Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Understanding the Reversible and Irreversible Two Stage Oxidation of Rubrene

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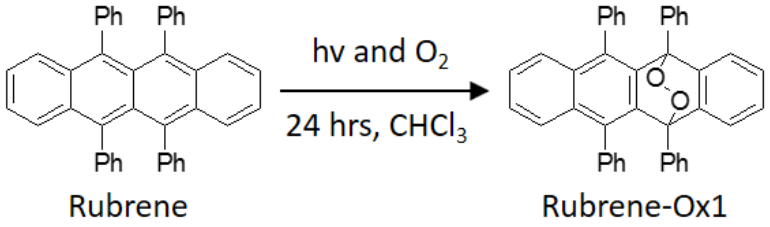
Contents

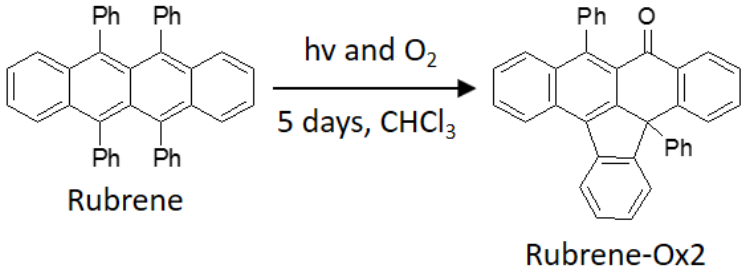
1. Synthesis

Rubrene-OX1



A solution of rubrene was prepared by dissolving 100 mg ($1.87x10^{-4}$ moles) of rubrene in 100 mL of $CHCl_3$ and allowed to stir in ambient laboratory conditions. Solution was exposed to both air and light for 24 hours and was dried under vacuo. The residue was purified via silica-gel column chromatography in hexanes. Product collected as a white solid in nearly quantitative yield (97%, 103 mg, $1.82x10^{-4}$ moles). ^{1}HNMR (CDCl3, 400MHz): σ 7.40 - 7.34(b, 6H), 7.22 – 7.17(b, 6H), 7.16 – 6.98(m, 12H), 6.86(t, 2H), 6.74(d, 2H).

Rubrene-OX2



A solution of rubrene was prepared by dissolving 100 mg ($1.87x10^{-4}$ moles) of rubrene in 100 mL of $CHCl_3$ and allowed to stir in ambient laboratory conditions. Solution was exposed to both air and light for 5 days and was dried under vacuo. The residue was purified via silica-gel column chromatography in hexanes. Product collected as a yellow solid (88%, 77 mg, $1.64x10^{-4}$ moles). ^{1}HNMR (CDCl3, 400MHz): σ 8.84(d, 1H), 8.46(d, 1H), 8.20(d, 1H), 7.91(d, 1H), 7.83(d, 1H), 7.78(t, 1H), 7.70(d, 1H), 7.58(dt, 4H), 7.50(m, 2H), 7.44(m, 3H).

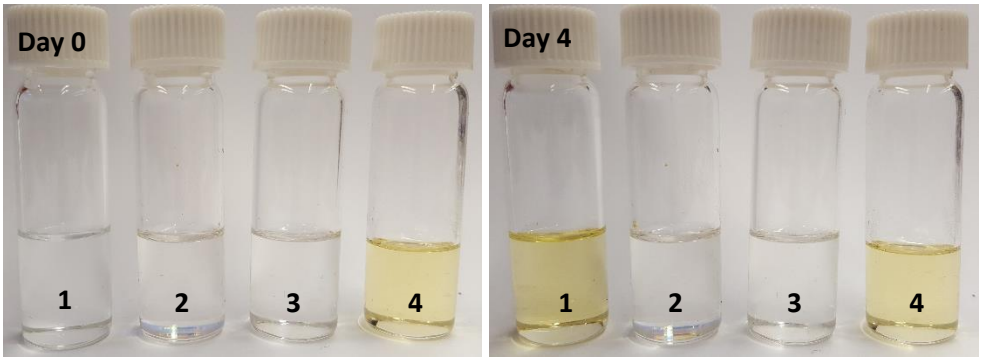


Figure S1. 5 mg of Rubrene-Ox1 were mixed dissolved in (1) chloroform, (2) toluene, (3) Na_2CO_3 treated chloroform, and (4) Na_2CO_3 treated choroform with Methanesulfonic acid.

2. ^{1}H NMR Spectra

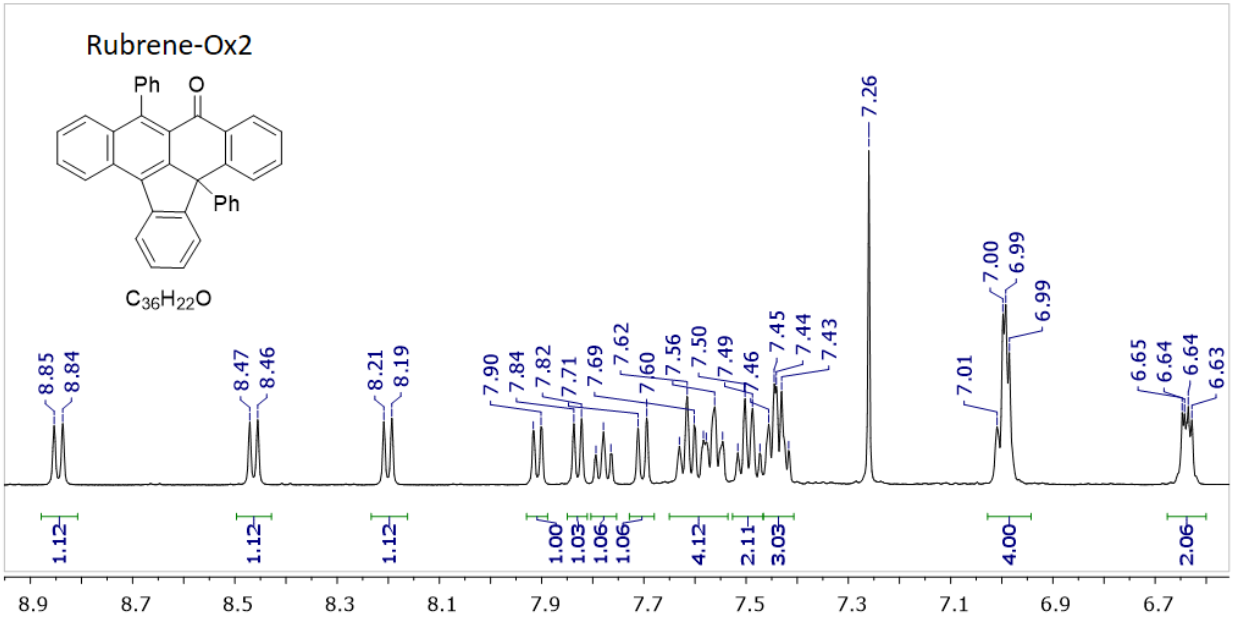


Figure S2. ^{1}H NMR of Rubrene-Ox2.

3. UV-Vis of oxidation of rubrene and half-life calculations

Half-life determination of rubrene was determined by monitoring the absorption profile over 160 minutes. Normalized peak absorbance versus time was plotted and fitted to an exponential decay to determine half-life time.

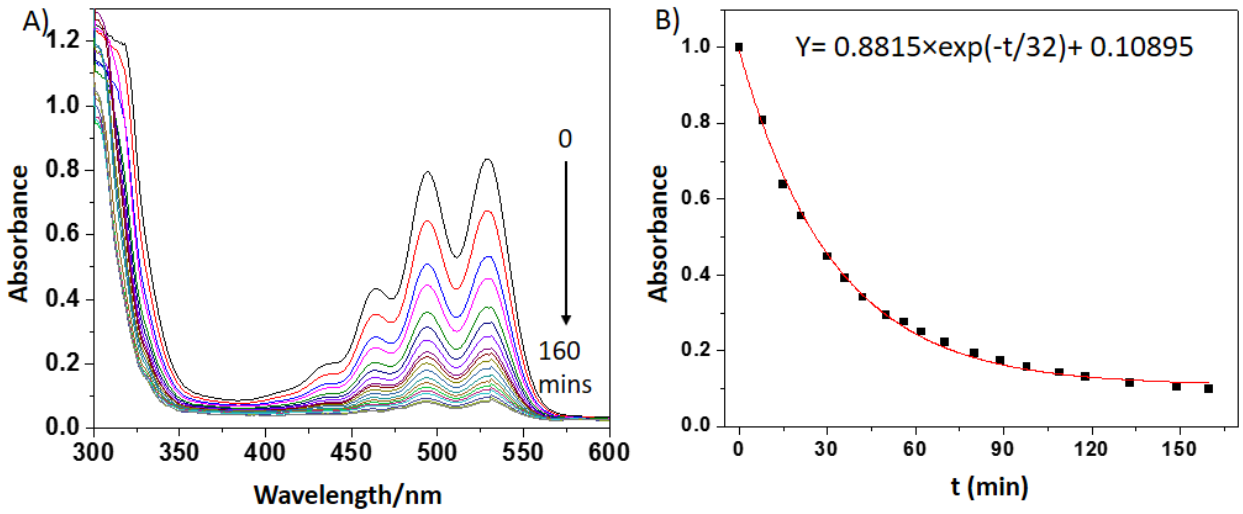


Figure S3. A)UV-vis spectra of rubrene in $CHCl_3$ recorded at regular interval (10 mins) during exposure to light, B) The absorbance intensity vs exposure time.

4. Rubrene-Ox2 Kinetics

Kinetic rate constant of rubrene-Ox1 with acid to form rubrene-Ox2 was determined by UV-Vis kinetics study. Below is the determined kinetic expression with the assumption of a bimolecular reaction of Rubene-Ox1 with acid.

[Rub-Ox1] + [H^+] → [Rub-Ox2]
if [Rub-Ox1] = [H^+], then
2[Rub-Ox1] → [Rub-Ox2]
then [Rub-Ox1] = [Rub-Ox2]/2
Plug into: Rate = k [Rub-Ox1]^2
Kinetic expression is therefore: [Rub-Ox2] = -4/(kt)

Once absorption coefficient of rubrene-Ox2 was determined, equimolar amounts of acid was added to a solution of rubrene-Ox1 and monitored over 40 minutes via UV-Vis. Peaks at 353 nm is unique to rubrene-Ox2. Known absorption values with absorption coefficient of rubrene-Ox2 allowed plotting concentration of the secondary product against inverse time to determine the kinetic rate constant as 7.91e-5 $M^{-1}min^{-1}$ or 1.32e-6 $M^{-1}min^{-1}$

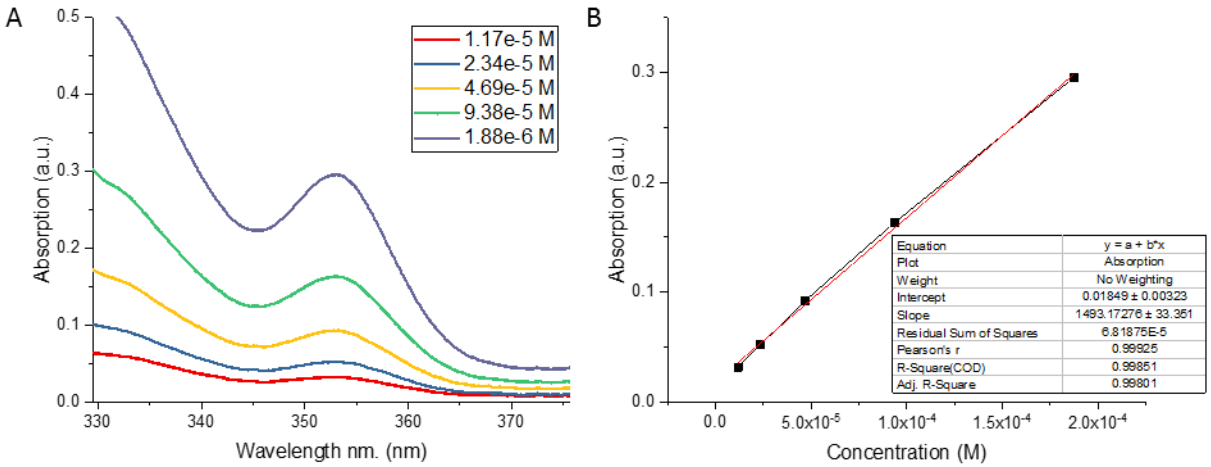


Figure S4. A) Rubrene-Ox2 concentration absorption sweep and B) Absorption coefficient of rubrene-Ox2 determined at 353 nm.

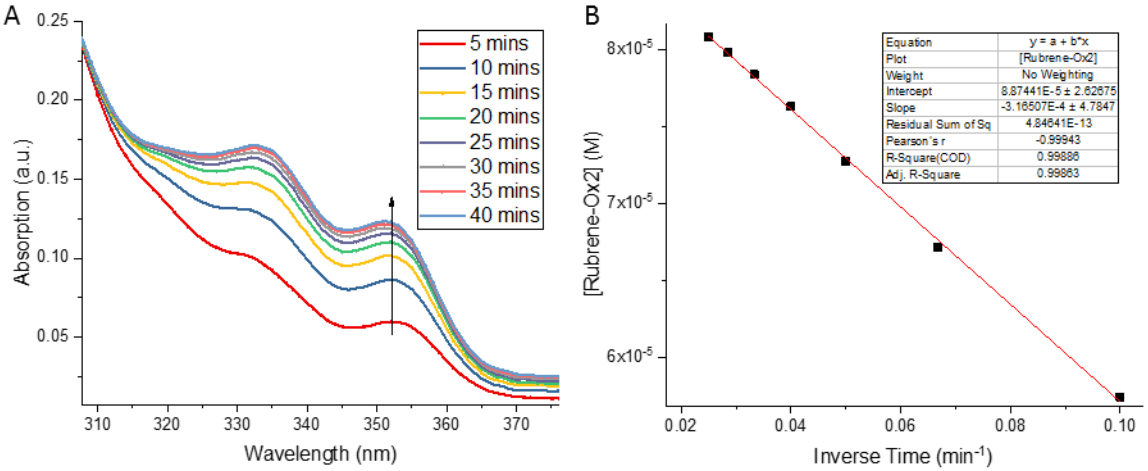


Figure S5. A) UV-Vis of rubrene-Ox1 to rubrene-Ox2 reaction with equimolar amounts of external acid and B) rubrene-Ox2 plotted against inverse time.

5. Output Characteristics

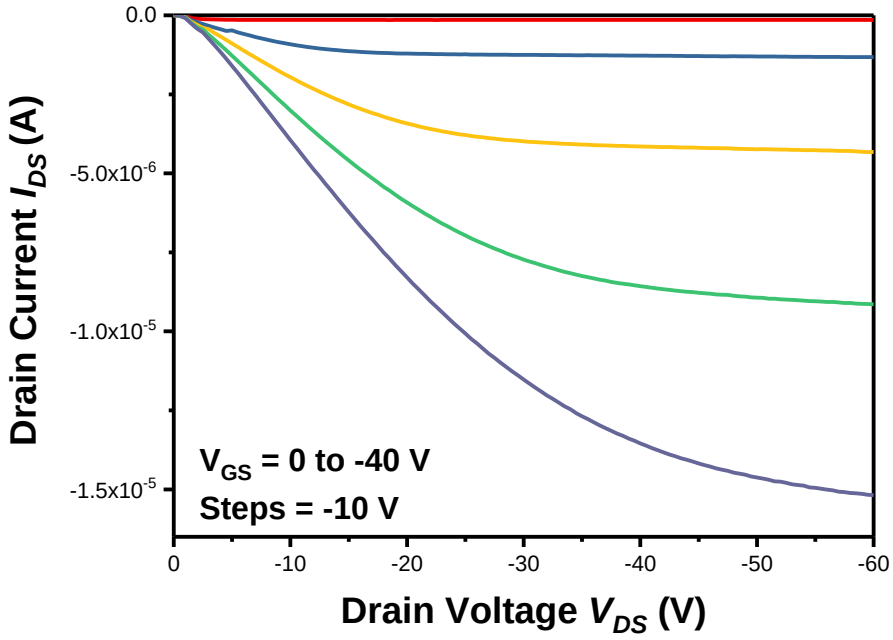


Figure S6. Output characteristics of rubrene single crystal transistor.

6. Rubrene-Ox2 Transistor

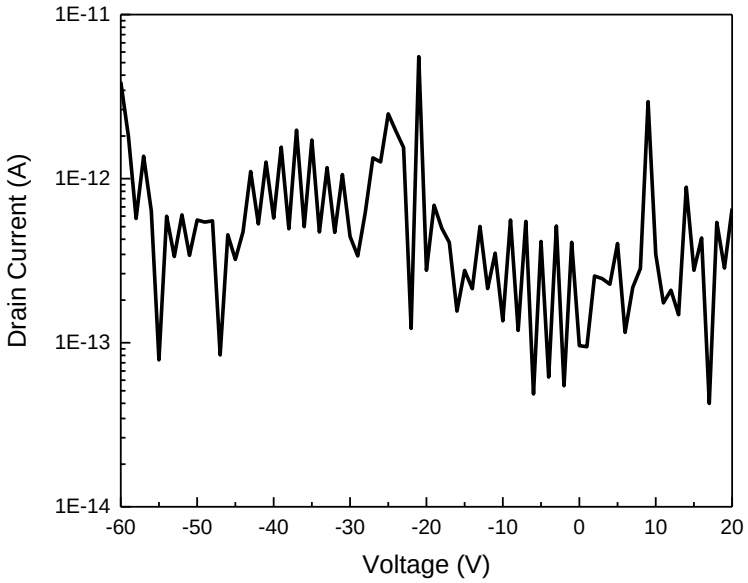


Figure S7. Transfer characteristics of **rubrene-Ox2** device.

7. DFT Analysis of Stage 1 and 2 Oxidation

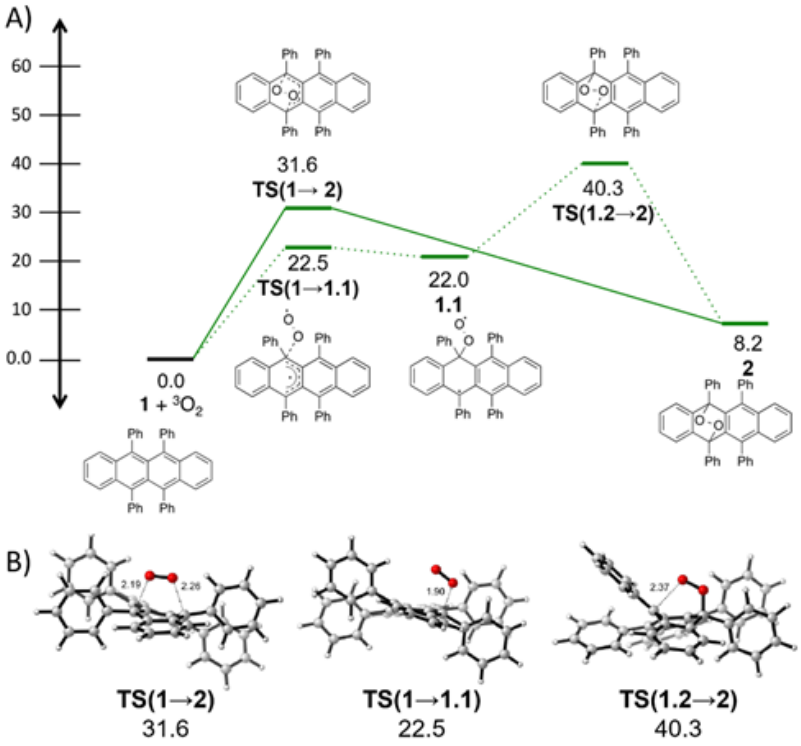


Figure S8. A) Potential surface energy in kcal mol^{-1} for the concerted (solid line) and stepwise (dashed line) oxidation of rubrene to *endo*-peroxide 2 and B) the key transition structures from stage 1 oxidation.

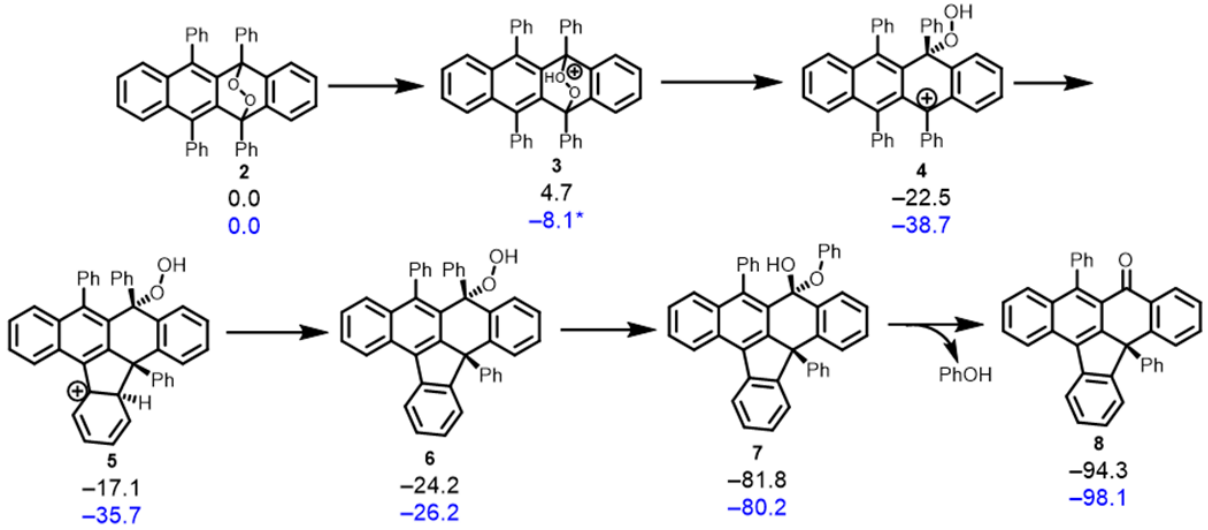


Figure S9. Computed thermodynamic analysis of the stages for the proposed rearrangement mechanism of Rubrene-Ox2 formation. The B3LYP-D3BJ/6-311+G(d,p)-IEFPCM^{CHCl3}//M06-2X/6-31G(d,p)-IEFPCM^{CHCl3} computational methodology was employed to simulate the energies of the states shown, which are reported in kcal mol^{-1}. All energies are reported relative to the isolated species: 4, H_3O^+, and H_2O.

8. Coordinates and Energies for Stationary Points

Rubrene

C	-1.40591600	1.23486600	-0.21571700
C	-0.70274800	2.44189800	-0.16489000
C	-1.34405800	3.70934300	-0.40491100
H	-2.37931500	3.71520800	-0.72491900
C	-0.68055100	4.88132400	-0.21986300
H	-1.18536900	5.82550900	-0.39659300
C	0.68045000	4.88132600	0.21998300
H	1.18524800	5.82551300	0.39676000
C	1.34398100	3.70935000	0.40496900
H	2.37923900	3.71522000	0.72497300
C	0.70269700	2.44190400	0.16488700
C	1.40588900	1.23488400	0.21565200
C	0.72227000	0.00001000	-0.00003700
C	1.40591600	-1.23486100	-0.21568800
C	0.70274600	-2.44189100	-0.16489100
C	1.34405400	-3.70933800	-0.40491000
H	2.37931200	-3.71520500	-0.72491400
C	0.68054500	-4.88131700	-0.21986100
H	1.18536200	-5.82550300	-0.39658700
C	-0.68045700	-4.88131800	0.21998500
H	-1.18525500	-5.82550400	0.39676500
C	-1.34398800	-3.70934100	0.40496600
H	-2.37924700	-3.71520900	0.72496700
C	-0.70270300	-2.44189600	0.16487600
C	-1.40589400	-1.23487700	0.21561700
C	-0.72226800	-0.00000200	-0.00007300
C	2.82744700	-1.25181400	-0.67585200
C	3.87092300	-1.74160200	0.11454500
C	3.10989200	-0.80794700	-1.97114000
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H	2.29906800	-0.43401300	-2.59021100
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H	-2.29898700	-0.43405000	2.59016600

C	-5.17445900	-1.75869100	0.37074600
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C	-3.10989900	0.80793600	-1.97115500
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C	-4.41255900	0.83534600	-2.46212500
H	-2.29907600	0.43401400	-2.59023400
C	-5.44909000	1.30535000	-1.66032100
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C	3.87089400	1.74164700	-0.11456200
C	4.41250800	0.83540100	2.46210100
H	2.29902900	0.43403700	2.59017800
C	5.17445200	1.75871800	0.37071600
H	3.65647900	2.08704600	-1.12183400
C	5.44904300	1.30542500	1.66031500
H	4.61680800	0.48768200	3.46994500
H	5.97858200	2.12348800	-0.26070800
H	6.46666700	1.32087400	2.03743500

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Thermal correction to Enthalpy= 0.600315
Thermal correction to Gibbs Free Energy= 0.506613
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Sum of electronic and thermal Energies= -1616.126062
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Sum of electronic and thermal Free Energies= -1616.218819

Rubrene-Ox1

O	0.71476100	-1.70257500	1.58077500
O	-0.71475200	-1.70257300	1.58077900
C	1.28048100	-1.29445100	0.30436300
C	0.69924900	-2.25713500	-0.72804900
C	1.39607800	-3.17485400	-1.50868300
H	2.47684500	-3.22423300	-1.47653900
C	0.69477700	-4.05820000	-2.32747400

H	1.24052500	-4.76147000	-2.94784000
C	-0.69477800	-4.05820400	-2.32747000
H	-1.24052700	-4.76147600	-2.94783100
C	-1.39607800	-3.17486100	-1.50867500
H	-2.47684500	-3.22424500	-1.47652300
C	-0.69924900	-2.25713800	-0.72804500
C	-1.28047800	-1.29445300	0.30436800
C	-0.72323900	0.12358300	0.06599700
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C	-0.70899000	2.54492800	-0.16137100
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C	0.70898500	2.54493000	-0.16136700
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C	-5.53770500	-1.84908900	0.78854800
H	-5.09121200	-2.27506000	2.84829100
H	-5.65803000	-1.36682200	-1.31014600
H	-6.60797500	-1.98742700	0.90396100
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C	3.31332500	-1.82416200	1.73228200
C	3.63650300	-1.32885300	-0.59971200
C	4.68848100	-2.00757400	1.87658300
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C	5.00569800	-1.50638600	-0.45427400
H	3.23054700	-1.04693100	-1.56675800
C	5.53771000	-1.84909200	0.78851800
H	5.09122600	-2.27508700	2.84825900
H	5.65802500	-1.36680300	-1.31017100
H	6.60798000	-1.98743200	0.90392400
C	2.92028700	1.43899500	-0.07325900

C	3.66734800	1.41691800	1.10524400
C	3.56504400	1.71506800	-1.28292000
C	5.04369300	1.62184000	1.06851300
H	3.16693300	1.21884700	2.04833200
C	4.93942500	1.92858700	-1.31975900
H	2.97924800	1.75951200	-2.19732300
C	5.68312000	1.87704300	-0.14291100
H	5.61727600	1.58210700	1.98917000
H	5.42871100	2.13598000	-2.26624200
H	6.75605900	2.03866200	-0.16850800
C	-2.92028900	1.43898800	-0.07327000
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H	-5.42870500	2.13594900	-2.26627000
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H	-6.75606000	2.03865400	-0.16853900

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Sum of electronic and thermal Free Energies= -1766.499964

2

O	-0.63300800	-1.61886900	-1.68025600
O	0.78562800	-1.69843600	-1.62856000
C	-1.34617800	-1.22308900	-0.14838300
C	-0.70952400	-2.27668200	0.69284900
C	-1.41804300	-3.25767700	1.38836600
H	-2.49951700	-3.28305600	1.36580900
C	-0.71939200	-4.21214800	2.11942500
H	-1.26489600	-4.96041900	2.68304700
C	0.67123100	-4.22399100	2.10072200
H	1.21470500	-4.98456200	2.65063400
C	1.37934600	-3.28377300	1.35414900
H	2.45829900	-3.34467600	1.30389100

C	0.68993600	-2.28638700	0.67341900
C	1.29725400	-1.27728900	-0.28768900
C	0.72436500	0.12694000	-0.04520000
C	1.43587800	1.30603800	0.04485200
C	0.71877600	2.55451300	0.14196900
C	1.41058500	3.79583700	0.18637900
H	2.49232200	3.80303200	0.16562500
C	0.72936200	4.98615700	0.23971200
H	1.27979200	5.92038500	0.26750200
C	-0.67965800	4.99914800	0.24583900
H	-1.21397200	5.94232900	0.27935400
C	-1.37719400	3.81933800	0.19766000
H	-2.45919300	3.83862800	0.18725400
C	-0.70014800	2.56894100	0.14831000
C	-1.43242000	1.33513100	0.06871900
C	-0.72639300	0.14596700	-0.01291000
C	2.79585500	-1.45960700	-0.44981800
C	3.37405300	-1.79146200	-1.67449400
C	3.60960800	-1.32828300	0.67974400
C	4.75326000	-1.97618800	-1.76716400
H	2.76846100	-1.90161700	-2.56522500
C	4.98290800	-1.50128200	0.58084100
H	3.16606700	-1.06622200	1.63613700
C	5.55964800	-1.82882300	-0.64615100
H	5.19169300	-2.23305400	-2.72555100
H	5.60298900	-1.37358100	1.46165200
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C	-3.32618700	-1.83395300	-1.64283700
C	-3.67983100	-1.28204500	0.68040000
C	-4.69861100	-2.03011900	-1.79460200
H	-2.68612700	-2.01366500	-2.49794300
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C	-4.93374200	1.96394400	1.34339800
H	-2.97084200	1.81435900	2.21936600
C	-5.67945800	1.89699600	0.16857900
H	-5.61913700	1.59230900	-1.96265800
H	-5.42189700	2.17821700	2.28837800

H	-6.75274700	2.05321800	0.19598100
C	2.92581600	1.43996900	0.07769100
C	3.54669600	1.72362400	1.29818500
C	3.68887700	1.41414100	-1.08937100
C	4.91940600	1.94028000	1.35580900
H	2.94627900	1.77258200	2.20259500
C	5.06428200	1.62122100	-1.02960800
H	3.20633000	1.21487100	-2.04148900
C	5.68200500	1.88348200	0.19130800
H	5.39232900	2.15430400	2.30868700
H	5.65317500	1.57934400	-1.94010200
H	6.75367700	2.04781200	0.23363300
H	-0.78698700	-0.83537000	-2.25328600

Zero-point correction= 0.591072
Thermal correction to Energy= 0.623559
Thermal correction to Enthalpy= 0.624504
Thermal correction to Gibbs Free Energy= 0.528324
Sum of electronic and zero-point Energies= -1766.802692
Sum of electronic and thermal Energies= -1766.770204
Sum of electronic and thermal Enthalpies= -1766.769260
Sum of electronic and thermal Free Energies= -1766.865440

3

O	2.12912300	-0.79418100	-1.96397700
O	1.11154100	-0.61153200	-2.94114000
C	1.47813600	-1.04464000	-0.71858500
C	0.62894400	-2.29457500	-0.87647600
C	1.21710500	-3.42463100	-1.42619300
H	2.22590300	-3.35829100	-1.81960000
C	0.52753700	-4.63262200	-1.44472300
H	0.99543400	-5.50881900	-1.88113300
C	-0.74145400	-4.73888200	-0.86262800
H	-1.24984300	-5.69533800	-0.83450300
C	-1.33718400	-3.62346700	-0.31198500
H	-2.30851400	-3.70959300	0.15684800
C	-0.68730900	-2.36264000	-0.37050300
C	-1.35494000	-1.15548800	0.01783200
C	-0.74611600	0.12438100	-0.18502500
C	-1.52456700	1.30930300	-0.16540300
C	-0.87219400	2.56399500	-0.04572700
C	-1.60315700	3.78764600	-0.02715000
H	-2.67686100	3.76617500	-0.16397600
C	-0.96094000	4.98300700	0.16498200
H	-1.52742200	5.90696300	0.18873800
C	0.44185200	5.01318000	0.31699400

H	0.94477000	5.96274100	0.46646000
C	1.18264400	3.85525600	0.24848000
H	2.26194200	3.89646500	0.32975500
C	0.55248700	2.60473600	0.05458400
C	1.32850600	1.40393300	-0.13501400
C	0.68803100	0.20262800	-0.32100000
C	2.57790000	-1.38147100	0.29155400
C	2.22309700	-1.51902400	1.63438300
H	1.18819300	-1.37622800	1.93916600
C	3.19222900	-1.81717000	2.58467600
H	2.91179400	-1.91653400	3.62803200
C	4.52082900	-1.98397100	2.19609600
H	5.27982700	-2.20964900	2.93767000
C	4.86891700	-1.86259100	0.85419400
H	5.90201100	-1.98672100	0.54638500
C	3.90032300	-1.57034700	-0.10402000
H	4.18025400	-1.45287900	-1.14457800
C	-2.62602800	-1.24008000	0.76674900
C	-3.79289200	-1.80625900	0.23636500
H	-3.80475200	-2.15461800	-0.79169700
C	-4.94963400	-1.84483300	1.00292900
H	-5.86175300	-2.24600800	0.57471800
C	-4.94105800	-1.36737600	2.31409000
H	-5.84530000	-1.41212800	2.91150900
C	-3.77638100	-0.82863700	2.85319900
H	-3.76465700	-0.46046100	3.87323200
C	-2.62560800	-0.74238300	2.07749300
H	-1.71990600	-0.30550800	2.48715100
C	-2.97869800	1.26037700	-0.46923800
C	-3.95547400	1.70828300	0.42681800
C	-5.29985400	1.62653300	0.08564000
H	-6.05401600	1.94673300	0.79670900
C	-5.67963200	1.12942300	-1.16163900
H	-6.73049900	1.07294000	-1.42489400
C	-4.71023700	0.70834700	-2.06698100
H	-4.99976600	0.32911300	-3.04123300
C	-3.36339300	0.76449800	-1.72028600
H	-2.60258200	0.42804600	-2.41901700
C	2.81936900	1.53283300	-0.09726300
C	3.46296400	1.53700600	1.14482300
H	2.87468400	1.42286200	2.05076200
C	4.84668000	1.64776600	1.21833400
H	5.33760500	1.62746200	2.18572100
C	5.59887900	1.77571800	0.05167700

H	6.67932100	1.85826400	0.10751200
C	4.96037800	1.80585600	-1.18492900
H	5.53987700	1.91849400	-2.09526100
C	3.57426700	1.68952700	-1.25989800
H	3.08273100	1.70823200	-2.22732600
H	1.08906200	0.35610500	-3.02317400
H	-3.65878300	2.07901600	1.40359000

Zero-point correction= 0.589022
Thermal correction to Energy= 0.622600
Thermal correction to Enthalpy= 0.623544
Thermal correction to Gibbs Free Energy= 0.525158
Sum of electronic and zero-point Energies= -1766.842476
Sum of electronic and thermal Energies= -1766.808898
Sum of electronic and thermal Enthalpies= -1766.807954
Sum of electronic and thermal Free Energies= -1766.906340

4

O	-1.97478400	-1.81943500	1.15107300
O	-2.31979900	-1.12869200	2.35461500
C	-0.73737700	-1.30609800	0.67572500
C	0.34234500	-1.52396200	1.75400600
C	0.13899500	-2.47299800	2.75728400
H	-0.79966600	-3.01388400	2.78988400
C	1.11089300	-2.70337300	3.72546400
H	0.93335400	-3.44269000	4.49898800
C	2.29812200	-1.97829800	3.70915100
H	3.05724800	-2.14778700	4.46490900
C	2.50603100	-1.02507500	2.71794600
H	3.43541800	-0.46346400	2.71104200
C	1.53848900	-0.79486300	1.73994400
C	1.74932900	0.20497300	0.62194500
C	0.41993500	0.87157100	0.35641300
C	0.52994800	2.25461400	0.20187600
C	-0.63239900	3.04138500	-0.08711000
C	-0.62199200	4.44878800	-0.18289600
H	0.27932000	5.00097000	0.04794700
C	-1.76123400	5.13700700	-0.53342800
H	-1.73746900	6.21891700	-0.60456500
C	-2.95267800	4.44014900	-0.80509900
H	-3.83908600	4.98329500	-1.11307400
C	-3.00267400	3.07355500	-0.66325500
H	-3.93006400	2.55064600	-0.85965100
C	-1.85778200	2.33468200	-0.26458300

C	-1.94006600	0.90828600	-0.02602900
C	-0.80430300	0.18344800	0.32166300
C	-0.45435900	-2.18770800	-0.55270100
C	-0.31720600	-1.66381500	-1.83873500
H	-0.40533300	-0.59550300	-2.00940100
C	-0.02897400	-2.49957700	-2.91470300
H	0.09564600	-2.07264500	-3.90439600
C	0.10938800	-3.87014400	-2.71822700
H	0.33601300	-4.52131500	-3.55610500
C	-0.04279100	-4.40180900	-1.43936700
H	0.05757400	-5.46991900	-1.27720900
C	-0.31812600	-3.56530700	-0.36290900
H	-0.42370900	-3.98465200	0.63211400
C	2.33164300	-0.45127400	-0.65273600
C	2.45052900	0.29730300	-1.82783000
H	2.11006200	1.32884600	-1.86510400
C	2.98270100	-0.27474500	-2.97907500
H	3.06220100	0.31807000	-3.88432700
C	3.39994900	-1.60360300	-2.97134300
H	3.80540000	-2.05338200	-3.87148400
C	3.28970700	-2.35016700	-1.80275000
H	3.60739500	-3.38745600	-1.78541000
C	2.76277000	-1.77792600	-0.64682700
H	2.66857500	-2.37896700	0.25105400
C	1.90648800	2.60444700	0.35322900
C	2.63118400	1.44865900	0.96091200
C	4.09524900	1.41100900	0.75914600
H	4.63631800	0.51012300	1.03313200
C	4.74892500	2.51471000	0.32543400
H	5.82767400	2.52597200	0.23051100
C	4.00550000	3.67810700	-0.04618900
H	4.55729400	4.54130000	-0.40658800
C	2.62474800	3.74010500	-0.04239100
H	2.13659900	4.61101700	-0.45635100
C	-3.28754100	0.27532700	-0.13566900
C	-3.58399800	-0.64342200	-1.14443100
H	-2.82196300	-0.91991000	-1.86490100
C	-4.85295900	-1.21014000	-1.22209900
H	-5.07283700	-1.92235500	-2.01017700
C	-5.83281300	-0.87534800	-0.29078000
H	-6.81694000	-1.32763900	-0.34951700
C	-5.54773400	0.04737900	0.71344800
H	-6.30732900	0.32050200	1.43813900
C	-4.28518200	0.63168500	0.78307500

H	-4.06463900	1.36767700	1.55226500
H	-3.21040200	-0.81889500	2.11610000
H	2.51591900	1.62292200	2.05363900

Zero-point correction= 0.590159
Thermal correction to Energy= 0.622717
Thermal correction to Enthalpy= 0.623661
Thermal correction to Gibbs Free Energy= 0.528569
Sum of electronic and zero-point Energies= -1766.837277
Sum of electronic and thermal Energies= -1766.804720
Sum of electronic and thermal Enthalpies= -1766.803776
Sum of electronic and thermal Free Energies= -1766.898868

5

O	-1.90070300	-1.65732200	1.35275900
O	-2.14761700	-0.86862300	2.51641200
C	-0.68676700	-1.22178500	0.73958700
C	0.46192200	-1.36935500	1.76061200
C	0.29733100	-2.21932600	2.85616400
H	-0.64598600	-2.73738800	2.98515600
C	1.31038400	-2.37780100	3.79615700
H	1.16052100	-3.04048100	4.64221400
C	2.49960400	-1.67013500	3.65902600
H	3.28929700	-1.77294200	4.39608100
C	2.67235200	-0.81797300	2.57274300
H	3.59366000	-0.25597200	2.47582500
C	1.66963300	-0.66843500	1.61519300
C	1.83162300	0.19759000	0.37618500
C	0.49679400	0.88060800	0.14602800
C	0.63785600	2.23910900	-0.03669500
C	-0.50782400	3.01481600	-0.37648300
C	-0.44020500	4.38697000	-0.73106600
H	0.51864000	4.88605700	-0.74193500
C	-1.56072800	5.07968400	-1.11343900
H	-1.48345500	6.12523400	-1.39286500
C	-2.80873100	4.42442300	-1.16861600
H	-3.69091900	4.96660600	-1.49257600
C	-2.90785500	3.09795100	-0.83220000
H	-3.86873700	2.60300100	-0.90424300
C	-1.77287400	2.34856300	-0.41190100
C	-1.89487200	0.95830900	-0.04097000
C	-0.75100900	0.22814300	0.24489400
C	-0.53208000	-2.23506100	-0.40732800
C	-0.50840000	-1.85014400	-1.74769200
H	-0.58383700	-0.80014600	-2.01209600
C	-0.35254000	-2.80152800	-2.75294400

H	-0.31228900	-2.48167300	-3.78921000
C	-0.23650000	-4.15000000	-2.42973000
H	-0.11333600	-4.89071300	-3.21342300
C	-0.27534700	-4.54300800	-1.09369200
H	-0.18969900	-5.59256700	-0.83095400
C	-0.41756400	-3.59103700	-0.08985800
H	-0.43453500	-3.90186500	0.94939000
C	2.26538600	-0.63886100	-0.85054300
C	2.25812800	-0.03844100	-2.11435500
H	1.93962800	0.99653600	-2.21250100
C	2.64231600	-0.75261300	-3.24204700
H	2.62454200	-0.27200600	-4.21527300
C	3.04638700	-2.08245500	-3.12377100
H	3.33995800	-2.64498800	-4.00432300
C	3.06908100	-2.68107500	-1.86946800
H	3.37747400	-3.71660500	-1.76488000
C	2.68668600	-1.96238200	-0.73650100
H	2.69284300	-2.44932900	0.23331400
C	2.05702900	2.58947200	0.19608800
C	2.76253100	1.39837700	0.45855700
C	4.13963600	1.40462000	0.62715800
H	4.68648400	0.47285200	0.73874400
C	4.81704200	2.62389800	0.63305700
H	5.89128000	2.64503500	0.78335300
C	4.11647900	3.81355500	0.44449900
H	4.64699500	4.75990900	0.46255600
C	2.74161000	3.80684300	0.21403900
H	2.23493900	4.75185000	0.06917100
C	-3.27409500	0.38541700	0.03002700
C	-3.69699900	-0.62482800	-0.83808500
H	-3.00430400	-1.02159400	-1.57286400
C	-4.99103300	-1.13035300	-0.75695400
H	-5.30239100	-1.91671500	-1.43685500
C	-5.88257900	-0.63753600	0.19366800
H	-6.88861300	-1.03867500	0.25787800
C	-5.47738900	0.37618000	1.05808600
H	-6.16518300	0.77255900	1.79786600
C	-4.18494700	0.89089900	0.96960600
H	-3.87256700	1.69790200	1.62845500
H	-2.97069100	-0.42407100	2.24839700

Zero-point correction= 0.579025
Thermal correction to Energy= 0.611262
Thermal correction to Enthalpy= 0.612206
Thermal correction to Gibbs Free Energy= 0.517528
Sum of electronic and zero-point Energies= -1766.475851
Sum of electronic and thermal Energies= -1766.443614

Sum of electronic and thermal Enthalpies= -1766.442670
Sum of electronic and thermal Free Energies= -1766.537348

6

O	-0.95699600	-1.53624200	-0.52719200
C	-0.25451800	-1.28614600	0.69114500
C	-1.08818900	-0.49277400	1.71191600
C	-1.60115800	-1.12960200	2.84123600
H	-1.39938000	-2.18245700	2.99091400
C	-2.33802900	-0.42314600	3.78816300
H	-2.73102100	-0.93783400	4.65858900
C	-2.54922100	0.93941200	3.62163000
H	-3.10833700	1.50382500	4.36079000
C	-2.02099300	1.59006400	2.50907200
H	-2.15502200	2.66034100	2.40332500
C	-1.29884100	0.88834200	1.54605100
C	-0.69087700	1.55905100	0.32055400
C	0.68093500	0.94985900	0.13904600
C	1.66739500	1.90209700	0.00800600
C	3.00910600	1.48076700	-0.23428600
C	4.08125000	2.37956300	-0.46867200
H	3.89761500	3.44434700	-0.45261900
C	5.34431500	1.92470300	-0.75291100
H	6.14577100	2.63244000	-0.93735800
C	5.59744000	0.53884700	-0.82449000
H	6.59308100	0.18193100	-1.06613400
C	4.58398800	-0.35852600	-0.60068600
H	4.78505400	-1.42098700	-0.67289900
C	3.26674700	0.07409900	-0.28378900
C	2.22133000	-0.87953600	-0.01308600
C	0.93880300	-0.43042500	0.23685700
C	1.04406500	3.23161400	0.19885300
C	-0.33565000	3.04056400	0.41696400
C	-1.19437300	4.12126800	0.55472600
H	-2.26683700	3.96835300	0.63608900
C	-0.66670100	5.41253200	0.56583900
H	-1.32570400	6.26483700	0.69332700
C	0.70299600	5.60815400	0.40514600
H	1.10906100	6.61431800	0.41711000
C	1.56256800	4.52824700	0.20917100
H	2.61759100	4.72628100	0.07597100
C	2.55002800	-2.33426500	-0.06168700
C	3.37010300	-2.92903100	0.90396200
H	3.77682200	-2.31724300	1.70379400

C	3.64843100	-4.29071400	0.84850000
H	4.27851600	-4.74257700	1.60762400
C	3.11310000	-5.07571100	-0.17254800
H	3.32847600	-6.13833600	-0.21134200
C	2.30084900	-4.49204200	-1.14101000
H	1.88262700	-5.09629800	-1.93931100
C	2.02282400	-3.12605000	-1.08958300
H	1.38206800	-2.66485000	-1.83568100
C	-1.60073100	1.42452600	-0.91789100
C	-2.98733600	1.50002300	-0.77991300
C	-1.05174800	1.37583900	-2.20255800
C	-3.81106900	1.54543200	-1.90412200
H	-3.43113000	1.51968400	0.21107100
C	-1.87437700	1.41283900	-3.32429100
H	0.02582000	1.31476500	-2.32450500
C	-3.25913300	1.50532400	-3.18024000
H	-4.88748700	1.60270300	-1.77636400
H	-1.43174700	1.37312200	-4.31466900
H	-3.89899100	1.53891900	-4.05607800
C	-2.21640100	-2.09403100	-0.53889900
C	-3.01443700	-1.70947000	-1.61644800
C	-2.68577800	-3.02867300	0.38532500
C	-4.28909400	-2.24183900	-1.76206800
H	-2.61630700	-0.98434900	-2.31819600
C	-3.97120400	-3.54735200	0.23097200
H	-2.05343000	-3.35778000	1.19784400
C	-4.77853400	-3.16052200	-0.83425100
H	-4.90352000	-1.92838800	-2.60061800
H	-4.33545400	-4.27108700	0.95345200
H	-5.77571400	-3.57347100	-0.94367100
O	0.10431100	-2.47800000	1.31445000
H	0.55176900	-3.03615000	0.66324900

Zero-point correction= 0.579843
Thermal correction to Energy= 0.612006
Thermal correction to Enthalpy= 0.612951
Thermal correction to Gibbs Free Energy= 0.517037
Sum of electronic and zero-point Energies= -1766.567585
Sum of electronic and thermal Energies= -1766.535421
Sum of electronic and thermal Enthalpies= -1766.534477
Sum of electronic and thermal Free Energies= -1766.630391

Rubrene-Ox2

O	-1.45911100	-2.70631700	0.09967000
C	-0.66481700	-1.85153000	-0.24042100
C	0.54052100	-2.19977000	-1.07372800
C	0.48680900	-3.36249100	-1.84062700
H	-0.39190000	-3.99424800	-1.76086600
C	1.53282600	-3.68275100	-2.70014200
H	1.48628300	-4.58260700	-3.30397100
C	2.63179800	-2.83297700	-2.79092900
H	3.44386600	-3.06633300	-3.47195400
C	2.70308600	-1.68101900	-2.00634000
H	3.56989800	-1.03398600	-2.07862900
C	1.66666500	-1.35872200	-1.13693700
C	1.70763200	-0.20490100	-0.14563000
C	0.32229000	0.39509700	-0.10454400
C	0.33059700	1.76003000	-0.25338600
C	-0.90861700	2.46525800	-0.16180900
C	-1.00377500	3.87838500	-0.21224700
H	-0.10484100	4.46884400	-0.32248200
C	-2.21340400	4.51579700	-0.08664900
H	-2.25885400	5.59940300	-0.11912600
C	-3.39410200	3.76751200	0.10109700
H	-4.34536300	4.27655900	0.21396100
C	-3.33871000	2.39745200	0.15440400
H	-4.24647000	1.82746500	0.31459300
C	-2.10725000	1.69964500	0.01745100
C	-2.07450300	0.25972600	0.05265000
C	-0.84870600	-0.38219000	-0.00895900
C	1.72940500	2.17502000	-0.51737500
C	2.54212700	1.02143000	-0.48069300
C	3.91837300	1.10784700	-0.62303500
H	4.54129600	0.22462700	-0.51409800
C	4.49563500	2.35097000	-0.88625500
H	5.56966400	2.43206100	-1.01570900
C	3.69575500	3.48765300	-0.97624800
H	4.15015500	4.45033700	-1.18623800
C	2.31628900	3.41290400	-0.78302500
H	1.73275500	4.32150100	-0.85258700
C	-3.36005400	-0.49352400	0.11174900
C	-3.72878400	-1.18185500	1.27019800
H	-3.05000800	-1.19538200	2.11710200
C	-4.94662900	-1.85044200	1.33269900
H	-5.22404000	-2.38067900	2.23798000
C	-5.80535200	-1.84556800	0.23466500
H	-6.75362300	-2.37105800	0.28340400
C	-5.44261300	-1.16563700	-0.92518400
H	-6.10535900	-1.16005400	-1.78451900
C	-4.22825300	-0.48639500	-0.98379900
H	-3.94622900	0.05410000	-1.88306400

C	2.12289800	-0.71584000	1.25496200
C	2.75393600	-1.94598200	1.43749900
C	1.90269800	0.10191100	2.36960500
C	3.15365200	-2.35309000	2.71155300
H	2.93464500	-2.59831800	0.58965600
C	2.29765100	-0.30551500	3.63725000
H	1.41718300	1.06537700	2.23918700
C	2.92583700	-1.53871400	3.81393900
H	3.64156200	-3.31464700	2.83506900
H	2.11392000	0.33999500	4.49016400
H	3.23288400	-1.85875700	4.80422700

Zero-point correction= 0.470328
Thermal correction to Energy= 0.496878
Thermal correction to Enthalpy= 0.497823
Thermal correction to Gibbs Free Energy= 0.412528
Sum of electronic and zero-point Energies= -1459.316261
Sum of electronic and thermal Energies= -1459.289711
Sum of electronic and thermal Enthalpies= -1459.288767
Sum of electronic and thermal Free Energies= -1459.374061