-1
80: 3204.45 cm**-1
81: 3208.90 cm**-1
82: 3240.56 cm**-1
83: 3272.98 cm**-1

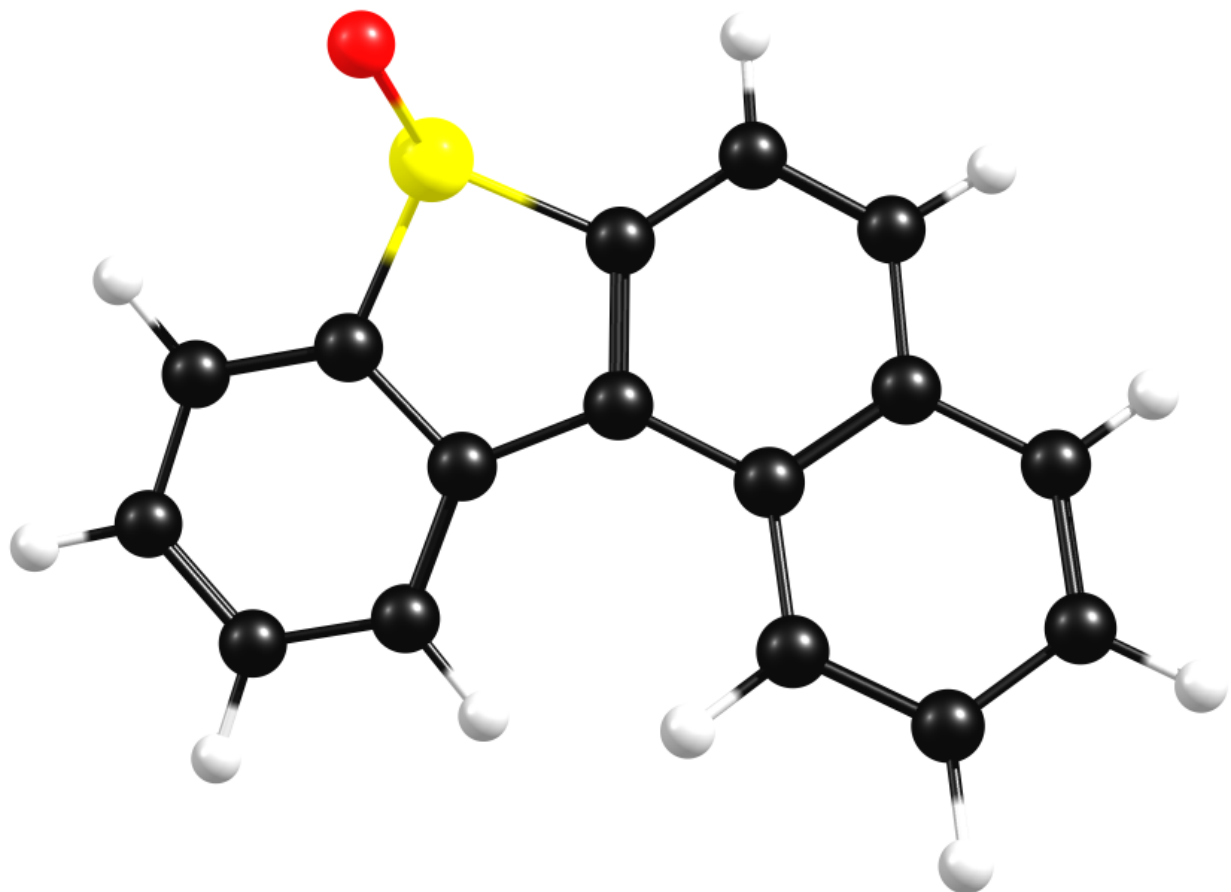
Electronic energy	-1088.61365334 hartree
Total thermal correction	0.01228467 hartree
Non-thermal (ZPE) correction	0.21133799 hartree
Total thermal energy	-1088.39003067 hartree
Total Enthalpy	-1088.38908646 hartree
Final Gibbs free enthalpy	-1088.43980394 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1088.496855603492 hartree
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Benzo[b]naphtho[1,2,d]thiophene S-oxide (1) S₁ state



TD-B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	1.809990	-1.708349	0.026990
C	1.231939	2.193216	-0.099752
C	1.020672	0.796006	-0.068973
C	2.517026	2.719183	-0.184821
H	2.637517	3.798766	-0.221954
C	2.213752	0.003190	-0.127507
C	3.659792	1.899287	-0.233512
H	4.650156	2.336148	-0.304517
C	3.503628	0.514978	-0.198725
H	4.364649	-0.146385	-0.227573
H	0.390105	2.872786	-0.096857
O	2.171981	-2.209015	1.463505
C	-0.182994	-0.004640	-0.059263
C	0.107657	-1.397660	-0.228480
C	-0.860531	-2.393472	-0.414980

C	-2.183782	-2.015973	-0.442646
C	-2.568403	-0.656612	-0.189636
C	-1.571650	0.361183	0.048248
C	-2.024665	1.661671	0.385130
C	-3.375180	1.973431	0.422850
C	-4.340059	0.993205	0.140491
C	-3.935258	-0.300014	-0.149053
H	-0.571513	-3.432450	-0.545678
H	-2.960187	-2.751306	-0.629568
H	-4.675331	-1.072560	-0.343487
H	-5.397018	1.243374	0.164504
H	-3.685055	2.981824	0.682779
H	-1.307031	2.424608	0.655706

Frequencies

0:	0.00	cm**-1
1:	0.00	cm**-1
2:	0.00	cm**-1
3:	0.00	cm**-1
4:	0.00	cm**-1
5:	0.00	cm**-1
6:	64.32	cm**-1
7:	73.04	cm**-1
8:	116.02	cm**-1
9:	143.11	cm**-1
10:	167.32	cm**-1
11:	184.58	cm**-1
12:	218.20	cm**-1
13:	276.76	cm**-1
14:	286.33	cm**-1
15:	319.62	cm**-1
16:	361.34	cm**-1
17:	401.86	cm**-1
18:	414.34	cm**-1
19:	421.16	cm**-1
20:	476.21	cm**-1
21:	487.20	cm**-1
22:	511.16	cm**-1
23:	515.29	cm**-1
24:	535.88	cm**-1
25:	563.50	cm**-1
26:	618.27	cm**-1
27:	624.76	cm**-1
28:	646.32	cm**-1
29:	697.55	cm**-1
30:	705.58	cm**-1
31:	722.86	cm**-1

32:	734.54	cm**-1
33:	741.27	cm**-1
34:	770.43	cm**-1
35:	789.10	cm**-1
36:	793.52	cm**-1
37:	834.04	cm**-1
38:	847.72	cm**-1
39:	871.65	cm**-1
40:	889.81	cm**-1
41:	925.27	cm**-1
42:	929.92	cm**-1
43:	938.37	cm**-1
44:	964.89	cm**-1
45:	970.08	cm**-1
46:	975.62	cm**-1
47:	1039.14	cm**-1
48:	1049.45	cm**-1
49:	1066.34	cm**-1
50:	1116.28	cm**-1
51:	1150.95	cm**-1
52:	1154.45	cm**-1
53:	1172.81	cm**-1
54:	1182.93	cm**-1
55:	1187.62	cm**-1
56:	1227.69	cm**-1
57:	1248.64	cm**-1
58:	1275.40	cm**-1
59:	1321.31	cm**-1
60:	1353.36	cm**-1
61:	1361.70	cm**-1
62:	1380.42	cm**-1
63:	1401.70	cm**-1
64:	1459.57	cm**-1
65:	1473.05	cm**-1
66:	1479.31	cm**-1
67:	1498.52	cm**-1
68:	1534.67	cm**-1
69:	1565.93	cm**-1
70:	1578.24	cm**-1
71:	1593.95	cm**-1
72:	1613.47	cm**-1
73:	1643.03	cm**-1
74:	3173.81	cm**-1
75:	3184.28	cm**-1
76:	3185.85	cm**-1
77:	3187.90	cm**-1
78:	3195.92	cm**-1
79:	3201.93	cm**-1

80: 3203.89 cm**-1
81: 3217.36 cm**-1
82: 3233.29 cm**-1
83: 3253.78 cm**-1

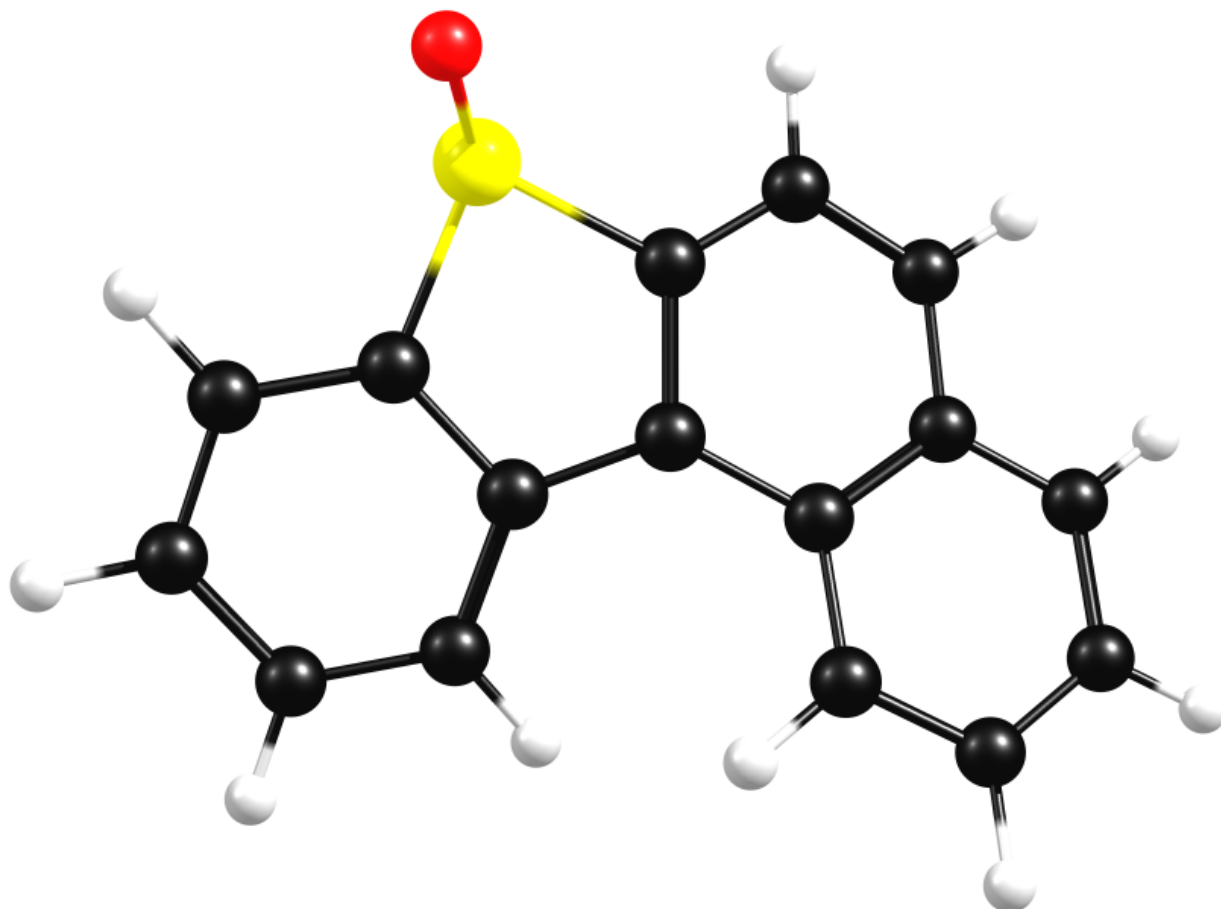
Electronic energy	-1088.50769084 hartree
Total thermal correction	0.01338923 hartree
Non-thermal (ZPE) correction	0.20890055 hartree
Total thermal energy	-1088.28540105 hartree
Total Enthalpy	-1088.28445684 hartree
Final Gibbs free enthalpy	-1088.33761622 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1088.504088267631 hartree
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Benzo[b]naphtho[1,2,d]thiophene S-oxide (1) T₁ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	1.905537	-1.822673	0.030657
C	1.187042	2.184565	-0.202323
C	1.012115	0.772344	-0.088063
C	2.459563	2.723328	-0.258478
H	2.577574	3.799528	-0.353110
C	2.200531	-0.036638	-0.091867
C	3.607878	1.904722	-0.213908
H	4.595902	2.353019	-0.254218
C	3.469795	0.513680	-0.138796
H	4.346702	-0.127665	-0.116330
H	0.327717	2.838004	-0.287348
O	2.225144	-2.309331	1.430580
C	-0.170982	-0.002276	-0.028420
C	0.150974	-1.440296	-0.156823
C	-0.811298	-2.377464	-0.407895

C	-2.164497	-1.976316	-0.485265
C	-2.562713	-0.619301	-0.211596
C	-1.569850	0.384405	0.074145
C	-2.010125	1.656911	0.457308
C	-3.380874	1.985284	0.488871
C	-4.331167	1.034089	0.156190
C	-3.918505	-0.266632	-0.182863
H	-0.546891	-3.423473	-0.540505
H	-2.936569	-2.709885	-0.697431
H	-4.661594	-1.023556	-0.420897
H	-5.388904	1.280319	0.169432
H	-3.681744	2.986907	0.781147
H	-1.290555	2.402824	0.771026

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	50.37	cm** ⁻¹
7:	79.72	cm** ⁻¹
8:	105.98	cm** ⁻¹
9:	141.80	cm** ⁻¹
10:	159.49	cm** ⁻¹
11:	183.72	cm** ⁻¹
12:	214.29	cm** ⁻¹
13:	274.29	cm** ⁻¹
14:	313.96	cm** ⁻¹
15:	329.56	cm** ⁻¹
16:	368.77	cm** ⁻¹
17:	380.05	cm** ⁻¹
18:	403.09	cm** ⁻¹
19:	442.50	cm** ⁻¹
20:	463.67	cm** ⁻¹
21:	478.01	cm** ⁻¹
22:	509.30	cm** ⁻¹
23:	524.51	cm** ⁻¹
24:	531.02	cm** ⁻¹
25:	542.39	cm** ⁻¹
26:	620.29	cm** ⁻¹
27:	620.57	cm** ⁻¹
28:	638.53	cm** ⁻¹
29:	684.57	cm** ⁻¹
30:	713.12	cm** ⁻¹
31:	722.66	cm** ⁻¹

32: 727.99 cm**-1
33: 757.37 cm**-1
34: 768.67 cm**-1
35: 777.88 cm**-1
36: 824.42 cm**-1
37: 862.15 cm**-1
38: 880.70 cm**-1
39: 885.78 cm**-1
40: 917.36 cm**-1
41: 935.05 cm**-1
42: 948.34 cm**-1
43: 961.42 cm**-1
44: 977.44 cm**-1
45: 981.99 cm**-1
46: 1029.47 cm**-1
47: 1045.21 cm**-1
48: 1046.27 cm**-1
49: 1058.44 cm**-1
50: 1071.66 cm**-1
51: 1116.04 cm**-1
52: 1130.33 cm**-1
53: 1145.32 cm**-1
54: 1178.13 cm**-1
55: 1187.17 cm**-1
56: 1217.87 cm**-1
57: 1233.40 cm**-1
58: 1274.15 cm**-1
59: 1302.60 cm**-1
60: 1315.40 cm**-1
61: 1355.34 cm**-1
62: 1374.10 cm**-1
63: 1399.28 cm**-1
64: 1427.07 cm**-1
65: 1453.96 cm**-1
66: 1463.62 cm**-1
67: 1483.33 cm**-1
68: 1509.47 cm**-1
69: 1554.66 cm**-1
70: 1572.16 cm**-1
71: 1586.99 cm**-1
72: 1602.98 cm**-1
73: 1624.09 cm**-1
74: 3179.44 cm**-1
75: 3184.48 cm**-1
76: 3185.39 cm**-1
77: 3191.17 cm**-1
78: 3191.79 cm**-1
79: 3200.74 cm**-1

80: 3207.42 cm**-1
81: 3209.18 cm**-1
82: 3221.94 cm**-1
83: 3237.61 cm**-1

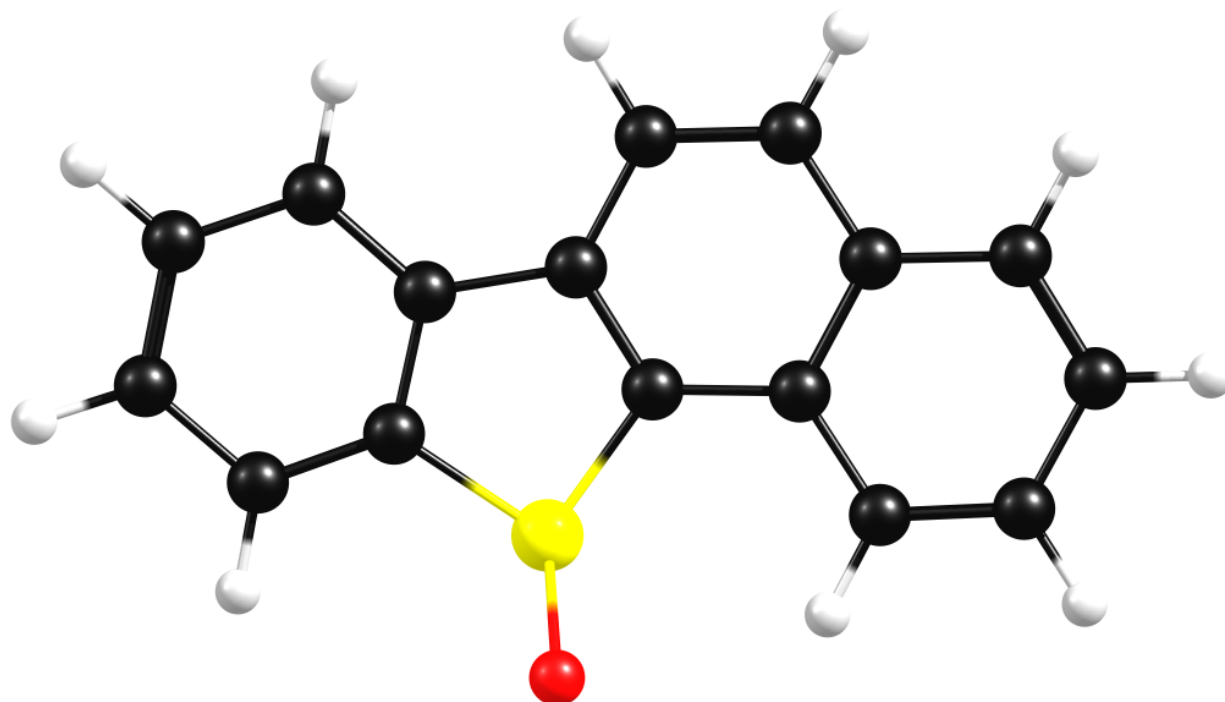
Electronic energy	-1088.53196884 hartree
Total thermal correction	0.01341380 hartree
Non-thermal (ZPE) correction	0.20838499 hartree
Total thermal energy	-1088.31017006 hartree
Total Enthalpy	-1088.30922585 hartree
Final Gibbs free enthalpy	-1088.36367402 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1088.497532967727 hartree
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Benzo[b]naphtho[2,1,d]thiophene S-oxide (2) S₀ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

C	-4.193226	1.233251	0.097503
C	-4.477574	-0.135427	0.040767
C	-3.440411	-1.067075	-0.078409
C	-2.875222	1.696815	0.056928
C	-2.136141	-0.594668	-0.110805
C	-1.828545	0.774165	-0.032925
H	-5.007945	1.947016	0.179591
H	-5.507320	-0.477409	0.087458
H	-3.647213	-2.132241	-0.130227
H	-2.671702	2.763020	0.107457
S	-0.665952	-1.620473	-0.385230
C	0.364986	-0.154200	-0.086336
C	-0.378339	1.017313	-0.033055
C	1.664697	2.299206	0.050385
C	1.781609	-0.165761	-0.050904
C	2.443992	1.107671	0.019898
C	0.289423	2.266155	0.027557
H	-0.281618	3.189355	0.059021
H	2.183423	3.253504	0.097648
C	3.863108	1.138372	0.058077
H	4.363249	2.102278	0.110701

C	3.937670	-1.281590	-0.026072
H	4.525990	-2.194688	-0.032767
C	2.562809	-1.353975	-0.063464
H	2.061317	-2.316596	-0.071835
C	4.594776	-0.028110	0.031342
H	5.680323	0.008624	0.061212
O	-0.498983	-2.701853	0.662455

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	53.01	cm** ⁻¹
7:	91.27	cm** ⁻¹
8:	113.01	cm** ⁻¹
9:	139.43	cm** ⁻¹
10:	156.72	cm** ⁻¹
11:	183.96	cm** ⁻¹
12:	211.43	cm** ⁻¹
13:	280.80	cm** ⁻¹
14:	314.88	cm** ⁻¹
15:	339.36	cm** ⁻¹
16:	373.43	cm** ⁻¹
17:	403.72	cm** ⁻¹
18:	431.39	cm** ⁻¹
19:	454.55	cm** ⁻¹
20:	469.19	cm** ⁻¹
21:	513.38	cm** ⁻¹
22:	525.62	cm** ⁻¹
23:	539.83	cm** ⁻¹
24:	556.96	cm** ⁻¹
25:	580.58	cm** ⁻¹
26:	590.08	cm** ⁻¹
27:	669.90	cm** ⁻¹
28:	681.52	cm** ⁻¹
29:	687.94	cm** ⁻¹
30:	726.00	cm** ⁻¹
31:	742.32	cm** ⁻¹
32:	761.26	cm** ⁻¹
33:	774.14	cm** ⁻¹
34:	794.20	cm** ⁻¹
35:	829.53	cm** ⁻¹
36:	834.38	cm** ⁻¹
37:	878.13	cm** ⁻¹

38: 888.09 cm**-1
39: 890.32 cm**-1
40: 946.33 cm**-1
41: 958.37 cm**-1
42: 970.75 cm**-1
43: 981.57 cm**-1
44: 988.38 cm**-1
45: 999.59 cm**-1
46: 1045.12 cm**-1
47: 1048.42 cm**-1
48: 1055.03 cm**-1
49: 1075.10 cm**-1
50: 1103.26 cm**-1
51: 1151.63 cm**-1
52: 1161.69 cm**-1
53: 1177.27 cm**-1
54: 1188.86 cm**-1
55: 1192.14 cm**-1
56: 1244.37 cm**-1
57: 1276.34 cm**-1
58: 1289.90 cm**-1
59: 1325.43 cm**-1
60: 1361.79 cm**-1
61: 1382.10 cm**-1
62: 1393.55 cm**-1
63: 1413.59 cm**-1
64: 1465.24 cm**-1
65: 1485.62 cm**-1
66: 1494.42 cm**-1
67: 1510.71 cm**-1
68: 1559.63 cm**-1
69: 1606.57 cm**-1
70: 1625.09 cm**-1
71: 1640.73 cm**-1
72: 1643.29 cm**-1
73: 1673.10 cm**-1
74: 3175.75 cm**-1
75: 3179.36 cm**-1
76: 3183.01 cm**-1
77: 3189.22 cm**-1
78: 3191.13 cm**-1
79: 3199.24 cm**-1
80: 3200.09 cm**-1
81: 3200.90 cm**-1
82: 3209.82 cm**-1
83: 3212.06 cm**-1

Electronic energy

-1088.62052781 hartree

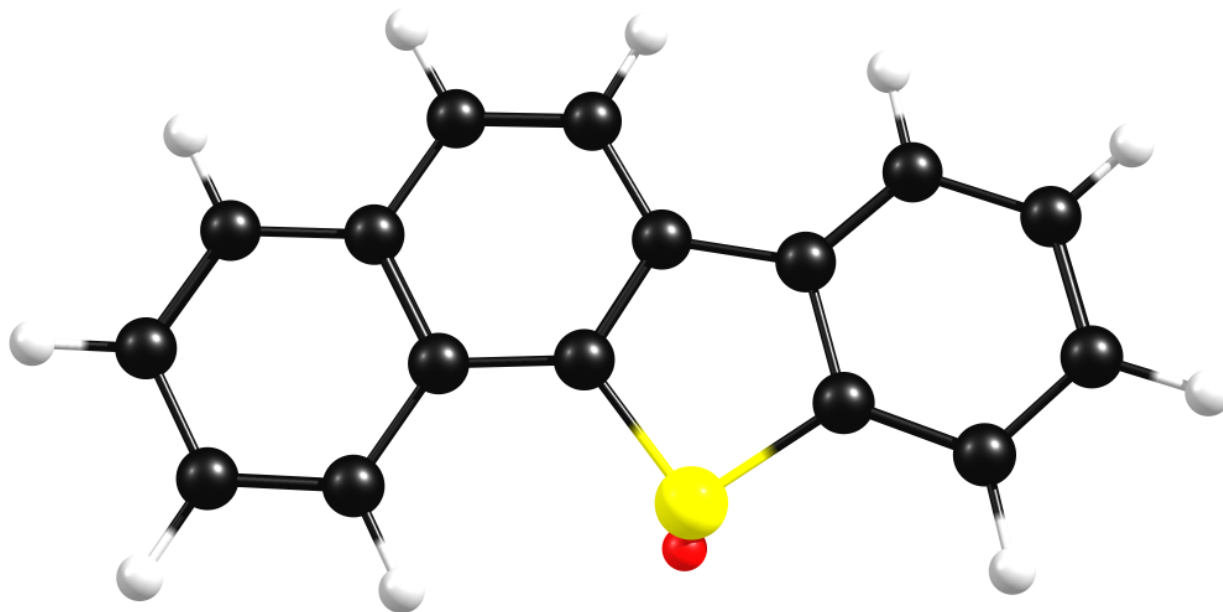
Total thermal correction	0.01306264 hartree
Non-thermal (ZPE) correction	0.21154128 hartree
Total thermal energy	-1088.39592389 hartree
Total Enthalpy	-1088.39497968 hartree
Final Gibbs free enthalpy	-1088.44764842 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1088.499372291350 hartree
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Benzo[b]naphtho[2,1,d]thiophene S-oxide (2) S₁ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

C	-4.203711	1.202870	-0.048614
C	-4.477163	-0.170875	-0.212732
C	-3.430047	-1.090865	-0.213683
C	-2.903903	1.677446	0.092864
C	-2.134243	-0.600477	-0.083220
C	-1.818402	0.782807	0.062422
H	-5.029214	1.908888	-0.031998
H	-5.499311	-0.513859	-0.334018
H	-3.620923	-2.155378	-0.313587
H	-2.724090	2.741225	0.222107
S	-0.668030	-1.572957	0.120661
C	0.374442	-0.171137	0.004197
C	-0.400094	1.023384	0.127869
C	1.671473	2.270954	0.166707
C	1.796692	-0.202296	-0.033615
C	2.457363	1.076699	0.031482
C	0.294616	2.246883	0.216488
H	-0.262669	3.175985	0.301962
H	2.196126	3.220713	0.226990
C	3.866096	1.116787	-0.036935
H	4.359329	2.084709	0.011933
C	3.970672	-1.289470	-0.205897
H	4.555737	-2.201141	-0.289625

C	2.587447	-1.370095	-0.140313
H	2.106813	-2.344671	-0.169370
C	4.617957	-0.043559	-0.157666
H	5.701682	0.010457	-0.207811
O	-0.677465	-2.240349	1.539369

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	51.38	cm** ⁻¹
7:	84.23	cm** ⁻¹
8:	125.38	cm** ⁻¹
9:	134.58	cm** ⁻¹
10:	151.17	cm** ⁻¹
11:	180.51	cm** ⁻¹
12:	208.68	cm** ⁻¹
13:	269.13	cm** ⁻¹
14:	285.46	cm** ⁻¹
15:	306.89	cm** ⁻¹
16:	374.73	cm** ⁻¹
17:	390.14	cm** ⁻¹
18:	415.28	cm** ⁻¹
19:	421.42	cm** ⁻¹
20:	479.48	cm** ⁻¹
21:	501.01	cm** ⁻¹
22:	507.79	cm** ⁻¹
23:	512.78	cm** ⁻¹
24:	548.96	cm** ⁻¹
25:	551.70	cm** ⁻¹
26:	587.57	cm** ⁻¹
27:	623.34	cm** ⁻¹
28:	676.15	cm** ⁻¹
29:	690.38	cm** ⁻¹
30:	700.54	cm** ⁻¹
31:	730.05	cm** ⁻¹
32:	741.40	cm** ⁻¹
33:	747.13	cm** ⁻¹
34:	763.31	cm** ⁻¹
35:	779.06	cm** ⁻¹
36:	805.03	cm** ⁻¹
37:	833.76	cm** ⁻¹
38:	851.69	cm** ⁻¹
39:	854.30	cm** ⁻¹

40: 891.61 cm**-1
41: 922.23 cm**-1
42: 931.48 cm**-1
43: 941.44 cm**-1
44: 965.28 cm**-1
45: 967.78 cm**-1
46: 969.97 cm**-1
47: 1035.78 cm**-1
48: 1047.74 cm**-1
49: 1057.05 cm**-1
50: 1083.51 cm**-1
51: 1148.14 cm**-1
52: 1153.93 cm**-1
53: 1165.57 cm**-1
54: 1185.78 cm**-1
55: 1189.04 cm**-1
56: 1243.98 cm**-1
57: 1260.62 cm**-1
58: 1285.76 cm**-1
59: 1332.97 cm**-1
60: 1345.39 cm**-1
61: 1359.68 cm**-1
62: 1387.62 cm**-1
63: 1410.13 cm**-1
64: 1461.48 cm**-1
65: 1474.28 cm**-1
66: 1481.21 cm**-1
67: 1510.57 cm**-1
68: 1530.68 cm**-1
69: 1565.10 cm**-1
70: 1584.87 cm**-1
71: 1592.20 cm**-1
72: 1615.16 cm**-1
73: 1640.26 cm**-1
74: 3172.19 cm**-1
75: 3175.13 cm**-1
76: 3178.09 cm**-1
77: 3184.33 cm**-1
78: 3190.81 cm**-1
79: 3194.40 cm**-1
80: 3196.49 cm**-1
81: 3201.13 cm**-1
82: 3204.68 cm**-1
83: 3216.89 cm**-1

Electronic energy	-1088.51267005 hartree
Total thermal correction	0.01346315 hartree
Non-thermal (ZPE) correction	0.20853621 hartree

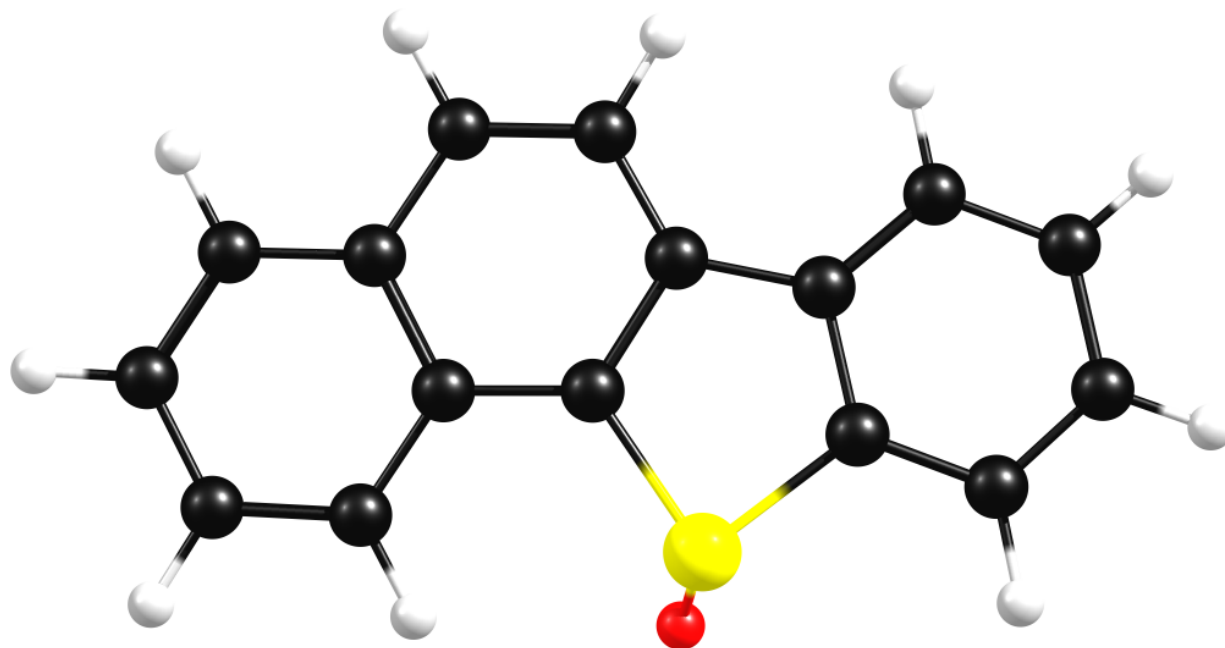
Total thermal energy	-1088.29067069 hartree
Total Enthalpy	-1088.28972648 hartree
Final Gibbs free enthalpy	-1088.34309351 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1088.504250500628 hartree
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Benzo[b]naphtho[2,1,d]thiophene S-oxide (2) T₁ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

C	-4.199947	1.228700	0.106841
C	-4.463714	-0.151500	-0.010127
C	-3.410669	-1.062041	-0.135924
C	-2.901023	1.711816	0.105752
C	-2.109747	-0.578607	-0.143589
C	-1.817970	0.807450	-0.015454
H	-5.029598	1.922842	0.206220
H	-5.489448	-0.507827	-0.004736
H	-3.604197	-2.127787	-0.220487
H	-2.712681	2.776306	0.215629
S	-0.646965	-1.640862	-0.340210
C	0.369185	-0.176862	-0.122069
C	-0.418176	1.077970	-0.022827
C	1.655748	2.310072	0.041754
C	1.779400	-0.183166	-0.055046
C	2.449852	1.095916	0.001960
C	0.265482	2.290032	0.043198
H	-0.284774	3.225729	0.094492
H	2.182219	3.258955	0.092197
C	3.837640	1.125407	0.021363
H	4.347208	2.085272	0.052800
C	3.967253	-1.298025	-0.024495
H	4.542861	-2.218772	-0.020277

C	2.560008	-1.362960	-0.040492
H	2.060785	-2.326045	-0.007593
C	4.605566	-0.072482	0.000467
H	5.689915	-0.012920	0.016417
O	-0.517032	-2.623931	0.810207

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	46.71	cm** ⁻¹
7:	90.30	cm** ⁻¹
8:	107.83	cm** ⁻¹
9:	138.98	cm** ⁻¹
10:	151.48	cm** ⁻¹
11:	177.15	cm** ⁻¹
12:	207.94	cm** ⁻¹
13:	271.25	cm** ⁻¹
14:	296.84	cm** ⁻¹
15:	316.32	cm** ⁻¹
16:	359.12	cm** ⁻¹
17:	380.41	cm** ⁻¹
18:	413.36	cm** ⁻¹
19:	430.97	cm** ⁻¹
20:	461.47	cm** ⁻¹
21:	488.86	cm** ⁻¹
22:	513.74	cm** ⁻¹
23:	517.96	cm** ⁻¹
24:	530.03	cm** ⁻¹
25:	542.39	cm** ⁻¹
26:	580.64	cm** ⁻¹
27:	611.46	cm** ⁻¹
28:	649.78	cm** ⁻¹
29:	678.66	cm** ⁻¹
30:	717.15	cm** ⁻¹
31:	727.62	cm** ⁻¹
32:	735.90	cm** ⁻¹
33:	755.73	cm** ⁻¹
34:	769.08	cm** ⁻¹
35:	781.25	cm** ⁻¹
36:	810.81	cm** ⁻¹
37:	866.46	cm** ⁻¹
38:	873.11	cm** ⁻¹
39:	883.76	cm** ⁻¹

40: 912.99 cm**-1
41: 924.01 cm**-1
42: 948.95 cm**-1
43: 958.40 cm**-1
44: 969.15 cm**-1
45: 982.22 cm**-1
46: 1006.89 cm**-1
47: 1021.82 cm**-1
48: 1039.30 cm**-1
49: 1056.08 cm**-1
50: 1073.55 cm**-1
51: 1084.55 cm**-1
52: 1111.95 cm**-1
53: 1145.33 cm**-1
54: 1167.67 cm**-1
55: 1186.59 cm**-1
56: 1207.94 cm**-1
57: 1233.49 cm**-1
58: 1280.86 cm**-1
59: 1296.74 cm**-1
60: 1317.08 cm**-1
61: 1363.29 cm**-1
62: 1383.69 cm**-1
63: 1403.13 cm**-1
64: 1441.50 cm**-1
65: 1451.23 cm**-1
66: 1475.05 cm**-1
67: 1490.60 cm**-1
68: 1498.86 cm**-1
69: 1524.29 cm**-1
70: 1565.14 cm**-1
71: 1584.16 cm**-1
72: 1596.15 cm**-1
73: 1623.67 cm**-1
74: 3178.93 cm**-1
75: 3181.59 cm**-1
76: 3183.65 cm**-1
77: 3191.79 cm**-1
78: 3192.37 cm**-1
79: 3198.65 cm**-1
80: 3200.14 cm**-1
81: 3204.94 cm**-1
82: 3210.62 cm**-1
83: 3214.58 cm**-1

Electronic energy	-1088.53329850 hartree
Total thermal correction	0.01352164 hartree
Non-thermal (ZPE) correction	0.20769622 hartree

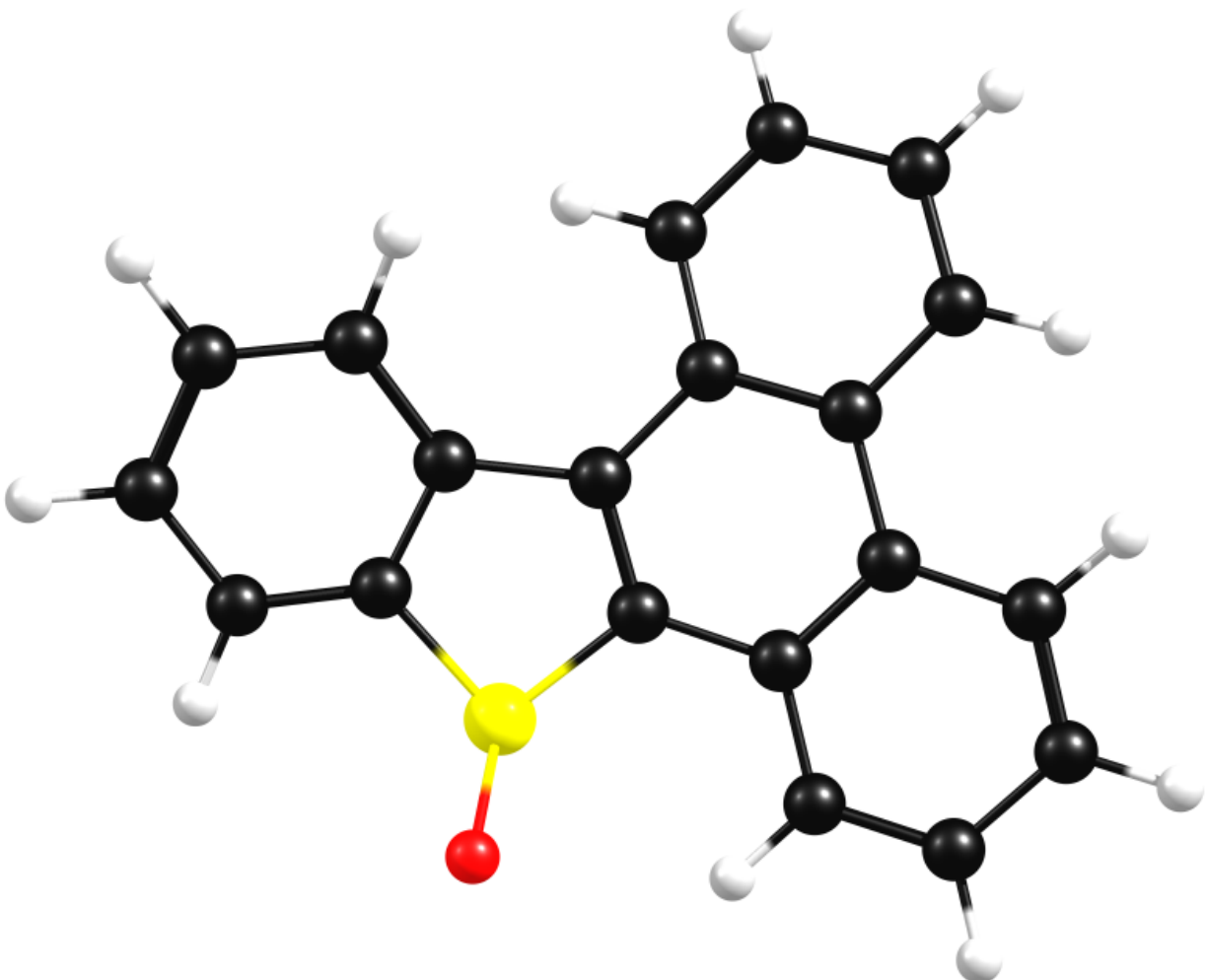
Total thermal energy	-1088.31208064 hartree
Total Enthalpy	-1088.31113643 hartree
Final Gibbs free enthalpy	-1088.36574320 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1088.501832961141 hartree
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Benzo[b]phenanthro[9,10,d]thiophene S-oxide (3) S₀ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	-1.371354	-1.945212	-0.621445
C	-4.718272	0.274205	0.155135
C	-4.130452	1.521602	0.376090
C	-3.912207	-0.825589	-0.154559
H	-4.754751	2.371268	0.637530
H	-4.338630	-1.813393	-0.303959
C	-2.746177	1.700376	0.288785
C	-2.542028	-0.632685	-0.233036
H	-2.333815	2.672632	0.521759
C	-1.918351	0.613264	-0.031142
H	-5.794118	0.153180	0.242058
C	1.706906	-2.598597	-0.108034

C	3.029188	-2.968924	0.036126
C	1.338506	-1.229826	-0.096086
C	4.018581	-1.983514	0.207530
C	2.335282	-0.221881	0.068990
C	3.676272	-0.643215	0.227914
C	-0.024669	-0.811925	-0.184445
C	-0.440816	0.499586	-0.098688
C	0.559163	1.548405	-0.079013
C	1.940612	1.183186	0.036607
H	0.932671	-3.353962	-0.191900
H	3.302453	-4.020175	0.031095
H	5.057804	-2.274436	0.332499
H	4.462821	0.088604	0.372701
C	0.230140	2.918405	-0.224697
C	2.901756	2.220513	0.080908
C	2.545671	3.552648	-0.016724
C	1.197663	3.904291	-0.192814
H	-0.795140	3.201286	-0.416727
H	3.953131	1.973604	0.174563
H	3.311987	4.321675	0.017683
H	0.914228	4.945552	-0.317205
O	-1.532706	-3.133314	0.305304

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	45.13	cm** ⁻¹
7:	70.43	cm** ⁻¹
8:	99.06	cm** ⁻¹
9:	108.84	cm** ⁻¹
10:	117.90	cm** ⁻¹
11:	151.50	cm** ⁻¹
12:	172.88	cm** ⁻¹
13:	220.42	cm** ⁻¹
14:	235.90	cm** ⁻¹
15:	260.92	cm** ⁻¹
16:	282.91	cm** ⁻¹
17:	323.11	cm** ⁻¹
18:	333.25	cm** ⁻¹
19:	390.10	cm** ⁻¹
20:	407.09	cm** ⁻¹
21:	418.60	cm** ⁻¹
22:	441.17	cm** ⁻¹

23:	449.92	cm**-1
24:	456.74	cm**-1
25:	488.60	cm**-1
26:	511.25	cm**-1
27:	536.15	cm**-1
28:	572.73	cm**-1
29:	585.43	cm**-1
30:	612.55	cm**-1
31:	625.32	cm**-1
32:	640.78	cm**-1
33:	666.23	cm**-1
34:	685.69	cm**-1
35:	711.76	cm**-1
36:	740.24	cm**-1
37:	746.54	cm**-1
38:	761.54	cm**-1
39:	764.58	cm**-1
40:	774.23	cm**-1
41:	784.73	cm**-1
42:	802.20	cm**-1
43:	811.62	cm**-1
44:	875.65	cm**-1
45:	883.60	cm**-1
46:	884.33	cm**-1
47:	906.23	cm**-1
48:	948.70	cm**-1
49:	953.44	cm**-1
50:	963.17	cm**-1
51:	986.67	cm**-1
52:	989.33	cm**-1
53:	994.28	cm**-1
54:	998.44	cm**-1
55:	1016.63	cm**-1
56:	1053.40	cm**-1
57:	1059.44	cm**-1
58:	1073.90	cm**-1
59:	1079.91	cm**-1
60:	1082.38	cm**-1
61:	1129.94	cm**-1
62:	1157.90	cm**-1
63:	1167.57	cm**-1
64:	1187.14	cm**-1
65:	1192.45	cm**-1
66:	1199.28	cm**-1
67:	1206.01	cm**-1
68:	1265.98	cm**-1
69:	1271.15	cm**-1
70:	1295.86	cm**-1

71: 1311.72 cm**⁻¹
72: 1335.31 cm**⁻¹
73: 1363.09 cm**⁻¹
74: 1371.34 cm**⁻¹
75: 1384.54 cm**⁻¹
76: 1402.60 cm**⁻¹
77: 1454.53 cm**⁻¹
78: 1473.41 cm**⁻¹
79: 1483.63 cm**⁻¹
80: 1491.08 cm**⁻¹
81: 1500.36 cm**⁻¹
82: 1537.91 cm**⁻¹
83: 1568.10 cm**⁻¹
84: 1611.33 cm**⁻¹
85: 1614.59 cm**⁻¹
86: 1626.12 cm**⁻¹
87: 1643.18 cm**⁻¹
88: 1659.26 cm**⁻¹
89: 1664.62 cm**⁻¹
90: 3182.67 cm**⁻¹
91: 3183.57 cm**⁻¹
92: 3184.94 cm**⁻¹
93: 3195.98 cm**⁻¹
94: 3198.62 cm**⁻¹
95: 3199.96 cm**⁻¹
96: 3207.73 cm**⁻¹
97: 3211.14 cm**⁻¹
98: 3214.99 cm**⁻¹
99: 3225.28 cm**⁻¹
100: 3239.82 cm**⁻¹
101: 3262.47 cm**⁻¹

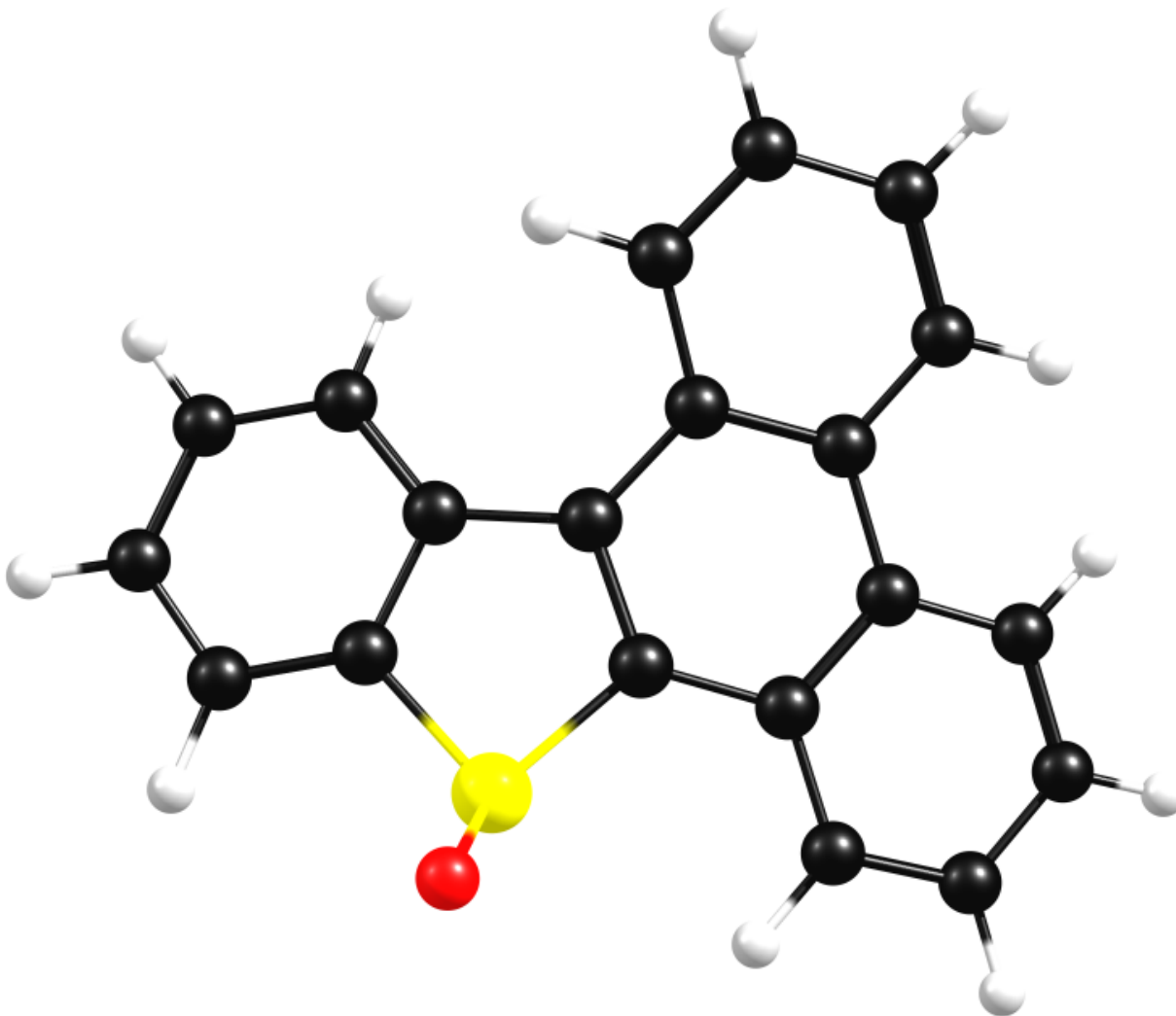
Electronic energy	-1241.88760845 hartree
Total thermal correction	0.01573228 hartree
Non-thermal (ZPE) correction	0.25887888 hartree
Total thermal energy	-1241.88760845 hartree
Total Enthalpy	-1241.88666424 hartree
Final Gibbs free enthalpy	-1241.94523425 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1242.045302825049 hartree
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Benzo[b]phenanthro[9,10,d]thiophene *S*-oxide (3) S_1 state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	-1.361367	-1.928496	0.438978
C	-4.724293	0.222599	-0.316891
C	-4.137154	1.497679	-0.390575
C	-3.910950	-0.886573	-0.085033
H	-4.766774	2.361138	-0.586947
H	-4.331149	-1.885940	-0.021333
C	-2.767886	1.693132	-0.231509
C	-2.546224	-0.675492	0.058716
H	-2.369962	2.693535	-0.337088

C	-1.903808	0.601152	0.007458
H	-5.793860	0.098146	-0.447536
C	1.730804	-2.633283	0.013032
C	3.053190	-2.986211	-0.185838
C	1.333277	-1.273537	0.038790
C	4.026109	-1.990077	-0.357861
C	2.325635	-0.248721	-0.095116
C	3.658304	-0.651507	-0.307986
C	-0.018129	-0.847541	0.149087
C	-0.463902	0.503343	0.132819
C	0.545012	1.530955	0.176036
C	1.927403	1.162784	0.028191
H	0.983978	-3.412182	0.142794
H	3.334239	-4.035446	-0.209162
H	5.064867	-2.260542	-0.521107
H	4.431276	0.097209	-0.439690
C	0.230332	2.897944	0.383778
C	2.890421	2.192130	0.034130
C	2.548254	3.527622	0.191618
C	1.205821	3.879518	0.383467
H	-0.791931	3.179032	0.597447
H	3.939994	1.942402	-0.069500
H	3.322431	4.289302	0.189816
H	0.928097	4.916872	0.548670
O	-1.530705	-2.363308	1.931153

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	41.61	cm** ⁻¹
7:	65.60	cm** ⁻¹
8:	96.95	cm** ⁻¹
9:	101.66	cm** ⁻¹
10:	121.97	cm** ⁻¹
11:	143.01	cm** ⁻¹
12:	175.23	cm** ⁻¹
13:	201.39	cm** ⁻¹
14:	240.28	cm** ⁻¹
15:	259.65	cm** ⁻¹
16:	285.64	cm** ⁻¹
17:	295.78	cm** ⁻¹
18:	332.09	cm** ⁻¹
19:	362.34	cm** ⁻¹

20:	399.89	cm**-1
21:	404.07	cm**-1
22:	413.57	cm**-1
23:	433.16	cm**-1
24:	441.05	cm**-1
25:	497.62	cm**-1
26:	505.39	cm**-1
27:	521.93	cm**-1
28:	529.25	cm**-1
29:	571.15	cm**-1
30:	600.30	cm**-1
31:	615.23	cm**-1
32:	625.50	cm**-1
33:	638.29	cm**-1
34:	683.38	cm**-1
35:	702.48	cm**-1
36:	719.38	cm**-1
37:	730.13	cm**-1
38:	743.34	cm**-1
39:	748.34	cm**-1
40:	761.21	cm**-1
41:	766.55	cm**-1
42:	783.01	cm**-1
43:	787.75	cm**-1
44:	841.96	cm**-1
45:	850.42	cm**-1
46:	856.00	cm**-1
47:	870.90	cm**-1
48:	909.72	cm**-1
49:	920.95	cm**-1
50:	932.67	cm**-1
51:	942.49	cm**-1
52:	969.24	cm**-1
53:	976.89	cm**-1
54:	977.73	cm**-1
55:	981.44	cm**-1
56:	1010.13	cm**-1
57:	1046.31	cm**-1
58:	1052.92	cm**-1
59:	1075.30	cm**-1
60:	1080.65	cm**-1
61:	1128.27	cm**-1
62:	1155.01	cm**-1
63:	1160.90	cm**-1
64:	1177.59	cm**-1
65:	1189.37	cm**-1
66:	1193.45	cm**-1
67:	1200.34	cm**-1

68:	1256.99	cm** ⁻¹
69:	1262.30	cm** ⁻¹
70:	1291.62	cm** ⁻¹
71:	1298.86	cm** ⁻¹
72:	1332.41	cm** ⁻¹
73:	1346.84	cm** ⁻¹
74:	1352.74	cm** ⁻¹
75:	1380.42	cm** ⁻¹
76:	1395.96	cm** ⁻¹
77:	1433.32	cm** ⁻¹
78:	1468.98	cm** ⁻¹
79:	1473.47	cm** ⁻¹
80:	1486.66	cm** ⁻¹
81:	1496.21	cm** ⁻¹
82:	1517.83	cm** ⁻¹
83:	1539.61	cm** ⁻¹
84:	1579.65	cm** ⁻¹
85:	1596.23	cm** ⁻¹
86:	1598.69	cm** ⁻¹
87:	1614.67	cm** ⁻¹
88:	1644.38	cm** ⁻¹
89:	1648.79	cm** ⁻¹
90:	3172.70	cm** ⁻¹
91:	3181.83	cm** ⁻¹
92:	3188.06	cm** ⁻¹
93:	3188.22	cm** ⁻¹
94:	3196.72	cm** ⁻¹
95:	3197.53	cm** ⁻¹
96:	3201.46	cm** ⁻¹
97:	3210.92	cm** ⁻¹
98:	3218.14	cm** ⁻¹
99:	3224.14	cm** ⁻¹
100:	3235.18	cm** ⁻¹
101:	3255.92	cm** ⁻¹

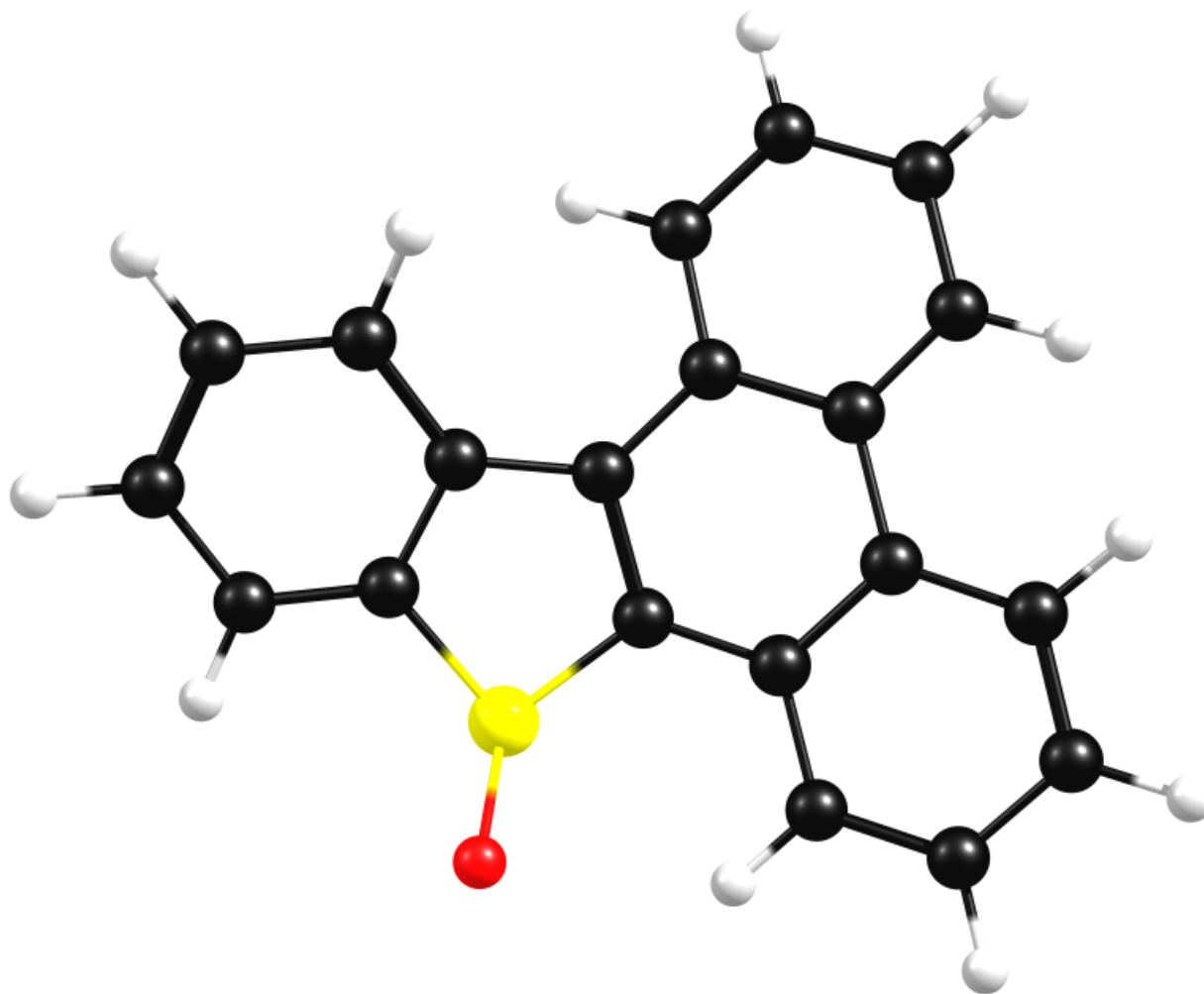
Electronic energy	-1241.78524970	hartree
Total thermal correction	0.01614497	hartree
Non-thermal (ZPE) correction	0.25591399	hartree
Total thermal energy	-1241.78524970	hartree
Total Enthalpy	-1241.78430550	hartree
Final Gibbs free enthalpy	-1241.84371438	hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1242.054010651	hartree
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Benzo[b]phenanthro[9,10,d]thiophene S-oxide (3) T₁ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	-1.371830	-1.963988	-0.757580
C	-4.681315	0.263345	0.184765
C	-4.086891	1.503811	0.493655
C	-3.878306	-0.818119	-0.196041
H	-4.714438	2.325924	0.826442
H	-4.315249	-1.790631	-0.404923
C	-2.717574	1.690494	0.410374
C	-2.510043	-0.632647	-0.288654
H	-2.288141	2.633162	0.726212
C	-1.873849	0.619369	-0.008171
H	-5.757879	0.142595	0.259039
C	1.700375	-2.624327	-0.137294
C	3.019150	-2.983727	0.082579

C	1.307308	-1.249770	-0.145834
C	3.981006	-1.995536	0.320803
C	2.305856	-0.229416	0.077424
C	3.614217	-0.639615	0.318778
C	-0.020306	-0.851386	-0.339099
C	-0.463834	0.553124	-0.144220
C	0.538195	1.581749	-0.125281
C	1.918740	1.204600	-0.003731
H	0.935776	-3.384206	-0.255486
H	3.298802	-4.033266	0.093605
H	5.012955	-2.269599	0.518372
H	4.387490	0.095013	0.515429
C	0.220667	2.954108	-0.270831
C	2.880278	2.218415	0.013930
C	2.538914	3.572302	-0.087152
C	1.202668	3.937834	-0.241472
H	-0.805883	3.240857	-0.460155
H	3.931376	1.963786	0.093195
H	3.319663	4.326789	-0.067638
H	0.925973	4.981590	-0.360081
O	-1.492522	-3.135005	0.201846

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	35.09	cm** ⁻¹
7:	72.31	cm** ⁻¹
8:	94.36	cm** ⁻¹
9:	103.55	cm** ⁻¹
10:	117.49	cm** ⁻¹
11:	147.69	cm** ⁻¹
12:	169.30	cm** ⁻¹
13:	218.64	cm** ⁻¹
14:	232.25	cm** ⁻¹
15:	261.79	cm** ⁻¹
16:	270.38	cm** ⁻¹
17:	295.87	cm** ⁻¹
18:	338.36	cm** ⁻¹
19:	374.06	cm** ⁻¹
20:	396.21	cm** ⁻¹
21:	402.97	cm** ⁻¹
22:	425.65	cm** ⁻¹
23:	440.21	cm** ⁻¹

24:	447.34	cm** -1
25:	465.57	cm** -1
26:	503.44	cm** -1
27:	520.28	cm** -1
28:	543.83	cm** -1
29:	559.66	cm** -1
30:	595.08	cm** -1
31:	607.83	cm** -1
32:	619.71	cm** -1
33:	634.99	cm** -1
34:	674.25	cm** -1
35:	695.84	cm** -1
36:	720.77	cm** -1
37:	729.25	cm** -1
38:	754.45	cm** -1
39:	759.19	cm** -1
40:	765.35	cm** -1
41:	769.47	cm** -1
42:	778.27	cm** -1
43:	810.36	cm** -1
44:	866.81	cm** -1
45:	878.40	cm** -1
46:	880.30	cm** -1
47:	906.89	cm** -1
48:	932.79	cm** -1
49:	943.27	cm** -1
50:	950.07	cm** -1
51:	966.03	cm** -1
52:	976.68	cm** -1
53:	983.37	cm** -1
54:	989.92	cm** -1
55:	999.38	cm** -1
56:	1032.15	cm** -1
57:	1042.25	cm** -1
58:	1058.61	cm** -1
59:	1071.32	cm** -1
60:	1076.39	cm** -1
61:	1114.72	cm** -1
62:	1130.64	cm** -1
63:	1147.78	cm** -1
64:	1153.91	cm** -1
65:	1179.80	cm** -1
66:	1181.96	cm** -1
67:	1199.36	cm** -1
68:	1237.59	cm** -1
69:	1245.88	cm** -1
70:	1291.39	cm** -1
71:	1315.38	cm** -1

72: 1326.73 cm**⁻¹
 73: 1331.18 cm**⁻¹
 74: 1335.46 cm**⁻¹
 75: 1360.13 cm**⁻¹
 76: 1391.02 cm**⁻¹
 77: 1426.52 cm**⁻¹
 78: 1452.75 cm**⁻¹
 79: 1467.51 cm**⁻¹
 80: 1479.87 cm**⁻¹
 81: 1481.66 cm**⁻¹
 82: 1494.52 cm**⁻¹
 83: 1524.71 cm**⁻¹
 84: 1568.71 cm**⁻¹
 85: 1574.75 cm**⁻¹
 86: 1598.37 cm**⁻¹
 87: 1599.54 cm**⁻¹
 88: 1606.38 cm**⁻¹
 89: 1629.75 cm**⁻¹
 90: 3185.10 cm**⁻¹
 91: 3186.02 cm**⁻¹
 92: 3187.47 cm**⁻¹
 93: 3193.38 cm**⁻¹
 94: 3198.45 cm**⁻¹
 95: 3202.47 cm**⁻¹
 96: 3208.24 cm**⁻¹
 97: 3210.59 cm**⁻¹
 98: 3219.45 cm**⁻¹
 99: 3221.38 cm**⁻¹
 100: 3225.01 cm**⁻¹
 101: 3241.87 cm**⁻¹

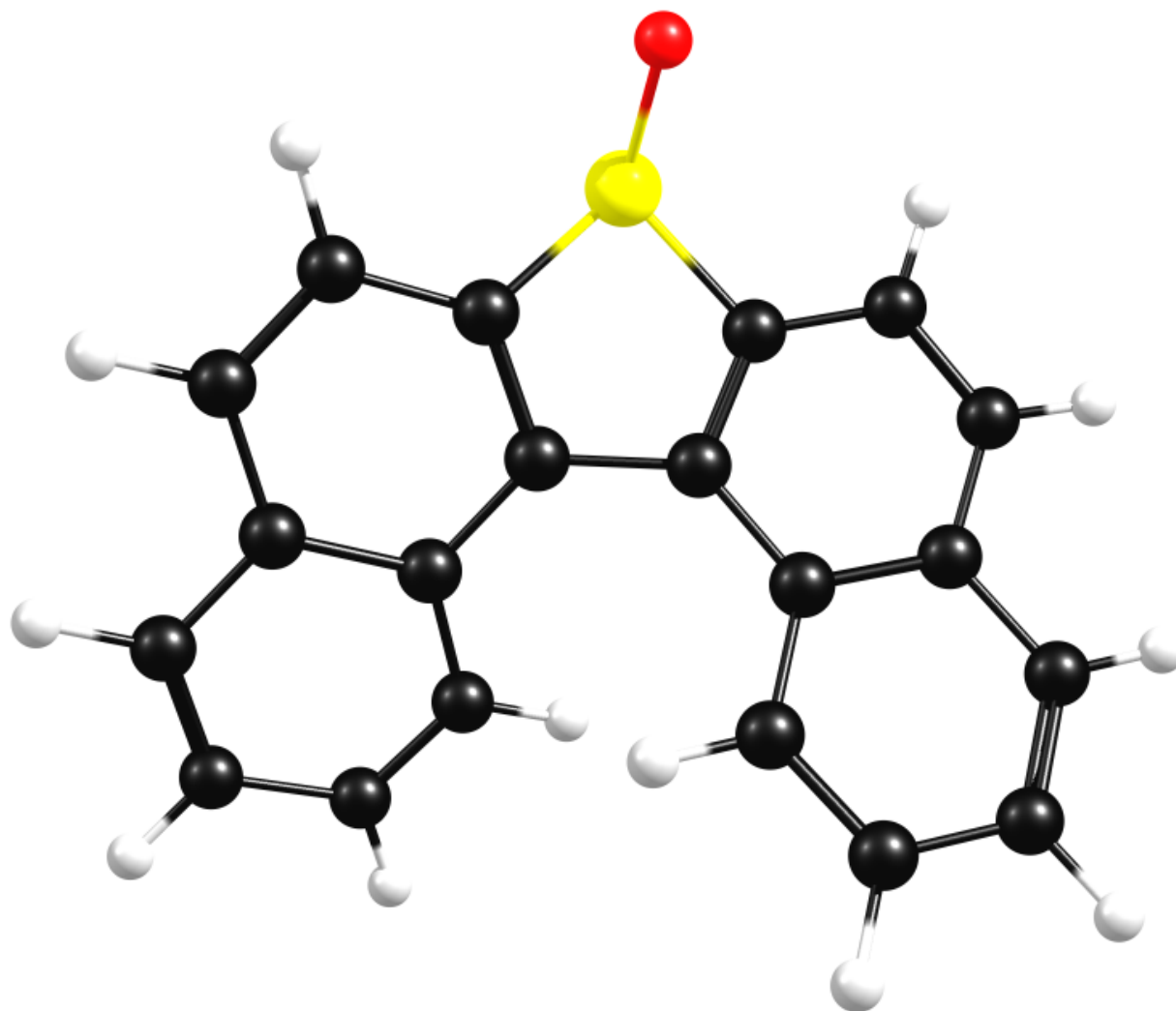
Electronic energy	-1242.08254200 hartree
Total thermal correction	0.01611358 hartree
Non-thermal (ZPE) correction	0.25568602 hartree
Total thermal energy	-1241.81074239 hartree
Total Enthalpy	-1241.80979819 hartree
Final Gibbs free enthalpy	-1241.87028893 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1242.042965691264 hartree
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dinaphtho[2,1-b:2',1'-d]thiophene S-oxide (4) S₀ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

H	-4.498640	1.303641	0.845057
C	-3.465428	1.124656	0.560470
C	-2.573676	2.168960	0.467442
C	-1.232590	1.879181	0.167881
C	-0.740098	0.585819	-0.015648
C	-1.702752	-0.474163	-0.151517
C	-3.070894	-0.193910	0.204511
C	-4.034902	-1.236012	0.123444
C	-3.702663	-2.477592	-0.366999
C	-2.385933	-2.721533	-0.821929

C	-1.415371	-1.748774	-0.716122
H	-2.881104	3.195217	0.645730
H	-0.423992	-1.943936	-1.105061
H	-2.139105	-3.679656	-1.270288
H	-4.454384	-3.258597	-0.437895
H	-5.055453	-1.019637	0.428667
C	0.742921	0.576924	-0.125717
C	1.233198	1.860997	-0.341039
C	2.588064	2.162834	-0.550590
C	3.497969	1.131783	-0.516051
C	3.088224	-0.186782	-0.177557
C	1.699260	-0.479766	0.074002
C	1.385729	-1.757705	0.617448
C	2.357044	-2.717762	0.802193
C	3.702632	-2.459556	0.453437
C	4.056321	-1.215142	-0.013494
H	2.899213	3.188368	-0.725528
H	4.553685	1.321561	-0.690845
H	5.094870	-0.985950	-0.238566
H	4.455988	-3.230599	0.587176
H	2.086424	-3.677314	1.233472
H	0.371699	-1.966746	0.931072
S	-0.035971	3.147142	-0.300081
O	0.264156	4.175301	0.768250

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	61.06	cm** ⁻¹
7:	66.34	cm** ⁻¹
8:	82.18	cm** ⁻¹
9:	91.87	cm** ⁻¹
10:	149.54	cm** ⁻¹
11:	181.89	cm** ⁻¹
12:	187.98	cm** ⁻¹
13:	192.51	cm** ⁻¹
14:	239.58	cm** ⁻¹
15:	247.12	cm** ⁻¹
16:	288.84	cm** ⁻¹
17:	324.98	cm** ⁻¹
18:	343.99	cm** ⁻¹
19:	397.29	cm** ⁻¹
20:	407.72	cm** ⁻¹

21:	427.44	cm** -1
22:	457.35	cm** -1
23:	467.35	cm** -1
24:	500.40	cm** -1
25:	518.06	cm** -1
26:	533.46	cm** -1
27:	544.94	cm** -1
28:	548.07	cm** -1
29:	555.70	cm** -1
30:	589.89	cm** -1
31:	607.00	cm** -1
32:	632.32	cm** -1
33:	651.47	cm** -1
34:	665.39	cm** -1
35:	691.29	cm** -1
36:	705.49	cm** -1
37:	761.49	cm** -1
38:	768.03	cm** -1
39:	781.56	cm** -1
40:	797.65	cm** -1
41:	799.09	cm** -1
42:	826.20	cm** -1
43:	828.99	cm** -1
44:	846.01	cm** -1
45:	866.35	cm** -1
46:	881.70	cm** -1
47:	887.06	cm** -1
48:	892.82	cm** -1
49:	953.37	cm** -1
50:	958.94	cm** -1
51:	961.24	cm** -1
52:	969.85	cm** -1
53:	978.76	cm** -1
54:	995.85	cm** -1
55:	1007.10	cm** -1
56:	1053.56	cm** -1
57:	1055.39	cm** -1
58:	1066.43	cm** -1
59:	1079.38	cm** -1
60:	1148.25	cm** -1
61:	1167.73	cm** -1
62:	1169.84	cm** -1
63:	1172.55	cm** -1
64:	1175.44	cm** -1
65:	1187.78	cm** -1
66:	1193.19	cm** -1
67:	1215.12	cm** -1
68:	1242.28	cm** -1

69: 1245.99 cm**-1
70: 1280.22 cm**-1
71: 1300.19 cm**-1
72: 1361.71 cm**-1
73: 1370.12 cm**-1
74: 1389.25 cm**-1
75: 1392.59 cm**-1
76: 1400.88 cm**-1
77: 1419.71 cm**-1
78: 1467.79 cm**-1
79: 1468.48 cm**-1
80: 1479.91 cm**-1
81: 1491.24 cm**-1
82: 1553.71 cm**-1
83: 1557.06 cm**-1
84: 1595.99 cm**-1
85: 1611.86 cm**-1
86: 1622.40 cm**-1
87: 1627.92 cm**-1
88: 1667.84 cm**-1
89: 1669.68 cm**-1
90: 3177.69 cm**-1
91: 3177.88 cm**-1
92: 3185.07 cm**-1
93: 3185.66 cm**-1
94: 3188.44 cm**-1
95: 3188.76 cm**-1
96: 3202.74 cm**-1
97: 3203.26 cm**-1
98: 3204.99 cm**-1
99: 3206.04 cm**-1
100: 3229.56 cm**-1
101: 3242.69 cm**-1

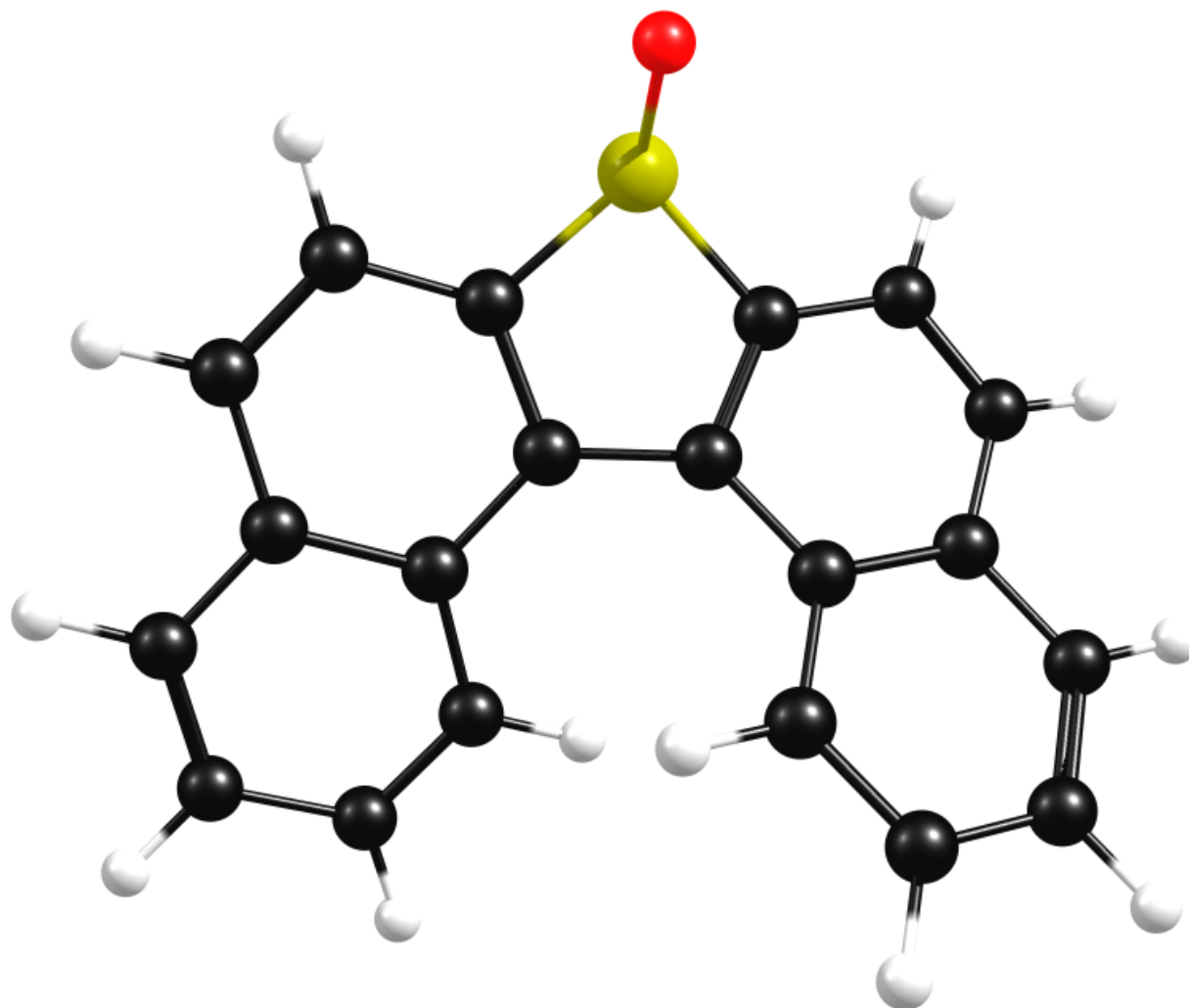
Electronic energy	-1242.14978060 hartree
Total thermal correction	0.01564831 hartree
Non-thermal (ZPE) correction	0.25837797 hartree
Total thermal energy	-1241.87575432 hartree
Total Enthalpy	-1241.87481011 hartree
Final Gibbs free enthalpy	-1241.93308271 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1242.043111554471 hartree
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dinaphtho[2,1-b:2',1'-d]thiophene S-oxide (4) S₁ state



TD-B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

H	-4.573780	1.402281	0.478546
C	-3.518199	1.196008	0.332504
C	-2.602699	2.222533	0.299807
C	-1.252107	1.899610	0.114736
C	-0.725637	0.582061	0.007613
C	-1.711647	-0.470708	-0.121982
C	-3.101704	-0.150331	0.093320
C	-4.068802	-1.182273	-0.001870
C	-3.719976	-2.467191	-0.366740
C	-2.377774	-2.758995	-0.677143
C	-1.403157	-1.785199	-0.558703
H	-2.913417	3.255293	0.425697

H	-0.385709	-2.023686	-0.837852
H	-2.103537	-3.751365	-1.023845
H	-4.479358	-3.240221	-0.443104
H	-5.108540	-0.931611	0.193232
C	0.722138	0.575420	-0.072542
C	1.249043	1.887813	-0.293753
C	2.580897	2.178313	-0.606707
C	3.472715	1.129654	-0.679939
C	3.077846	-0.182865	-0.268335
C	1.714044	-0.461296	0.114472
C	1.446968	-1.707338	0.736631
C	2.423399	-2.680697	0.860873
C	3.725842	-2.446465	0.381413
C	4.043074	-1.214007	-0.157683
H	2.896401	3.200448	-0.795479
H	4.503486	1.301348	-0.973232
H	5.059827	-1.003778	-0.480229
H	4.485303	-3.218799	0.464250
H	2.182041	-3.624883	1.340990
H	0.461002	-1.892090	1.144470
S	0.045694	3.090573	0.137306
O	0.220761	3.663693	1.578603

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	61.35	cm** ⁻¹
7:	66.96	cm** ⁻¹
8:	85.16	cm** ⁻¹
9:	99.67	cm** ⁻¹
10:	145.45	cm** ⁻¹
11:	177.32	cm** ⁻¹
12:	192.87	cm** ⁻¹
13:	200.46	cm** ⁻¹
14:	229.32	cm** ⁻¹
15:	248.32	cm** ⁻¹
16:	281.74	cm** ⁻¹
17:	305.21	cm** ⁻¹
18:	342.31	cm** ⁻¹
19:	371.13	cm** ⁻¹
20:	390.44	cm** ⁻¹
21:	412.26	cm** ⁻¹
22:	448.25	cm** ⁻¹

23:	472.68	cm**-1
24:	490.52	cm**-1
25:	500.90	cm**-1
26:	507.66	cm**-1
27:	517.65	cm**-1
28:	537.59	cm**-1
29:	550.29	cm**-1
30:	579.32	cm**-1
31:	605.52	cm**-1
32:	633.36	cm**-1
33:	643.25	cm**-1
34:	646.66	cm**-1
35:	666.52	cm**-1
36:	693.74	cm**-1
37:	737.44	cm**-1
38:	743.28	cm**-1
39:	768.19	cm**-1
40:	776.87	cm**-1
41:	786.72	cm**-1
42:	794.26	cm**-1
43:	801.55	cm**-1
44:	805.06	cm**-1
45:	852.41	cm**-1
46:	864.42	cm**-1
47:	876.30	cm**-1
48:	886.83	cm**-1
49:	904.25	cm**-1
50:	922.66	cm**-1
51:	929.80	cm**-1
52:	943.75	cm**-1
53:	951.55	cm**-1
54:	966.16	cm**-1
55:	982.18	cm**-1
56:	999.94	cm**-1
57:	1058.52	cm**-1
58:	1061.27	cm**-1
59:	1075.54	cm**-1
60:	1135.05	cm**-1
61:	1151.65	cm**-1
62:	1155.54	cm**-1
63:	1168.08	cm**-1
64:	1173.43	cm**-1
65:	1183.55	cm**-1
66:	1188.05	cm**-1
67:	1211.03	cm**-1
68:	1238.53	cm**-1
69:	1252.90	cm**-1
70:	1279.13	cm**-1

71: 1302.93 cm**⁻¹
72: 1346.29 cm**⁻¹
73: 1355.16 cm**⁻¹
74: 1359.77 cm**⁻¹
75: 1372.83 cm**⁻¹
76: 1381.59 cm**⁻¹
77: 1431.53 cm**⁻¹
78: 1461.12 cm**⁻¹
79: 1463.94 cm**⁻¹
80: 1477.29 cm**⁻¹
81: 1482.03 cm**⁻¹
82: 1537.50 cm**⁻¹
83: 1550.65 cm**⁻¹
84: 1561.14 cm**⁻¹
85: 1576.60 cm**⁻¹
86: 1594.04 cm**⁻¹
87: 1603.49 cm**⁻¹
88: 1647.46 cm**⁻¹
89: 1653.71 cm**⁻¹
90: 3175.32 cm**⁻¹
91: 3176.04 cm**⁻¹
92: 3186.58 cm**⁻¹
93: 3187.69 cm**⁻¹
94: 3189.28 cm**⁻¹
95: 3192.84 cm**⁻¹
96: 3202.15 cm**⁻¹
97: 3203.37 cm**⁻¹
98: 3206.41 cm**⁻¹
99: 3208.95 cm**⁻¹
100: 3228.11 cm**⁻¹
101: 3244.26 cm**⁻¹

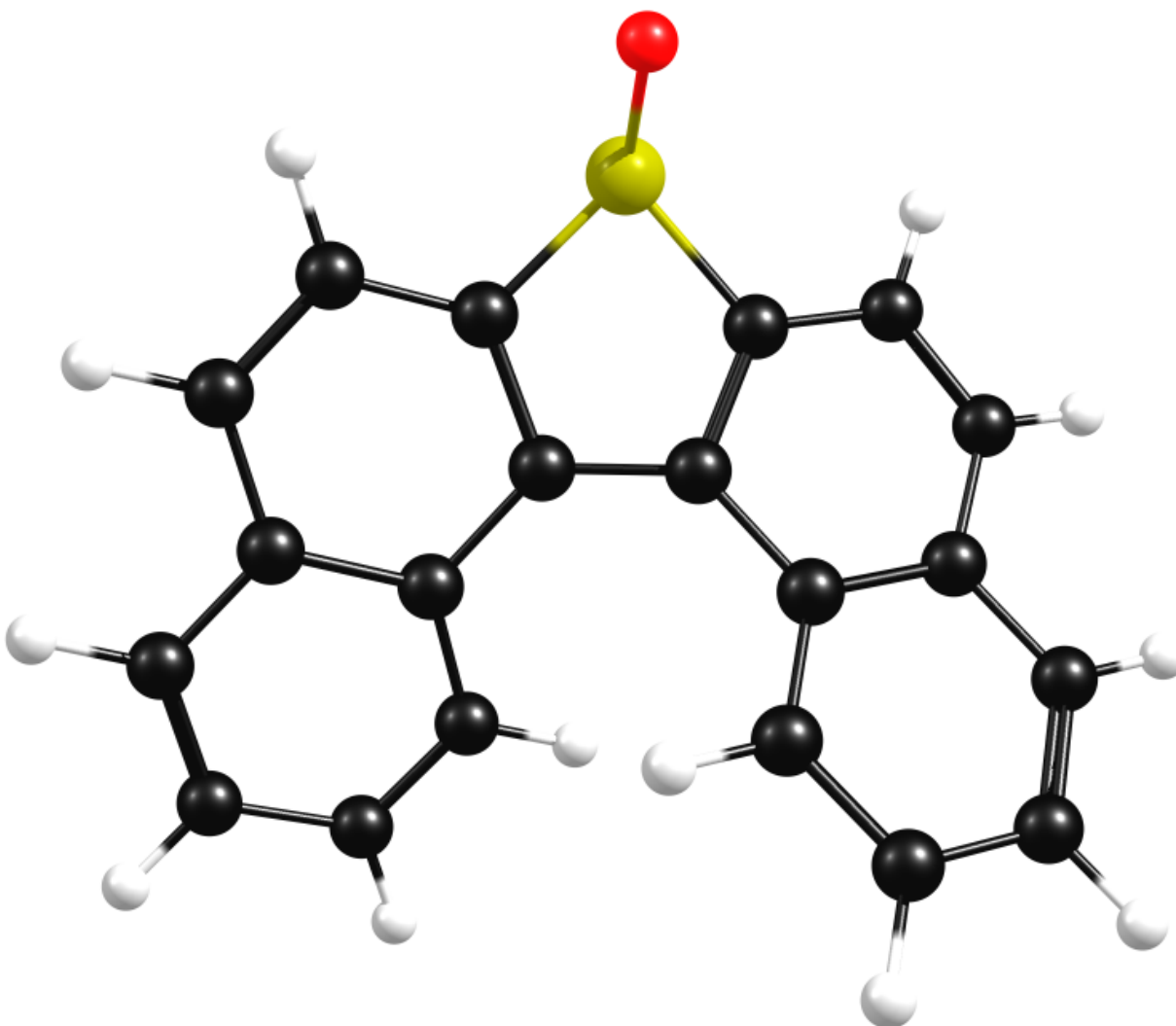
Electronic energy	-1242.04794786 hartree
Total thermal correction	0.01595420 hartree
Non-thermal (ZPE) correction	0.25581501 hartree
Total thermal energy	-1241.77617865 hartree
Total Enthalpy	-1241.77523444 hartree
Final Gibbs free enthalpy	-1241.83389259 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p) -1242.053750417977 hartree

dinaphtho[2,1-b:2',1'-d]thiophene S-oxide (4) T₁ state



TD-B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

H	-4.474351	1.404206	0.771922
C	-3.434402	1.214545	0.522877
C	-2.529761	2.271188	0.421378
C	-1.205440	2.007101	0.127928
C	-0.678316	0.651101	0.022432
C	-1.667467	-0.425156	-0.108059
C	-3.035503	-0.128036	0.206365
C	-4.000912	-1.152841	0.121362
C	-3.665704	-2.424848	-0.327766
C	-2.350974	-2.689455	-0.723463
C	-1.371975	-1.701348	-0.615681

H	-2.857183	3.293757	0.588329
H	-0.364615	-1.922571	-0.946623
H	-2.085037	-3.664558	-1.120957
H	-4.425338	-3.198423	-0.393887
H	-5.028476	-0.922707	0.391211
C	0.722372	0.647414	0.024343
C	1.247226	1.994945	-0.184584
C	2.562146	2.234535	-0.526033
C	3.459781	1.165017	-0.593989
C	3.069884	-0.150794	-0.171209
C	1.711686	-0.420857	0.204775
C	1.429906	-1.651548	0.819074
C	2.410403	-2.634197	0.969031
C	3.711351	-2.404907	0.512227
C	4.035232	-1.170591	-0.040902
H	2.897611	3.246172	-0.738964
H	4.490480	1.333002	-0.891862
H	5.054680	-0.965621	-0.357421
H	4.471638	-3.174389	0.611519
H	2.155313	-3.576502	1.444915
H	0.433235	-1.839997	1.199677
S	0.032487	3.314648	0.023239
O	0.179337	4.007888	1.364023

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	39.86	cm** ⁻¹
7:	66.49	cm** ⁻¹
8:	79.32	cm** ⁻¹
9:	90.83	cm** ⁻¹
10:	146.51	cm** ⁻¹
11:	172.16	cm** ⁻¹
12:	175.03	cm** ⁻¹
13:	189.04	cm** ⁻¹
14:	234.96	cm** ⁻¹
15:	238.35	cm** ⁻¹
16:	288.63	cm** ⁻¹
17:	323.40	cm** ⁻¹
18:	348.32	cm** ⁻¹
19:	374.39	cm** ⁻¹
20:	383.87	cm** ⁻¹

21:	407.17	cm**-1
22:	436.67	cm**-1
23:	465.07	cm**-1
24:	471.26	cm**-1
25:	505.81	cm**-1
26:	514.23	cm**-1
27:	526.50	cm**-1
28:	533.80	cm**-1
29:	536.83	cm**-1
30:	554.10	cm**-1
31:	606.80	cm**-1
32:	624.58	cm**-1
33:	633.54	cm**-1
34:	642.37	cm**-1
35:	682.55	cm**-1
36:	688.95	cm**-1
37:	734.73	cm**-1
38:	747.97	cm**-1
39:	765.75	cm**-1
40:	775.93	cm**-1
41:	786.15	cm**-1
42:	793.05	cm**-1
43:	800.95	cm**-1
44:	840.44	cm**-1
45:	870.36	cm**-1
46:	885.13	cm**-1
47:	887.12	cm**-1
48:	894.62	cm**-1
49:	925.69	cm**-1
50:	930.25	cm**-1
51:	943.58	cm**-1
52:	955.69	cm**-1
53:	968.49	cm**-1
54:	984.68	cm**-1
55:	996.97	cm**-1
56:	1049.55	cm**-1
57:	1056.06	cm**-1
58:	1058.50	cm**-1
59:	1077.40	cm**-1
60:	1089.94	cm**-1
61:	1126.14	cm**-1
62:	1134.71	cm**-1
63:	1145.71	cm**-1
64:	1149.32	cm**-1
65:	1182.58	cm**-1
66:	1188.32	cm**-1
67:	1207.04	cm**-1
68:	1217.23	cm**-1

69:	1242.83	cm** ⁻¹
70:	1254.32	cm** ⁻¹
71:	1290.63	cm** ⁻¹
72:	1306.62	cm** ⁻¹
73:	1328.11	cm** ⁻¹
74:	1347.21	cm** ⁻¹
75:	1374.35	cm** ⁻¹
76:	1377.72	cm** ⁻¹
77:	1428.57	cm** ⁻¹
78:	1442.19	cm** ⁻¹
79:	1464.92	cm** ⁻¹
80:	1473.09	cm** ⁻¹
81:	1488.98	cm** ⁻¹
82:	1505.23	cm** ⁻¹
83:	1521.98	cm** ⁻¹
84:	1529.50	cm** ⁻¹
85:	1558.01	cm** ⁻¹
86:	1596.78	cm** ⁻¹
87:	1605.35	cm** ⁻¹
88:	1625.33	cm** ⁻¹
89:	1630.22	cm** ⁻¹
90:	3179.65	cm** ⁻¹
91:	3180.05	cm** ⁻¹
92:	3185.80	cm** ⁻¹
93:	3188.39	cm** ⁻¹
94:	3191.42	cm** ⁻¹
95:	3191.73	cm** ⁻¹
96:	3201.79	cm** ⁻¹
97:	3202.91	cm** ⁻¹
98:	3205.62	cm** ⁻¹
99:	3206.29	cm** ⁻¹
100:	3224.88	cm** ⁻¹
101:	3231.30	cm** ⁻¹

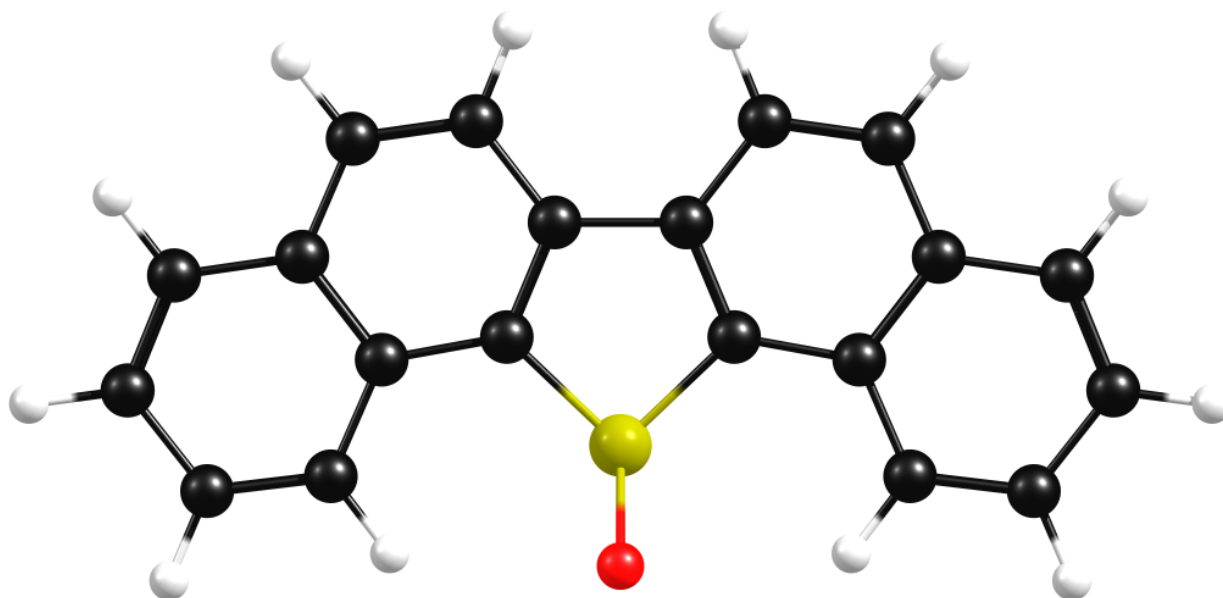
Electronic energy	-1242.07908244	hartree
Total thermal correction	0.01608455	hartree
Non-thermal (ZPE) correction	0.25500261	hartree
Total thermal energy	-1241.80799528	hartree
Total Enthalpy	-1241.80705107	hartree
Final Gibbs free enthalpy	-1241.86747772	hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p)	-1242.040583540381	hartree
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dinaphtho[1,2-b:2',1'-d]thiophene *S*-oxide (5) S_0 state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	0.000007	-1.278872	-0.443526
H	5.591324	1.516477	0.107662
C	4.936785	0.650913	0.040470
C	5.462247	-0.621196	-0.007751
C	4.603761	-1.745404	-0.085458
C	3.236373	-1.586191	-0.119976
C	2.665892	-0.283909	-0.084427
C	3.532434	0.859782	0.004831
C	2.964352	2.164573	0.053637
C	1.602780	2.364268	0.032542
C	0.734739	1.246217	-0.041174
C	1.272646	-0.031418	-0.111298
H	6.538514	-0.768026	0.020159
H	5.030567	-2.744159	-0.110289
H	2.580547	-2.450629	-0.145358
H	1.195447	3.370108	0.076876
H	3.635996	3.017365	0.113070
H	-3.636003	3.017353	0.113029
C	-2.964356	2.164562	0.053605
C	-1.602785	2.364262	0.032525
C	-0.734739	1.246214	-0.041183
C	-1.272641	-0.031423	-0.111311
C	-2.665886	-0.283919	-0.084456
C	-3.532433	0.859769	0.004794

C	-4.936783	0.650897	0.040419
C	-5.462241	-0.621214	-0.007808
C	-4.603751	-1.745419	-0.085508
C	-3.236363	-1.586202	-0.120013
H	-1.195458	3.370105	0.076858
H	-2.580535	-2.450639	-0.145390
H	-5.030553	-2.744175	-0.110345
H	-6.538508	-0.768048	0.020093
H	-5.591325	1.516460	0.107605
O	0.000004	-2.430803	0.543257

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	38.10	cm** ⁻¹
7:	67.65	cm** ⁻¹
8:	99.61	cm** ⁻¹
9:	105.93	cm** ⁻¹
10:	115.29	cm** ⁻¹
11:	169.61	cm** ⁻¹
12:	183.89	cm** ⁻¹
13:	213.92	cm** ⁻¹
14:	214.53	cm** ⁻¹
15:	255.91	cm** ⁻¹
16:	275.37	cm** ⁻¹
17:	335.75	cm** ⁻¹
18:	337.04	cm** ⁻¹
19:	377.39	cm** ⁻¹
20:	413.06	cm** ⁻¹
21:	450.30	cm** ⁻¹
22:	451.49	cm** ⁻¹
23:	471.72	cm** ⁻¹
24:	484.07	cm** ⁻¹
25:	502.21	cm** ⁻¹
26:	527.01	cm** ⁻¹
27:	541.17	cm** ⁻¹
28:	549.38	cm** ⁻¹
29:	554.48	cm** ⁻¹
30:	582.74	cm** ⁻¹
31:	585.62	cm** ⁻¹
32:	646.34	cm** ⁻¹
33:	665.00	cm** ⁻¹
34:	671.05	cm** ⁻¹

35:	690.48	cm** -1
36:	698.08	cm** -1
37:	759.05	cm** -1
38:	767.51	cm** -1
39:	789.16	cm** -1
40:	789.79	cm** -1
41:	819.53	cm** -1
42:	831.19	cm** -1
43:	832.92	cm** -1
44:	838.32	cm** -1
45:	841.34	cm** -1
46:	886.75	cm** -1
47:	888.28	cm** -1
48:	932.34	cm** -1
49:	957.10	cm** -1
50:	959.67	cm** -1
51:	969.91	cm** -1
52:	972.06	cm** -1
53:	976.08	cm** -1
54:	997.75	cm** -1
55:	999.23	cm** -1
56:	1003.94	cm** -1
57:	1049.83	cm** -1
58:	1053.27	cm** -1
59:	1063.36	cm** -1
60:	1140.88	cm** -1
61:	1160.50	cm** -1
62:	1164.65	cm** -1
63:	1175.22	cm** -1
64:	1182.10	cm** -1
65:	1191.63	cm** -1
66:	1192.46	cm** -1
67:	1242.31	cm** -1
68:	1247.17	cm** -1
69:	1286.38	cm** -1
70:	1288.89	cm** -1
71:	1342.32	cm** -1
72:	1353.65	cm** -1
73:	1377.34	cm** -1
74:	1395.92	cm** -1
75:	1400.59	cm** -1
76:	1406.23	cm** -1
77:	1421.95	cm** -1
78:	1465.67	cm** -1
79:	1476.19	cm** -1
80:	1492.46	cm** -1
81:	1506.40	cm** -1
82:	1555.88	cm** -1

83: 1559.59 cm**-1
84: 1601.37 cm**-1
85: 1611.05 cm**-1
86: 1632.99 cm**-1
87: 1644.13 cm**-1
88: 1671.04 cm**-1
89: 1674.68 cm**-1
90: 3175.23 cm**-1
91: 3175.26 cm**-1
92: 3178.76 cm**-1
93: 3180.30 cm**-1
94: 3187.36 cm**-1
95: 3187.39 cm**-1
96: 3198.32 cm**-1
97: 3200.42 cm**-1
98: 3200.69 cm**-1
99: 3203.34 cm**-1
100: 3212.99 cm**-1
101: 3213.05 cm**-1

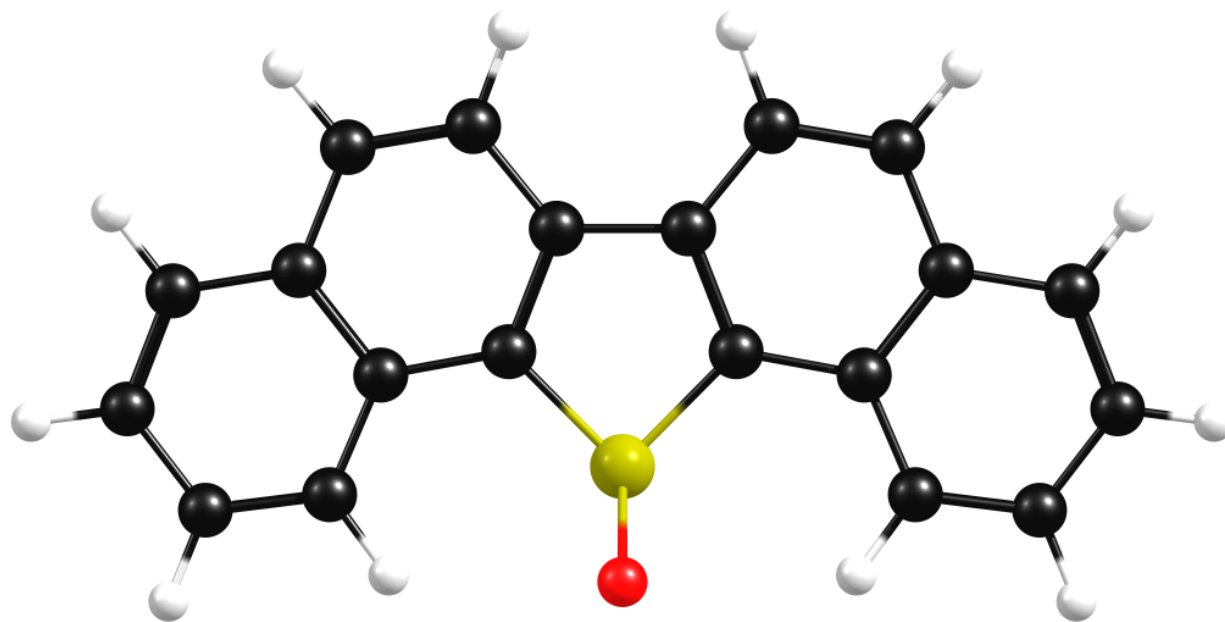
Electronic energy	-1242.16824869 hartree
Total thermal correction	0.01574963 hartree
Non-thermal (ZPE) correction	0.25840643 hartree
Total thermal energy	-1241.89409263 hartree
Total Enthalpy	-1241.89314842 hartree
Final Gibbs free enthalpy	-1241.95186989 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p) -1242.073319530190 hartree

dinaphtho[1,2-b:2',1'-d]thiophene S-oxide (5) S₁ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	0.000006	-1.308082	-0.290604
H	5.570279	1.489960	-0.056218
C	4.902248	0.632250	-0.071213
C	5.428379	-0.659028	-0.146415
C	4.570212	-1.767655	-0.151398
C	3.193318	-1.589185	-0.093785
C	2.631394	-0.284724	-0.064629
C	3.514330	0.851962	-0.019175
C	2.960400	2.174913	0.073578
C	1.603095	2.393280	0.118061
C	0.710543	1.298992	0.056830
C	1.239549	-0.030549	-0.081477
H	6.504510	-0.802974	-0.183663
H	4.981708	-2.772342	-0.178693
H	2.531283	-2.446656	-0.021971
H	1.215303	3.404773	0.197948
H	3.647949	3.015104	0.120579
H	-3.647958	3.015091	0.120535
C	-2.960405	2.174902	0.073543
C	-1.603101	2.393274	0.118042
C	-0.710544	1.298989	0.056821
C	-1.239544	-0.030553	-0.081491

C	-2.631389	-0.284733	-0.064660
C	-3.514330	0.851950	-0.019217
C	-4.902245	0.632233	-0.071271
C	-5.428371	-0.659047	-0.146480
C	-4.570200	-1.767672	-0.151453
C	-3.193308	-1.589196	-0.093822
H	-1.215314	3.404768	0.197934
H	-2.531271	-2.446665	-0.022001
H	-4.981692	-2.772360	-0.178753
H	-6.504501	-0.802997	-0.183741
H	-5.570280	1.489940	-0.056284
O	0.000001	-2.300286	0.880698

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	31.25	cm** ⁻¹
7:	56.74	cm** ⁻¹
8:	91.95	cm** ⁻¹
9:	104.46	cm** ⁻¹
10:	106.79	cm** ⁻¹
11:	146.00	cm** ⁻¹
12:	173.82	cm** ⁻¹
13:	200.68	cm** ⁻¹
14:	207.55	cm** ⁻¹
15:	247.45	cm** ⁻¹
16:	257.05	cm** ⁻¹
17:	294.82	cm** ⁻¹
18:	325.97	cm** ⁻¹
19:	363.52	cm** ⁻¹
20:	375.45	cm** ⁻¹
21:	398.71	cm** ⁻¹
22:	424.94	cm** ⁻¹
23:	468.20	cm** ⁻¹
24:	474.64	cm** ⁻¹
25:	493.05	cm** ⁻¹
26:	496.40	cm** ⁻¹
27:	515.24	cm** ⁻¹
28:	521.73	cm** ⁻¹
29:	531.00	cm** ⁻¹
30:	559.03	cm** ⁻¹
31:	569.36	cm** ⁻¹
32:	595.04	cm** ⁻¹

33:	621.83	cm**-1
34:	640.94	cm**-1
35:	658.25	cm**-1
36:	683.64	cm**-1
37:	740.73	cm**-1
38:	749.69	cm**-1
39:	762.13	cm**-1
40:	765.25	cm**-1
41:	773.82	cm**-1
42:	804.90	cm**-1
43:	810.44	cm**-1
44:	825.57	cm**-1
45:	831.93	cm**-1
46:	877.71	cm**-1
47:	880.97	cm**-1
48:	921.46	cm**-1
49:	930.38	cm**-1
50:	938.72	cm**-1
51:	940.76	cm**-1
52:	947.89	cm**-1
53:	951.10	cm**-1
54:	954.80	cm**-1
55:	980.79	cm**-1
56:	983.02	cm**-1
57:	1002.12	cm**-1
58:	1056.73	cm**-1
59:	1063.10	cm**-1
60:	1102.93	cm**-1
61:	1144.55	cm**-1
62:	1145.92	cm**-1
63:	1165.82	cm**-1
64:	1166.78	cm**-1
65:	1186.51	cm**-1
66:	1189.47	cm**-1
67:	1241.08	cm**-1
68:	1243.98	cm**-1
69:	1289.16	cm**-1
70:	1292.12	cm**-1
71:	1306.36	cm**-1
72:	1353.51	cm**-1
73:	1367.04	cm**-1
74:	1370.84	cm**-1
75:	1383.16	cm**-1
76:	1392.28	cm**-1
77:	1428.55	cm**-1
78:	1459.96	cm**-1
79:	1469.01	cm**-1
80:	1471.09	cm**-1

81: 1510.08 cm**-1
82: 1528.63 cm**-1
83: 1564.16 cm**-1
84: 1567.78 cm**-1
85: 1579.39 cm**-1
86: 1587.98 cm**-1
87: 1602.55 cm**-1
88: 1628.55 cm**-1
89: 1633.90 cm**-1
90: 3178.04 cm**-1
91: 3178.21 cm**-1
92: 3181.00 cm**-1
93: 3183.90 cm**-1
94: 3191.03 cm**-1
95: 3191.04 cm**-1
96: 3198.50 cm**-1
97: 3202.01 cm**-1
98: 3202.67 cm**-1
99: 3202.73 cm**-1
100: 3212.45 cm**-1
101: 3212.70 cm**-1

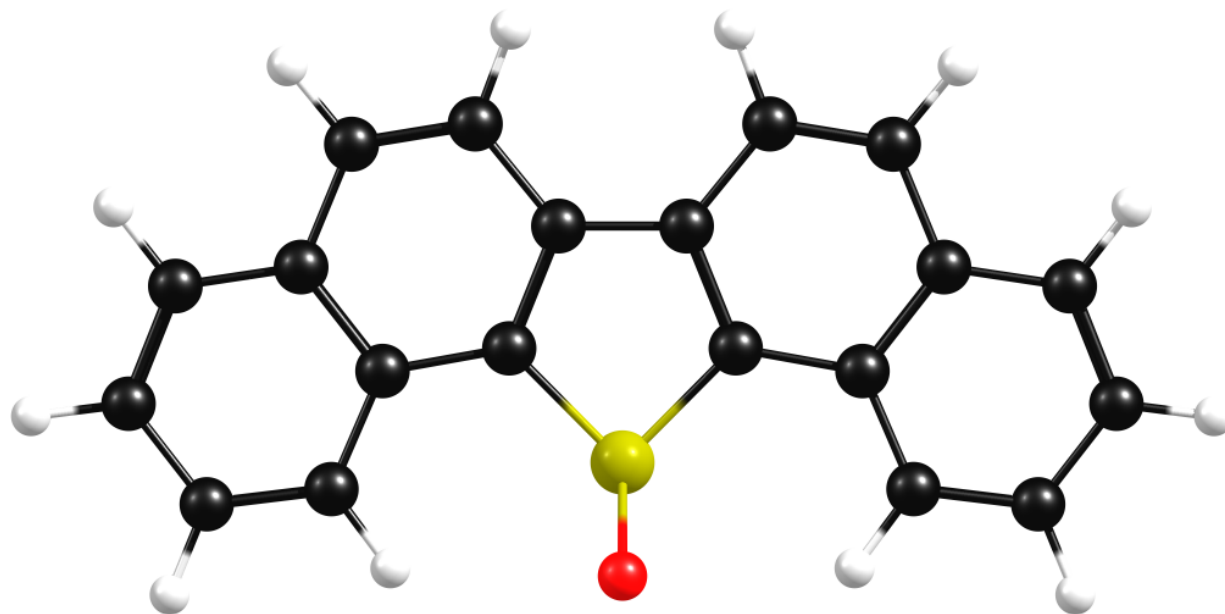
Electronic energy	-1242.05324828 hartree
Total thermal correction	0.01557150 hartree
Non-thermal (ZPE) correction	0.25471212 hartree
Total thermal energy	-1241.78296466 hartree
Total Enthalpy	-1241.78202045 hartree
Final Gibbs free enthalpy	-1241.83966639 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p) -1242.062499617344 hartree

dinaphtho[1,2-b:2',1'-d]thiophene *S*-oxide (5) T₁ state



B3LYP/6-31G(d,p) optimization and Hessian

Coordinates

S	-0.000008	-1.329352	-0.332518
H	5.563165	1.500827	0.013387
C	4.900070	0.640006	-0.026961
C	5.437379	-0.652195	-0.091682
C	4.586511	-1.762761	-0.128530
C	3.206718	-1.593364	-0.112767
C	2.639692	-0.292183	-0.079001
C	3.518329	0.847730	-0.012917
C	2.948720	2.179376	0.065764
C	1.601203	2.396870	0.084871
C	0.699618	1.293858	0.011173
C	1.249300	-0.043192	-0.107365
H	6.514911	-0.789864	-0.100103
H	5.003844	-2.765220	-0.156013
H	2.549446	-2.456427	-0.086119
H	1.209667	3.407608	0.156145
H	3.636093	3.019563	0.120840
H	-3.635834	3.019606	0.119643
C	-2.948484	2.179395	0.064871
C	-1.600771	2.396898	0.084090
C	-0.699347	1.294301	0.010908
C	-1.249393	-0.043755	-0.107764
C	-2.639752	-0.292557	-0.079079
C	-3.518363	0.847532	-0.013378

C	-4.899759	0.639997	-0.027319
C	-5.437537	-0.652592	-0.091532
C	-4.587053	-1.762974	-0.127922
C	-3.206900	-1.593576	-0.112211
H	-1.209471	3.407764	0.155012
H	-2.549742	-2.456716	-0.085170
H	-5.004284	-2.765482	-0.155019
H	-6.515117	-0.789840	-0.099884
H	-5.562909	1.500792	0.012649
O	0.000113	-2.322392	0.820060

Frequencies

0:	0.00	cm** ⁻¹
1:	0.00	cm** ⁻¹
2:	0.00	cm** ⁻¹
3:	0.00	cm** ⁻¹
4:	0.00	cm** ⁻¹
5:	0.00	cm** ⁻¹
6:	38.56	cm** ⁻¹
7:	75.61	cm** ⁻¹
8:	96.99	cm** ⁻¹
9:	106.92	cm** ⁻¹
10:	119.35	cm** ⁻¹
11:	176.18	cm** ⁻¹
12:	184.37	cm** ⁻¹
13:	203.93	cm** ⁻¹
14:	224.42	cm** ⁻¹
15:	253.11	cm** ⁻¹
16:	267.54	cm** ⁻¹
17:	312.10	cm** ⁻¹
18:	325.38	cm** ⁻¹
19:	375.80	cm** ⁻¹
20:	401.17	cm** ⁻¹
21:	419.85	cm** ⁻¹
22:	431.35	cm** ⁻¹
23:	465.91	cm** ⁻¹
24:	467.18	cm** ⁻¹
25:	497.69	cm** ⁻¹
26:	498.76	cm** ⁻¹
27:	527.24	cm** ⁻¹
28:	530.39	cm** ⁻¹
29:	536.50	cm** ⁻¹
30:	559.89	cm** ⁻¹
31:	586.07	cm** ⁻¹
32:	619.02	cm** ⁻¹
33:	643.17	cm** ⁻¹
34:	653.70	cm** ⁻¹

35:	662.58	cm**-1
36:	686.28	cm**-1
37:	747.08	cm**-1
38:	760.01	cm**-1
39:	775.34	cm**-1
40:	776.42	cm**-1
41:	806.22	cm**-1
42:	817.02	cm**-1
43:	817.90	cm**-1
44:	819.97	cm**-1
45:	831.32	cm**-1
46:	886.95	cm**-1
47:	887.61	cm**-1
48:	930.60	cm**-1
49:	933.65	cm**-1
50:	943.41	cm**-1
51:	944.28	cm**-1
52:	963.09	cm**-1
53:	968.20	cm**-1
54:	983.76	cm**-1
55:	985.25	cm**-1
56:	990.68	cm**-1
57:	1004.14	cm**-1
58:	1036.30	cm**-1
59:	1059.39	cm**-1
60:	1062.09	cm**-1
61:	1139.05	cm**-1
62:	1141.12	cm**-1
63:	1153.53	cm**-1
64:	1162.84	cm**-1
65:	1173.18	cm**-1
66:	1187.63	cm**-1
67:	1211.75	cm**-1
68:	1233.78	cm**-1
69:	1248.37	cm**-1
70:	1275.36	cm**-1
71:	1294.84	cm**-1
72:	1298.95	cm**-1
73:	1351.97	cm**-1
74:	1362.28	cm**-1
75:	1388.78	cm**-1
76:	1397.63	cm**-1
77:	1439.21	cm**-1
78:	1456.73	cm**-1
79:	1473.97	cm**-1
80:	1477.51	cm**-1
81:	1486.30	cm**-1
82:	1504.39	cm**-1

83: 1537.18 cm**-1
84: 1571.18 cm**-1
85: 1572.24 cm**-1
86: 1594.01 cm**-1
87: 1602.94 cm**-1
88: 1615.92 cm**-1
89: 1617.87 cm**-1
90: 3176.35 cm**-1
91: 3176.58 cm**-1
92: 3178.96 cm**-1
93: 3181.12 cm**-1
94: 3189.23 cm**-1
95: 3189.30 cm**-1
96: 3197.64 cm**-1
97: 3201.89 cm**-1
98: 3203.55 cm**-1
99: 3203.72 cm**-1
100: 3214.98 cm**-1
101: 3215.19 cm**-1

Electronic energy	-1242.08680353 hartree
Total thermal correction	0.01606305 hartree
Non-thermal (ZPE) correction	0.25510173 hartree
Total thermal energy	-1241.81563874 hartree
Total Enthalpy	-1241.81469453 hartree
Final Gibbs free enthalpy	-1241.87483412 hartree

Energy Calculations at above geometry

T₂

TD-B3LYP/6-31G(d,p) -1242.059131602872 hartree

Calculations for Redox Potentials

Benzene

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	1.400085000	0.000000000
C	1.212517000	0.700047000	0.000000000
C	-1.212517000	0.700047000	0.000000000
H	2.154413000	1.243851000	0.000000000
H	-2.154413000	1.243851000	0.000000000
C	1.212509000	-0.700042000	0.000000000
C	-1.212509000	-0.700042000	0.000000000
H	2.154355000	-1.243818000	0.000000000
H	-2.154355000	-1.243818000	0.000000000
C	0.000000000	-1.400095000	0.000000000
H	0.000000000	-2.487702000	0.000000000
H	0.000000000	2.487635000	0.000000000

Frequencies --	409.7782	415.5598	618.6244
Frequencies --	619.2990	687.2321	711.0817
Frequencies --	866.5322	869.0279	989.5069
Frequencies --	992.6293	1009.4777	1016.7938
Frequencies --	1020.8952	1059.6523	1059.7315
Frequencies --	1169.4011	1190.9070	1190.9764
Frequencies --	1349.5236	1382.8354	1516.2483
Frequencies --	1516.4586	1639.0265	1639.2820
Frequencies --	3179.3616	3187.4418	3187.6026
Frequencies --	3201.3062	3201.4794	3211.0159

Zero-point correction=	0.100487 (Hartree/Particle)
Thermal correction to Energy=	0.104886
Thermal correction to Enthalpy=	0.105830
Thermal correction to Gibbs Free Energy=	0.074704
Sum of electronic and zero-point Energies=	-232.167162
Sum of electronic and thermal Energies=	-232.162763
Sum of electronic and thermal Enthalpies=	-232.161819
Sum of electronic and thermal Free Energies=	-232.192945

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	-1.437392000	0.000000000
C	0.000000000	-0.725761000	1.195131000
C	0.000000000	-0.725761000	-1.195131000
H	0.000000000	-1.243387000	2.149464000
H	0.000000000	-1.243387000	-2.149464000
C	0.000000000	0.725761000	1.195131000
C	0.000000000	0.725761000	-1.195131000

H	0.000000000	1.243387000	2.149464000
H	0.000000000	1.243387000	-2.149464000
C	0.000000000	1.437392000	0.000000000
H	0.000000000	2.522117000	0.000000000
H	0.000000000	-2.522117000	0.000000000

Frequencies --	-331.8249	289.4009	340.3673
Frequencies --	388.8371	605.6877	674.9401
Frequencies --	837.2804	873.6286	909.8273
Frequencies --	962.5705	979.1845	1005.7063
Frequencies --	1007.4918	1009.6457	1012.5694
Frequencies --	1083.4778	1181.8660	1193.2366
Frequencies --	1319.7589	1384.8317	1411.7519
Frequencies --	1465.4875	1532.6882	1587.7194
Frequencies --	3231.2769	3236.7627	3237.4881
Frequencies --	3243.5037	3248.7125	3252.3074

Zero-point correction=	0.096840 (Hartree/Particle)
Thermal correction to Energy=	0.101584
Thermal correction to Enthalpy=	0.102529
Thermal correction to Gibbs Free Energy=	0.068400
Sum of electronic and zero-point Energies=	-231.927018
Sum of electronic and thermal Energies=	-231.922274
Sum of electronic and thermal Enthalpies=	-231.921330
Sum of electronic and thermal Free Energies=	-231.955458

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	0.000000000	1.406317000
C	0.000000000	1.230181000	0.731717000
C	0.000000000	-1.230181000	0.731717000
H	0.000000000	2.166433000	1.287228000
H	0.000000000	-2.166433000	1.287228000
C	0.000000000	1.230181000	-0.731717000
C	0.000000000	-1.230181000	-0.731717000
H	0.000000000	2.166433000	-1.287228000
H	0.000000000	-2.166433000	-1.287228000
C	0.000000000	0.000000000	-1.406317000
H	0.000000000	0.000000000	-2.498905000
H	0.000000000	0.000000000	2.498905000

Frequencies --	46.0699	84.5636	381.0710
Frequencies --	460.7227	534.5246	538.2177
Frequencies --	556.4992	611.1768	618.2030
Frequencies --	637.5427	910.9838	926.0146
Frequencies --	931.8640	952.0685	996.9096
Frequencies --	1042.7222	1141.2986	1148.7017

Frequencies --	1288.7336	1355.7158	1366.1427
Frequencies --	1471.3792	1476.8182	1528.6903
Frequencies --	3119.3952	3121.6113	3147.7158
Frequencies --	3160.0376	3169.0707	3179.1265

Zero-point correction=	0.090907 (Hartree/Particle)
Thermal correction to Energy=	0.097305
Thermal correction to Enthalpy=	0.098249
Thermal correction to Gibbs Free Energy=	0.061320
Sum of electronic and zero-point Energies=	-232.207954
Sum of electronic and thermal Energies=	-232.201555
Sum of electronic and thermal Enthalpies=	-232.200611
Sum of electronic and thermal Free Energies=	-232.237540

Naphthalene

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

H	0.000000000	1.243919000	2.494531000
C	0.000000000	1.246744000	1.406378000
C	0.000000000	2.438007000	0.709952000
C	0.000000000	2.438007000	-0.709952000
C	0.000000000	1.246744000	-1.406378000
C	0.000000000	0.000000000	-0.718028000
C	0.000000000	0.000000000	0.718028000
C	0.000000000	-1.246744000	1.406378000
C	0.000000000	-2.438007000	0.709952000
C	0.000000000	-2.438007000	-0.709952000
C	0.000000000	-1.246744000	-1.406378000
H	0.000000000	3.383327000	1.247082000
H	0.000000000	3.383327000	-1.247082000
H	0.000000000	1.243919000	-2.494531000
H	0.000000000	-1.243919000	-2.494531000
H	0.000000000	-3.383327000	-1.247082000
H	0.000000000	-3.383327000	1.247082000
H	0.000000000	-1.243919000	2.494531000

Frequencies --	179.4871	186.4270	361.4902
Frequencies --	401.2306	477.3184	493.8790
Frequencies --	515.8416	516.9887	630.5417
Frequencies --	631.3627	732.3576	769.7859
Frequencies --	775.6532	801.6907	804.8667
Frequencies --	857.6402	899.1474	945.7773
Frequencies --	967.7125	986.7163	1001.7027
Frequencies --	1007.7461	1035.0440	1043.9893
Frequencies --	1144.7400	1168.4852	1172.5532
Frequencies --	1175.4267	1232.1785	1273.5988
Frequencies --	1284.3212	1400.9541	1408.7467
Frequencies --	1419.9244	1491.7453	1493.4544

Frequencies --	1553.6946	1616.4429	1640.7189
Frequencies --	1673.8564	3179.7572	3181.0548
Frequencies --	3182.8472	3185.0476	3196.1269
Frequencies --	3196.7015	3207.8104	

Zero-point correction=	0.147428 (Hartree/Particle)
Thermal correction to Energy=	0.154243
Thermal correction to Enthalpy=	0.155187
Thermal correction to Gibbs Free Energy=	0.117531
Sum of electronic and zero-point Energies=	-385.772436
Sum of electronic and thermal Energies=	-385.765622
Sum of electronic and thermal Enthalpies=	-385.764678
Sum of electronic and thermal Free Energies=	-385.802334

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

H	0.000000000	1.238093000	2.491374000
C	0.000000000	1.235245000	1.404735000
C	0.000000000	2.451145000	0.696513000
C	0.000000000	2.451145000	-0.696513000
C	0.000000000	1.235245000	-1.404735000
C	0.000000000	0.000000000	-0.716170000
C	0.000000000	0.000000000	0.716170000
C	0.000000000	-1.235245000	1.404735000
C	0.000000000	-2.451145000	0.696513000
C	0.000000000	-2.451145000	-0.696513000
C	0.000000000	-1.235245000	-1.404735000
H	0.000000000	3.389199000	1.242807000
H	0.000000000	3.389199000	-1.242807000
H	0.000000000	1.238093000	-2.491374000
H	0.000000000	-1.238093000	-2.491374000
H	0.000000000	-3.389199000	-1.242807000
H	0.000000000	-3.389199000	1.242807000
H	0.000000000	-1.238093000	2.491374000

Frequencies --	146.3046	176.5095	355.1879
Frequencies --	378.1804	426.1977	433.9010
Frequencies --	474.0994	512.9954	557.5090
Frequencies --	604.4171	725.1879	748.7720
Frequencies --	771.3298	774.8724	808.6317
Frequencies --	877.0342	934.9670	939.7784
Frequencies --	982.3060	1004.7347	1021.8322
Frequencies --	1025.4607	1039.1938	1062.4895
Frequencies --	1118.5042	1120.4248	1182.2581
Frequencies --	1186.8619	1233.1387	1263.6799
Frequencies --	1299.7048	1422.3738	1425.3344
Frequencies --	1431.5455	1469.9243	1497.4547
Frequencies --	1513.5827	1551.1613	1569.3707
Frequencies --	1631.7492	3215.1913	3216.7656
Frequencies --	3217.9014	3219.6978	3227.9936

Frequencies -- 3228.2780 3237.7398 3238.3691

Zero-point correction= 0.146944 (Hartree/Particle)
Thermal correction to Energy= 0.154044
Thermal correction to Enthalpy= 0.154988
Thermal correction to Gibbs Free Energy= 0.116097
Sum of electronic and zero-point Energies= -385.562287
Sum of electronic and thermal Energies= -385.555187
Sum of electronic and thermal Enthalpies= -385.554242
Sum of electronic and thermal Free Energies= -385.593134

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

H	0.00000000	1.25606000	2.49643000
C	0.00000000	1.25333100	1.40674400
C	0.00000000	2.47672500	0.69752700
C	0.00000000	2.47672500	-0.69752700
C	0.00000000	1.25333100	-1.40674400
C	0.00000000	0.00000000	-0.72745000
C	0.00000000	0.00000000	0.72745000
C	0.00000000	-1.25333100	1.40674400
C	0.00000000	-2.47672500	0.69752700
C	0.00000000	-2.47672500	-0.69752700
C	0.00000000	-1.25333100	-1.40674400
H	0.00000000	3.41815200	1.24536000
H	0.00000000	3.41815200	-1.24536000
H	0.00000000	1.25606000	-2.49643000
H	0.00000000	-1.25606000	-2.49643000
H	0.00000000	-3.41815200	-1.24536000
H	0.00000000	-3.41815200	1.24536000
H	0.00000000	-1.25606000	2.49643000

Frequencies --	158.1512	187.9081	295.5008
Frequencies --	361.8278	482.0022	508.5978
Frequencies --	509.8695	514.2735	587.9666
Frequencies --	606.7362	658.9045	718.1069
Frequencies --	718.6763	732.4088	746.7213
Frequencies --	779.7898	792.7845	803.9701
Frequencies --	804.6131	894.4677	899.2477
Frequencies --	908.5834	1007.8466	1051.0470
Frequencies --	1061.9030	1102.7459	1153.6694
Frequencies --	1160.4758	1204.7334	1223.9536
Frequencies --	1264.6765	1374.3336	1402.8716
Frequencies --	1405.2204	1412.9554	1447.6577
Frequencies --	1475.2386	1523.0765	1533.1119
Frequencies --	1596.5144	3143.6739	3145.9548
Frequencies --	3147.4572	3151.6203	3160.5353
Frequencies --	3161.9731	3177.1364	3179.2369

Zero-point correction=	0.142023 (Hartree/Particle)
Thermal correction to Energy=	0.149323
Thermal correction to Enthalpy=	0.150267
Thermal correction to Gibbs Free Energy=	0.111157
Sum of electronic and zero-point Energies=	-385.839543
Sum of electronic and thermal Energies=	-385.832242
Sum of electronic and thermal Enthalpies=	-385.831298
Sum of electronic and thermal Free Energies=	-385.870408

Chrysene

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	1.258721000	1.437146000	0.000000000
C	2.487395000	0.705708000	0.000000000
C	-0.001537000	0.709934000	0.000000000
C	2.447014000	-0.723107000	0.000000000
C	0.001537000	-0.709934000	0.000000000
C	1.258721000	-1.399075000	0.000000000
C	-1.258721000	1.399075000	0.000000000
C	-2.447014000	0.723107000	0.000000000
C	-2.487395000	-0.705708000	0.000000000
C	-1.258721000	-1.437146000	0.000000000
C	-3.724756000	-1.400688000	0.000000000
C	-3.763282000	-2.782036000	0.000000000
C	-1.334653000	-2.855918000	0.000000000
C	-2.553894000	-3.512118000	0.000000000
C	1.334653000	2.855918000	0.000000000
C	3.724756000	1.400688000	0.000000000
H	3.387154000	-1.270341000	0.000000000
H	1.279197000	-2.483165000	0.000000000
H	-1.279197000	2.483165000	0.000000000
H	-3.387154000	1.270341000	0.000000000
H	-4.645903000	-0.821742000	0.000000000
H	-4.715924000	-3.305772000	0.000000000
H	-0.428575000	-3.451581000	0.000000000
H	-2.578181000	-4.599150000	0.000000000
C	2.553894000	3.512118000	0.000000000
C	3.763282000	2.782036000	0.000000000
H	0.428575000	3.451581000	0.000000000
H	4.645903000	0.821742000	0.000000000
H	2.578181000	4.599150000	0.000000000
H	4.715924000	3.305772000	0.000000000

Frequencies --	57.1936	90.7959	150.2217
Frequencies --	179.7679	191.6234	242.7825
Frequencies --	294.8805	299.7292	382.7548
Frequencies --	399.4319	442.9837	485.1963

Frequencies --	486.3254	489.7749	524.3346
Frequencies --	543.4714	571.1310	575.2526
Frequencies --	577.6420	595.7946	687.9239
Frequencies --	688.2408	691.4128	749.9201
Frequencies --	755.6529	776.0850	779.6948
Frequencies --	791.5348	833.2725	841.9869
Frequencies --	861.6819	882.2938	886.6597
Frequencies --	890.3790	891.1931	970.8015
Frequencies --	972.3558	988.7175	991.5857
Frequencies --	1004.8660	1005.4848	1035.2862
Frequencies --	1057.6978	1063.3318	1100.3604
Frequencies --	1156.4761	1173.8235	1179.3989
Frequencies --	1184.4170	1207.7159	1217.7615
Frequencies --	1255.3834	1268.6077	1281.0208
Frequencies --	1283.4005	1327.2799	1362.0706
Frequencies --	1393.4579	1398.4482	1403.1858
Frequencies --	1459.8611	1467.2970	1471.2149
Frequencies --	1489.7770	1528.2853	1560.4010
Frequencies --	1566.7020	1609.8993	1640.0981
Frequencies --	1649.6611	1661.1187	1664.2725
Frequencies --	3183.7421	3183.7984	3187.5894
Frequencies --	3187.9713	3193.5268	3193.7193
Frequencies --	3207.0266	3207.2712	3217.7434
Frequencies --	3217.9093	3236.7298	3237.1839

Zero-point correction=	0.241702 (Hartree/Particle)
Thermal correction to Energy=	0.253759
Thermal correction to Enthalpy=	0.254704
Thermal correction to Gibbs Free Energy=	0.204186
Sum of electronic and zero-point Energies=	-692.984031
Sum of electronic and thermal Energies=	-692.971973
Sum of electronic and thermal Enthalpies=	-692.971029
Sum of electronic and thermal Free Energies=	-693.021547

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	1.250793000	1.465358000	0.000000000
C	2.481262000	0.739652000	0.000000000
C	-0.009403000	0.723800000	0.000000000
C	2.447560000	-0.678747000	0.000000000
C	0.009403000	-0.723800000	0.000000000
C	1.250793000	-1.383379000	0.000000000
C	-1.250793000	1.383379000	0.000000000
C	-2.447560000	0.678747000	0.000000000
C	-2.481262000	-0.739652000	0.000000000
C	-1.250793000	-1.465358000	0.000000000
C	-3.718316000	-1.429319000	0.000000000
C	-3.752133000	-2.818080000	0.000000000

C	-1.316626000	-2.870417000	0.000000000
C	-2.547104000	-3.534260000	0.000000000
C	1.316626000	2.870417000	0.000000000
C	3.718316000	1.429319000	0.000000000
H	3.387441000	-1.224554000	0.000000000
H	1.297732000	-2.465602000	0.000000000
H	-1.297732000	2.465602000	0.000000000
H	-3.387441000	1.224554000	0.000000000
H	-4.638812000	-0.851601000	0.000000000
H	-4.702227000	-3.344060000	0.000000000
H	-0.413006000	-3.468616000	0.000000000
H	-2.561413000	-4.620622000	0.000000000
C	2.547104000	3.534260000	0.000000000
C	3.752133000	2.818080000	0.000000000
H	0.413006000	3.468616000	0.000000000
H	4.638812000	0.851601000	0.000000000
H	2.561413000	4.620622000	0.000000000
H	4.702227000	3.344060000	0.000000000

Frequencies --	54.3195	77.6361	146.5563
Frequencies --	168.3212	193.3001	226.4026
Frequencies --	290.4032	294.1155	376.2536
Frequencies --	383.7856	424.1050	460.6469
Frequencies --	477.2644	478.2566	500.9007
Frequencies --	523.5743	541.1846	556.3161
Frequencies --	561.8927	571.6541	685.3627
Frequencies --	685.8186	686.8102	738.5119
Frequencies --	763.0466	771.6399	774.1235
Frequencies --	779.3763	853.1167	861.3892
Frequencies --	863.2636	887.2913	893.6568
Frequencies --	899.9395	906.9875	984.1097
Frequencies --	985.4781	1001.8224	1004.4899
Frequencies --	1018.4943	1019.3740	1034.9062
Frequencies --	1067.4457	1072.1267	1110.4096
Frequencies --	1149.3563	1162.7625	1172.6333
Frequencies --	1185.4883	1200.8053	1252.5042
Frequencies --	1261.3931	1278.6820	1293.5850
Frequencies --	1300.8782	1324.7077	1361.4203
Frequencies --	1362.2374	1386.8823	1406.5887
Frequencies --	1464.4200	1465.4438	1470.2367
Frequencies --	1479.9988	1534.1459	1536.0607
Frequencies --	1548.7813	1581.4595	1587.4024
Frequencies --	1611.5622	1619.7633	1637.5667
Frequencies --	3206.7471	3206.7538	3211.9369
Frequencies --	3212.4995	3213.7205	3213.9565
Frequencies --	3224.8693	3225.2231	3232.5522
Frequencies --	3232.6110	3252.8799	3253.0689

Zero-point correction=	0.241439 (Hartree/Particle)
Thermal correction to Energy=	0.253729
Thermal correction to Enthalpy=	0.254673
Thermal correction to Gibbs Free Energy=	0.202912
Sum of electronic and zero-point Energies=	-692.783394
Sum of electronic and thermal Energies=	-692.771104

Sum of electronic and thermal Enthalpies= -692.770160
Sum of electronic and thermal Free Energies= -692.821921

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	1.258604000	1.468451000	0.000000000
C	2.499747000	0.736693000	0.000000000
C	-0.012376000	0.728527000	0.000000000
C	2.469184000	-0.692106000	0.000000000
C	0.012376000	-0.728527000	0.000000000
C	1.258604000	-1.382418000	0.000000000
C	-1.258604000	1.382418000	0.000000000
C	-2.469184000	0.692106000	0.000000000
C	-2.499747000	-0.736693000	0.000000000
C	-1.258604000	-1.468451000	0.000000000
C	-3.725207000	-1.455232000	0.000000000
C	-3.756908000	-2.849048000	0.000000000
C	-1.331100000	-2.879809000	0.000000000
C	-2.552673000	-3.566343000	0.000000000
C	1.331100000	2.879809000	0.000000000
C	3.725207000	1.455232000	0.000000000
H	3.410598000	-1.238246000	0.000000000
H	1.297099000	-2.468413000	0.000000000
H	-1.297099000	2.468413000	0.000000000
H	-3.410598000	1.238246000	0.000000000
H	-4.655976000	-0.889637000	0.000000000
H	-4.710737000	-3.372992000	0.000000000
H	-0.417760000	-3.467187000	0.000000000
H	-2.558561000	-4.654241000	0.000000000
C	2.552673000	3.566343000	0.000000000
C	3.756908000	2.849048000	0.000000000
H	0.417760000	3.467187000	0.000000000
H	4.655976000	0.889637000	0.000000000

Frequencies --	31.9179	90.5074	128.1269
Frequencies --	182.6442	186.6103	227.4737
Frequencies --	289.1913	295.2445	349.2648
Frequencies --	371.7391	427.9271	475.2949
Frequencies --	476.7287	493.5912	525.0731
Frequencies --	539.1123	549.4998	562.0844
Frequencies --	570.1943	572.7783	660.6260
Frequencies --	674.6412	677.3628	701.3106
Frequencies --	710.2251	748.0776	752.0155
Frequencies --	762.9731	766.4092	771.9417
Frequencies --	845.8342	846.6514	847.8340
Frequencies --	872.7290	885.4175	900.1309
Frequencies --	900.6833	909.0679	910.2131
Frequencies --	958.9210	959.2356	1014.6587
Frequencies --	1057.3423	1063.2737	1093.5540

Frequencies --	1111.5399	1132.0658	1135.8604
Frequencies --	1168.9953	1176.0069	1216.5575
Frequencies --	1224.6323	1255.1430	1265.2935
Frequencies --	1270.6351	1293.3693	1303.7861
Frequencies --	1311.4820	1349.3170	1372.9142
Frequencies --	1444.0601	1448.0775	1450.2420
Frequencies --	1463.7419	1491.8861	1515.1898
Frequencies --	1523.6326	1550.0822	1569.0881
Frequencies --	1585.3321	1595.4556	1619.8552
Frequencies --	3160.9260	3161.1939	3165.4157
Frequencies --	3165.7968	3174.7279	3175.5551
Frequencies --	3184.3957	3185.3189	3192.0899
Frequencies --	3192.4825	3208.2149	3208.9706

Zero-point correction=	0.236145 (Hartree/Particle)
Thermal correction to Energy=	0.248721
Thermal correction to Enthalpy=	0.249665
Thermal correction to Gibbs Free Energy=	0.197130
Sum of electronic and zero-point Energies=	-693.059379
Sum of electronic and thermal Energies=	-693.046802
Sum of electronic and thermal Enthalpies=	-693.045858
Sum of electronic and thermal Free Energies=	-693.098393

Pyrimidine

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

N	0.000000000	1.195227000	-0.716529000
N	0.000000000	-1.195227000	-0.716529000
C	0.000000000	0.000000000	-1.319160000
C	0.000000000	1.185927000	0.626351000
C	0.000000000	0.000000000	1.358229000
C	0.000000000	-1.185927000	0.626351000
H	0.000000000	0.000000000	-2.406122000
H	0.000000000	2.154358000	1.121715000
H	0.000000000	0.000000000	2.443467000
H	0.000000000	-2.154358000	1.121715000

Frequencies --	352.0457	407.5571	632.9315
Frequencies --	688.5240	729.7075	824.5215
Frequencies --	972.8020	1012.2727	1014.4423
Frequencies --	1027.4241	1079.1502	1094.5858
Frequencies --	1157.3733	1225.0574	1267.1551
Frequencies --	1393.3103	1440.8879	1497.5692
Frequencies --	1616.6301	1621.1917	3198.0108
Frequencies --	3200.5959	3209.0271	3235.4090

Zero-point correction=	0.077226 (Hartree/Particle)
Thermal correction to Energy=	0.081422
Thermal correction to Enthalpy=	0.082366
Thermal correction to Gibbs Free Energy=	0.050510
Sum of electronic and zero-point Energies=	-264.272049
Sum of electronic and thermal Energies=	-264.267853
Sum of electronic and thermal Enthalpies=	-264.266909
Sum of electronic and thermal Free Energies=	-264.298765

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

N	0.000000000	1.113065000	0.687402000
N	0.000000000	-1.113065000	0.687402000
C	0.000000000	0.000000000	1.410414000
C	0.000000000	1.174887000	-0.632269000
C	0.000000000	0.000000000	-1.390323000
C	0.000000000	-1.174887000	-0.632269000
H	0.000000000	0.000000000	2.492180000
H	0.000000000	2.164415000	-1.087514000
H	0.000000000	0.000000000	-2.474100000
H	0.000000000	-2.164415000	-1.087514000

Frequencies --	369.4716	447.1430	497.0739
Frequencies --	566.1348	652.7146	831.9342
Frequencies --	909.6801	937.6002	967.5842
Frequencies --	1006.0799	1045.6469	1062.1023
Frequencies --	1160.2249	1171.5801	1223.3155
Frequencies --	1332.6669	1444.8368	1463.4569
Frequencies --	1501.6555	1623.3561	3202.3266
Frequencies --	3202.8769	3272.7439	3308.0069

Zero-point correction=	0.075636	(Hartree/Particle)
Thermal correction to Energy=	0.080003	
Thermal correction to Enthalpy=	0.080947	
Thermal correction to Gibbs Free Energy=	0.048231	
Sum of electronic and zero-point Energies=	-264.024377	
Sum of electronic and thermal Energies=	-264.020009	
Sum of electronic and thermal Enthalpies=	-264.019065	
Sum of electronic and thermal Free Energies=	-264.051781	

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

N	0.000000000	1.209997000	-0.752177000
N	0.000000000	-1.209997000	-0.752177000
C	0.000000000	0.000000000	-1.319692000
C	0.000000000	1.203265000	0.660013000
C	0.000000000	0.000000000	1.363828000
C	0.000000000	-1.203265000	0.660013000
H	0.000000000	0.000000000	-2.413637000
H	0.000000000	2.171992000	1.152486000
H	0.000000000	0.000000000	2.454170000
H	0.000000000	-2.171992000	1.152486000

Frequencies --	226.7615	386.4862	557.6109
Frequencies --	571.2509	586.3829	658.0274
Frequencies --	681.3935	918.0754	928.1660
Frequencies --	958.3569	967.1460	1035.1266
Frequencies --	1058.7343	1120.6306	1283.4075
Frequencies --	1346.7986	1369.8535	1401.2866

Frequencies --	1472.8843	1514.3800	3103.7382
Frequencies --	3153.0429	3183.4103	3194.4711

Zero-point correction=	0.072166 (Hartree/Particle)
Thermal correction to Energy=	0.076937
Thermal correction to Enthalpy=	0.077882
Thermal correction to Gibbs Free Energy=	0.044394
Sum of electronic and zero-point Energies=	-264.345347
Sum of electronic and thermal Energies=	-264.340576
Sum of electronic and thermal Enthalpies=	-264.339632
Sum of electronic and thermal Free Energies=	-264.373120

Quinoline

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	1.231524000	1.410304000	-0.000033000
C	-0.014922000	0.725055000	-0.000010000
C	-0.026256000	-0.708058000	0.000025000
C	1.211130000	-1.407986000	-0.000008000
C	2.404698000	-0.715171000	-0.000002000
C	2.416819000	0.704421000	0.000004000
C	-1.267765000	1.394050000	0.000029000
C	-2.428471000	0.653506000	-0.000052000
N	-1.192308000	-1.427967000	0.000070000
H	1.231954000	2.498173000	-0.000028000
H	1.190578000	-2.494811000	-0.000024000
H	3.346656000	-1.257895000	-0.000032000
H	3.366603000	1.232952000	0.000050000
H	-1.293320000	2.481552000	0.000085000
H	-3.405367000	1.128152000	0.000230000
H	-3.244816000	-1.359331000	-0.000098000
C	-2.334446000	-0.761625000	-0.000065000

Frequencies --	175.5279	183.6697	382.2218
Frequencies --	402.4494	477.3642	492.7188
Frequencies --	526.3636	528.8584	623.3862
Frequencies --	639.3360	749.3089	769.9672
Frequencies --	792.7213	824.3233	826.4259
Frequencies --	883.5447	950.0343	977.0942
Frequencies --	980.0510	1007.9128	1011.7097
Frequencies --	1037.7683	1059.1010	1142.5487
Frequencies --	1163.7383	1169.8663	1237.9694
Frequencies --	1259.5654	1287.0278	1364.7868
Frequencies --	1400.9887	1426.6652	1469.5684
Frequencies --	1501.8221	1545.4971	1611.1442
Frequencies --	1640.3795	1664.5726	3176.1112
Frequencies --	3186.9684	3194.2693	3195.2590
Frequencies --	3204.7190	3213.7211	3218.8081

Zero-point correction=	0.135728 (Hartree/Particle)
Thermal correction to Energy=	0.142412
Thermal correction to Enthalpy=	0.143357
Thermal correction to Gibbs Free Energy=	0.104574
Sum of electronic and zero-point Energies=	-401.824770

Sum of electronic and thermal Energies=	-401.818086
Sum of electronic and thermal Enthalpies=	-401.817142
Sum of electronic and thermal Free Energies=	-401.855924

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	1.214290000	1.406466000	-0.000170000
C	-0.031039000	0.726160000	-0.000127000
C	-0.038389000	-0.700687000	-0.000006000
C	1.209062000	-1.399523000	-0.000010000
C	2.432224000	-0.697240000	0.000085000
C	2.437009000	0.690313000	0.000108000
C	-1.270439000	1.396766000	-0.000011000
C	-2.440337000	0.636045000	0.000125000
N	-1.175240000	-1.427301000	0.000006000
H	1.225209000	2.493283000	-0.000401000
H	1.193711000	-2.485492000	-0.000083000
H	3.365103000	-1.251551000	0.000174000
H	3.372960000	1.239316000	0.000347000
H	-1.304796000	2.482610000	-0.000048000
H	-3.416113000	1.110371000	0.001073000
H	-3.239606000	-1.372955000	-0.000255000
C	-2.340680000	-0.762379000	-0.000134000

Frequencies --	150.8505	168.3159	369.6786
Frequencies --	371.7610	413.6254	430.6612
Frequencies --	470.9094	506.3057	519.1852
Frequencies --	604.0180	726.5150	763.4326
Frequencies --	773.5949	812.6962	826.6435
Frequencies --	897.2566	939.7603	984.3062
Frequencies --	993.8298	1021.7731	1026.9920
Frequencies --	1045.2039	1068.7663	1097.5912
Frequencies --	1140.0121	1182.9885	1234.2121
Frequencies --	1254.9499	1271.1516	1346.0885
Frequencies --	1422.3399	1431.1567	1457.0571
Frequencies --	1464.1867	1488.4908	1550.7721
Frequencies --	1568.6292	1628.2498	3216.9103
Frequencies --	3223.1571	3225.4647	3232.8564
Frequencies --	3239.4613	3242.8122	3247.1104

Zero-point correction=	0.134530 (Hartree/Particle)
Thermal correction to Energy=	0.141588
Thermal correction to Enthalpy=	0.142533
Thermal correction to Gibbs Free Energy=	0.102383
Sum of electronic and zero-point Energies=	-401.598368
Sum of electronic and thermal Energies=	-401.591309
Sum of electronic and thermal Enthalpies=	-401.590365
Sum of electronic and thermal Free Energies=	-401.630515

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-1.239957000	1.401904000	-0.000186000
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C	0.014094000	0.735728000	-0.000081000
C	0.028539000	-0.716737000	-0.000122000
C	-1.212395000	-1.399658000	0.000229000
C	-2.439024000	-0.707289000	0.000221000
C	-2.452514000	0.690413000	-0.000106000
C	1.270818000	1.408861000	0.000122000
C	2.458520000	0.640784000	0.000318000
N	1.199076000	-1.442030000	-0.000335000
H	-1.249577000	2.491661000	-0.000291000
H	-1.196034000	-2.488525000	0.000390000
H	-3.373530000	-1.265585000	0.000414000
H	-3.397264000	1.231281000	-0.000230000
H	1.302343000	2.496816000	0.000162000
H	3.434229000	1.123558000	0.000521000
H	3.279706000	-1.350325000	0.000278000
C	2.373019000	-0.744785000	-0.000212000

Frequencies --	155.9159	187.8659	310.3089
Frequencies --	383.6065	480.6179	516.0465
Frequencies --	516.0827	523.0379	595.6580
Frequencies --	600.3816	675.3236	731.9161
Frequencies --	744.8677	747.1914	776.2011
Frequencies --	813.2420	814.8670	855.4792
Frequencies --	902.9520	913.5124	928.3404
Frequencies --	1026.5672	1064.6120	1081.3757
Frequencies --	1110.1807	1161.4558	1193.0087
Frequencies --	1229.0356	1271.3663	1302.9285
Frequencies --	1362.6338	1403.5513	1433.9536
Frequencies --	1454.7554	1471.1963	1532.3991
Frequencies --	1551.4125	1597.3033	3141.3104
Frequencies --	3151.1015	3159.5043	3164.5832
Frequencies --	3171.0696	3182.4655	3186.9515

Zero-point correction=	0.131173 (Hartree/Particle)
Thermal correction to Energy=	0.138244
Thermal correction to Enthalpy=	0.139188
Thermal correction to Gibbs Free Energy=	0.099110
Sum of electronic and zero-point Energies=	-401.905488
Sum of electronic and thermal Energies=	-401.898416
Sum of electronic and thermal Enthalpies=	-401.897472
Sum of electronic and thermal Free Energies=	-401.937551

Pyridine

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000950000	1.386190000	0.000008000
C	-1.200482000	0.674287000	0.000004000
C	-1.149141000	-0.722004000	-0.000098000
N	-0.001044000	-1.420621000	0.000083000
C	1.147909000	-0.723817000	-0.000042000
C	1.201685000	0.672255000	-0.000004000
H	0.002539000	2.473269000	0.000092000
H	-2.160035000	1.183750000	0.000111000
H	-2.067249000	-1.306168000	0.000025000

H	2.065275000	-1.309503000	0.000064000
H	2.161254000	1.181547000	-0.000079000

Frequencies --	385.7442	416.6276	614.1705
Frequencies --	664.3685	714.1422	759.3619
Frequencies --	897.7606	964.6580	1004.2025
Frequencies --	1011.1962	1024.9558	1044.3434
Frequencies --	1081.3805	1090.5700	1167.4107
Frequencies --	1236.6570	1303.4258	1391.1526
Frequencies --	1475.3449	1520.0443	1624.1651
Frequencies --	1635.6658	3184.0944	3186.9266
Frequencies --	3202.2324	3214.0625	3221.6993

Zero-point correction=	0.088931 (Hartree/Particle)
Thermal correction to Energy=	0.093213
Thermal correction to Enthalpy=	0.094157
Thermal correction to Gibbs Free Energy=	0.061520
Sum of electronic and zero-point Energies=	-248.217755
Sum of electronic and thermal Energies=	-248.213474
Sum of electronic and thermal Enthalpies=	-248.212529
Sum of electronic and thermal Free Energies=	-248.245167

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-0.664923324	1.507824804	-1.147990687
C	-0.625160534	1.378500355	-2.535544683
C	-0.730213682	2.532554935	-3.313828093
N	-0.872853062	3.739016347	-2.848587708
C	-0.904152321	3.870852495	-1.470567750
C	-0.807642107	2.782527916	-0.601753274
H	-0.586436367	0.634662555	-0.506625605
H	-0.515375669	0.407573001	-3.008381305
H	-0.702592054	2.465093061	-4.400109265
H	-1.016336583	4.879068112	-1.075299735
H	-0.843839516	2.934799647	0.472411602

Frequencies --	297.8456	389.7748	543.0014
Frequencies --	567.0264	588.7866	625.4156
Frequencies --	730.1169	916.5734	964.5177
Frequencies --	970.0080	1000.9283	1028.9211
Frequencies --	1070.9546	1076.2392	1157.7133
Frequencies --	1162.4747	1272.3379	1320.0998
Frequencies --	1447.7816	1472.2215	1532.7192
Frequencies --	1622.4617	3218.4090	3222.8014
Frequencies --	3229.9662	3240.5015	3243.6108

Zero-point correction=	0.086373 (Hartree/Particle)
Thermal correction to Energy=	0.091075
Thermal correction to Enthalpy=	0.092019
Thermal correction to Gibbs Free Energy=	0.058089
Sum of electronic and zero-point Energies=	-247.973278
Sum of electronic and thermal Energies=	-247.968576

Sum of electronic and thermal Enthalpies= -247.967632
Sum of electronic and thermal Free Energies= -248.001562

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-0.664923324	1.507824804	-1.147990687
C	-0.625160534	1.378500355	-2.535544683
C	-0.730213682	2.532554935	-3.313828093
N	-0.872853062	3.739016347	-2.848587708
C	-0.904152321	3.870852495	-1.470567750
C	-0.807642107	2.782527916	-0.601753274
H	-0.586436367	0.634662555	-0.506625605
H	-0.515375669	0.407573001	-3.008381305
H	-0.702592054	2.465093061	-4.400109265
H	-1.016336583	4.879068112	-1.075299735
H	-0.843839516	2.934799647	0.472411602

Frequencies --	212.8039	418.0987	419.0986
Frequencies --	572.0990	640.0567	652.5090
Frequencies --	704.4321	782.4739	868.2522
Frequencies --	902.3554	912.6062	934.3315
Frequencies --	972.8611	1031.2589	1047.9416
Frequencies --	1209.4496	1215.6941	1347.7433
Frequencies --	1381.5073	1459.7177	1497.7576
Frequencies --	1623.5049	3124.2552	3127.8852
Frequencies --	3153.6996	3154.1207	3198.1108

Zero-point correction= 0.083300 (Hartree/Particle)
Thermal correction to Energy= 0.088280
Thermal correction to Enthalpy= 0.089225
Thermal correction to Gibbs Free Energy= 0.054733
Sum of electronic and zero-point Energies= -248.276292
Sum of electronic and thermal Energies= -248.271312
Sum of electronic and thermal Enthalpies= -248.270368
Sum of electronic and thermal Free Energies= -248.304860

Pyrole

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	0.714833000	-0.987381000
C	0.000000000	1.126271000	0.334650000
N	0.000000000	0.000000000	1.121946000
C	0.000000000	-1.126271000	0.334650000
C	0.000000000	-0.714833000	-0.987381000
H	0.000000000	1.365366000	-1.853688000
H	0.000000000	2.113822000	0.775913000
H	0.000000000	-2.113822000	0.775913000
H	0.000000000	-1.365366000	-1.853688000
H	0.000000000	0.000000000	2.134699000

Frequencies --	510.8027	623.7195	642.5736
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Frequencies --	702.7963	728.4066	838.8210
Frequencies --	875.9610	877.5829	895.9354
Frequencies --	1028.7091	1065.6960	1088.6026
Frequencies --	1151.7089	1171.3696	1314.3545
Frequencies --	1421.8071	1452.5246	1502.7052
Frequencies --	1571.2410	3239.7639	3252.0033
Frequencies --	3276.8543	3280.1091	3626.4377

Zero-point correction=	0.082334 (Hartree/Particle)
Thermal correction to Energy=	0.086281
Thermal correction to Enthalpy=	0.087225
Thermal correction to Gibbs Free Energy=	0.056601
Sum of electronic and zero-point Energies=	-210.108057
Sum of electronic and thermal Energies=	-210.104110
Sum of electronic and thermal Enthalpies=	-210.103166
Sum of electronic and thermal Free Energies=	-210.133790

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	0.687090000	-1.017527000
C	0.000000000	1.108752000	0.354408000
N	0.000000000	0.000000000	1.139167000
C	0.000000000	-1.108752000	0.354408000
C	0.000000000	-0.687090000	-1.017527000
H	0.000000000	1.357841000	-1.866088000
H	0.000000000	2.104014000	0.779586000
H	0.000000000	-2.104014000	0.779586000
H	0.000000000	-1.357841000	-1.866088000
H	0.000000000	0.000000000	2.156270000

Frequencies --	481.4945	512.6685	629.4660
Frequencies --	736.8693	751.2720	866.7420
Frequencies --	892.9907	901.7117	951.5997
Frequencies --	1002.8945	1045.0320	1077.9159
Frequencies --	1088.8493	1179.5787	1271.4113
Frequencies --	1326.9311	1475.1481	1484.5063
Frequencies --	1557.9966	3283.1491	3293.9362
Frequencies --	3298.8190	3304.2455	3583.3259

Zero-point correction=	0.082011 (Hartree/Particle)
Thermal correction to Energy=	0.086024
Thermal correction to Enthalpy=	0.086968
Thermal correction to Gibbs Free Energy=	0.055578
Sum of electronic and zero-point Energies=	-209.904409
Sum of electronic and thermal Energies=	-209.900396
Sum of electronic and thermal Enthalpies=	-209.899452
Sum of electronic and thermal Free Energies=	-209.930841

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	0.714721000	-0.991185000
C	0.000000000	1.119649000	0.336259000

N	0.000000000	0.000000000	1.118307000
C	0.000000000	-1.119649000	0.336259000
C	0.000000000	-0.714721000	-0.991185000
H	0.000000000	1.368948000	-1.857964000
H	0.000000000	2.104411000	0.789873000
H	0.000000000	-2.104411000	0.789873000
H	0.000000000	-1.368948000	-1.857964000
H	0.000000000	0.000000000	2.167145000

Frequencies --	498.3911	606.8782	642.1498
Frequencies --	698.3493	713.9140	831.9143
Frequencies --	863.8334	869.8225	882.9917
Frequencies --	1002.2353	1015.8818	1065.5734
Frequencies --	1074.2750	1171.3923	1298.7636
Frequencies --	1417.4384	1436.6523	1498.0724
Frequencies --	1545.4726	2695.3405	3197.9597
Frequencies --	3209.5306	3216.5321	3225.1821

Zero-point correction=	0.079004 (Hartree/Particle)
Thermal correction to Energy=	0.083006
Thermal correction to Enthalpy=	0.083950
Thermal correction to Gibbs Free Energy=	0.052598
Sum of electronic and zero-point Energies=	-210.121506
Sum of electronic and thermal Energies=	-210.117504
Sum of electronic and thermal Enthalpies=	-210.116560
Sum of electronic and thermal Free Energies=	-210.147912

Thiophene

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	0.716317000	-1.275196000
C	0.000000000	1.246432000	-0.011103000
S	0.000000000	0.000000000	1.201456000
C	0.000000000	-1.246432000	-0.011103000
C	0.000000000	-0.716317000	-1.275196000
H	0.000000000	1.322171000	-2.176071000
H	0.000000000	2.289486000	0.282215000
H	0.000000000	-2.289486000	0.282215000
H	0.000000000	-1.322171000	-2.176071000

Frequencies --	453.9050	570.0957	608.7824
Frequencies --	697.3997	726.3703	740.0162
Frequencies --	830.6085	878.9032	890.2359
Frequencies --	926.4327	1052.3747	1104.0739
Frequencies --	1109.1450	1280.3549	1399.6012
Frequencies --	1456.1698	1560.1511	3217.7752
Frequencies --	3229.9554	3267.5014	3269.1808

Zero-point correction=	0.066680 (Hartree/Particle)
Thermal correction to Energy=	0.070760
Thermal correction to Enthalpy=	0.071704
Thermal correction to Gibbs Free Energy=	0.040087

Sum of electronic and zero-point Energies=	-552.951960
Sum of electronic and thermal Energies=	-552.947879
Sum of electronic and thermal Enthalpies=	-552.946935
Sum of electronic and thermal Free Energies=	-552.978553

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	0.000000000	0.690651000	-1.315364000
C	0.000000000	1.225015000	-0.000041000
S	0.000000000	0.000000000	1.227145000
C	0.000000000	-1.225015000	-0.000041000
C	0.000000000	-0.690651000	-1.315364000
H	0.000000000	1.322475000	-2.196167000
H	0.000000000	2.276196000	0.271432000
H	0.000000000	-2.276196000	0.271432000
H	0.000000000	-1.322475000	-2.196167000

Frequencies --	362.9843	460.4253	549.0398
Frequencies --	613.9797	713.1400	816.1888
Frequencies --	849.7125	851.6258	884.4706
Frequencies --	969.7679	1025.7957	1081.7784
Frequencies --	1115.8481	1257.1585	1365.5283
Frequencies --	1366.6360	1522.9220	3259.6292
Frequencies --	3268.2182	3271.6999	3277.7891

Zero-point correction=	0.065803 (Hartree/Particle)
Thermal correction to Energy=	0.070109
Thermal correction to Enthalpy=	0.071053
Thermal correction to Gibbs Free Energy=	0.038400
Sum of electronic and zero-point Energies=	-552.723423
Sum of electronic and thermal Energies=	-552.719117
Sum of electronic and thermal Enthalpies=	-552.718173
Sum of electronic and thermal Free Energies=	-552.750827

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-0.128490000	1.295250000	0.699899000
C	-0.128490000	0.001383000	1.286624000
S	0.190234000	-1.219040000	0.000000000
C	-0.128490000	0.001383000	-1.286624000
C	-0.128490000	1.295250000	-0.699899000
H	-0.199927000	2.201311000	1.299944000
H	0.219933000	-0.228793000	2.290425000
H	0.219933000	-0.228793000	-2.290425000
H	-0.199927000	2.201311000	-1.299944000

Frequencies --	269.5392	288.8198	480.3788
Frequencies --	507.7665	575.2265	656.6338
Frequencies --	690.7371	745.1831	791.2511
Frequencies --	850.4130	1030.2363	1046.0885
Frequencies --	1087.7345	1222.1815	1303.7159
Frequencies --	1391.3604	1470.8144	3158.9328

Frequencies --	3171.8815	3182.1757	3189.8711
Zero-point correction=			0.061763 (Hartree/Particle)
Thermal correction to Energy=			0.066740
Thermal correction to Enthalpy=			0.067684
Thermal correction to Gibbs Free Energy=			0.033217
Sum of electronic and zero-point Energies=			-552.996935
Sum of electronic and thermal Energies=			-552.991958
Sum of electronic and thermal Enthalpies=			-552.991014
Sum of electronic and thermal Free Energies=			-553.025482

Dibenzothiophene S-oxide

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	-0.000186000	1.765101000	-0.344149000
C	1.610688000	-1.894035000	0.097842000
C	0.736127000	-0.808117000	-0.015295000
C	2.991007000	-1.663321000	0.097731000
H	3.672445000	-2.504804000	0.190568000
C	1.273207000	0.484944000	-0.139926000
C	3.506254000	-0.365914000	-0.020619000
H	4.580703000	-0.204779000	-0.016522000
C	2.641501000	0.728835000	-0.152191000
H	3.035533000	1.736494000	-0.255347000
H	1.224282000	-2.905685000	0.187841000
C	-2.990765000	-1.663641000	0.097433000
C	-3.506106000	-0.366237000	-0.020372000
C	-1.610405000	-1.894236000	0.097280000
H	-4.580555000	-0.205106000	-0.015840000
H	-1.223866000	-2.905904000	0.186512000
C	-2.641462000	0.728600000	-0.151954000
C	-0.735990000	-0.808199000	-0.015417000
H	-3.035653000	1.736214000	-0.254991000
C	-1.273116000	0.484895000	-0.139930000
H	-3.672120000	-2.505208000	0.190076000
O	-0.000429000	2.716966000	0.860825000

Frequencies --	77.6518	85.1165	121.4508
Frequencies --	178.2918	193.6185	282.5932
Frequencies --	339.6205	394.9898	396.9583
Frequencies --	426.0507	449.7883	478.3989
Frequencies --	490.7074	558.3971	565.3901
Frequencies --	624.1192	696.0320	698.3116
Frequencies --	724.4894	732.6580	767.1985
Frequencies --	772.6153	782.6559	879.5200
Frequencies --	887.4484	962.6003	968.5693
Frequencies --	979.9069	1006.5792	1010.8854
Frequencies --	1015.6203	1040.4333	1043.1461
Frequencies --	1071.4947	1080.1154	1134.4505
Frequencies --	1146.3962	1181.0674	1181.1236
Frequencies --	1244.6268	1300.4811	1318.7115
Frequencies --	1340.9440	1381.7064	1466.1315
Frequencies --	1480.2598	1499.5025	1511.4464
Frequencies --	1617.0709	1625.9911	1633.4646

Frequencies --	1635.2204	3188.0589	3195.7374
Frequencies --	3199.1209	3201.8350	3206.8507
Frequencies --	3208.9626	3217.4405	3218.2326

Zero-point correction=	0.164297 (Hartree/Particle)
Thermal correction to Energy=	0.174822
Thermal correction to Enthalpy=	0.175766
Thermal correction to Gibbs Free Energy=	0.127613
Sum of electronic and zero-point Energies=	-935.344154
Sum of electronic and thermal Energies=	-935.333629
Sum of electronic and thermal Enthalpies=	-935.332685
Sum of electronic and thermal Free Energies=	-935.380839

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	0.000046000	1.652146000	-0.273780000
C	1.614779000	-1.895512000	0.053086000
C	0.737625000	-0.817510000	-0.026617000
C	2.999994000	-1.655142000	0.074381000
H	3.678568000	-2.501147000	0.131435000
C	1.300610000	0.476422000	-0.067289000
C	3.523556000	-0.357165000	0.020946000
H	4.597282000	-0.200510000	0.039889000
C	2.668644000	0.744366000	-0.072987000
H	3.052954000	1.757714000	-0.138897000
H	1.234974000	-2.910797000	0.112342000
C	-3.000115000	-1.655040000	0.073948000
C	-3.523586000	-0.357027000	0.021200000
C	-1.614904000	-1.895483000	0.052411000
H	-4.597294000	-0.200275000	0.040381000
H	-1.235167000	-2.910840000	0.110820000
C	-2.668603000	0.744512000	-0.072500000
C	-0.737699000	-0.817480000	-0.026680000
H	-3.052891000	1.757885000	-0.138137000
C	-1.300622000	0.476472000	-0.067015000
H	-3.678722000	-2.501044000	0.130634000
O	0.000186000	2.915775000	0.539340000

Frequencies --	29.7036	97.2373	129.2552
Frequencies --	190.2137	191.4469	262.5689
Frequencies --	331.1014	386.5963	396.2125
Frequencies --	419.5087	433.4167	436.2175
Frequencies --	497.0668	504.9212	546.1482
Frequencies --	596.6984	688.5813	699.2477
Frequencies --	699.6937	718.1195	765.8473
Frequencies --	766.9840	769.5398	863.6021
Frequencies --	888.9712	972.2915	980.6553
Frequencies --	983.2399	1011.4686	1016.8092
Frequencies --	1021.5619	1025.9864	1043.8338
Frequencies --	1054.6723	1087.1646	1131.6362
Frequencies --	1146.4952	1174.1127	1187.3173
Frequencies --	1235.3196	1289.2305	1316.7408
Frequencies --	1325.3431	1392.8996	1453.4531
Frequencies --	1458.8519	1484.3861	1512.5141
Frequencies --	1568.2803	1592.6120	1601.0883

Frequencies --	1606.5392	3201.1970	3216.1105
Frequencies --	3219.9091	3222.6756	3226.0734
Frequencies --	3227.7376	3235.4229	3235.9189

Zero-point correction=	0.163501 (Hartree/Particle)
Thermal correction to Energy=	0.174259
Thermal correction to Enthalpy=	0.175203
Thermal correction to Gibbs Free Energy=	0.125401
Sum of electronic and zero-point Energies=	-935.111026
Sum of electronic and thermal Energies=	-935.100267
Sum of electronic and thermal Enthalpies=	-935.099323
Sum of electronic and thermal Free Energies=	-935.149125

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	3.508237000	-0.343447000	-0.163803000
C	2.625530000	0.725681000	-0.312643000
C	3.002794000	-1.647588000	0.099349000
H	3.007159000	1.728578000	-0.498357000
H	3.697762000	-2.475244000	0.224205000
C	1.246730000	0.498209000	-0.213622000
C	1.635882000	-1.880371000	0.197074000
H	1.270195000	-2.887443000	0.391018000
C	0.716330000	-0.816488000	0.037435000
H	4.580224000	-0.180869000	-0.244041000
C	-1.636089000	-1.880192000	0.197377000
C	-0.716457000	-0.816421000	0.037681000
C	-3.002978000	-1.647365000	0.099491000
H	-3.698021000	-2.474949000	0.224393000
C	-1.246756000	0.498435000	-0.213318000
C	-3.508333000	-0.343191000	-0.163918000
H	-4.580304000	-0.180649000	-0.244444000
C	-2.625586000	0.725876000	-0.312647000
H	-3.007139000	1.728799000	-0.498407000
H	-1.270508000	-2.887264000	0.391549000
S	-0.000039000	1.778997000	-0.261276000
O	0.000680000	2.590781000	1.087970000

Frequencies --	87.9597	121.4383	126.3644
Frequencies --	155.2121	205.3386	279.1892
Frequencies --	301.5507	398.8087	407.2539
Frequencies --	418.7900	422.8549	451.2266
Frequencies --	488.2832	520.1755	549.5554
Frequencies --	615.2821	679.6275	687.8600
Frequencies --	692.2566	709.6564	718.3184
Frequencies --	737.3616	763.9474	817.7486
Frequencies --	827.1563	833.2763	937.9996
Frequencies --	939.6559	957.4345	958.2664
Frequencies --	981.4245	1017.3115	1019.3577
Frequencies --	1032.2629	1062.2236	1135.5647
Frequencies --	1146.7101	1169.7846	1170.4430
Frequencies --	1201.7102	1283.9421	1346.4399
Frequencies --	1352.2534	1376.5601	1443.3529
Frequencies --	1462.1796	1471.9967	1499.8728
Frequencies --	1532.4467	1532.9742	1564.6790

Frequencies --	1594.2498	3165.6454	3167.0908
Frequencies --	3170.4197	3171.5787	3183.4471
Frequencies --	3184.0251	3197.7849	3198.2415

Zero-point correction=	0.160943 (Hartree/Particle)
Thermal correction to Energy=	0.171698
Thermal correction to Enthalpy=	0.172642
Thermal correction to Gibbs Free Energy=	0.123778
Sum of electronic and zero-point Energies=	-935.430589
Sum of electronic and thermal Energies=	-935.419834
Sum of electronic and thermal Enthalpies=	-935.418890
Sum of electronic and thermal Free Energies=	-935.467753

Benzo[b]naphtha-[1,2,d]thiophene S-oxide (1)

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	1.861152000	-1.726497000	-0.314001000
C	1.223279000	2.215363000	0.023956000
C	1.036832000	0.826092000	-0.061060000
C	2.516159000	2.752909000	0.067310000
H	2.631795000	3.830853000	0.142488000
C	2.204033000	0.033522000	-0.123736000
C	3.648376000	1.936260000	0.016066000
H	4.643200000	2.370812000	0.054867000
C	3.492096000	0.549667000	-0.095156000
H	4.357650000	-0.105331000	-0.152460000
H	0.391091000	2.903924000	0.062299000
O	2.361906000	-2.514066000	0.905630000
C	-0.200082000	-0.003037000	-0.080514000
C	0.099920000	-1.361991000	-0.153221000
C	-0.856459000	-2.391948000	-0.157492000
C	-2.185357000	-2.043577000	-0.074236000
C	-2.576297000	-0.677588000	-0.012358000
C	-1.588057000	0.375941000	-0.023591000
C	-2.063653000	1.717834000	0.025759000
C	-3.412727000	2.004852000	0.088248000
C	-4.374420000	0.967310000	0.104788000
C	-3.958351000	-0.344793000	0.054601000
H	-0.550857000	-3.432937000	-0.217774000
H	-2.956633000	-2.809597000	-0.061601000
H	-4.682808000	-1.155889000	0.062135000
H	-5.433185000	1.207714000	0.155053000
H	-3.736438000	3.041874000	0.124820000
H	-1.369242000	2.544153000	0.012955000

Frequencies --	49.1119	70.9966	103.5204
Frequencies --	156.2641	170.9699	190.7516
Frequencies --	215.0759	285.5731	302.1262
Frequencies --	351.3497	377.8974	411.9059
Frequencies --	421.4071	442.9906	471.9556
Frequencies --	506.6525	530.1523	537.7836
Frequencies --	548.2887	583.1985	621.5512
Frequencies --	642.9751	675.3703	699.3458
Frequencies --	720.5849	740.9367	753.9102

Frequencies --	761.3708	791.5345	828.3633
Frequencies --	832.7575	873.9394	877.7946
Frequencies --	883.7976	962.4667	973.3107
Frequencies --	973.5733	982.6636	985.4554
Frequencies --	1006.8431	1010.4912	1049.9094
Frequencies --	1061.4764	1068.6254	1133.7549
Frequencies --	1153.6872	1167.2360	1176.0919
Frequencies --	1184.8282	1191.7239	1226.2268
Frequencies --	1243.3926	1282.8277	1328.2449
Frequencies --	1354.9882	1371.7863	1397.4643
Frequencies --	1402.5063	1467.0975	1475.6473
Frequencies --	1491.6135	1504.4287	1555.6707
Frequencies --	1602.3735	1616.6365	1624.5239
Frequencies --	1635.9426	1664.1269	3190.9778
Frequencies --	3197.7630	3199.1639	3200.1403
Frequencies --	3204.0899	3212.9853	3214.1165
Frequencies --	3217.7416	3262.6917	3304.1202

Zero-point correction=	0.211787 (Hartree/Particle)
Thermal correction to Energy=	0.224861
Thermal correction to Enthalpy=	0.225805
Thermal correction to Gibbs Free Energy=	0.171863
Sum of electronic and zero-point Energies=	-1088.941470
Sum of electronic and thermal Energies=	-1088.928396
Sum of electronic and thermal Enthalpies=	-1088.927452
Sum of electronic and thermal Free Energies=	-1088.981394

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	1.904211000	-1.697297000	-0.422649000
C	1.133048000	2.221181000	0.191613000
C	0.998293000	0.832810000	-0.035365000
C	2.401293000	2.790428000	0.251887000
H	2.495120000	3.856215000	0.437034000
C	2.191223000	0.070428000	-0.167754000
C	3.556866000	2.009947000	0.093828000
H	4.536801000	2.475012000	0.146054000
C	3.455503000	0.627001000	-0.119174000
H	4.346998000	0.016990000	-0.233337000
H	0.272600000	2.853719000	0.360573000
O	2.493527000	-2.501908000	0.730800000
C	-0.195236000	0.003581000	-0.090161000
C	0.137992000	-1.381757000	-0.145304000
C	-0.782359000	-2.401735000	-0.025046000
C	-2.132105000	-2.056107000	0.138891000
C	-2.549466000	-0.706381000	0.102725000
C	-1.590639000	0.357561000	-0.059919000
C	-2.087057000	1.669068000	-0.209445000
C	-3.458970000	1.938516000	-0.140121000
C	-4.382142000	0.910008000	0.069818000
C	-3.930921000	-0.403239000	0.182728000
H	-0.481075000	-3.444643000	-0.050465000
H	-2.878251000	-2.836833000	0.256837000
H	-4.635904000	-1.218195000	0.320569000
H	-5.444047000	1.128593000	0.126288000

H	-3.801124000	2.961859000	-0.261853000
H	-1.418657000	2.491431000	-0.420917000

Frequencies --	49.0136	65.7750	93.1074
Frequencies --	146.1442	156.8176	194.8606
Frequencies --	209.5331	276.5523	292.4457
Frequencies --	344.9459	373.1607	399.7816
Frequencies --	413.6438	435.1521	445.2307
Frequencies --	495.6528	517.3028	524.6910
Frequencies --	528.2024	546.2172	612.3588
Frequencies --	634.6918	672.7485	686.0612
Frequencies --	711.5434	723.4628	756.7823
Frequencies --	761.4036	791.1236	835.6045
Frequencies --	849.7112	872.3519	878.2456
Frequencies --	905.4289	972.6178	975.6840
Frequencies --	985.7391	998.3813	1009.2548
Frequencies --	1017.4987	1025.2218	1048.0371
Frequencies --	1065.2531	1066.9323	1129.5909
Frequencies --	1145.1489	1153.4923	1159.9593
Frequencies --	1187.9939	1192.7137	1235.9889
Frequencies --	1264.5726	1281.3199	1327.5807
Frequencies --	1366.5259	1394.8510	1397.4554
Frequencies --	1403.5431	1459.5403	1469.8393
Frequencies --	1481.2684	1491.3595	1533.9844
Frequencies --	1566.2820	1585.6139	1589.4334
Frequencies --	1603.0168	1626.6340	3213.5376
Frequencies --	3216.9104	3220.1226	3222.6102
Frequencies --	3223.1319	3229.6707	3232.8425
Frequencies --	3233.8719	3261.2435	3285.1430

Zero-point correction=	0.211303 (Hartree/Particle)
Thermal correction to Energy=	0.224601
Thermal correction to Enthalpy=	0.225545
Thermal correction to Gibbs Free Energy=	0.170379
Sum of electronic and zero-point Energies=	-1088.731211
Sum of electronic and thermal Energies=	-1088.717912
Sum of electronic and thermal Enthalpies=	-1088.716968
Sum of electronic and thermal Free Energies=	-1088.772135

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	1.866018000	-1.770836000	-0.127015000
C	1.241725000	2.206847000	-0.040213000
C	1.023341000	0.802845000	-0.060888000
C	2.531095000	2.731595000	-0.100021000
H	2.657621000	3.812132000	-0.085364000
C	2.203228000	-0.011190000	-0.156121000
C	3.667988000	1.900812000	-0.186862000
H	4.664785000	2.331108000	-0.234107000
C	3.491790000	0.514348000	-0.217011000
H	4.352148000	-0.149103000	-0.284787000
H	0.412981000	2.902742000	0.001802000
O	2.238119000	-2.340879000	1.282340000
C	-0.182006000	0.005261000	-0.062570000
C	0.130017000	-1.386390000	-0.222606000

C	-0.848396000	-2.377319000	-0.379926000
C	-2.185396000	-2.023633000	-0.364078000
C	-2.578236000	-0.658143000	-0.147991000
C	-1.579008000	0.376626000	0.022083000
C	-2.048650000	1.692602000	0.278782000
C	-3.406960000	1.997558000	0.332755000
C	-4.369827000	0.993575000	0.138067000
C	-3.950165000	-0.312541000	-0.092272000
H	-0.557621000	-3.418306000	-0.512464000
H	-2.959726000	-2.775842000	-0.495825000
H	-4.685226000	-1.103755000	-0.230834000
H	-5.430431000	1.231391000	0.175385000
H	-3.716487000	3.021101000	0.532976000
H	-1.342516000	2.491816000	0.459986000

Frequencies --	56.2275	75.9729	103.6796
Frequencies --	145.1626	170.8197	181.9589
Frequencies --	215.4181	287.6793	307.3580
Frequencies --	333.9029	362.8389	397.5989
Frequencies --	410.6258	434.5229	473.2093
Frequencies --	499.5129	515.6834	531.6803
Frequencies --	533.4134	565.3642	623.7210
Frequencies --	632.6533	637.0842	693.9056
Frequencies --	715.5941	718.6254	725.3086
Frequencies --	736.3813	768.0952	782.0713
Frequencies --	823.9082	835.8315	858.8180
Frequencies --	861.9630	879.9785	932.0070
Frequencies --	935.4641	941.5288	964.9480
Frequencies --	970.1869	974.5372	1032.9698
Frequencies --	1048.8142	1059.2462	1112.3510
Frequencies --	1142.6555	1144.9876	1158.7287
Frequencies --	1172.9770	1177.6416	1221.3146
Frequencies --	1240.2630	1273.6880	1322.3814
Frequencies --	1338.6391	1352.9324	1372.4859
Frequencies --	1389.5199	1451.4323	1460.2258
Frequencies --	1476.3373	1481.5815	1524.7056
Frequencies --	1542.9954	1567.4759	1583.6094
Frequencies --	1601.7773	1621.9800	3168.7822
Frequencies --	3170.4466	3175.8680	3181.1900
Frequencies --	3181.6728	3189.0282	3198.7500
Frequencies --	3202.7858	3231.9014	3267.9216

Zero-point correction=	0.208355 (Hartree/Particle)
Thermal correction to Energy=	0.221698
Thermal correction to Enthalpy=	0.222642
Thermal correction to Gibbs Free Energy=	0.167750
Sum of electronic and zero-point Energies=	-1089.038800
Sum of electronic and thermal Energies=	-1089.025458
Sum of electronic and thermal Enthalpies=	-1089.024514
Sum of electronic and thermal Free Energies=	-1089.079405

Benzo[b]naphtho[2,1,d]-thiophene S-oxide (2),

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-4.486093000	-0.120748000	-0.058706000
C	-4.192862000	1.245044000	0.041152000
C	-3.451306000	-1.061784000	-0.159873000
H	-5.004363000	1.964649000	0.110665000
H	-3.672794000	-2.122172000	-0.249087000
C	-2.868868000	1.700331000	0.053472000
C	-2.143719000	-0.594276000	-0.134608000
H	-2.655218000	2.763020000	0.129043000
H	-5.519561000	-0.455908000	-0.064079000
C	-1.827725000	0.770019000	-0.026906000
S	-0.668997000	-1.639233000	-0.289562000
C	-0.375886000	1.008099000	-0.003325000
H	2.182539000	3.244582000	0.182274000
C	1.664969000	2.291180000	0.108695000
C	0.287554000	2.257240000	0.085420000
C	0.369568000	-0.161247000	-0.077435000
C	1.788164000	-0.174326000	-0.069233000
C	2.445955000	1.101656000	0.036890000
C	3.867044000	1.143564000	0.061569000
C	4.609685000	-0.015937000	-0.021844000
C	3.959672000	-1.271197000	-0.134025000
C	2.582411000	-1.352384000	-0.155013000
H	-0.288003000	3.176986000	0.137255000
H	2.102577000	-2.323664000	-0.233978000
H	4.553466000	-2.179003000	-0.202753000
H	5.695512000	0.027830000	-0.004030000
H	4.357831000	2.110554000	0.144959000
O	-0.552427000	-2.571317000	0.925669000

Frequencies --	51.3517	84.3327	108.0562
Frequencies --	141.8266	157.9743	183.7313
Frequencies --	216.0193	278.9798	318.7201
Frequencies --	335.7321	372.2082	404.6943
Frequencies --	435.3382	454.6258	468.6168
Frequencies --	511.1104	522.2685	538.7145
Frequencies --	556.9310	573.2885	589.2766
Frequencies --	667.9003	676.9626	686.7164
Frequencies --	727.1775	739.2991	758.1668
Frequencies --	768.6690	784.3946	827.2329
Frequencies --	838.7651	880.5670	886.9846
Frequencies --	890.6027	968.0590	971.8170
Frequencies --	973.8345	983.8329	989.6952
Frequencies --	1007.3152	1009.1966	1045.0148
Frequencies --	1048.0178	1061.0751	1104.0957
Frequencies --	1149.6386	1160.6959	1181.2743
Frequencies --	1184.4494	1195.1082	1245.1180
Frequencies --	1277.4732	1291.9736	1329.3710
Frequencies --	1365.0711	1381.9331	1391.4535
Frequencies --	1406.5902	1463.3317	1482.6853
Frequencies --	1495.4224	1510.9837	1557.8761
Frequencies --	1601.3357	1620.4748	1633.6325
Frequencies --	1637.2611	1665.5756	3189.3712
Frequencies --	3195.6572	3196.6474	3197.9873
Frequencies --	3204.5340	3207.5177	3211.0869
Frequencies --	3215.3367	3215.8436	3220.1781

Zero-point correction=

0.211601 (Hartree/Particle)

Thermal correction to Energy=

0.224694

Thermal correction to Enthalpy=	0.225638
Thermal correction to Gibbs Free Energy=	0.171805
Sum of electronic and zero-point Energies=	-1088.947187
Sum of electronic and thermal Energies=	-1088.934094
Sum of electronic and thermal Enthalpies=	-1088.933150
Sum of electronic and thermal Free Energies=	-1088.986983

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-4.460445000	-0.132437000	-0.000178000
C	-4.178512000	1.242396000	0.075150000
C	-3.427274000	-1.077647000	-0.112232000
H	-4.996366000	1.952330000	0.154271000
H	-3.653050000	-2.137669000	-0.184893000
C	-2.865806000	1.704584000	0.051709000
C	-2.126522000	-0.606726000	-0.126833000
H	-2.652090000	2.767025000	0.115891000
H	-5.491911000	-0.471885000	0.018437000
C	-1.817139000	0.770287000	-0.041773000
S	-0.661470000	-1.660221000	-0.324659000
C	-0.393970000	1.029933000	-0.039931000
H	2.154016000	3.259827000	0.164239000
C	1.637096000	2.307452000	0.087193000
C	0.256980000	2.274796000	0.042409000
C	0.377027000	-0.168018000	-0.112363000
C	1.776437000	-0.167548000	-0.073777000
C	2.424510000	1.114434000	0.038830000
C	3.824150000	1.165650000	0.085764000
C	4.587861000	-0.012696000	0.022775000
C	3.963887000	-1.261608000	-0.093909000
C	2.577206000	-1.348132000	-0.140009000
H	-0.317439000	3.194175000	0.082296000
H	2.105795000	-2.322254000	-0.220954000
H	4.561349000	-2.166203000	-0.146176000
H	5.671084000	0.051225000	0.061794000
H	4.319204000	2.129252000	0.166410000
O	-0.506248000	-2.587575000	0.875786000

Frequencies --	44.3305	87.9886	99.9112
Frequencies --	142.1289	154.9806	185.3147
Frequencies --	203.8465	270.0169	306.0252
Frequencies --	328.2950	367.2587	394.1634
Frequencies --	419.1641	435.9071	452.1489
Frequencies --	500.4867	515.9006	522.4324
Frequencies --	529.8045	552.3195	579.8990
Frequencies --	648.9683	663.5830	675.8580
Frequencies --	720.1571	727.7603	742.9568
Frequencies --	770.5206	786.2631	820.1354
Frequencies --	843.4092	886.2366	891.9660
Frequencies --	898.1780	971.1576	982.0897
Frequencies --	983.8156	1002.4144	1007.1782
Frequencies --	1019.4119	1021.1825	1042.5560
Frequencies --	1052.7646	1062.0117	1099.0373
Frequencies --	1145.1035	1155.2212	1174.9093
Frequencies --	1186.1270	1199.4934	1246.5663

Frequencies --	1282.7842	1292.8159	1338.8492
Frequencies --	1364.5453	1384.0352	1399.8859
Frequencies --	1430.6839	1463.4620	1474.6137
Frequencies --	1488.4778	1508.9205	1522.2026
Frequencies --	1561.9731	1576.1025	1594.2146
Frequencies --	1600.9909	1626.6675	3214.5358
Frequencies --	3216.8538	3219.9896	3221.0916
Frequencies --	3222.8856	3227.6491	3229.9276
Frequencies --	3233.0260	3237.6995	3239.9782

Zero-point correction=	0.211173 (Hartree/Particle)
Thermal correction to Energy=	0.224482
Thermal correction to Enthalpy=	0.225426
Thermal correction to Gibbs Free Energy=	0.170415
Sum of electronic and zero-point Energies=	-1088.732775
Sum of electronic and thermal Energies=	-1088.719466
Sum of electronic and thermal Enthalpies=	-1088.718522
Sum of electronic and thermal Free Energies=	-1088.773534

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

C	-4.475470000	-0.146194000	-0.273148000
C	-4.204084000	1.226054000	-0.061820000
C	-3.421210000	-1.061964000	-0.333560000
H	-5.029326000	1.933124000	-0.012668000
H	-3.621056000	-2.120659000	-0.488144000
C	-2.898410000	1.689036000	0.080825000
C	-2.113018000	-0.597549000	-0.184274000
H	-2.711425000	2.749923000	0.234046000
H	-5.500970000	-0.488052000	-0.387454000
C	-1.816842000	0.782684000	0.019158000
S	-0.652953000	-1.647742000	-0.158985000
C	-0.399613000	1.019988000	0.094241000
H	2.189720000	3.237084000	0.280143000
C	1.667596000	2.286886000	0.188288000
C	0.286338000	2.248905000	0.218479000
C	0.358661000	-0.183643000	-0.059327000
C	1.785531000	-0.186366000	-0.085734000
C	2.454021000	1.090063000	0.030867000
C	3.865838000	1.131328000	-0.011568000
C	4.626753000	-0.027699000	-0.160592000
C	3.978477000	-1.271720000	-0.262414000
C	2.589064000	-1.350798000	-0.219132000
H	-0.278509000	3.173535000	0.323933000
H	2.110545000	-2.324936000	-0.285429000
H	4.563560000	-2.182850000	-0.368790000
H	5.712317000	0.029575000	-0.189820000
H	4.358728000	2.098484000	0.075637000
O	-0.631015000	-2.454426000	1.185070000

Frequencies --	50.4269	76.5655	114.5992
Frequencies --	139.3644	150.9371	173.8440
Frequencies --	212.9859	275.2516	307.5852
Frequencies --	313.7621	369.4627	393.5837

Frequencies --	421.1713	437.5382	467.3018
Frequencies --	507.8700	511.5497	522.4813
Frequencies --	545.4537	556.6827	587.8088
Frequencies --	626.8499	666.5175	684.9557
Frequencies --	715.4669	724.8318	734.4555
Frequencies --	744.1543	760.6353	790.3697
Frequencies --	816.1526	850.8072	851.6728
Frequencies --	856.0665	882.6935	927.8677
Frequencies --	943.0526	946.0674	969.1723
Frequencies --	970.4345	972.8696	1024.0289
Frequencies --	1045.5173	1050.4605	1076.5281
Frequencies --	1138.4470	1142.4037	1151.0234
Frequencies --	1173.0932	1176.2003	1234.2756
Frequencies --	1251.4496	1280.2495	1326.4824
Frequencies --	1330.4730	1354.6581	1376.2766
Frequencies --	1395.6551	1450.2288	1467.3162
Frequencies --	1472.1468	1484.5049	1517.6882
Frequencies --	1545.7321	1570.4697	1576.9321
Frequencies --	1605.5058	1616.0089	3167.5735
Frequencies --	3170.1572	3175.2148	3176.0469
Frequencies --	3179.8670	3187.3165	3188.7966
Frequencies --	3190.6829	3200.0375	3203.2983

Zero-point correction=	0.207869 (Hartree/Particle)
Thermal correction to Energy=	0.221301
Thermal correction to Enthalpy=	0.222245
Thermal correction to Gibbs Free Energy=	0.167133
Sum of electronic and zero-point Energies=	-1089.043024
Sum of electronic and thermal Energies=	-1089.029593
Sum of electronic and thermal Enthalpies=	-1089.028648
Sum of electronic and thermal Free Energies=	-1089.083761

Benzo[b]phenanthro[9,10-d]thiophene S-oxide (3)

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	-1.377951000	-1.995596000	-0.389736000
C	-4.744481000	0.270552000	0.078688000
C	-4.162881000	1.528387000	0.254841000
C	-3.925355000	-0.843884000	-0.140115000
H	-4.793939000	2.393170000	0.441485000
H	-4.354260000	-1.834617000	-0.265979000
C	-2.773963000	1.705979000	0.205498000
C	-2.552149000	-0.648711000	-0.172969000
H	-2.385328000	2.699546000	0.378362000
C	-1.930644000	0.606835000	-0.022738000
H	-5.823505000	0.152209000	0.120538000
C	1.720039000	-2.603673000	-0.155636000
C	3.048211000	-2.973779000	-0.054063000
C	1.340073000	-1.237944000	-0.092085000
C	4.037587000	-1.986745000	0.123997000
C	2.339396000	-0.229991000	0.060720000
C	3.688124000	-0.647373000	0.178980000
C	-0.025031000	-0.816081000	-0.136603000

C	-0.446282000	0.495503000	-0.071489000
C	0.557857000	1.544369000	-0.051578000
C	1.941756000	1.174910000	0.051805000
H	0.961249000	-3.371281000	-0.270789000
H	3.325119000	-4.023445000	-0.103776000
H	5.081791000	-2.273975000	0.215712000
H	4.476178000	0.084458000	0.313245000
C	0.235213000	2.921014000	-0.166061000
C	2.910642000	2.207376000	0.105560000
C	2.558985000	3.543772000	0.030167000
C	1.208964000	3.903325000	-0.124449000
H	-0.788515000	3.226414000	-0.321033000
H	3.961851000	1.957242000	0.189178000
H	3.329850000	4.309046000	0.069610000
H	0.925948000	4.948180000	-0.220898000
O	-1.503199000	-2.977556000	0.784416000

Frequencies --	36.5796	62.1082	92.7288
Frequencies --	101.1351	112.0611	156.9968
Frequencies --	170.8813	219.1725	234.7822
Frequencies --	257.3649	283.4789	324.3791
Frequencies --	331.5362	384.1034	405.8176
Frequencies --	414.2917	437.8619	452.4896
Frequencies --	458.1405	484.5536	508.5964
Frequencies --	531.7645	565.4661	579.1500
Frequencies --	611.1260	625.3928	639.1012
Frequencies --	661.9855	684.1086	712.5043
Frequencies --	731.8317	739.0568	759.0111
Frequencies --	761.2791	768.8994	777.9502
Frequencies --	785.1526	807.7903	875.1828
Frequencies --	876.3471	885.6904	903.2411
Frequencies --	965.1054	968.6756	973.9500
Frequencies --	978.8445	985.9605	1005.2415
Frequencies --	1008.3459	1009.1947	1013.9964
Frequencies --	1057.8151	1070.3914	1070.7179
Frequencies --	1077.5326	1128.2965	1155.1978
Frequencies --	1164.9486	1182.3046	1187.0937
Frequencies --	1190.1638	1204.2794	1257.9091
Frequencies --	1264.6303	1298.5252	1312.6088
Frequencies --	1338.0650	1359.9960	1368.8895
Frequencies --	1382.1641	1393.6577	1448.0640
Frequencies --	1472.3429	1480.2487	1487.5732
Frequencies --	1502.3390	1534.5655	1564.6511
Frequencies --	1606.9808	1609.2395	1620.8014
Frequencies --	1636.5889	1651.8100	1658.1340
Frequencies --	3196.6167	3197.4809	3198.9171
Frequencies --	3205.8807	3207.3410	3210.5384
Frequencies --	3218.3616	3218.6453	3223.6488
Frequencies --	3240.1812	3264.7403	3301.6844

Zero-point correction=	0.258670 (Hartree/Particle)
Thermal correction to Energy=	0.274530
Thermal correction to Enthalpy=	0.275474
Thermal correction to Gibbs Free Energy=	0.215299
Sum of electronic and zero-point Energies=	-1242.543998
Sum of electronic and thermal Energies=	-1242.528138
Sum of electronic and thermal Enthalpies=	-1242.527194
Sum of electronic and thermal Free Energies=	-1242.587369

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	1.392100000	-1.978921000	0.575178000
C	4.673674000	0.312967000	-0.257079000
C	4.063600000	1.550477000	-0.514359000
C	3.899159000	-0.803589000	0.091258000
H	4.673906000	2.396362000	-0.816040000
H	4.365129000	-1.768453000	0.268856000
C	2.684857000	1.710089000	-0.409825000
C	2.530256000	-0.633659000	0.182027000
H	2.244706000	2.663646000	-0.670856000
C	1.884278000	0.610133000	-0.030418000
H	5.751348000	0.211203000	-0.344806000
C	-1.703237000	-2.626975000	0.112129000
C	-3.016554000	-2.991958000	-0.080585000
C	-1.321499000	-1.247188000	0.079614000
C	-3.983689000	-1.995261000	-0.321414000
C	-2.319496000	-0.225293000	-0.129018000
C	-3.639914000	-0.642024000	-0.342175000
C	0.012421000	-0.839709000	0.199361000
C	0.439581000	0.510717000	0.099429000
C	-0.550973000	1.548645000	0.117483000
C	-1.928957000	1.184556000	-0.050485000
H	-0.948786000	-3.390615000	0.264896000
H	-3.303654000	-4.038529000	-0.060318000
H	-5.018567000	-2.278919000	-0.490518000
H	-4.426102000	0.081188000	-0.522209000
C	-0.215466000	2.910220000	0.333619000
C	-2.883493000	2.214330000	-0.097051000
C	-2.519792000	3.552435000	0.062601000
C	-1.185369000	3.901212000	0.301784000
H	0.803456000	3.182458000	0.574490000
H	-3.932870000	1.984110000	-0.236603000
H	-3.288002000	4.319851000	0.029433000
H	-0.908815000	4.936579000	0.476253000
O	1.524790000	-3.079611000	-0.469601000

Frequencies --	40.1855	65.3719	91.8885
Frequencies --	103.9334	118.2903	147.9171
Frequencies --	173.8078	213.2284	234.4350
Frequencies --	252.7394	271.7522	306.9994
Frequencies --	336.7396	382.6190	398.0860
Frequencies --	413.4499	427.1201	444.7762
Frequencies --	450.0329	466.5782	498.5784
Frequencies --	518.4560	543.0153	557.9486
Frequencies --	602.5174	612.1872	631.2666
Frequencies --	668.6770	676.8280	700.7430
Frequencies --	712.3172	733.1653	753.2967
Frequencies --	757.6182	775.1545	781.3825
Frequencies --	789.2527	809.4970	885.2221
Frequencies --	890.5276	899.9405	903.5788
Frequencies --	971.8204	981.6684	985.4166
Frequencies --	992.2676	1007.9829	1014.1492
Frequencies --	1018.0533	1020.4483	1021.5758

Frequencies --	1053.0601	1065.6811	1068.9868
Frequencies --	1080.6845	1127.7151	1156.8196
Frequencies --	1164.7004	1181.6616	1187.2247
Frequencies --	1196.5071	1199.9218	1258.0580
Frequencies --	1268.6975	1302.0134	1320.7216
Frequencies --	1338.3034	1353.3076	1369.2084
Frequencies --	1392.3367	1411.0590	1442.2133
Frequencies --	1465.9490	1474.0845	1481.3080
Frequencies --	1488.3817	1503.8126	1552.6528
Frequencies --	1561.6059	1584.6643	1594.7743
Frequencies --	1609.0572	1623.3750	1638.2905
Frequencies --	3212.6636	3213.8217	3217.1442
Frequencies --	3219.7694	3225.8191	3228.2524
Frequencies --	3229.6010	3239.7071	3241.2865
Frequencies --	3254.8063	3256.0654	3273.0895

Zero-point correction=	0.258306 (Hartree/Particle)
Thermal correction to Energy=	0.274292
Thermal correction to Enthalpy=	0.275236
Thermal correction to Gibbs Free Energy=	0.214312
Sum of electronic and zero-point Energies=	-1242.334565
Sum of electronic and thermal Energies=	-1242.318579
Sum of electronic and thermal Enthalpies=	-1242.317635
Sum of electronic and thermal Free Energies=	-1242.378560

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	1.364077000	-2.046291000	0.085981000
C	4.734904000	0.210625000	-0.409434000
C	4.164341000	1.498973000	-0.415302000
C	3.896654000	-0.899214000	-0.268765000
H	4.805308000	2.368663000	-0.543250000
H	4.309795000	-1.906112000	-0.271164000
C	2.791362000	1.694036000	-0.272259000
C	2.525632000	-0.701590000	-0.124645000
H	2.418751000	2.709305000	-0.319022000
C	1.911148000	0.592015000	-0.107843000
H	5.807846000	0.080088000	-0.522355000
C	-1.739625000	-2.620806000	-0.145210000
C	-3.072530000	-2.968955000	-0.298611000
C	-1.326914000	-1.258464000	-0.091306000
C	-4.054543000	-1.967388000	-0.395372000
C	-2.332459000	-0.235154000	-0.150557000
C	-3.677060000	-0.628087000	-0.316211000
C	0.038634000	-0.861754000	-0.009049000
C	0.470098000	0.497581000	0.005070000
C	-0.535329000	1.534221000	0.085886000
C	-1.928736000	1.176590000	-0.007799000
H	-0.992652000	-3.406723000	-0.071679000
H	-3.353809000	-4.018866000	-0.344376000
H	-5.101611000	-2.230225000	-0.523033000
H	-4.455952000	0.123934000	-0.387653000
C	-0.220178000	2.906768000	0.285384000
C	-2.894598000	2.202992000	0.067667000
C	-2.551009000	3.541783000	0.233467000

C	-1.198025000	3.890106000	0.353104000
H	0.809476000	3.205150000	0.423685000
H	-3.948700000	1.954023000	0.007248000
H	-3.327560000	4.300814000	0.286896000
H	-0.907589000	4.926376000	0.511794000
O	1.512607000	-2.623930000	1.533490000

Frequencies --	38.3458	60.4295	90.1472
Frequencies --	94.7591	112.0657	144.7052
Frequencies --	177.4788	199.3511	240.8142
Frequencies --	265.7798	285.9294	326.2483
Frequencies --	329.7623	360.0541	401.8035
Frequencies --	405.9241	420.6221	438.3829
Frequencies --	450.9847	491.4248	507.3510
Frequencies --	528.9269	544.8354	573.4450
Frequencies --	608.9113	611.1192	624.1698
Frequencies --	638.1127	679.2227	708.2530
Frequencies --	721.0108	723.7079	736.7001
Frequencies --	746.0509	758.2125	759.3966
Frequencies --	771.4730	810.6472	843.8173
Frequencies --	848.7399	856.9433	864.1403
Frequencies --	904.1192	940.6267	943.6501
Frequencies --	946.4373	972.0423	976.0459
Frequencies --	977.8249	981.6884	1002.8262
Frequencies --	1040.3522	1054.2152	1070.6474
Frequencies --	1075.9852	1120.6424	1146.8708
Frequencies --	1154.1662	1171.3067	1179.0394
Frequencies --	1186.0055	1190.6674	1251.5486
Frequencies --	1252.8808	1290.9059	1299.6319
Frequencies --	1327.1537	1338.6945	1346.3086
Frequencies --	1371.8784	1385.7175	1423.2784
Frequencies --	1461.1265	1467.6835	1477.3471
Frequencies --	1485.0934	1511.2837	1528.2958
Frequencies --	1569.4809	1581.5536	1588.5744
Frequencies --	1603.5721	1627.6265	1633.9797
Frequencies --	3178.1536	3179.2856	3182.7857
Frequencies --	3183.9411	3191.5116	3197.2572
Frequencies --	3201.1819	3203.3251	3210.3866
Frequencies --	3227.8676	3237.2108	3274.6405

Zero-point correction=	0.255443 (Hartree/Particle)
Thermal correction to Energy=	0.271578
Thermal correction to Enthalpy=	0.272522
Thermal correction to Gibbs Free Energy=	0.211200
Sum of electronic and zero-point Energies=	-1242.644566
Sum of electronic and thermal Energies=	-1242.628430
Sum of electronic and thermal Enthalpies=	-1242.627486
Sum of electronic and thermal Free Energies=	-1242.688808

Dinaphtho[2,1-b:2',1'-d]thiophene S-oxide (4)

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

H	-4.502281000	1.236388000	0.749293000
C	-3.467138000	1.017592000	0.499933000

C	-2.541215000	2.034245000	0.399881000
C	-1.204356000	1.690513000	0.136474000
C	-0.745479000	0.380669000	-0.016247000
C	-1.738053000	-0.652985000	-0.139314000
C	-3.103547000	-0.321733000	0.189157000
C	-4.102086000	-1.334346000	0.117811000
C	-3.800127000	-2.599230000	-0.337092000
C	-2.482502000	-2.895805000	-0.764816000
C	-1.480967000	-1.951789000	-0.665456000
H	-2.831105000	3.072945000	0.534442000
H	-0.491783000	-2.193827000	-1.033868000
H	-2.258842000	-3.873112000	-1.184958000
H	-4.574920000	-3.358891000	-0.400952000
H	-5.120201000	-1.075488000	0.399029000
C	0.738251000	0.327027000	-0.131575000
C	1.267406000	1.587477000	-0.390951000
C	2.623867000	1.844312000	-0.649341000
C	3.502684000	0.783517000	-0.604471000
C	3.060079000	-0.507935000	-0.205345000
C	1.667804000	-0.749479000	0.088542000
C	1.327644000	-1.997688000	0.685314000
C	2.277085000	-2.978433000	0.888616000
C	3.623641000	-2.773760000	0.500240000
C	4.004478000	-1.557924000	-0.023739000
H	2.966581000	2.849334000	-0.879731000
H	4.557565000	0.932382000	-0.820487000
H	5.044001000	-1.366289000	-0.279504000
H	4.356943000	-3.562373000	0.647421000
H	1.988615000	-3.913165000	1.362619000
H	0.315381000	-2.170315000	1.027479000
S	0.045772000	2.917235000	-0.291494000
O	0.406609000	3.835148000	0.884676000

Frequencies --	56.7175	64.9562	79.9369
Frequencies --	92.7365	156.8958	179.8438
Frequencies --	188.1865	195.4311	240.5224
Frequencies --	246.6912	293.5123	328.5037
Frequencies --	345.6536	395.4843	409.6054
Frequencies --	426.7417	460.0075	467.8857
Frequencies --	499.3311	518.1482	532.7712
Frequencies --	541.3763	547.1980	552.4979
Frequencies --	591.8829	611.3022	632.4513
Frequencies --	650.5165	663.4926	689.6149
Frequencies --	709.4573	758.3849	765.0730
Frequencies --	782.9742	795.4168	805.7894
Frequencies --	825.1269	826.5335	846.8069
Frequencies --	864.5811	883.7283	885.5779
Frequencies --	895.6180	954.0206	970.8213
Frequencies --	972.9183	983.0261	985.5661
Frequencies --	994.5688	1007.5842	1017.2540
Frequencies --	1050.0714	1051.4010	1068.8976
Frequencies --	1147.9090	1161.3853	1163.3151
Frequencies --	1171.6471	1174.5957	1183.9746
Frequencies --	1187.3087	1213.6070	1242.1838
Frequencies --	1245.7836	1281.6260	1304.1958
Frequencies --	1359.7823	1367.1709	1387.0184
Frequencies --	1392.2051	1399.3571	1418.4913
Frequencies --	1464.8825	1465.3514	1480.8050

Frequencies --	1489.7678	1550.1350	1553.9030
Frequencies --	1593.2510	1607.4755	1614.0273
Frequencies --	1618.7332	1661.3861	1662.9404
Frequencies --	3189.5194	3190.6612	3196.8438
Frequencies --	3197.7429	3197.9539	3198.7745
Frequencies --	3210.9313	3211.8075	3212.4201
Frequencies --	3212.7141	3239.3487	3249.2142

Zero-point correction=	0.258420	(Hartree/Particle)
Thermal correction to Energy=	0.274061	
Thermal correction to Enthalpy=	0.275005	
Thermal correction to Gibbs Free Energy=	0.215661	
Sum of electronic and zero-point Energies=	-1242.533068	
Sum of electronic and thermal Energies=	-1242.517427	
Sum of electronic and thermal Enthalpies=	-1242.516483	
Sum of electronic and thermal Free Energies=	-1242.575827	

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

H	-4.445168000	1.224174000	0.836266000
C	-3.421271000	1.003788000	0.547196000
C	-2.495974000	2.040121000	0.417219000
C	-1.191978000	1.708083000	0.090122000
C	-0.725886000	0.373331000	-0.062276000
C	-1.727014000	-0.663064000	-0.169769000
C	-3.075957000	-0.329499000	0.211302000
C	-4.085656000	-1.323941000	0.160359000
C	-3.806261000	-2.591461000	-0.325667000
C	-2.513671000	-2.886993000	-0.793141000
C	-1.492461000	-1.945366000	-0.712153000
H	-2.795316000	3.073105000	0.567872000
H	-0.516403000	-2.198929000	-1.107222000
H	-2.304502000	-3.860105000	-1.228323000
H	-4.588515000	-3.343391000	-0.373830000
H	-5.090831000	-1.061439000	0.478707000
C	0.723896000	0.319597000	-0.118318000
C	1.273066000	1.604143000	-0.364758000
C	2.613409000	1.843561000	-0.623054000
C	3.488689000	0.760709000	-0.580598000
C	3.043493000	-0.527911000	-0.193119000
C	1.652111000	-0.769433000	0.094929000
C	1.309669000	-2.011733000	0.673786000
C	2.268658000	-2.997008000	0.881866000
C	3.608778000	-2.792049000	0.508283000
C	3.991691000	-1.567495000	-0.013202000
H	2.974724000	2.840573000	-0.856319000
H	4.542717000	0.906928000	-0.800315000
H	5.030604000	-1.371366000	-0.263987000
H	4.342852000	-3.578750000	0.655488000
H	1.972539000	-3.934803000	1.343277000
H	0.295255000	-2.200447000	1.000059000
S	0.060261000	2.949304000	-0.313295000
O	0.374236000	3.853913000	0.873376000

Frequencies --	47.7957	65.4814	80.0550
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Frequencies --	93.2138	153.0331	172.5113
Frequencies --	186.7799	190.4763	234.1656
Frequencies --	241.5986	293.2400	324.0191
Frequencies --	346.2864	389.9102	403.0972
Frequencies --	412.6481	444.2533	466.5040
Frequencies --	485.3519	505.5732	519.1644
Frequencies --	530.5806	536.9689	546.9424
Frequencies --	563.1276	605.9157	629.0128
Frequencies --	645.9546	659.6121	687.7206
Frequencies --	703.6300	761.8118	772.8586
Frequencies --	774.4760	794.9580	795.7775
Frequencies --	842.0454	844.4228	851.2679
Frequencies --	867.5428	885.8933	899.2958
Frequencies --	912.5619	953.5897	983.5642
Frequencies --	988.2294	995.9221	1006.1340
Frequencies --	1011.1949	1018.4284	1026.8387
Frequencies --	1060.0512	1061.3407	1080.2838
Frequencies --	1148.2312	1154.9089	1162.1985
Frequencies --	1165.5760	1171.9041	1186.2980
Frequencies --	1186.8694	1218.2110	1256.6226
Frequencies --	1261.8613	1290.3331	1313.6406
Frequencies --	1326.9456	1356.7395	1382.0173
Frequencies --	1394.6115	1402.9006	1429.7285
Frequencies --	1462.4256	1464.6237	1473.2083
Frequencies --	1481.7329	1538.9057	1543.3964
Frequencies --	1564.8149	1573.0865	1576.6345
Frequencies --	1603.5685	1623.0344	1628.3242
Frequencies --	3207.5740	3208.1003	3213.6853
Frequencies --	3214.0913	3215.5206	3216.8895
Frequencies --	3225.9190	3226.4768	3227.6136
Frequencies --	3229.1199	3245.9974	3255.9298

Zero-point correction=	0.258306 (Hartree/Particle)
Thermal correction to Energy=	0.274098
Thermal correction to Enthalpy=	0.275042
Thermal correction to Gibbs Free Energy=	0.214613
Sum of electronic and zero-point Energies=	-1242.330524
Sum of electronic and thermal Energies=	-1242.314733
Sum of electronic and thermal Enthalpies=	-1242.313789
Sum of electronic and thermal Free Energies=	-1242.374218

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

Dinaphtho[1,2-b:2',1'-d]thiophene S-oxide (5)

Charge 0 multiplicity 1

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	-0.000027000	-1.331674000	-0.203454000
H	5.588127000	1.532808000	0.048186000
C	4.942572000	0.659245000	-0.005446000
C	5.481724000	-0.608110000	-0.080419000
C	4.631624000	-1.741069000	-0.155095000

C	3.259909000	-1.594530000	-0.147947000
C	2.673005000	-0.299813000	-0.069265000
C	3.533560000	0.852608000	-0.000526000
C	2.960716000	2.155445000	0.061407000
C	1.595819000	2.349589000	0.061120000
C	0.735605000	1.224828000	0.009721000
C	1.277696000	-0.051067000	-0.051352000
H	6.559955000	-0.743900000	-0.085343000
H	5.066653000	-2.735105000	-0.217796000
H	2.624245000	-2.473871000	-0.199558000
H	1.181997000	3.352884000	0.102166000
H	3.629723000	3.011470000	0.106488000
H	-3.629761000	3.011326000	0.108672000
C	-2.960742000	2.155344000	0.062881000
C	-1.595840000	2.349563000	0.062485000
C	-0.735599000	1.224894000	0.010083000
C	-1.277678000	-0.051009000	-0.051102000
C	-2.672957000	-0.299839000	-0.069159000
C	-3.533550000	0.852551000	0.000046000
C	-4.942566000	0.659223000	-0.005253000
C	-5.481701000	-0.608083000	-0.081022000
C	-4.631569000	-1.741008000	-0.156102000
C	-3.259859000	-1.594509000	-0.148557000
H	-1.182116000	3.352860000	0.104479000
H	-2.624220000	-2.473855000	-0.200491000
H	-5.066584000	-2.735010000	-0.219433000
H	-6.559928000	-0.743881000	-0.086286000
H	-5.588109000	1.532776000	0.048722000
O	-0.000071000	-2.243404000	1.033309000

Frequencies --	35.7963	56.1720	81.0218
Frequencies --	107.1821	110.3786	165.7576
Frequencies --	175.3400	209.1342	211.4721
Frequencies --	259.2890	266.9917	331.4945
Frequencies --	338.0057	383.6176	409.6936
Frequencies --	442.1089	442.7569	482.6167
Frequencies --	482.8015	499.8096	526.4092
Frequencies --	541.4990	543.1349	551.9435
Frequencies --	579.1495	583.1843	644.1851
Frequencies --	656.8977	668.7285	690.4417
Frequencies --	690.6082	753.9688	763.1503
Frequencies --	778.6164	783.2697	816.9003
Frequencies --	829.6535	833.4242	835.7574
Frequencies --	842.5755	880.2371	880.5999
Frequencies --	928.8292	971.3929	971.4651
Frequencies --	971.7600	976.1910	987.3268
Frequencies --	991.4115	1006.3442	1007.9339
Frequencies --	1007.9513	1044.0094	1047.5549
Frequencies --	1138.7465	1153.6343	1160.3918
Frequencies --	1172.2264	1181.9555	1183.3549
Frequencies --	1205.7476	1241.3870	1250.2844
Frequencies --	1279.6528	1283.4280	1343.8368
Frequencies --	1362.5932	1373.9397	1393.4295
Frequencies --	1395.7199	1401.8302	1415.8453
Frequencies --	1462.3765	1471.4683	1489.4982
Frequencies --	1506.6968	1552.4797	1560.1808
Frequencies --	1597.8347	1605.2233	1627.0053
Frequencies --	1636.6509	1663.5457	1667.4408

Frequencies --	3188.6474	3188.7025	3193.8432
Frequencies --	3195.4589	3196.0196	3196.7833
Frequencies --	3205.5927	3205.6482	3209.4308
Frequencies --	3214.4407	3214.4761	3220.0035

Zero-point correction=	0.258083 (Hartree/Particle)
Thermal correction to Energy=	0.273987
Thermal correction to Enthalpy=	0.274931
Thermal correction to Gibbs Free Energy=	0.214546
Sum of electronic and zero-point Energies=	-1242.550606
Sum of electronic and thermal Energies=	-1242.534703
Sum of electronic and thermal Enthalpies=	-1242.533758
Sum of electronic and thermal Free Energies=	-1242.594143

Charge 1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	-0.000038000	-1.355004000	-0.219127000
H	5.560326000	1.530267000	0.054194000
C	4.907387000	0.663314000	0.003329000
C	5.448130000	-0.619325000	-0.071439000
C	4.609550000	-1.750017000	-0.147170000
C	3.234621000	-1.601091000	-0.141958000
C	2.652667000	-0.300520000	-0.066388000
C	3.513531000	0.854364000	0.006892000
C	2.941646000	2.165583000	0.066566000
C	1.581440000	2.368187000	0.056447000
C	0.721593000	1.245207000	0.000394000
C	1.270103000	-0.056118000	-0.065913000
H	6.526479000	-0.748652000	-0.073473000
H	5.044954000	-2.742794000	-0.207077000
H	2.599020000	-2.480023000	-0.187128000
H	1.170478000	3.371297000	0.096208000
H	3.616511000	3.015701000	0.117838000
H	-3.616477000	3.015917000	0.114283000
C	-2.941630000	2.165711000	0.064203000
C	-1.581434000	2.368275000	0.054280000
C	-0.721590000	1.245231000	-0.000260000
C	-1.270074000	-0.056167000	-0.066141000
C	-2.652621000	-0.300511000	-0.066432000
C	-3.513500000	0.854442000	0.005864000
C	-4.907361000	0.663370000	0.002774000
C	-5.448106000	-0.619316000	-0.070582000
C	-4.609517000	-1.750107000	-0.145433000
C	-3.234633000	-1.601174000	-0.140719000
H	-1.170449000	3.371417000	0.093067000
H	-2.599038000	-2.480151000	-0.185127000
H	-5.044943000	-2.742945000	-0.204156000
H	-6.526452000	-0.748664000	-0.072163000
H	-5.560279000	1.530385000	0.052905000
O	-0.000092000	-2.230964000	1.029596000

Frequencies --	28.7786	41.5571	80.3589
Frequencies --	103.2365	112.0229	166.6936
Frequencies --	172.5025	197.9836	202.9667
Frequencies --	257.7950	263.0531	323.4764

Frequencies --	335.1161	380.4935	398.5997
Frequencies --	428.4470	432.6519	476.6225
Frequencies --	478.8060	479.9995	517.0272
Frequencies --	521.0699	534.8467	544.5896
Frequencies --	566.1854	580.9088	637.0062
Frequencies --	650.5919	658.3164	675.8414
Frequencies --	684.3963	741.1546	757.5329
Frequencies --	778.3234	778.5643	812.5790
Frequencies --	824.5160	828.3845	833.6081
Frequencies --	840.8672	892.0857	892.7776
Frequencies --	931.7462	969.0698	980.6255
Frequencies --	981.2644	997.3790	999.6984
Frequencies --	1005.2817	1014.1089	1017.9344
Frequencies --	1018.3056	1050.4645	1053.8119
Frequencies --	1125.5893	1147.6486	1155.5450
Frequencies --	1168.8038	1179.6242	1183.9573
Frequencies --	1212.5095	1249.9316	1252.2922
Frequencies --	1286.4714	1290.3477	1307.1286
Frequencies --	1338.8908	1380.4672	1391.7062
Frequencies --	1392.2094	1402.7721	1436.7290
Frequencies --	1458.7120	1471.1212	1475.9316
Frequencies --	1503.3145	1519.3456	1551.3094
Frequencies --	1555.3954	1572.5935	1583.6849
Frequencies --	1608.3593	1618.3018	1632.9408
Frequencies --	3208.3926	3208.4439	3212.7329
Frequencies --	3214.0528	3214.6185	3215.3555
Frequencies --	3221.5512	3221.6046	3227.2835
Frequencies --	3229.4859	3230.1306	3242.5303

Zero-point correction=	0.257505 (Hartree/Particle)
Thermal correction to Energy=	0.273630
Thermal correction to Enthalpy=	0.274574
Thermal correction to Gibbs Free Energy=	0.212700
Sum of electronic and zero-point Energies=	-1242.341441
Sum of electronic and thermal Energies=	-1242.325317
Sum of electronic and thermal Enthalpies=	-1242.324373
Sum of electronic and thermal Free Energies=	-1242.386247

Charge -1 multiplicity 2

SMD-B3LYP/6-31+G(d) solvent=acetonitrile

S	0.040730000	1.174347000	-0.027006000
H	-5.335626000	-2.014808000	-0.005160000
C	-4.749394000	-1.098333000	-0.011110000
C	-5.374175000	0.133517000	-0.024772000
C	-4.601430000	1.319652000	-0.030223000
C	-3.219437000	1.265248000	-0.023581000
C	-2.552494000	0.008739000	-0.012591000
C	-3.332514000	-1.198717000	-0.004217000
C	-2.679512000	-2.471571000	0.011785000
C	-1.310257000	-2.575545000	0.019035000
C	-0.511029000	-1.397139000	0.007799000
C	-1.133257000	-0.142914000	-0.008705000
H	-6.459640000	0.195543000	-0.030145000
H	-5.099488000	2.285587000	-0.038877000
H	-2.653348000	2.200338000	-0.024138000

H	-0.831682000	-3.551188000	0.032214000
H	-3.295996000	-3.367490000	0.018990000
H	3.965485000	-2.870119000	0.047064000
C	3.232388000	-2.066971000	0.030791000
C	1.889545000	-2.356673000	0.030035000
C	0.935868000	-1.299208000	0.009515000
C	1.380173000	0.027468000	-0.009376000
C	2.765115000	0.368601000	-0.010958000
C	3.704951000	-0.716979000	0.010729000
C	5.093841000	-0.417229000	0.011004000
C	5.541229000	0.889691000	-0.009137000
C	4.611435000	1.957531000	-0.030661000
C	3.253387000	1.702628000	-0.031269000
H	1.549947000	-3.388793000	0.045516000
H	2.551915000	2.533601000	-0.047775000
H	4.968364000	2.984117000	-0.046696000
H	6.607306000	1.102206000	-0.008717000
H	5.803234000	-1.241956000	0.027407000
O	-2.511092000	4.344081000	0.114733000

Frequencies --	37.3307	47.7925	70.9238
Frequencies --	73.5198	82.7252	115.9224
Frequencies --	121.8788	137.0085	211.9632
Frequencies --	219.4258	248.0865	251.2902
Frequencies --	261.9561	328.8624	396.8445
Frequencies --	421.2293	423.2901	426.6297
Frequencies --	484.5523	502.4613	503.3689
Frequencies --	529.9297	541.0514	547.3831
Frequencies --	558.5498	563.7775	592.5640
Frequencies --	648.4096	648.9110	676.5860
Frequencies --	692.3105	698.9166	754.5974
Frequencies --	764.6564	776.0884	784.0834
Frequencies --	818.8014	824.2580	836.7690
Frequencies --	838.0170	843.5254	879.8478
Frequencies --	884.3098	942.5790	969.7264
Frequencies --	970.9501	981.9587	982.8144
Frequencies --	983.1250	1003.8787	1005.3420
Frequencies --	1012.5153	1048.6750	1051.9742
Frequencies --	1143.8928	1154.8381	1161.2620
Frequencies --	1176.4999	1181.6812	1182.6989
Frequencies --	1190.5390	1238.6536	1242.4176
Frequencies --	1283.4652	1287.3703	1331.3600
Frequencies --	1365.6400	1367.3800	1386.2020
Frequencies --	1391.4052	1408.1962	1421.0272
Frequencies --	1462.0499	1468.8852	1487.7748
Frequencies --	1499.0767	1550.5156	1558.7663
Frequencies --	1583.6381	1595.5164	1631.7137
Frequencies --	1636.4246	1658.6721	1662.9989
Frequencies --	3096.4587	3182.8972	3184.6063
Frequencies --	3187.2060	3188.9204	3191.4959
Frequencies --	3196.9549	3200.0501	3207.7821
Frequencies --	3209.3865	3210.7989	3211.4133

Zero-point correction=	0.255160 (Hartree/Particle)
Thermal correction to Energy=	0.272118
Thermal correction to Enthalpy=	0.273062
Thermal correction to Gibbs Free Energy=	0.208816
Sum of electronic and zero-point Energies=	-1242.632950

Sum of electronic and thermal Energies=	-1242.615993
Sum of electronic and thermal Enthalpies=	-1242.615049
Sum of electronic and thermal Free Energies=	-1242.679295

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