Supporting Information

Light-controlled pKa Value of Chiral Brønsted Acid Catalysts in Enantioselective Aza-Friedel–Crafts Reaction

Chandu G. Krishnan,[a] Masaru Kondo,*[b] Osamu Yasuda,[a] Duona Fan,[a] Kento Nakamura,[a] Yoshitomo Wakabayashi,[a] Hiroaki Sasai,[a,c] and Shinobu Takizawa*[a]

[a] SANKEN, Osaka University, Mihogaoka, Ibaraki-shi, Osaka 567-0047, Japan.
[b] Graduate School of Science and Engineering, Ibaraki University, Hitachi-shi, Ibaraki 316-8511, Japan.
[c] Graduate School of Pharmaceutical Sciences, Osaka University, Suita-shi, Osaka 565-0871, Japan

E-mail: masaru.kondo.fg74@vc.ibaraki.ac.jp, taki@sanken.osaka-u.ac.jp

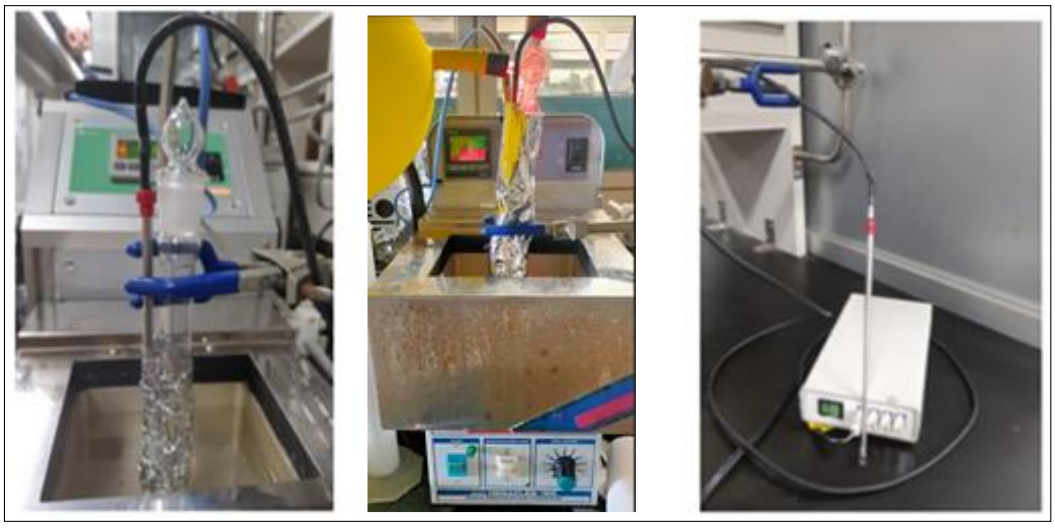
CONTENTS

1. General information

^{1}H- and ^{13}C-NMR spectra were recorded with a JEOL JMN ECS400 FT NMR (^{1}H-NMR 400 MHz, ^{13}C-NMR 100 MHz). ^{1}H-NMR spectra are reported as follows: chemical shift in ppm relative to the chemical shift of $CHCl_3$ at 7.26 ppm, integration, multiplicities (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constants (Hz). ^{13}C-NMR spectra reported in ppm relative to the central line of triplet for $CDCl_3$ at 77 ppm. ESI-MS spectra were obtained with JMS-T100LC (JEOL). HPLC analysis were performed on a JASCO HPLC system (JASCO PU 980 pump and UV-975 UV/Vis detector). UV spectra were recorded on JASCO v-770. FT-IR spectra were recorded on a JASCO FT-IR system (FT/IR4100). Column chromatography on SiO_2 was performed with Kanto Silica Gel 60 (40-100 μm). Commercially available organic and inorganic compounds were used without further purification. UV and visible light irradiations were performed with LED lamp (PER-AMP, Techno Sigma Co., Ltd.).

2. Reaction setup

The reaction setup is depicted in Figure S1. A self-constructed light source configuration made from Thermo Scientific UC reactors forms the reaction setup. Commercial LED lamps (PER-AMP, Techno Sigma Co., Ltd.) are used to photoirradiate the Schlenk tube at a distance of 0.5 cm from the aluminum foil-covered test tube. The setup is cooled by keeping it in water for the reaction. A Thermo-stainless-steel chamber ensures constant at 25 °C during the reaction. Temperature inside the chamber was monitored during the experiment to ensure no fluctuations and did not exceed 25 °C.

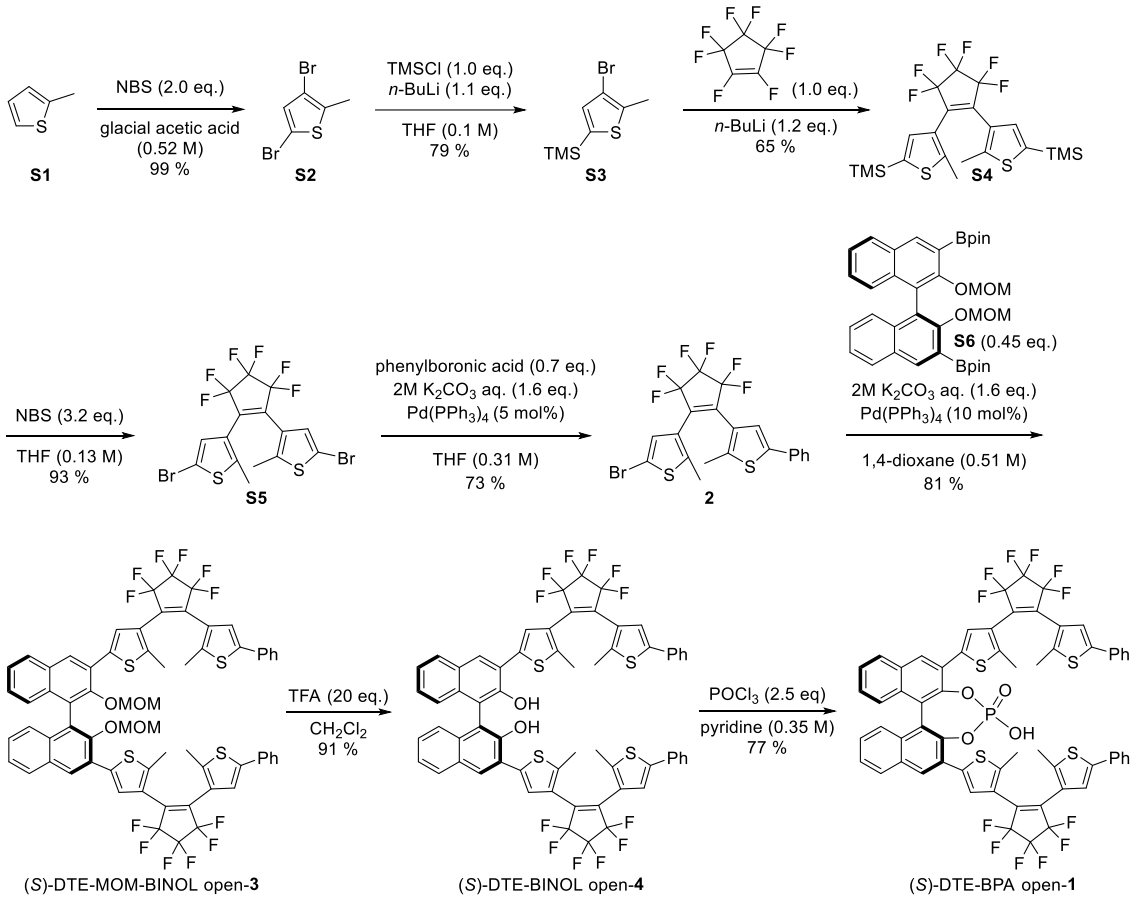


Reaction setup using UC reactor and LED

LED Apparatus (PER-AMP)

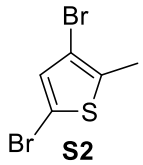
Figure S1. Reaction setup for photochemical reaction**.**

3. Synthesis procedure for (*S*)-DTE-BPA open-1



Scheme S1. Synthesis route for (*S*)-DTE-BPA open-**1**.

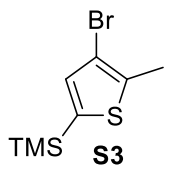
3-1. Synthesis of 3,5-dibromo-2-methylthiophene (S2)



To a solution of 1.0 g (10.2 mmol) of 2-methylthiophene (**S1**) in glacial acetic acid (20 mL), 3.6 g (20.4 mmol) of NBS was added in portion. Then, the reaction mixture was stirred at room temperature for 48 h. After that the crude mixture was extracted with dichloromethane (DCM) and the organic phase was washed with 1 M aqueous NaOH (200 mL). The organic phase was collected, dried over Na_2SO_4 and the solvent was removed *in vacuo* to afford the product **S2** in 99 % yield (2.59 g) as a pale-yellow liquid. If trace amount of impurities is there, SiO_2 column chromatography can be performed with *n*-hexane as an eluent. Spectroscopic data agree with those reported in the literature.[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 1 H), 2.34 (s, 3 H).

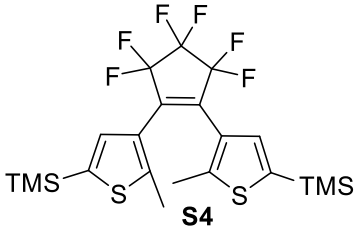
3-2. Synthesis of 3-bromo-2-methyl-5-trimethylsilylthiophene (S3)



A dry THF solution (13.0 mL) of **S2** (3.2 mmol, 0.77 g) in a flame-dried two-neck round bottom flask with a magnetic stirrer bar was degassed with nitrogen for 5 min and kept under nitrogen atmosphere at –78 °C. Then, *n*-BuLi (1.60 mol/L in *n*-hexane, 3.33 mmol) was added dropwise *via* nitrogen fleshed needle and the solution turned yellow. The mixture was then stirred for 1.5 h at –78 °C, followed by slow addition of trimethylsilyl

chloride (7.56 mmol, 0.97 mL) *via* syringe. After further 2.5 h of stirring at –78 °C, solution was allowed to cool to 25 °C. The reaction mixture was quenched by adding aqueous saturated solution of NH_4Cl and then poured into water, and the organic layer was separated and extracted with chloroform (3 × 10.0 mL). The organic layer was dried over Na_2SO_4 and concentrated under vacuum. The crude mixture was separated using SiO_2 column chromatography with *n*-hexane as an eluent to afford **S3** as a colorless clear liquid (0.590 g, 79%). Spectroscopic data agree with those reported in the literature.[2]
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 (s, 1 H), 2.42 (s, 3 H), 0.28 (s, 9 H).

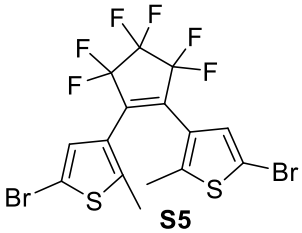
3-3. Synthesis of 1,2-bis(2'-methyl-5'-trimethylsilylthien-3'-yl) hexafluorocyclopent-1-ene (S4)



S4

A dry THF solution (22.0 mL) of **S3** (2.45 mmol, 0.61 g) in a flame-dried two-neck round bottom flask with a magnetic stirrer bar was degassed with nitrogen for 5 min and kept under nitrogen atmosphere at –78 °C. The mixture was stirred and added *n*-BuLi (1.6 mol/L in *n*-hexane, 2.69 mmol) dropwise *via* syringe under nitrogen atmosphere. The mixture was then stirred at –78 °C for 2 h. After that, octafluorocyclopentene (1.10 mmol, 0.15 mL) in THF (1.0 mL) was added at –78 °C slowly *via* syringe. After addition of octafluorocyclopentene, the reaction mixture turned to a red-brownish color. The solution was then stirred at –78 °C for 4 h and the solution was stirred for another 24 h at 25 °C. Then, the reaction was quenched with aqueous saturated solution of NH_4Cl and then poured into water, and the organic layer was separated and extracted with chloroform (3 × 10.0 mL). The organic layer was dried using Na_2SO_4 and concentrated under vacuum. And the crude mixture residue was purified by SiO_2 column chromatography with *n*-hexane as an eluent to afford **S4** as a white solid (0.42 g, 65%). Spectroscopic data agree with those reported in the literature.[2]
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.05 (s, 2 H), 1.91 (s, 6 H), 0.27 (s, 18 H).

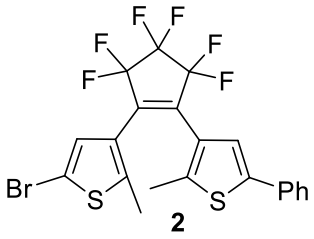
3-4. Synthesis of 3,3'-(perfluorocyclopent-1-ene-1,2-diyl) bis(5-bromo-2-methylthiophene) (S5)



S5

A solution of **S4** (1.05 g, 2.05 mmol) and NBS (0.802 g, 4.50 mmol) in THF (16 mL) were placed in a flame dried round-bottom flask with a magnetic stirrer bar. The mixture was covered with aluminium foil and stirred for 3 h in an ice-water bath under nitrogen atmosphere. Then, the reaction was stirred overnight at 25 °C and quenched with acetone (1.2 mL). After evaporation of the solvent, the mixture was washed with brine and extracted with chloroform. The organic layer was then dried over anhydrous Na_2SO_4 and the solvent was removed *in vacuo* and the crude product was purified by SiO_2 column chromatography with petroleum ether or *n*-hexane as an eluent to afford **S5** as a pale-pink powder (0.99 g, 92 %). Spectroscopic data agree with those reported in the literature.[1]
^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.01 (s, 2H), 1.89 (s, 6H).

3-5. Synthesis of 5-bromo-3-(3,3,4,4,5,5-hexafluoro-2-(2-methyl-5-phenylthiophen-3-yl) cyclopent-1-enyl)-2-methylthiophene (2)

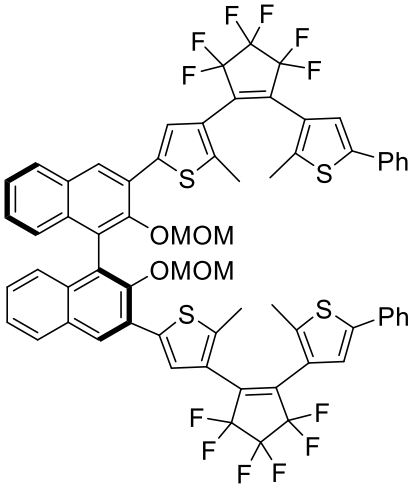


2

Compound **S5** (2.0 g, 3.8 mmol) and phenylboronic acid (1.02 g, 1.1 eq. 4.18 mmol) were placed into a 100 mL two-necked round-bottom flask under nitrogen atmosphere. A solution of toluene (40 mL) and K_2CO_3 aqueous solution (10 mL, 2.0 M) were added to the flask and the solution was degassed with nitrogen for 10 min after that $Pd(PPh_3)_4$ (0.22 g, 0.19 mmol) was added. The reaction mixture was covered with aluminium foil and stirred at 85 °C for 48 h under a nitrogen atmosphere. After bringing to 25 °C, the mixture was evaporated under reduced pressure and the remaining residue was extracted with DCM and washed with brine. The organic layer was dried over Na_2SO_4, and the solvent was evaporated under *vacuo*. The crude product was purified by SiO_2 column chromatography with *n*-hexane as an eluent to afford **2** as a pale-blue powder (1.44 g, 73 %). Spectroscopic data agree with those reported in the literature.[1]

^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.52-7.54 (d, 2H), 7.37-7.40 (t, 2H), 7.31 (t, J = 7.1, 1.1 Hz, 1H), 7.24 (s, 1H), 7.06 (s, 1H), 1.96 (s, 3H), 1.88 (s, J = 0.9 Hz, 3H).

3-6. Synthesis of (*S*)-DTE-MOM-BINOL open-3



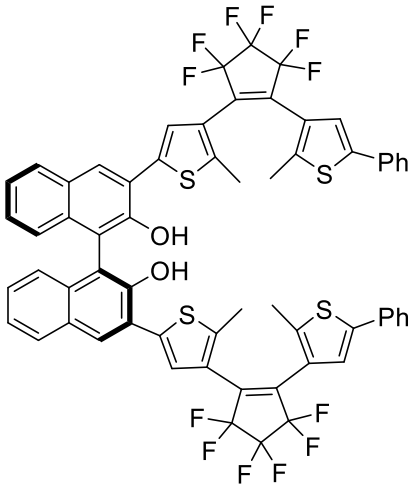
(*S*)-DTE-MOM-BINOL open-**3**

To a solution of compound **2** (270 mg, 0.52 mmol, 1.0 eq.) in 1,4-dioxane (0.37 M, 1.4 mL) kept under nitrogen atmosphere in a round bottom flask with a magnetic stirrer bar was added with (*S*)-BINOL boronic acid ester **S6** (147 mg, 0.24 mmol, 0.46 eq.), K_2CO_3 aq. (2 M, 0.2 mL). The solution was then degassed under nitrogen for 10 min. After that, $Pd(PPh_3)_4$ (27.0 mg, 0.02 mmol, 10 mol%) was added to the solution and stirred for 28 h at 90 °C. After confirming the starting material consumption by TLC analysis, sat. NH_4Cl aq (2.0 mL) was poured into the flask and an extraction was performed by EtOAc. The collected organic layer was dried over Na_2SO_4. After filtration, concentrated residue was purified using SiO_2 column chromatography with *n*-hexane as an eluent to afford the desired product (*S*)-DTE-MOM-BINOL open-**3** (243 mg, 81% yield) as a blue solid.

m.p. 106 °C; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 2H), 7.88 (d, J = 8.2 Hz, 2H), 7.61 (s, 2H), 7.54 (d, J = 7.8 Hz, 4H), 7.45-7.22 (m, 14H), 4.54 (dd, J = 53.8, 5.3 Hz, 4H), 2.45 (s, 6H), 2.04 (d, J = 5.5 Hz, 12H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 151.1, 150.3, 149.7, 148.4, 143.0, 142.6, 142.5, 141.5, 141.3, 138.1, 137.7, 137.6, 137.1, 136.5 (t, $^2J_{CF}$ = 19.12Hz, CF_2C=CCF_2), 136.4 (t, $^2J_{CF}$ = 19.12Hz, CF_2C=CCF_2), 133.8, 133.4, 132.7, 130.9, 129.5, 129.4, 129.2, 128.7, 128.1, 127.4, 127.0, 126.8, 126.6, 126.4, 126.1, 125.9, 125.7, 125.5, 125.1, 124.1, 122.7, 116.4 (t,$^1J_{CF}$ = 211.8 Hz, t, $^2J_{CF}$ = 19.25 Hz, $CF_2CF_2CF_2$,and $CF_2CF_2CF_2$), 117.5, 111.3 (t, $^1J_{CF}$ = 225.0 Hz, quint, $^2J_{CF}$ = 21.5 Hz, $CF_2CF_2CF_2$), 112.0, 111.6, 111.5, 111.3, 111.1, 111.0, 109.8, 109.7, 109.5, 109.4, 109.2, 98.6 (OCH_2OMe), 60.3, 56.1(OMe), 20.7, 14.7, 14.6, 14.5, 14.3; HRMS (ESI) *m/z* $[M+Na]^+$ Calcd for $C_{66}H_{46}F_{12}O_4S_4$: m/z ($[M+Na]^+$) 1281.1980, found 1281.1996; IR

(KBr) 3064, 2961, 2924, 1737, 1601, 1551, 1499, 1440, 1336, 1272, 1190, 1055, 987, 901, 753 cm^{-1}.

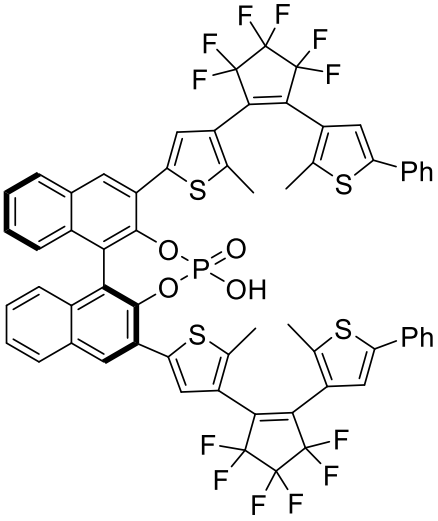
3-7. Synthesis of (*S*)-DTE-BINOL open-4


(*S*)-DTE-BINOL open-**4**

To a solution of compound (*S*)-DTE-MOM-BINOL open-**3** (243 mg, 0.19 mmol, 1.0 eq.) in a round bottom flask kept under nitrogen atmosphere in dry DCM (0.01M, 17 mL), trifluoracetic acid (TFA) (433 mg, 3.8 mmol, 20 eq.) was slowly added at 0 °C and brought to 25 °C. The solution was continued stirring for 18 h at 25 °C. After evaporation of solvent, water was added and the organic phase was collected after separation, dried over Na_2SO_4 and the residue was purified by SiO_2 column chromatography with hexane/DCM = 7/3 as an eluent to afford the product (*S*)-DTE-BINOL open-**4** (203 mg, 91% yield) as a blue solid.

m.p. 144 ℃; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 2H), 7.90 (d, J = 7.8 Hz, 2H), 7.71 (s, 2H), 7.53 (d, J = 7.3 Hz, 4H), 7.42-7.28 (m, 12H), 7.12 (d, J = 8.2 Hz, 2H), 5.55 (s, 2H), 2.00 (d, J = 2.3 Hz, 12H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 149.6, 142.6, 142.4, 141.5, 137.0, 136.5 (t, $^2J_{CF}$ = 20.25 Hz, CF_2C=CCF_2), 136.3 (t, $^2J_{CF}$ = 19.12Hz, CF_2C=CCF_2), 133.5, 132.6, 129.5, 129.3, 129.2, 128.7, 128.1, 126.7, 126.0, 125.7, 125.5, 125.1, 124.1, 122.6, 122.6, 116.4 (t,$^1J_{CF}$ = 211.8 Hz, t, $^2J_{CF}$ = 20.25 Hz, $CF_2CF_2CF_2$,and $CF_2CF_2CF_2$), 111.9, 111.3 (t, $^1J_{CF}$ = 225.0 Hz, quint, $^2J_{CF}$ = 20.4 Hz, $CF_2CF_2CF_2$), 31.8, 29.9, 22.8, 14.8, 14.5, 14.2; FTMS (APCI) calcd for $C_{62}H_{38}F_{12}O_2S_4$: m/z ([M+H]$^+$) 1171.1636, found 1171.1720; IR (KBr) 3500, 3060, 2920, 2852, 1722, 1598, 1502, 1433, 1358, 1337, 1272, 1192, 1138, 1118, 1054, 986, 891, 750 cm^{-1};

3-8. Synthesis of (*S*)-DTE-BPA open-1


(*S*)-DTE-BPA open-**1**

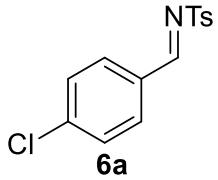
To a solution of compound (*S*)-DTE-BINOL open-**4** (203 mg, 0.17 mmol, 1.0 eq.) in pyridine (0.5 mL) was slowly added $POCl_3$ (65.9 mg, 0.43 mmol, 2.5 eq.) at 25 °C. The solution was stirred for 12 h at 95 °C. After addition of water (1.0 mL), the mixture was still stirred for 6 h at 95 °C. Then, HCl aq (1M, 2 mL) was poured into the flask and extracted with EtOAc. The collected organic layer was dried over Na_2SO_4. After filtration, concentrated residue was purified by SiO_2 column chromatography with *n*-hexane/EtOAc = 3/1 as an eluent to give the product (*S*)-DTE-BPA open-**1** (161 mg, 77% yield) as a blue solid.

m.p. 158 ℃; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.26 (s, 2H), 7.95 (d, J = 8.2 Hz, 2H), 7.55 (s, 2H), 7.51-7.46 (m, 2H), 7.36 (d, J = 7.6 Hz, 2H), 7.19 (s, 12H), 7.14 (s, 2H), 5.76 (br, 1H), 1.72 (d, J = 11.4 Hz, 12H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ 145.6,

145.5, 144.3, 142.8, 142.2, 141.9, 141.6, 137.2, 136.1 (t, $^{2}J_{CF}$ = 18.0Hz, CF_2C=CCF_2 and CF_2C=CCF_2), 133.4, 132.2, 131.0, 129.1, 128.4, 128.0, 126.9, 126.7, 126.5, 126.3, 126.1, 125.8, 125.7, 125.6, 125.0, 123.6, 122.2, 116.34 (t,$^{1}J_{CF}$ = 211.8 Hz, t, $^{2}J_{CF}$ = 19.12 Hz, $CF_2CF_2CF_2$), 116.26 (t,$^{1}J_{CF}$ = 211.9 Hz, t, $^{2}J_{CF}$ = 19.12 Hz, $CF_2CF_2CF_2$), 111.2 (t, $^{1}J_{CF}$ = 223.8 Hz, quint, $^{2}J_{CF}$ = 20.3 Hz, $CF_2CF_2CF_2$), 60.5, 29.8, 21.1, 14.7, 14.3; ^{31}P-NMR (189 MHz, $CDCl_3$) δ = 4.61 ppm; FTMS (APCI) calcd for $C_{62}H_{37}F_{12}O_4PS_4$: m/z ($[M+H]^+$) 1233.1193, found 1233.1198; IR (KBr) 3064, 2957, 2922, 2853, 2364, 2345, 1335, 1269, 1189, 1115, 1048, 1021, 985, 952, 894, 751 cm^{-1}.

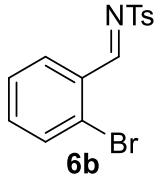
4. Synthesis of aldimines 6[3]

According to the literature,[3] aldimines can be synthesized from the corresponding aldehydes and toluene sulfonamide in the presence of pyrrolidine as a catalyst.



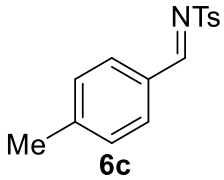
6a

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 7.87 (t, *J* = 8.0 Hz, 4H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.35 (d, *J* = 7.8 Hz, 2H), 2.44 (s, 3H). All data in accordance with literature.[4]



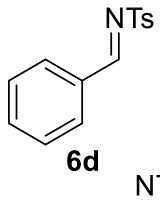
6b

^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.43 (s, 1H), 8.15 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.90 (d, *J* = 7.8 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.36-7.44 (m, 4H), 2.45 (s, 3H). All data in accordance with literature.[4]



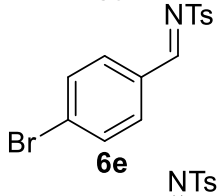
6c

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 7.88 (d, 2H, J= 8.3,), 7.82 (d, 2H, *J*= 8.2,), 7.34 (d, 2H, *J*= 8.1,), 7.29 (d, 2H, *J*= 8.0), 2.43-2.44 (6H) All data in accordance with literature. [4]



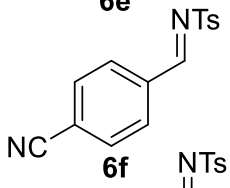
6d

^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 7.91 (m, 4H), 7.62 (t, 1H, *J* =7.5), 7.49 (t, 2H, *J*= 7.7), 7.35 (d, 2H, J =8.1), 2.44 (s, 3H). All data in accordance with literature.[4]



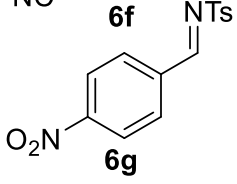
6e

^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.88 (d, 2H, *J*= 8.3), 7.78 (d, 2H, *J* = 8.5), 7.63 (d, 2H, *J* = 8.5,), 7.35 (d, 2H, *J* = 8.5,), 2.44 (s, 3H). All data in accordance with literature. [4, 5]



6f

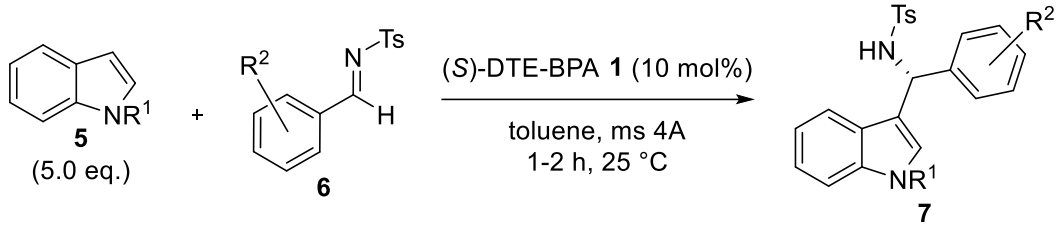
^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.02 (dd, *J* = 6.4, 1.8 Hz, 2H), 7.87-7.89 (m, 2H), 7.77 (dd, *J* = 6.9, 1.8 Hz, 2H), 7.36 (d, *J* = 7.8 Hz, 2H), 2.44 (s, 3H). All data in accordance with literature.[5]

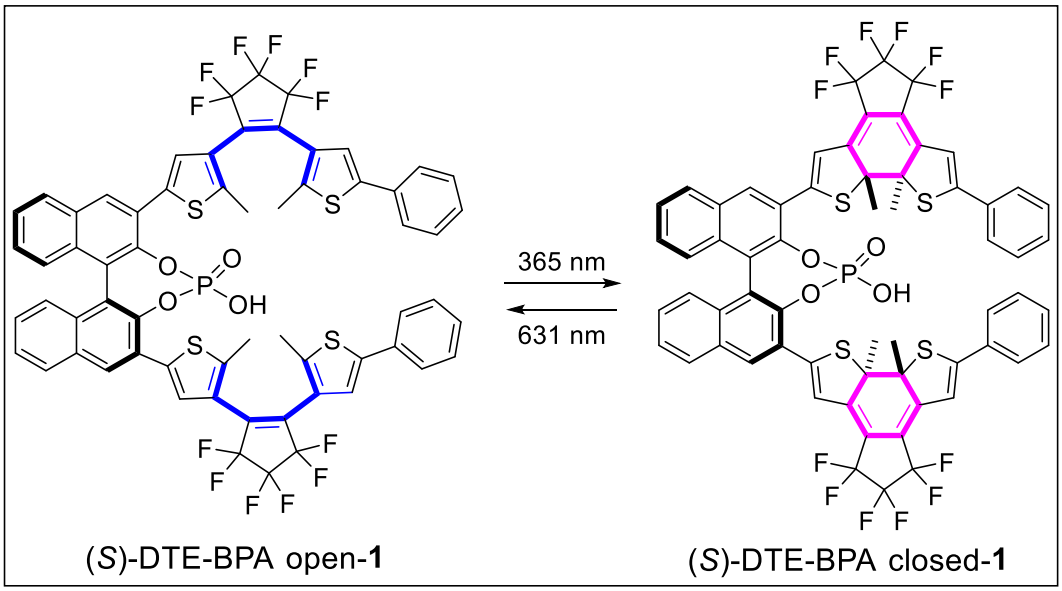


6g

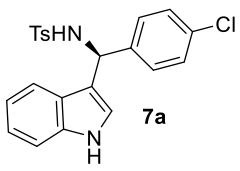
^{1}H-NMR (400 MHz, $CDCl_3$) δ 9.11 (s, 1H), 8.34 (d, *J* = 9.2 Hz, 2H), 8.10-8.12 (m, 2H), 7.90-7.92 (m, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 2.46 (s, 3H). All data in accordance with literature.[5]

5. General procedure for the enantioselective aza-Friedel Crafts reaction

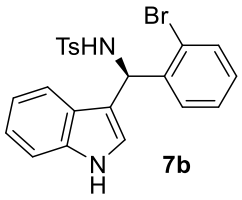




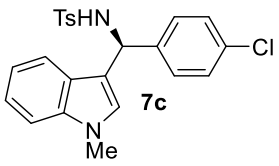
A well flame dried Schlenk flask was equipped with a magnetic stirrer bar, following the addition of activated MS4A. Under nitrogen atmosphere, 10 mol% of catalyst (*S*)-DTE-BPA **1** (12.4 mg) in toluene (2.5 mL) was added to the flask covered with aluminum foil. The flask was then exposed to 365 nm UV light for 12 h. After a removing of UV lamp, indoles **5** (0.5 mmol, 5.0 eq.) was added and the mixture was stirred for 1 h at 25 ^{o}C under nitrogen atmosphere. Then, imine **6** (0.1 mmol, 1.0 eq.) was added to the flask, and stirred until completely consuming of the starting material **6** by TLC monitoring with *n*-hexane/EtOAc = 3/1 as an eluent. Then saturated $NaHCO_3$ (2 mL), EtOAc (2 mL) and water (1 mL) were added to the mixture. The organic layer was separated and filtered using FILTSTAR syringe filter 13 mm from Hawach Scientific. The obtained organic solution was then dried by Na_2SO_4, then, filtered, and concentrated under reduced pressure to afford desired product **7**. Absolute configuration of **7** was determined by comparing the retention time of HPLC of products with those of literature data.



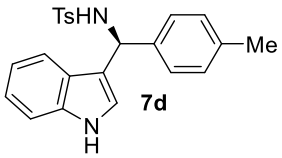
White solid; 47% yield, 68:32 er (under dark); 86% yield, 84:16 er (under 365 nm); ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.02 (s, Br, 1H), 7.56 (d, J = 8.2 Hz, 2H), 7.31 (d, J = 8.9 Hz, 1H), 7.23-7.09 (m, J = 18.5, 8.0 Hz, 8H), 7.01 (t, J = 7.6 Hz, 1H), 6.64 (d, J = 2.3 Hz, 1H), 5.82 (d, J = 6.4 Hz, 1H), 5.05 (d, J = 6.4 Hz, 1H), 2.41 (d, J = 11.4 Hz, 3H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3 as an eluent, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 15.2 min, t_{minor} = 31.9 min). All data in accordance with literature. [7,8]



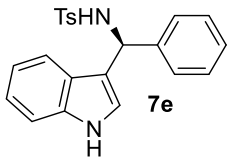
White solid; 62% yield, 56:44 er (under dark); 74% yield, 78:22 er (under 365 nm); [1] H-NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.70 (d, *J* = 8.1 Hz, 2H), 7.55 (dd, *J* = 7.7 Hz 1H), 7.45 (d, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.25-7.20 (m, 3H), 7.20-7.12 (m, 2H), 7.09 (m, *J* = 7.7 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.55 (d, *J* = 2.4 Hz, 1H), 6.19 (d, *J* = 5.6 Hz, 1H), 5.07 (d, *J* = 5.8 Hz, 1H), 2.41 (s, 3H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3, flow rate = 1.0 mL/min, λ = 254 nm, t_{minor} = 6.2 min, t_{major} = 14.9 min. All data in accordance with literature. [7,8]



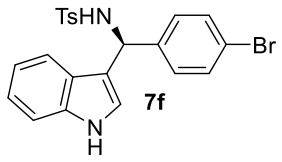
White solid; 34% yield, 68:32 er (under dark); 90% yield, 84:16 er (under 365 nm); [1]H-NMR (400 MHz, CDCl3) δ 7.48 (d, *J* = 8.2 Hz, 2H), 7.06-7.18 (m, 9H), 6.91-6.95 (m, 1H), 6.38 (s, 1H), 5.72 (d, *J* = 6.4 Hz, 1H), 4.97 (d, *J* = 6.9 Hz, 1H), 3.56 (s, 3H), 2.33 (s, 3H). Enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 15.4 min, t_{minor} = 32.2 min. All data in accordance with literature.[8]



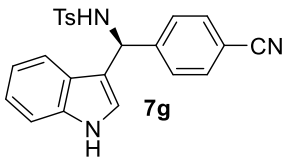
White solid; 49% yield, 61:39 er (under dark); 88% yield, 85:15 er (under 365 nm); [1]H-NMR (400 MHz,$CDCl_3$) δ 7.97 (br, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.24 – 6.94 (m, 9H), 6.71 (d, *J* = 2.5 Hz, 1H), 5.80 (d, *J* = 6.8 Hz, 1H), 5.03 (d, J = 6.8 Hz, 1H), 2.37 (s, 3H), 2.29 (s, 3H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3, flow rate = 0.5 mL/min, λ = 254 nm, t_{major} = 13.1 min, t_{minor} = 23.8 min. All data in accordance with literature.[9]



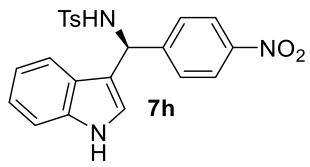
White solid; 52% yield, 58:42 er (under dark); 88% yield, 70:30 er (under 365 nm); [1]H-NMR (400 MHz, $CDCl_3$) δ 2.37 (s, 3H), 5.01 (d, *J* = 6.8 Hz, 1H), 5.85 (d, *J* = 7.2 Hz, 1H), 6.68 (d, *J* = 0.8 Hz, 1H), 7.01-7.11 (t, *J* = 7.2 Hz, 1H), 7.24 (d, J = 7.6 Hz, 2H), 7.26-7.29 (m, 6H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.17 (br, 1H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3, flow rate = 0.5 mL/min, λ = 254 nm, t_{major} = 17.1 min, t_{minor} = 32.8 min. All data in accordance with literature.[7]



White solid; 44% yield, 90:10 er (under dark); 87% yield, 97:3 er (under 365 nm); [1]H-NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.30-7.33 (m, 4H), 7.09-7.19 (m, 6H), 6.95-7.03 (m, 1H), 6.60-6.65 (d, 1H), 5.76-5.80 (d, 1H), 4.96 (d, *J* = 6.4 Hz, 1H), 2.40 (s, 3H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 14.4 min, t_{minor} = 27.4 min. All data in accordance with literature.[7]



White solid; 39% yield, 59:11 er (under dark); 96% yield, 71:29 er (365 nm); ^{1}H^NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.59-7.62 (m, 2H), 7.54 (dd, *J* = 6.4, 1.8 Hz, 2H), 7.46 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 8.2 Hz, 1H), 7.19-7.22 (m, 3H), 7.10 (d, *J* = 7.8 Hz, 1H), 7.00-7.04 (m, 1H), 6.58 (d, *J* = 2.3 Hz, 1H), 5.87 (d, *J* = 6.0 Hz, 1H), 5.06 (d, *J* = 6.0 Hz, 1H), 2.43 (s, 3H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 7/3, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 17.0 min, t_{minor} = 30.0 min. All data in accordance with literature.[10]



White solid; 42% yield, 59:11 er (under dark); 92% yield, 71:29 er (under 365 nm); ^{1}H NMR (400 MHz, $CDCl_3$): 2.41 (s, 3H), 5.10 (d, *J* = 6.0 Hz, 1H), 5.91 (d, *J* = 6.0 Hz, 1H), 6.59 (d, *J* = 2.4 Hz, 1H), 6.99–7.04 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 1H), 7.21 (m, 3H), 7.34 (d, *J* = 11.7 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 8.07–8.09 (m, 2H), 8.10 (s, 1H); enantioselectivity was determined by HPLC (Daicel Chiralcel OD-H, *n*-hexane/*i*-propanol = 9/1, flow rate = 1.0 mL/min, λ = 254 nm, t_{major} = 9.7 min, t_{minor} = 16.9 min. All data in accordance with literature.[10]

6. Photoisomerization experiments

6-1. Photoisomerization studies of (*S*)-DTE-BPA 1

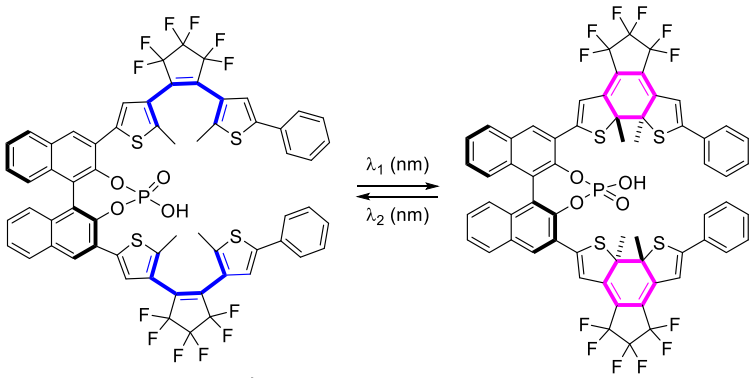


Table S1. Photoisomerization of (*S*)-DTE-BPA **1** under various wavelengths (35 min, 0 °C, $CDCl_3$).

Entry	Wavelength (nm)		% of (*S*)-DTE-BPA closed-**1**[a]
	λ_1	λ_2	
1	Normal		0
2	310		8
3	340		31
4	**365**		**50 (56[b])**
5	385		25 (27[b])
6	395		15[b]
7		**631**	**0**
8		**521**	**0**
9		448	12[b]

[a]Determined by ^{1}H-NMR. [b]Irradiation for 60 min.

Table S2. Solvent effect on the photostationary state (PSS) ratio of (*S*)-DTE-BPA **1** (365 nm, 0 °C).

Entry	Solvent	Photoirradiation time (h)	(*S*)-DTE-BPA closed-**1** (%)[a]
1	$CDCl_3$	0.5	45
2	$CDCl_3$	1	55
3	$CDCl_3$	1.5	65
4	$CDCl_3$	12	77
5	toluene-d_8	1	75
10	toluene-d_8	0.25	34
11	toluene-d_8	0.5	53
12	toluene-d_8	0.75	65
8	**toluene-d_8**	**2**	**77**
9	toluene-d_8	12	77
6	acetone-d_6	1	62
7	CD_3CN	1	44

[a]Determined by ^{1}H-NMR.

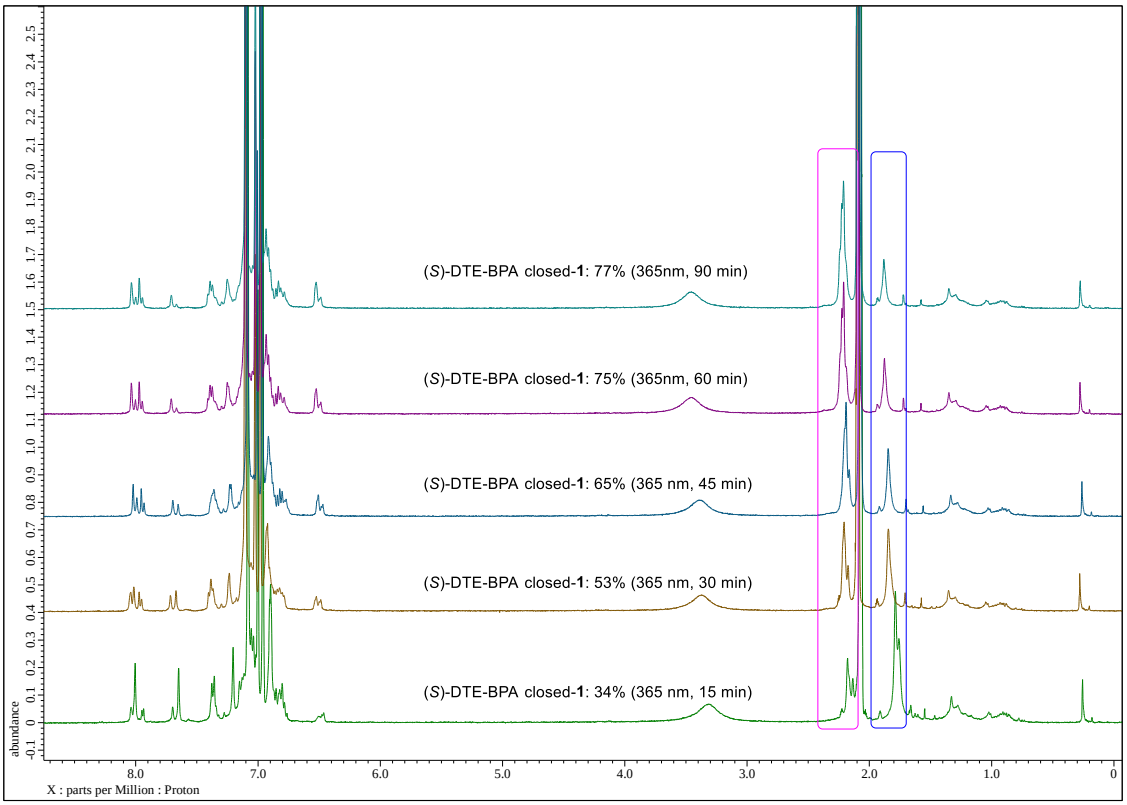


Figure S2. Photoisomerization experiments of DTE-BPA **1** for different photoirradiation time under 365 nm LED light (toluene-d_8).

Note: Photoirradiation about 2 h is enough to achieve the PSS ratio of open-closed-**1**/closed-**1** = 23/77 in toluene-d_8. Further irradiation did not improve the isomerization ratio.

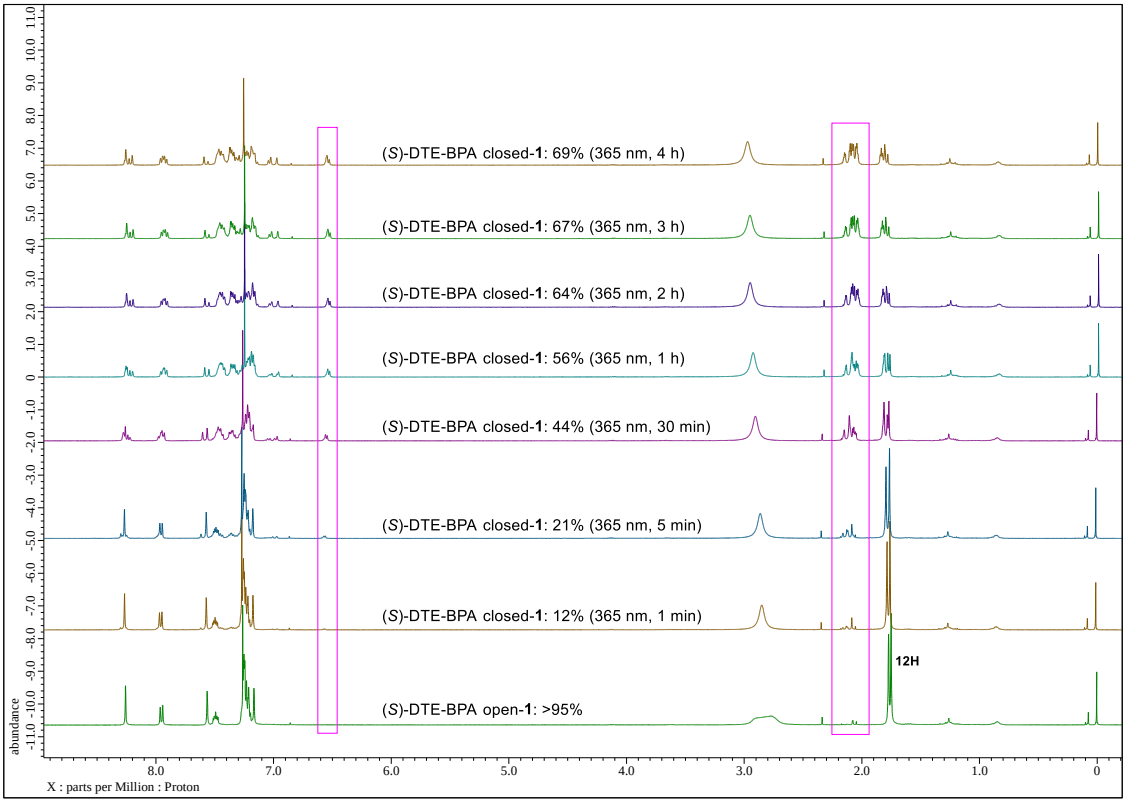


Figure S3. Photoisomerization experiments of DTE-BPA **1** for different photoirradiation time under 365 nm LED light ($CDCl_3$).

Note: Photoirradiation about 12 h in $CDCl_3$ achieved the closed isomer up to 77%. Further irradiation did not improve the isomerization ratio.

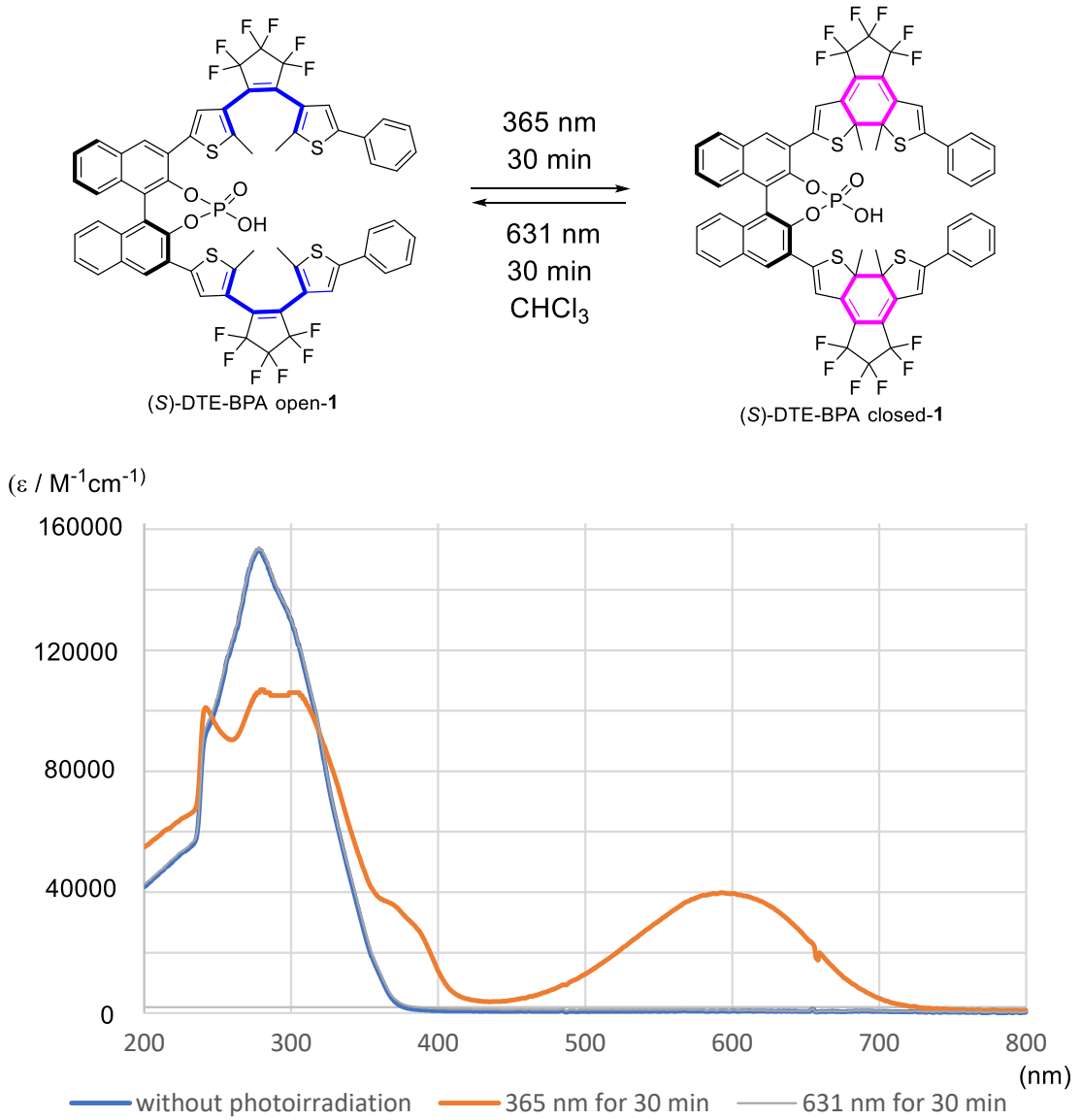
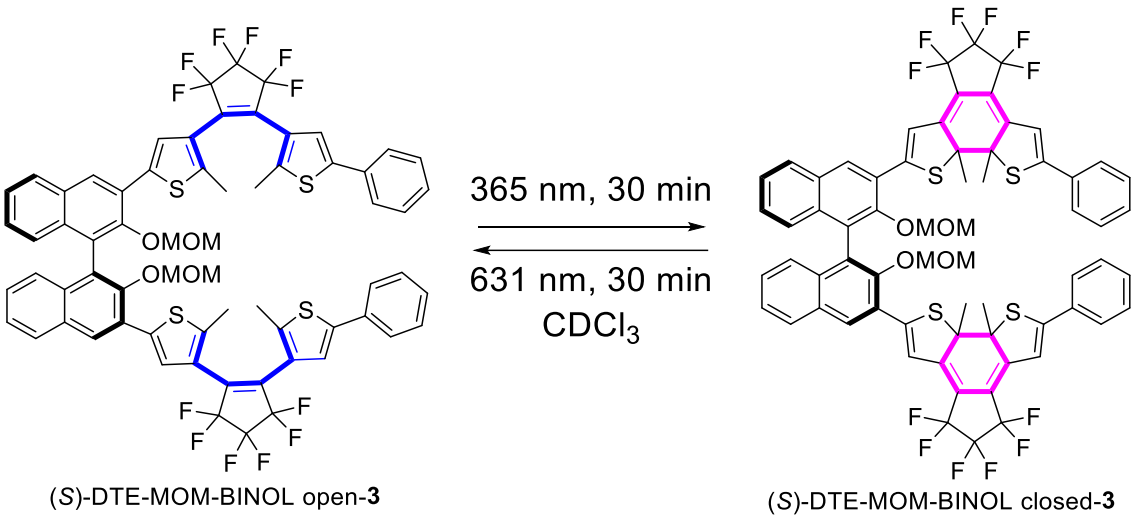


Figure S4. Photoisomerization studies of (*S*)-DTE-BPA **1** by UV-Vis spectroscopy ($CHCl_3$, 20 μM)

6-2. Photoisomerization studies of (*S*)-DTE-MOM-BINOL 3 by NMR



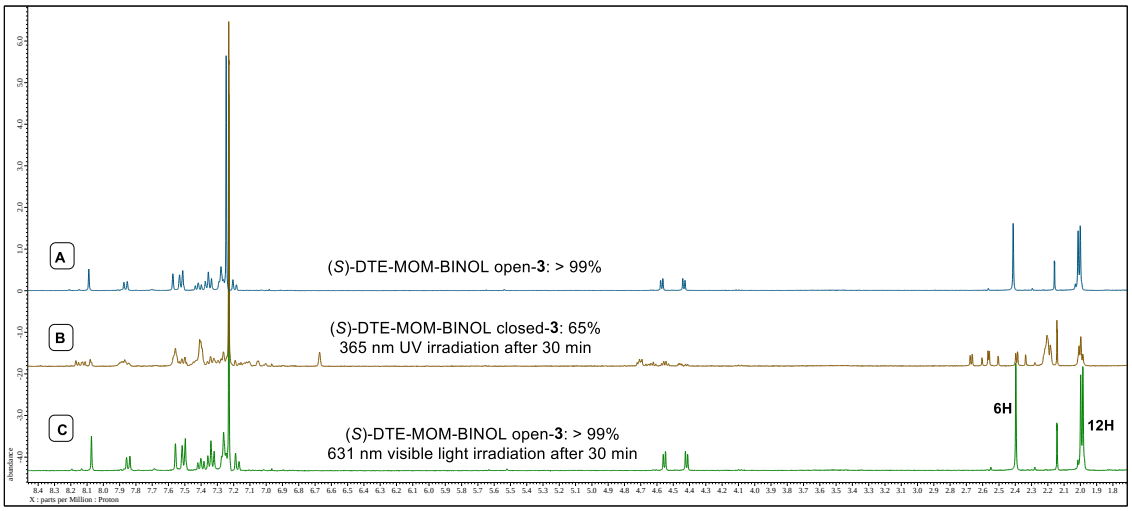


Figure S5. Photoisomerization experiments of (*S*)-DTE-MOM-BINOL **3** under different wavelengths ($CDCl_3$). (A) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL open-**3**. (B) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL closed-**3** after irradiation with UV light (395 nm, for 30 min). (C) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL open-**3** after irradiation with UV light (385 nm, for 30 min).

6-3. Photoisomerization studies of (*S*)-DTE-BINOL 4

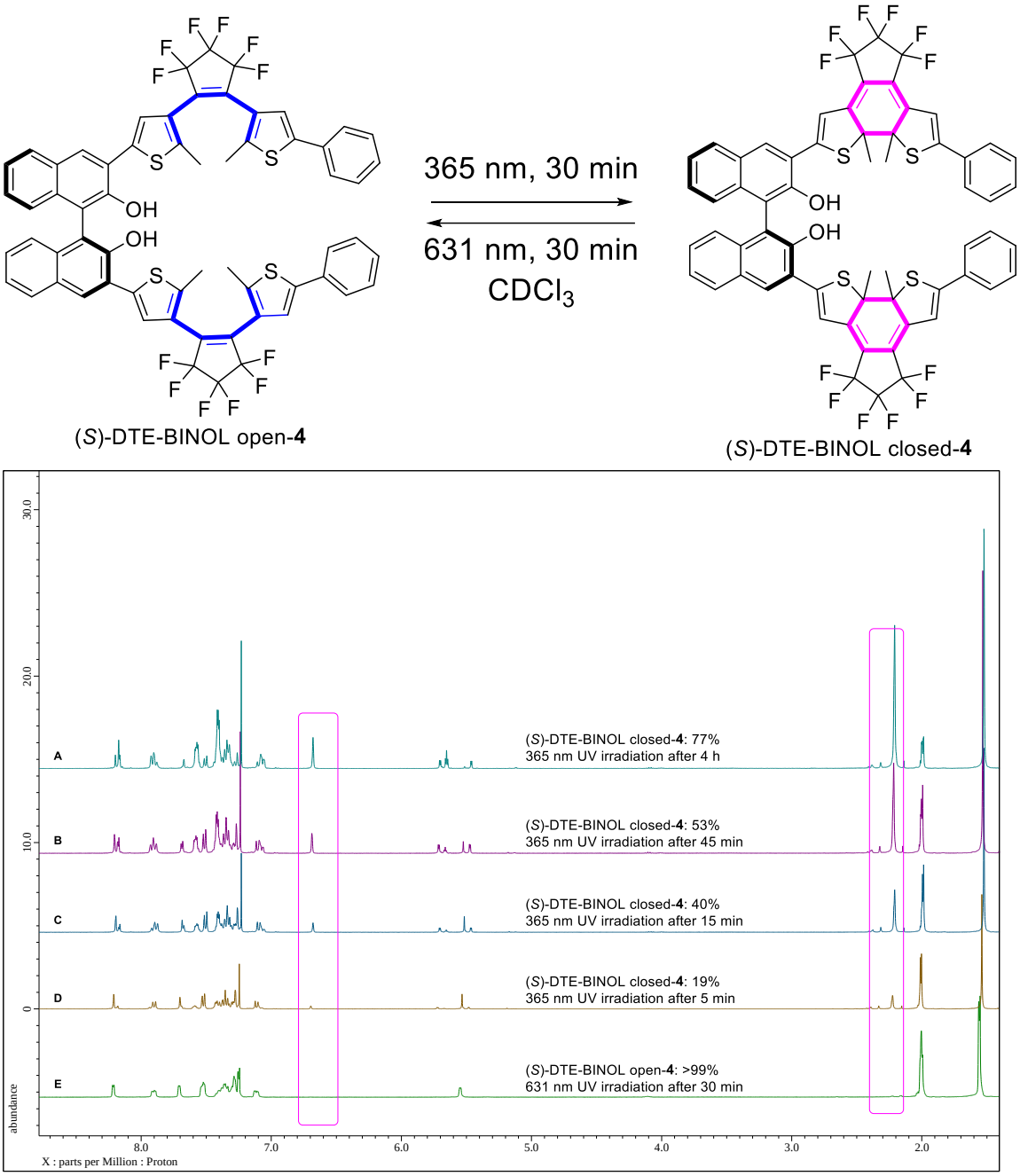


Figure S6. Photoisomerization experiments of (*S*)-DTE-BINOL **4** under different wavelengths ($CDCl_3$). (A) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL closed-**4** after irradiation with UV light (385 nm, for 4 h). (B) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL closed-**4** after irradiation with UV light (385 nm, for 45 min). (C) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL closed-**4** after irradiation with UV light (385 nm, for 15 min). (D) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL closed-**4** after irradiation with UV light (385 nm, for 5 min). (E) ^{1}H-NMR spectra of (*S*)-DTE-MOM-BINOL open-**4** after irradiation with UV light (631 nm, for 30 min).

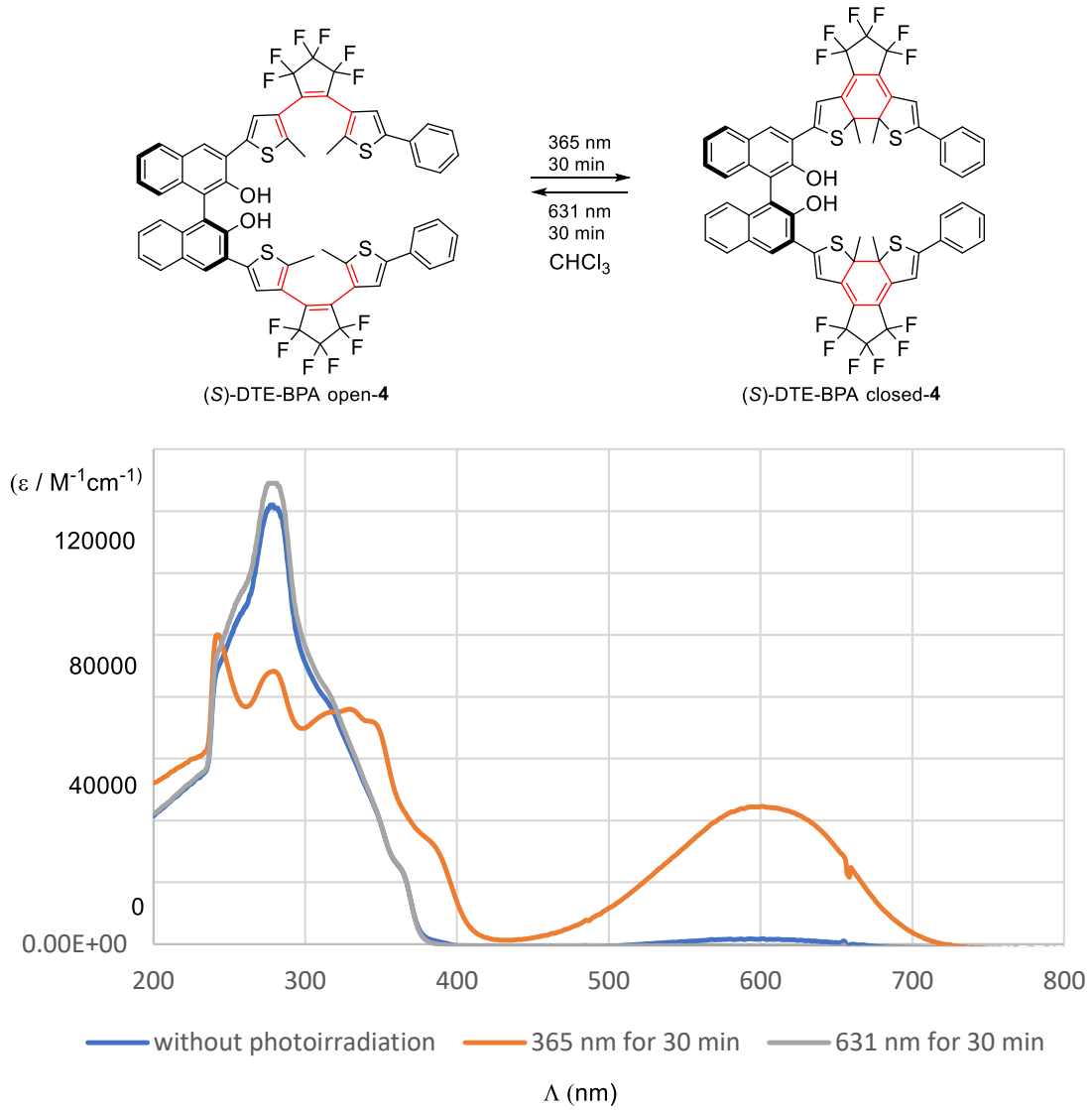


Figure S7. Photoisomerization studies of (*S*)-DTE-BINOL **4** by UV-Vis spectroscopy ($CHCl_3$, 20 μM).

Table S3. Solvent effect on the photostationary state (PSS) ratio of (*S*)-DTE-BINOL **4**.[a]

Entry	Solvent	(*S*)-DTE-BINOL closed-**4** (%)
1	$CDCl_3$	75
2	Toluene-d_8	75
3	THF-d_8	83
4	CD_3CN	44

[a]365 nm UV irradiation after 30 min.

7. Fatigue resistance testing of (*S*)-DTE-BPA 1

A solution of (*S*)-DTE-BPA **1** was cyclically irradiated with 365 nm UV light and 631 nm visible light radiation to test its fatigue resistance. Minimal changes where observed in UV-vis spectra by switching between (*S*)-DTE-BPA open-**1** and (*S*)-DTE-BPA closed-**1** state over several cycles without any decomposition.

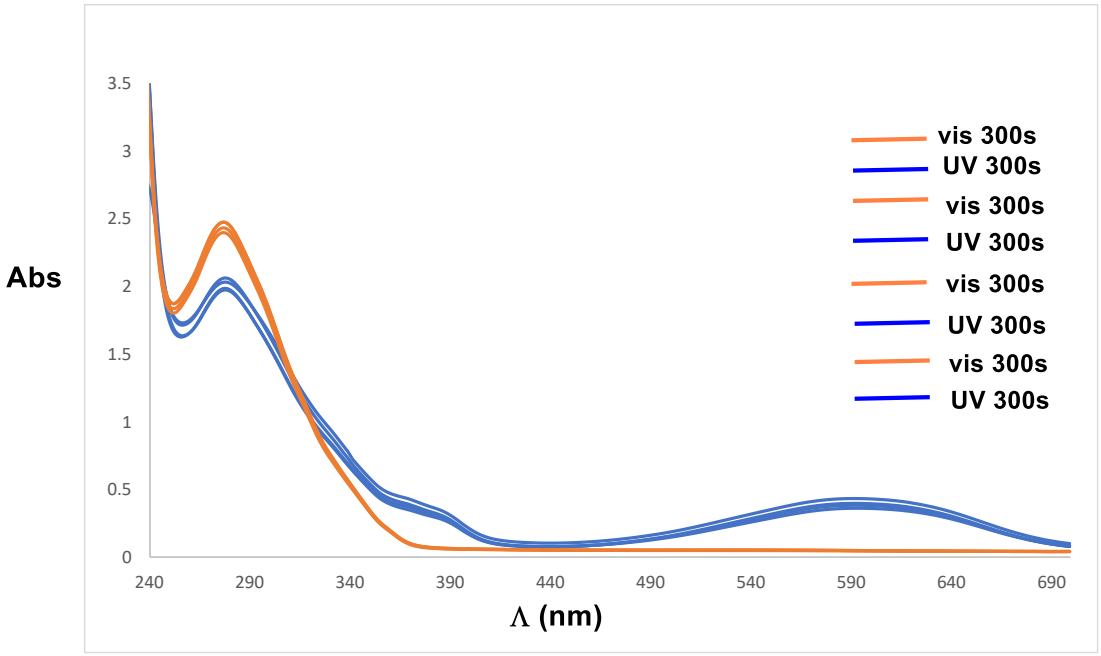
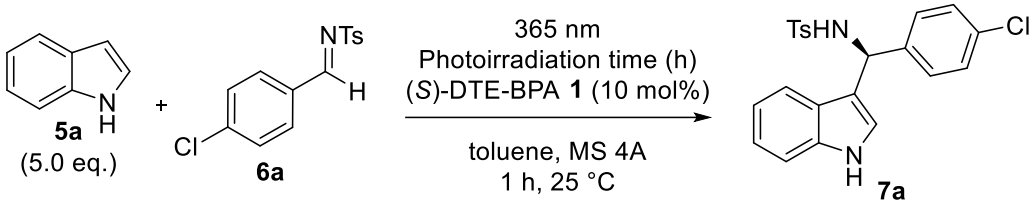


Figure S9. UV-vis spectra of (*S*)-DTE-BPA **1** ($CHCl_3$, 40 μM)

8. Control experiment

Table S4. Influence of PSS ratio of (*S*)-DTE-BPA **1** towards reactivity and selectivity



Entry	365 nm Photoirradiation time (h)	(*S*)-DTE-BPA **1** (10 mol%)	^{1}H-NMR yield (%)[b]	er[c]
1	0	open-**1**: >99%	47	68:32
2	0.25	closed-**1**: 34%	79	75:25
3	0.5	closed-**1**: 53%	86	81:19
4	0.75	closed-**1**: 65%	89	83:17
5	2	closed-**1**: 77%	89 (86[d])	86:14

[a]Reaction conditions: **5a** (58.2 mg, 0.5 mmol), **6a** (33.6 mg, 0.1 mmol), (*S*)-DTE-BPA **1** (12.4 mg) in dry toluene (2.5 mL) under the photoirradiation with 365 nm. [b]Use of 1,3,5-trimethoxybenzene as an internal standard. [c]Determined by HPLC (Daicel Chiralpak OD-H). [d]Isolated yield.

9. DFT calculations

DFT computational calculations were conducted for both isomeric forms using the SMD/B3LYP/6-31+G(d)//B3LYP/6-31+G(d) method to elucidate the influence of the photocyclization of BINOL-DTEs on their acidities. Since a mixture of half- and fully-closed isomers is present after 365 nm photoirradiation, experimental measurements are unreliable for determining their acidity. Therefore, to understand the trend in the acidities of photoresponsive DTE-BPA **1** using computational methods, the proton-exchange method[26] was utilized with respect to the experimental value of (*S*)-1,1'-binaphthyl-2,2'-diyl hydrogen phosphate (**8**) as a reference acid ($pK_{a\ (DMSO,\ experimental)}$ = 3.37). The exchanged free energy in DMSO was determined using the following equation:

$$\Delta G^*_{exchange} = \Delta G^*_{gas,exchange} + \Delta G^*_{solv((S)\text{-DTE-BPA}\mathbf{1}(anion))} + \Delta G^*_{solv(\mathbf{8})} - \Delta G^*_{solv((S)\text{-DTE-BPA}\mathbf{1})} - \Delta G^*_{solv(\mathbf{8'})}.$$

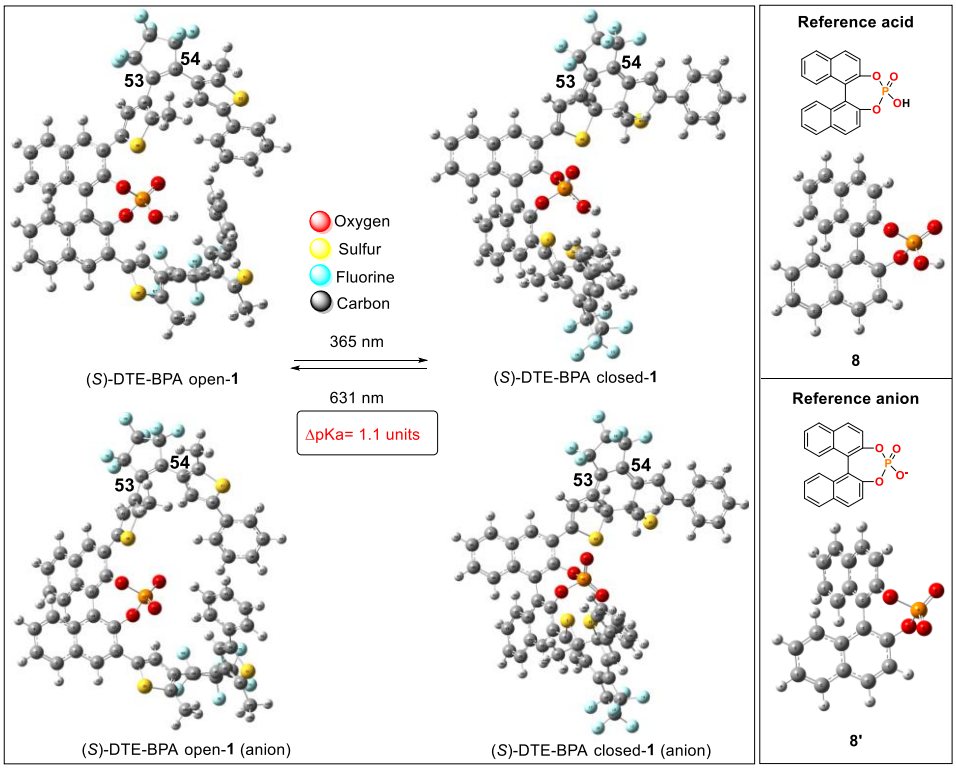


Figure S10 DFT optimised geometries of (S)-DTE-BPA open-1 and closed-1 (SMD/B3LYP/6-31+G(d)//B3LYP/6-31+G(d), DMSO)

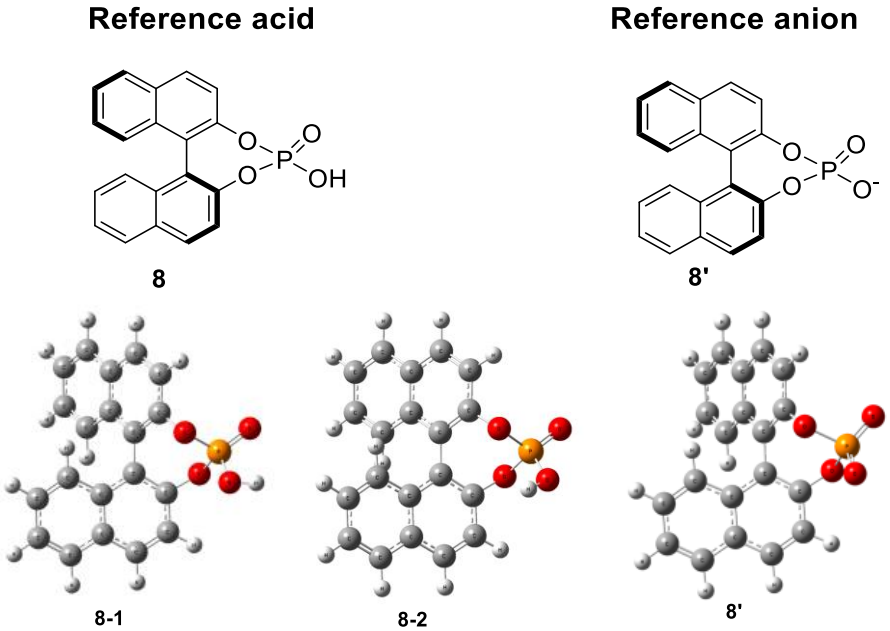
The ΔpK_a was then calculated using $\Delta pK_a = (\Delta G^*_{exchange,\ close} - \Delta G^*_{exchange,\ open})/RTln10$, where R is the universal gas constant and T = 298.15 K.

We conducted a preliminary conformational screening of the DTEs to investigate the conformational distribution of both isomers (fully open and fully closed forms). As a result of our initial screening using molecular mechanics, a systematic ring, and the spin-stepped method with the Merck molecular force field, we screened 182 probable conformers of (*S*)-DTE-BPA closed-**1** and 291 probable conformers of (*S*)-DTE-BPA open-**1** from 82,994 candidates. Geometry optimisation was performed by improving the level of theory to eliminate higher-energy conformations. A semiempirical PM6 method followed by a restricted Hartree-Fock (HF) SCF calculation (geometry cycles = 1,000) was performed using Pulay DIIS (RHF/3-21G(d)) to select the 100 most stable conformations, followed by a restricted hybrid HF-DFT SCF calculation (B3LYP/6-31G(d)) for further geometry minimisation using the Spartan 20 program. The B3LYP/6-31+G(d) method was also employed using the Gaussian 16 program package. In the optimised geometry of (*S*)-DTE-BPA **1** in DMSO, the bond length between C (53) and C (54) shifted from 1.36 Å in the open form to 1.45 Å in the closed form, indicating that photoirradiation can achieve ring cyclisation in these systems (Figure S10). As an outcome of the aforementioned computational calculations with the selected most stable optimised geometries, a difference of 1.1 pK_a units was observed between the open and closed forms of the DTEs. Enhanced acidity was expected based on the extended π-conjugation through the DTE photochromic unit after photocyclisation. The photoisomerisation ability and the enhanced acidity after photochemical isomerisation of our designed photoresponsive chiral catalyst (*S*)-DTE-BPA **1** prompted us to further

study their catalytic activity modulation behaviour and asymmetric induction ability with and without photoirradiation.

9-1. Major conformers and of (S)-1,1'-binaphthyl-2,2'-diyl hydrogen phosphate (8) and their anion 8' cartesian coordinates.

All the DFT calculations were performed using Gaussian 16 program package. Visualization of the final output were done with Gauss View software. The DFT calculations were performed for geometry optimization using the B3LYP/6-31+G(d) methods in gas-phase. Frequency calculations at the same level of theory was employed to understand the nature of the stationary points and thermal corrections to Gibbs free energy (ZPG). SMD calculation (B3LYP/6-31+G(d)) with the gas-phase optimized geometries were employed with thermal corrections to the Gibbs free energies (G) to obtain the energies in solution phase (E). It should be noted that some conformers with higher energy weren't considered in the following analogues.



Level of Theory Associated with Free Energy (G) values:
SMD/B3LYP 6-31+G(d)//B3LYP 6-31+G(d)
[Unit of G is in Hatree. ($1E_h$= 627.50 Kcal/mol)]

	ZPG	**E_{gas} (8) (hatree)**	**E_{sol} (8') (hatree)**
8-1	0.236479	**-1412.347701**	**-1412.374916**
8-2	0.236459	-1412.346034	-1412.374009
8'	0.226023	**-1411.840724**	**-1411.933547**

8-1 (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.204234	5.174983	0.158499
2	6	0	-1.418547	4.164574	-0.182678
3	6	0	-1.930559	1.557632	-1.071380
4	6	0	-2.512181	3.914108	-0.981419
5	6	0	-0.534227	3.118357	0.199066
6	6	0	-0.805305	1.774249	-0.226894
7	6	0	-2.758628	2.597431	-1.439196
8	1	0	-2.131942	0.558411	-1.440701
9	1	0	-3.176593	4.723433	-1.272195
10	1	0	-3.605943	2.403702	-2.091839
11	6	0	0.082739	0.711347	0.172881
12	6	0	1.239159	1.065868	0.849754
13	6	0	1.517177	2.383420	1.270424
14	6	0	0.629469	3.387239	0.969477
15	1	0	2.429944	2.570611	1.826625
16	1	0	0.823848	4.406131	1.295196
17	6	0	-0.173936	-0.718009	-0.161728
18	6	0	-0.574673	-3.419334	-0.956468
19	6	0	-1.377591	-1.407673	0.228966
20	6	0	0.792286	-1.450107	-0.832378
21	6	0	0.606897	-2.783738	-1.251159
22	6	0	-1.581401	-2.763880	-0.196632
23	1	0	-0.738824	-4.445117	-1.276929
24	1	0	1.407214	-3.276762	-1.793136
25	6	0	-2.774567	-3.441376	0.177384
26	6	0	-3.721682	-2.828326	0.967208
27	6	0	-3.504241	-1.506240	1.424216
28	6	0	-2.366123	-0.815390	1.064401
29	1	0	-2.917806	-4.464794	-0.162129
30	1	0	-4.625901	-3.359477	1.252278
31	1	0	-4.238435	-1.031940	2.070290
32	1	0	-2.214119	0.192655	1.433471
33	8	0	2.181903	0.089936	1.192422
34	8	0	2.015018	-0.847228	-1.156711
35	15	0	3.081417	-0.617971	0.043468
36	8	0	3.846156	-1.771739	0.553788
37	8	0	3.963886	0.554801	-0.625036
38	1	0	4.911448	0.370663	-0.510225

Zero-point correction=	0.283247 (Hartree/Particle)
Thermal correction to Energy=	0.301789
Thermal correction to Enthalpy=	0.302733
Thermal correction to Gibbs Free Energy=	0.237223
Sum of electronic and zero-point Energies=	-1412.064454
Sum of electronic and thermal Energies=	-1412.045912
Sum of electronic and thermal Enthalpies=	-1412.044968
Sum of electronic and thermal Free Energies=	-1412.110478

8-1 (SMD)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.889001	5.236405	0.164544
2	6	0	-1.164434	4.242382	-0.180664
3	6	0	-1.831195	1.669080	-1.076825
4	6	0	-2.269918	4.058329	-0.982784
5	6	0	-0.346069	3.142459	0.200819
6	6	0	-0.696624	1.817319	-0.229064
7	6	0	-2.594141	2.758912	-1.444509
8	1	0	-2.093675	0.685910	-1.452036
9	1	0	-2.884758	4.906164	-1.273662
10	1	0	-3.450278	2.618615	-2.099663
11	6	0	0.126145	0.703596	0.172762
12	6	0	1.296790	0.991218	0.856480
13	6	0	1.654762	2.287504	1.280794
14	6	0	0.828722	3.343008	0.975971
15	1	0	2.573853	2.425962	1.842028
16	1	0	1.080721	4.348673	1.302795
17	6	0	-0.213022	-0.709241	-0.161802
18	6	0	-0.774557	-3.383812	-0.960743
19	6	0	-1.454869	-1.327658	0.230638
20	6	0	0.704919	-1.498884	-0.835042
21	6	0	0.442510	-2.817882	-1.257862
22	6	0	-1.737774	-2.669907	-0.196547
23	1	0	-1.002065	-4.396262	-1.284519
24	1	0	1.205045	-3.359130	-1.809578
25	6	0	-2.968042	-3.279307	0.177905
26	6	0	-3.877396	-2.611813	0.969579
27	6	0	-3.583175	-1.304028	1.427776
28	6	0	-2.406840	-0.678590	1.067389
29	1	0	-3.168764	-4.292102	-0.164067
30	1	0	-4.811338	-3.089036	1.255065
31	1	0	-4.289046	-0.788855	2.074503
32	1	0	-2.199043	0.318375	1.440322
33	8	0	2.177349	-0.048333	1.199553
34	8	0	1.965696	-0.967072	-1.162142
35	15	0	3.035851	-0.787156	0.038671
36	8	0	3.723572	-1.986389	0.568724
37	8	0	3.968322	0.318477	-0.659275
38	1	0	4.896332	0.263049	-0.356305

Zero-point correction= 0.282483 (Hartree/Particle)
Thermal correction to Energy= 0.301056
Thermal correction to Enthalpy= 0.302000
Thermal correction to Gibbs Free Energy= 0.236479
Sum of electronic and zero-point Energies= -1412.092433
Sum of electronic and thermal Energies= -1412.073861
Sum of electronic and thermal Enthalpies= -1412.072917
Sum of electronic and thermal Free Energies= -1412.138437

8-2 (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.166133	5.300570	0.168827
2	6	0	-0.572074	4.352281	-0.176323
3	6	0	-1.582565	1.896947	-1.072309
4	6	0	-1.688699	4.321995	-0.981798
5	6	0	0.086765	3.152088	0.208811
6	6	0	-0.441036	1.887548	-0.221702
7	6	0	-2.187235	3.079727	-1.442931
8	1	0	-1.975593	0.956729	-1.442339
9	1	0	-2.179594	5.246273	-1.274383
10	1	0	-3.053174	3.057156	-2.099390
11	6	0	0.217996	0.670091	0.180129
12	6	0	1.416933	0.787621	0.868601
13	6	0	1.945103	2.026167	1.294841
14	6	0	1.275242	3.186154	0.987713
15	1	0	2.868227	2.028049	1.865958
16	1	0	1.662057	4.146265	1.320337
17	6	0	-0.310063	-0.681642	-0.160138
18	6	0	-1.216651	-3.256770	-0.953906
19	6	0	-1.624797	-1.126581	0.226730
20	6	0	0.500374	-1.584552	-0.829493
21	6	0	0.065124	-2.859010	-1.247030
22	6	0	-2.082329	-2.419556	-0.198783
23	1	0	-1.572457	-4.233346	-1.272528
24	1	0	0.758316	-3.496988	-1.785345
25	6	0	-3.384178	-2.856069	0.171451
26	6	0	-4.199689	-2.072017	0.956856
27	6	0	-3.735636	-0.814883	1.413187
28	6	0	-2.485158	-0.354727	1.057308
29	1	0	-3.718869	-3.834005	-0.167232
30	1	0	-5.189546	-2.420387	1.239212
31	1	0	-4.368077	-0.208164	2.056055
32	1	0	-2.144950	0.606177	1.426840
33	8	0	2.145953	-0.353653	1.210268
34	8	0	1.814063	-1.223363	-1.153096
35	15	0	2.923788	-1.187225	0.046418
36	8	0	3.479308	-2.451472	0.546482
37	8	0	4.012780	-0.203301	-0.612094
38	1	0	3.621582	0.505471	-1.152046

Zero-point correction= 0.283261 (Hartree/Particle)
Thermal correction to Energy= 0.301758
Thermal correction to Enthalpy= 0.302702
Thermal correction to Gibbs Free Energy= 0.237325
Sum of electronic and zero-point Energies= -1412.062773
Sum of electronic and thermal Energies= -1412.044276
Sum of electronic and thermal Enthalpies= -1412.043332
Sum of electronic and thermal Free Energies= -1412.108709

8-2 (SMD)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.166133	5.300570	0.168827
2	6	0	-0.572074	4.352281	-0.176323
3	6	0	-1.582565	1.896947	-1.072309
4	6	0	-1.688699	4.321995	-0.981798
5	6	0	0.086765	3.152088	0.208811
6	6	0	-0.441036	1.887548	-0.221702
7	6	0	-2.187235	3.079727	-1.442931
8	1	0	-1.975593	0.956729	-1.442339
9	1	0	-2.179594	5.246273	-1.274383
10	1	0	-3.053174	3.057156	-2.099390
11	6	0	0.217996	0.670091	0.180129
12	6	0	1.416933	0.787621	0.868601
13	6	0	1.945103	2.026167	1.294841
14	6	0	1.275242	3.186154	0.987713
15	1	0	2.868227	2.028049	1.865958
16	1	0	1.662057	4.146265	1.320337
17	6	0	-0.310063	-0.681642	-0.160138
18	6	0	-1.216651	-3.256770	-0.953906
19	6	0	-1.624797	-1.126581	0.226730
20	6	0	0.500374	-1.584552	-0.829493
21	6	0	0.065124	-2.859010	-1.247030
22	6	0	-2.082329	-2.419556	-0.198783
23	1	0	-1.572457	-4.233346	-1.272528
24	1	0	0.758316	-3.496988	-1.785345
25	6	0	-3.384178	-2.856069	0.171451
26	6	0	-4.199689	-2.072017	0.956856
27	6	0	-3.735636	-0.814883	1.413187
28	6	0	-2.485158	-0.354727	1.057308
29	1	0	-3.718869	-3.834005	-0.167232
30	1	0	-5.189546	-2.420387	1.239212
31	1	0	-4.368077	-0.208164	2.056055
32	1	0	-2.144950	0.606177	1.426840
33	8	0	2.145953	-0.353653	1.210268
34	8	0	1.814063	-1.223363	-1.153096
35	15	0	2.923788	-1.187225	0.046418
36	8	0	3.479308	-2.451472	0.546482
37	8	0	4.012780	-0.203301	-0.612094
38	1	0	3.621582	0.505471	-1.152046

Zero-point correction=	0.282291 (Hartree/Particle)
Thermal correction to Energy=	0.300376
Thermal correction to Enthalpy=	0.301320
Thermal correction to Gibbs Free Energy=	0.236459
Sum of electronic and zero-point Energies=	-1412.091718
Sum of electronic and thermal Energies=	-1412.073633
Sum of electronic and thermal Enthalpies=	-1412.072689
Sum of electronic and thermal Free Energies=	-1412.137549

8' (Gas phase)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.021273	4.921069	0.158970
2	6	0	-2.075168	3.886264	-0.176010
3	6	0	-2.166372	1.231698	-1.050382
4	6	0	-3.126629	3.461117	-0.960314
5	6	0	-1.027871	3.001326	0.199078
6	6	0	-1.078740	1.626869	-0.218251
7	6	0	-3.159936	2.118966	-1.410899
8	1	0	-2.202672	0.211139	-1.415648
9	1	0	-3.916674	4.152624	-1.245019
10	1	0	-3.971831	1.784573	-2.053299
11	6	0	-0.029177	0.724371	0.173250
12	6	0	1.075182	1.244653	0.848613
13	6	0	1.125512	2.605277	1.247919
14	6	0	0.089661	3.455691	0.951949
15	1	0	2.010998	2.940827	1.778440
16	1	0	0.126593	4.498609	1.261916
17	6	0	-0.034610	-0.724308	-0.173232
18	6	0	0.063471	-3.456479	-0.951913
19	6	0	-1.091007	-1.618824	0.218241
20	6	0	1.065820	-1.252978	-0.848526
21	6	0	1.105775	-2.613955	-1.247820
22	6	0	-1.050588	-2.993630	-0.199077
23	1	0	0.092495	-4.499643	-1.261893
24	1	0	1.988697	-2.956243	-1.778306
25	6	0	-2.104581	-3.870594	0.176005
26	6	0	-3.152783	-3.437480	0.960305
27	6	0	-3.175895	-2.095107	1.410879
28	6	0	-2.175625	-1.215412	1.050361
29	1	0	-2.058538	-4.905774	-0.158983
30	1	0	-3.948055	-4.122964	1.245023
31	1	0	-3.985227	-1.754561	2.053285
32	1	0	-2.204176	-0.194609	1.415627
33	8	0	2.116068	0.438892	1.192314
34	8	0	2.112882	-0.455354	-1.192320
35	15	0	3.258723	-0.011995	-0.000003
36	8	0	3.928331	-1.235647	0.534337
37	8	0	3.936492	1.207118	-0.534473

Zero-point correction= 0.270923 (Hartree/Particle)
Thermal correction to Energy= 0.288991
Thermal correction to Enthalpy= 0.289935
Thermal correction to Gibbs Free Energy= 0.225233
Sum of electronic and zero-point Energies= -1411.569801
Sum of electronic and thermal Energies= -1411.551734
Sum of electronic and thermal Enthalpies= -1411.550790
Sum of electronic and thermal Free Energies= -1411.615492

8' (SMD) Standard orientation:

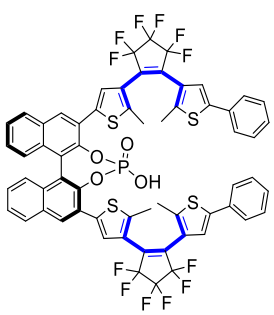
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.061770	-4.900509	0.159386
2	6	0	2.100167	-3.868763	-0.183839
3	6	0	2.154695	-1.211185	-1.073304
4	6	0	3.136915	-3.433264	-0.981643
5	6	0	1.047565	-2.989699	0.196603
6	6	0	1.080073	-1.617736	-0.229895
7	6	0	3.152081	-2.092552	-1.439875
8	1	0	2.182558	-0.192925	-1.446282
9	1	0	3.932528	-4.115191	-1.271100
10	1	0	3.954866	-1.755145	-2.091171
11	6	0	0.020861	-0.726074	0.169120
12	6	0	-1.065878	-1.264288	0.851435
13	6	0	-1.098458	-2.616224	1.271185
14	6	0	-0.052164	-3.454888	0.969321
15	1	0	-1.960377	-2.965772	1.832222
16	1	0	-0.065798	-4.491986	1.296519
17	6	0	0.020081	0.726076	-0.169192
18	6	0	-0.055905	3.454823	-0.969339
19	6	0	1.078315	1.618882	0.229858
20	6	0	-1.067242	1.263125	-0.851497
21	6	0	-1.101284	2.615030	-1.271227
22	6	0	1.044318	2.990817	-0.196613
23	1	0	-0.070670	4.491915	-1.296506
24	1	0	-1.963585	2.963659	-1.832250
25	6	0	2.095950	3.871021	0.183870
26	6	0	3.133147	3.436642	0.981701
27	6	0	3.149764	2.095941	1.439914
28	6	0	2.153352	1.213491	1.073297
29	1	0	2.056435	4.902732	-0.159333
30	1	0	3.928003	4.119437	1.271197
31	1	0	3.952893	1.759405	2.091235
32	1	0	2.182306	0.195260	1.446269
33	8	0	-2.131775	-0.460575	1.191316
34	8	0	-2.132292	0.458275	-1.191348
35	15	0	-3.232008	-0.001723	0.000007
36	8	0	-3.947887	1.194318	0.559729
37	8	0	-3.946662	-1.198530	-0.559643

Zero-point correction= 0.271512 (Hartree/Particle)
Thermal correction to Energy= 0.289447
Thermal correction to Enthalpy= 0.290392
Thermal correction to Gibbs Free Energy= 0.226023
Sum of electronic and zero-point Energies= -1411.662035
Sum of electronic and thermal Energies= -1411.644100
Sum of electronic and thermal Enthalpies= -1411.643156
Sum of electronic and thermal Free Energies= -1411.707525

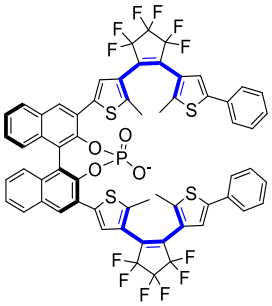
9-2. Major conformers of (*S*)-DTE-BPA open-1 and closed-1.

9-2-1. Preliminary lowest energy calculations

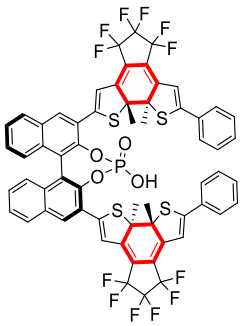
All the DFT calculations were performed using Gaussian 16 program package. Visualization of the final output were done with Gauss View software. The geometry optimization was performed using the B3LYP/6-31+G(d) methods in gas-phase. Frequency calculations at the same level of theory was employed to understand the nature of the stationary points and thermal corrections to Gibbs free energy (ZPG). Due to the higher flexibility of (*S*)-DTE-BPA **1**, conformational screening was performed to obtain the most stable conformer for preliminary lowest energy calculations. Among the 291 possible conformers of (*S*)-DTE-BPA open-**1** analyzed, 5 conformers with lowest energy were selected for further calculation. It should be noted that some conformers with higher energy weren't considered in the following analogues.



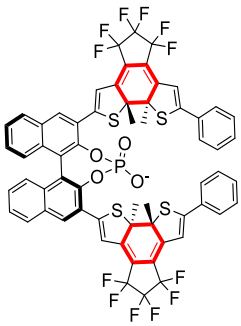
(*S*)-DTE-BPA open-**1**



(*S*)-DTE-BPA open-**1 anion**



(*S*)-DTE-BPA closed-**1**

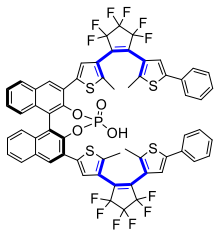


(*S*)-DTE-BPA closed-**1 anion**

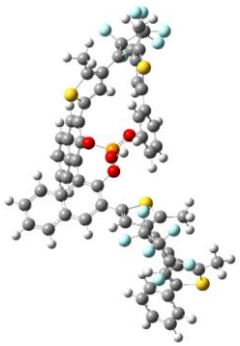
Free Energy Value for Each Optimized structure of (*S*)-DTE-BPA open-1 in Gas and Solvent Phase.

N.B.-Values in green color indicate gas phase free energy values. Whereas,values in blue color indicate solvent phase free energy values.

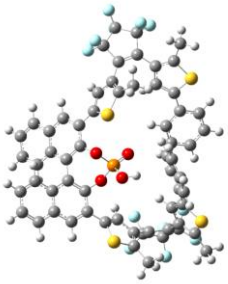
General Structure



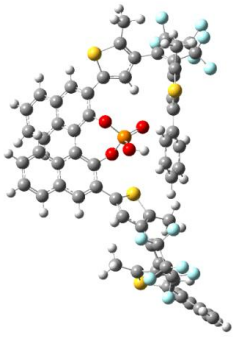
(*S*)-DTE-BPA open-**1**



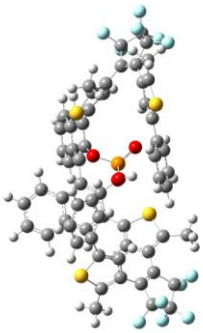
M0107- *open isomer* (Hartree/Particle)
G = -5817.495583
ZPG = 0.725739
G= -5817.549053
ZPG= 0.840600



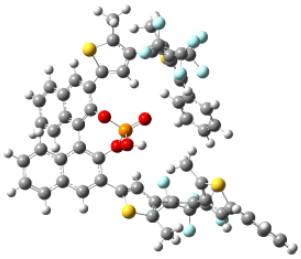
M022- *open isomer* (Hartree/Particle)
G = -5817.495846
ZPG = 0.842542
G = -5817.548783
ZPG =0.840477



M0242- *open isomer* (Hartree/Particle)
G = -5817.496645
ZPG = 0.842078
G = -5817.550156
ZPG = 0.840379



M008- *open isomer* (Hartree/Particle)
G = -5817.492051
ZPG = 0.842840
G= -5817.549769
ZPG= 0.840594



M0258- *open isomer* (Hartree/Particle)
G = -5817.495112
ZPG = 0.841933
G = -5817.549852
ZPG = 0.840419

M0107[open] (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.270383	6.297923	-4.095315
2	6	0	2.661901	5.742194	-3.410566
3	6	0	1.030140	4.303056	-1.642606
4	6	0	1.308933	6.101874	-3.228183
5	6	0	3.177142	4.684582	-2.737197
6	6	0	2.371271	3.926019	-1.849888
7	6	0	0.518864	5.410708	-2.367300
8	1	0	0.905000	6.928157	-3.777914
9	1	0	4.200571	4.397723	-2.877626
10	1	0	-0.506615	5.682835	-2.242685
11	6	0	2.883614	2.777088	-1.200489
12	6	0	2.086829	1.981055	-0.437905
13	6	0	0.740426	2.373266	-0.247187
14	6	0	0.222014	3.520066	-0.758391
15	1	0	3.917945	2.527012	-1.334838
16	6	0	-1.179096	3.905973	-0.420903
17	6	0	-3.846412	4.539551	0.145105
18	6	0	-1.485961	5.156919	0.206283
19	6	0	-2.190026	3.030421	-0.653068
20	6	0	-3.543129	3.329350	-0.384630
21	6	0	-2.832824	5.471331	0.473383
22	1	0	-4.868974	4.783490	0.348055
23	6	0	-3.149359	6.695225	1.112823
24	6	0	-2.170968	7.556413	1.485398
25	6	0	-0.818232	7.234116	1.240847
26	6	0	-0.484475	6.073458	0.620180
27	1	0	-4.180171	6.916600	1.306542
28	1	0	-2.418515	8.473716	1.979269
29	1	0	-0.049603	7.912491	1.554481
30	1	0	0.541874	5.830740	0.450873
31	6	0	2.610235	0.738533	0.161449
32	6	0	3.356854	-0.197703	-0.462700
33	6	0	3.797064	-1.242810	0.421506
34	6	0	3.351665	-1.085565	1.688065
35	16	0	2.398693	0.336101	1.835844
36	1	0	3.582776	-0.181034	-1.508133
37	6	0	-4.569713	2.293566	-0.601043
38	16	0	-5.126701	1.821323	-2.171502
39	6	0	-6.161227	0.613760	-1.511798
40	6	0	-6.069495	0.582029	-0.160908
41	6	0	-5.160346	1.567822	0.361189
42	1	0	-4.954671	1.678305	1.401497
43	8	0	-1.905551	1.755751	-1.147807
44	8	0	-0.085922	1.500893	0.469236
45	6	0	7.570166	-2.146736	1.948586
46	6	0	6.846985	-1.770530	0.866617
47	6	0	5.885764	-2.614538	0.151342
48	6	0	4.599946	-2.376415	-0.041796
49	6	0	7.126861	-0.422007	0.442849
50	6	0	8.054524	0.187956	1.203044
51	16	0	8.604609	-0.867259	2.464931
52	1	0	6.657300	0.036757	-0.399821
53	6	0	-6.784488	-0.342353	0.710497

54	6	0	-6.757318	-1.669761	0.710570
55	6	0	-5.915740	-2.548772	-0.103112
56	6	0	-6.358208	-3.649232	-0.761576
57	16	0	-5.073135	-4.426316	-1.601783
58	6	0	-3.913147	-3.255695	-1.052774
59	6	0	-4.496524	-2.324580	-0.272622
60	1	0	-3.956766	-1.507309	0.160767
61	6	0	-7.723313	-2.186938	1.747406
62	6	0	-7.835777	-1.023855	2.718198
63	6	0	-7.689304	0.173038	1.795920
64	6	0	3.954713	-3.439102	-0.870019
65	6	0	5.031047	-4.510794	-1.048903
66	6	0	6.328682	-3.833101	-0.606251
67	9	0	2.852036	-3.955272	-0.249632
68	9	0	3.534839	-2.965379	-2.085493
69	9	0	5.093976	-4.965306	-2.319377
70	9	0	4.767237	-5.541892	-0.203277
71	9	0	7.064375	-3.478850	-1.699242
72	9	0	7.090131	-4.685254	0.133666
73	9	0	-7.172714	1.255598	2.442898
74	9	0	-8.920671	0.527483	1.320765
75	9	0	-6.773168	-1.055393	3.567846
76	9	0	-8.979737	-1.023063	3.434530
77	9	0	-8.977612	-2.385290	1.216776
78	9	0	-7.343016	-3.347814	2.332448
79	6	0	-2.489053	-3.355457	-1.431475
80	6	0	0.202577	-3.501478	-2.147853
81	6	0	-2.117707	-3.550575	-2.757953
82	6	0	-1.496569	-3.244074	-0.461924
83	6	0	-0.159303	-3.315956	-0.820694
84	6	0	-0.782557	-3.622901	-3.112213
85	1	0	1.238409	-3.541542	-2.411482
86	1	0	-2.875266	-3.628775	-3.512589
87	1	0	-1.773199	-3.097659	0.562106
88	1	0	0.606383	-3.250470	-0.076219
89	1	0	-0.512246	-3.769533	-4.137886
90	6	0	8.568952	1.563261	1.062937
91	6	0	9.511092	4.164753	0.791541
92	6	0	9.935496	1.817364	1.044653
93	6	0	7.679353	2.624361	0.942527
94	6	0	8.149082	3.917488	0.804904
95	6	0	10.402299	3.112252	0.912514
96	1	0	9.875035	5.167918	0.691244
97	1	0	10.629126	1.003060	1.118769
98	1	0	6.625829	2.432042	0.981233
99	1	0	7.453951	4.728956	0.719037
100	1	0	11.458167	3.297592	0.894382
101	6	0	3.599930	-2.001285	2.857495
102	1	0	3.692513	-3.024161	2.512511
103	1	0	4.516864	-1.722139	3.364551
104	1	0	2.789491	-1.954035	3.573432
105	6	0	7.543461	-3.460028	2.692033
106	1	0	7.522971	-3.291838	3.761728
107	1	0	6.670008	-4.029248	2.415781
108	1	0	8.415987	-4.056494	2.452281
109	6	0	-7.015828	-0.246943	-2.402166
110	1	0	-7.354282	0.305989	-3.269550

111	1	0	-7.884603	-0.593354	-1.859877
112	1	0	-6.459997	-1.113848	-2.739581
113	6	0	-7.758915	-4.210442	-0.793477
114	1	0	-8.487118	-3.413899	-0.830690
115	1	0	-7.946524	-4.784988	0.106373
116	1	0	-7.903743	-4.857258	-1.649473
117	15	0	-1.205654	0.631261	-0.269016
118	8	0	-2.046968	-0.115771	0.647807
119	8	0	-0.440570	-0.173629	-1.351969
120	1	0	-0.415161	-1.143630	-1.362909

Zero-point correction=	0.842537 (Hartree/Particle)
Thermal correction to Energy=	0.914814
Thermal correction to Enthalpy=	0.915758
Thermal correction to Gibbs Free Energy=	0.725739
Sum of electronic and zero-point Energies=	-5817.378784
Sum of electronic and thermal Energies=	-5817.306508
Sum of electronic and thermal Enthalpies=	-5817.305563
Sum of electronic and thermal Free Energies=	-5817.495583

M022[open] (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.261059	8.705035	2.419924
2	6	0	-2.872093	7.809928	1.977846
3	6	0	-1.815689	5.493304	0.805985
4	6	0	-1.492171	7.713532	1.694104
5	6	0	-3.694245	6.767350	1.703131
6	6	0	-3.184371	5.574896	1.128559
7	6	0	-0.978523	6.594067	1.122554
8	1	0	-0.845705	8.531823	1.940464
9	1	0	-4.741516	6.821385	1.927800
10	1	0	0.067246	6.528022	0.913974
11	6	0	-4.025935	4.459594	0.905069
12	6	0	-3.536080	3.278793	0.440927
13	6	0	-2.157980	3.222844	0.116621
14	6	0	-1.318203	4.283339	0.220302
15	1	0	-5.068637	4.550705	1.136357
16	6	0	0.092669	4.172390	-0.262573
17	6	0	2.789252	4.042968	-0.986193
18	6	0	0.604872	5.096073	-1.230769
19	6	0	0.909583	3.180666	0.183019
20	6	0	2.281239	3.088075	-0.158817

21	6	0	1.969965	5.035301	-1.567708
22	1	0	3.833663	4.040991	-1.221648
23	6	0	2.498903	5.957241	-2.508056
24	6	0	1.695526	6.866862	-3.111598
25	6	0	0.316286	6.900178	-2.807659
26	6	0	-0.213503	6.046824	-1.894595
27	1	0	3.544311	5.907940	-2.742005
28	1	0	2.096060	7.552759	-3.830803
29	1	0	-0.316485	7.604500	-3.309433
30	1	0	-1.258039	6.076053	-1.673634
31	6	0	-4.379634	2.080515	0.304775
32	6	0	-4.326517	1.117708	-0.637097
33	6	0	-5.279578	0.062785	-0.416882
34	6	0	-6.057741	0.264215	0.670198
35	16	0	-5.622862	1.728465	1.467875
36	1	0	-3.642408	1.114556	-1.455242
37	6	0	3.146039	2.003984	0.341159
38	16	0	2.983956	1.251069	1.899881
39	6	0	4.386293	0.285834	1.661993
40	6	0	4.936691	0.510194	0.443747
41	6	0	4.223608	1.509703	-0.305493
42	1	0	4.522385	1.812637	-1.283464
43	8	0	0.408620	2.189648	1.035480
44	8	0	-1.638620	1.988288	-0.291759
45	6	0	-5.141825	-3.827869	1.039626
46	6	0	-4.526704	-2.859931	0.320134
47	6	0	-4.969827	-2.359589	-0.984304
48	6	0	-5.294709	-1.111758	-1.288361
49	6	0	-3.372187	-2.312850	0.985269
50	6	0	-3.139819	-2.870596	2.189208
51	16	0	-4.323670	-4.094257	2.534948
52	1	0	-2.770461	-1.536657	0.564404
53	6	0	6.127060	-0.154974	-0.083890
54	6	0	6.362326	-1.454388	-0.234503
55	6	0	5.405850	-2.550008	-0.054153
56	6	0	5.608363	-3.712323	0.613469
57	16	0	4.209050	-4.720033	0.530701
58	6	0	3.338183	-3.565396	-0.432197
59	6	0	4.094597	-2.474494	-0.654119
60	1	0	3.771964	-1.643965	-1.243067
61	6	0	7.759250	-1.664452	-0.759057
62	6	0	8.116944	-0.318095	-1.368708
63	6	0	7.302015	0.661394	-0.543574
64	6	0	-5.555132	-0.966651	-2.758741
65	6	0	-5.765768	-2.398999	-3.222566
66	6	0	-4.963494	-3.214907	-2.222318
67	9	0	-6.622615	-0.178222	-3.039143
68	9	0	-4.467107	-0.433755	-3.398669
69	9	0	-5.414629	-2.614066	-4.505976
70	9	0	-7.082134	-2.708844	-3.049327
71	9	0	-3.691827	-3.382000	-2.705197
72	9	0	-5.490295	-4.455484	-2.042866
73	9	0	6.924672	1.740922	-1.289698
74	9	0	8.055824	1.127757	0.493363
75	9	0	7.661295	-0.290115	-2.650414
76	9	0	9.441485	-0.059428	-1.355370
77	9	0	8.658016	-1.903987	0.256825

78	9	0	7.864609	-2.683453	-1.642954
79	6	0	1.965049	-3.808077	-0.911794
80	6	0	-0.622676	-4.213649	-1.859001
81	6	0	1.052689	-2.759384	-0.940244
82	6	0	1.564607	-5.064911	-1.353956
83	6	0	0.278168	-5.264476	-1.821577
84	6	0	-0.228565	-2.962442	-1.418484
85	1	0	-1.619126	-4.356135	-2.221542
86	1	0	1.315475	-1.789916	-0.573565
87	1	0	2.262468	-5.879191	-1.347769
88	1	0	-0.017734	-6.236921	-2.162418
89	1	0	-0.905327	-2.134225	-1.427921
90	6	0	-2.068560	-2.516450	3.138418
91	6	0	-0.055822	-1.758185	4.912514
92	6	0	-0.807166	-2.158711	2.663506
93	6	0	-2.301917	-2.499809	4.510033
94	6	0	-1.300899	-2.129011	5.389160
95	6	0	0.186455	-1.772866	3.549119
96	1	0	0.716281	-1.464508	5.594886
97	1	0	-0.597291	-2.192705	1.613795
98	1	0	-3.270773	-2.760224	4.887217
99	1	0	-1.497877	-2.119789	6.442557
100	1	0	1.149465	-1.498860	3.166741
101	6	0	-7.156466	-0.615149	1.204572
102	1	0	-7.494781	-1.294429	0.434202
103	1	0	-6.801451	-1.201804	2.044492
104	1	0	-8.003212	-0.022792	1.530413
105	6	0	-6.377066	-4.617129	0.686221
106	1	0	-7.029333	-4.714988	1.545151
107	1	0	-6.922086	-4.128948	-0.107405
108	1	0	-6.109931	-5.608573	0.340898
109	6	0	4.843694	-0.675102	2.726176
110	1	0	4.684739	-0.261870	3.714936
111	1	0	5.897923	-0.884635	2.609507
112	1	0	4.302890	-1.611649	2.648309
113	6	0	6.815233	-4.169101	1.393764
114	1	0	7.618798	-3.457816	1.308938
115	1	0	7.169058	-5.126625	1.027881
116	1	0	6.565585	-4.282010	2.443680
117	15	0	-0.705546	1.121815	0.650440
118	8	0	-0.260389	-0.115518	0.034663
119	8	0	-1.500195	0.966328	1.978528
120	1	0	-1.459707	0.154867	2.508740

Zero-point correction=	0.842542 (Hartree/Particle)
Thermal correction to Energy=	0.914945
Thermal correction to Enthalpy=	0.915890
Thermal correction to Gibbs Free Energy=	0.727590
Sum of electronic and zero-point Energies=	-5817.380895
Sum of electronic and thermal Energies=	-5817.308491
Sum of electronic and thermal Enthalpies=	-5817.307547
Sum of electronic and thermal Free Energies=	-5817.495846

M008[open] (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.872363	7.207073	1.788210
2	6	0	-3.190500	6.500701	1.358816
3	6	0	-1.367267	4.688891	0.239439
4	6	0	-1.799759	6.682508	1.528416
5	6	0	-3.653480	5.428337	0.671267
6	6	0	-2.754145	4.485018	0.109391
7	6	0	-0.914774	5.807864	0.986103
8	1	0	-1.444179	7.517154	2.098456
9	1	0	-4.707143	5.267042	0.552921
10	1	0	0.135321	5.948464	1.123924
11	6	0	-3.231716	3.330892	-0.551103
12	6	0	-2.385475	2.370174	-1.014335
13	6	0	-0.995161	2.609536	-0.900687
14	6	0	-0.474546	3.739600	-0.352852
15	1	0	-4.289168	3.206864	-0.665804
16	6	0	1.002156	3.957736	-0.357208
17	6	0	3.784123	4.298821	-0.260054
18	6	0	1.589016	5.131347	-0.936012
19	6	0	1.828916	3.008467	0.149986
20	6	0	3.232608	3.151447	0.207828
21	6	0	2.985464	5.304510	-0.856987
22	1	0	4.846325	4.432309	-0.217338
23	6	0	3.579248	6.459619	-1.426093
24	6	0	2.822705	7.380568	-2.072321
25	6	0	1.428513	7.189770	-2.186953
26	6	0	0.828299	6.103486	-1.636367
27	1	0	4.641803	6.581018	-1.347008
28	1	0	3.276530	8.246669	-2.510403
29	1	0	0.841217	7.909897	-2.720471
30	1	0	-0.226175	5.964434	-1.734949
31	6	0	-2.915813	1.113604	-1.573109
32	6	0	-4.043088	0.500595	-1.158813
33	6	0	-4.368644	-0.692984	-1.899202
34	6	0	-3.455408	-0.939873	-2.882464
35	16	0	-2.202091	0.233714	-2.885934
36	1	0	-4.632171	0.852938	-0.344575
37	6	0	4.057665	2.016598	0.661857
38	16	0	4.094591	1.442239	2.295839
39	6	0	5.153792	0.146601	1.885063
40	6	0	5.449087	0.160238	0.561938
41	6	0	4.824953	1.256038	-0.135402
42	1	0	4.930350	1.417930	-1.184010
43	8	0	1.295687	1.790888	0.596417
44	8	0	-0.138075	1.607230	-1.374499
45	6	0	-6.690724	-0.042839	1.446215
46	6	0	-5.854601	-0.941787	0.874472
47	6	0	-6.150688	-1.623656	-0.388025
48	6	0	-5.531851	-1.515988	-1.564246
49	6	0	-4.629839	-1.119248	1.611126
50	6	0	-4.562446	-0.354008	2.716862
51	16	0	-6.001323	0.602255	2.890842
52	1	0	-3.854649	-1.789093	1.308834
53	6	0	6.305016	-0.802723	-0.121809

53	6	0	6.305016	-0.802723	-0.121809
54	6	0	6.216672	-2.129174	-0.155789
55	6	0	5.138494	-2.979324	0.352853
56	6	0	5.307403	-4.184610	0.955508
57	16	0	3.794351	-4.911141	1.329284
58	6	0	2.906872	-3.575629	0.662560
59	6	0	3.742229	-2.629299	0.189236
60	1	0	3.401279	-1.719724	-0.261709
61	6	0	7.404095	-2.685718	-0.901295
62	6	0	7.841641	-1.526686	-1.777482
63	6	0	7.482315	-0.322980	-0.926962
64	6	0	-6.247096	-2.382229	-2.576069
65	6	0	-7.612824	-2.596027	-1.948902
66	6	0	-7.282092	-2.613015	-0.476050
67	9	0	-6.333519	-1.818212	-3.808760
68	9	0	-5.665504	-3.616280	-2.724587
69	9	0	-8.247781	-3.696739	-2.397372
70	9	0	-8.382672	-1.495490	-2.193512
71	9	0	-6.882236	-3.874347	-0.128127
72	9	0	-8.355009	-2.303547	0.296884
73	9	0	7.179462	0.759947	-1.699570
74	9	0	8.548887	0.018809	-0.147132
75	9	0	7.077994	-1.515439	-2.902750
76	9	0	9.146048	-1.576619	-2.120869
77	9	0	8.454485	-2.951919	-0.050400
78	9	0	7.146447	-3.818813	-1.595274
79	6	0	1.432403	-3.598226	0.624093
80	6	0	-1.353125	-3.702007	0.510869
81	6	0	0.753640	-3.104544	-0.487667
82	6	0	0.697051	-4.133067	1.677350
83	6	0	-0.684197	-4.185837	1.620889
84	6	0	-0.630777	-3.154755	-0.539623
85	1	0	-2.422074	-3.759061	0.458278
86	1	0	1.304811	-2.675781	-1.298111
87	1	0	1.204965	-4.498312	2.547753
88	1	0	-1.234445	-4.599182	2.442126
89	1	0	-1.140458	-2.783765	-1.406996
90	6	0	-3.435311	-0.250545	3.665036
91	6	0	-1.281188	-0.070838	5.411185
92	6	0	-2.153232	-0.029101	3.177478
93	6	0	-3.632108	-0.371271	5.035758
94	6	0	-2.558555	-0.282333	5.903140
95	6	0	-1.081708	0.056658	4.047633
96	1	0	-0.450865	-0.002070	6.085639
97	1	0	-1.990121	0.094997	2.127736
98	1	0	-4.618440	-0.549605	5.416848
99	1	0	-2.718237	-0.383992	6.958297
100	1	0	-0.102022	0.236267	3.651790
101	6	0	-3.399390	-2.057408	-3.898167
102	1	0	-3.642998	-3.005560	-3.445355
103	1	0	-4.115361	-1.872787	-4.687763
104	1	0	-2.412688	-2.125685	-4.337800
105	6	0	-8.031193	0.427901	0.938115
106	1	0	-8.095101	1.508972	0.968941
107	1	0	-8.182990	0.100904	-0.079675
108	1	0	-8.833381	0.018286	1.539646
109	6	0	5.632398	-0.820216	2.934547
110	1	0	5.787400	-0.317695	3.881339

111	1	0	6.567227	-1.269061	2.628360
112	1	0	4.906336	-1.612257	3.078617
113	6	0	6.584255	-4.922146	1.272320
114	1	0	7.411488	-4.239570	1.370643
115	1	0	6.818009	-5.615461	0.471538
116	1	0	6.486936	-5.482163	2.194008
117	15	0	0.759035	0.699649	-0.421751
118	8	0	1.737253	-0.096239	-1.140903
119	8	0	-0.241211	-0.092264	0.476400
120	1	0	-0.287436	-1.061879	0.425919

Zero-point correction=	0.842840	(Hartree/Particle)
Thermal correction to Energy=	0.914975	
Thermal correction to Enthalpy=	0.915919	
Thermal correction to Gibbs Free Energy=	0.726685	
Sum of electronic and zero-point Energies=	-5817.375895	
Sum of electronic and thermal Energies=	-5817.303760	
Sum of electronic and thermal Enthalpies=	-5817.302816	
Sum of electronic and thermal Free Energies=	-5817.492051	

M0258[open] (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.756306	8.264287	-3.980353
2	6	0	-2.626577	7.378478	-3.391473
3	6	0	-2.336828	5.064487	-1.836057
4	6	0	-3.760478	6.704883	-2.886861
5	6	0	-1.385210	6.893864	-3.142523
6	6	0	-1.209141	5.716273	-2.371521
7	6	0	-3.623455	5.584759	-2.132379
8	1	0	-4.738172	7.082978	-3.107913
9	1	0	-0.516442	7.386381	-3.533009
10	1	0	-4.486570	5.077492	-1.759832
11	6	0	0.080343	5.178075	-2.151177
12	6	0	0.256808	4.007662	-1.482665
13	6	0	-0.888676	3.367392	-0.955123
14	6	0	-2.141944	3.879405	-1.054464
15	1	0	0.930851	5.700137	-2.542491
16	6	0	-3.284071	3.202856	-0.368673
17	6	0	-5.507071	1.941314	0.755825
18	6	0	-4.100586	3.920418	0.564744
19	6	0	-3.555841	1.890863	-0.606599
20	6	0	-4.684795	1.229145	-0.060826
21	6	0	-5.231948	3.282261	1.105550
22	1	0	-6.365666	1.464465	1.184665
23	6	0	-6.056350	3.980951	2.024921
24	6	0	-5.748835	5.244337	2.407588
25	6	0	-4.592446	5.873456	1.895626
26	6	0	-3.793608	5.235883	1.002618
27	1	0	-6.921380	3.483803	2.417925
28	1	0	-6.370524	5.767095	3.106386
29	1	0	-4.342768	6.862561	2.223003
30	1	0	-2.917888	5.717390	0.625583

31	6	0	1.590046	3.407544	-1.311491
32	6	0	2.150407	2.927694	-0.186174
33	6	0	3.482398	2.419395	-0.394250
34	6	0	3.901700	2.541635	-1.676947
35	16	0	2.676651	3.253872	-2.655768
36	1	0	1.664835	2.909685	0.764001
37	6	0	-4.973038	-0.186547	-0.358594
38	16	0	-6.554306	-0.678152	-0.886784
39	6	0	-6.109449	-2.341195	-0.901500
40	6	0	-4.817249	-2.502425	-0.517741
41	6	0	-4.165653	-1.250650	-0.212993
42	1	0	-3.142023	-1.185733	0.081418
43	8	0	-2.691425	1.146481	-1.417946
44	8	0	-0.708717	2.117275	-0.343167
45	6	0	3.744971	-1.007660	-0.609837
46	6	0	4.866058	-0.437274	-0.098633
47	6	0	4.890874	0.706975	0.810450
48	6	0	4.278931	1.879563	0.705278
49	6	0	6.076111	-1.102728	-0.519730
50	6	0	5.852305	-2.140209	-1.348559
51	16	0	4.149486	-2.348269	-1.614638
52	1	0	7.046993	-0.785700	-0.212405
53	6	0	-4.084970	-3.765107	-0.436893
54	6	0	-3.153189	-4.096805	0.450708
55	6	0	-2.728333	-3.369309	1.644896
56	6	0	-3.523319	-3.097014	2.706217
57	16	0	-2.664183	-2.190551	3.895747
58	6	0	-1.215825	-2.168521	2.937657
59	6	0	-1.396462	-2.843325	1.787715
60	1	0	-0.658870	-2.911115	1.021184
61	6	0	-2.500830	-5.399260	0.087085
62	6	0	-2.910797	-5.607752	-1.360228
63	6	0	-4.239355	-4.874869	-1.441693
64	6	0	4.458222	2.710682	1.938749
65	6	0	5.531969	1.988332	2.752704
66	6	0	5.689936	0.621571	2.078936
67	9	0	4.829797	3.988067	1.664589
68	9	0	3.292623	2.777197	2.659760
69	9	0	5.172464	1.857515	4.055203
70	9	0	6.697718	2.677708	2.679854
71	9	0	5.262562	-0.370913	2.911663
72	9	0	7.012372	0.375835	1.821669
73	9	0	-5.221569	-5.764731	-1.072479
74	9	0	-4.531647	-4.449043	-2.696037
75	9	0	-2.992717	-6.905170	-1.722579
76	9	0	-2.018197	-4.969447	-2.166191
77	9	0	-1.146409	-5.354051	0.223115
78	9	0	-2.957525	-6.442758	0.839730
79	6	0	0.000509	-1.435449	3.334022
80	6	0	2.324402	-0.000928	3.877209
81	6	0	1.248295	-2.024766	3.166299
82	6	0	-0.071268	-0.128888	3.804450
83	6	0	1.084158	0.580715	4.075098
84	6	0	2.401363	-1.308773	3.429005
85	1	0	3.216367	0.557607	4.054668
86	1	0	1.309439	-3.040405	2.829380

87	1	0	-1.027953	0.339865	3.923263
88	1	0	1.019430	1.594745	4.416346
89	1	0	3.359801	-1.757119	3.273518
90	6	0	6.854971	-3.024537	-1.970557
91	6	0	8.777384	-4.668389	-3.134758
92	6	0	6.717925	-3.448968	-3.287799
93	6	0	7.964045	-3.440458	-1.241231
94	6	0	8.921078	-4.250790	-1.822655
95	6	0	7.671679	-4.267480	-3.863813
96	1	0	9.516803	-5.301739	-3.582692
97	1	0	5.873771	-3.126669	-3.864648
98	1	0	8.063398	-3.142704	-0.216828
99	1	0	9.770491	-4.563726	-1.248357
100	1	0	7.554303	-4.585293	-4.880751
101	6	0	5.227031	2.139613	-2.268481
102	1	0	5.997762	2.169254	-1.510293
103	1	0	5.179110	1.129487	-2.658751
104	1	0	5.513212	2.807925	-3.071206
105	6	0	2.303356	-0.632899	-0.388222
106	1	0	1.655555	-1.496833	-0.444284
107	1	0	2.170479	-0.193637	0.589707
108	1	0	1.978415	0.084865	-1.131696
109	6	0	-7.102192	-3.387697	-1.341802
110	1	0	-8.117613	-3.068409	-1.145627
111	1	0	-6.927636	-4.320323	-0.829320
112	1	0	-6.996135	-3.570185	-2.405138
113	6	0	-4.965689	-3.480294	2.904567
114	1	0	-5.200622	-4.359254	2.319423
115	1	0	-5.619123	-2.674806	2.586910
116	1	0	-5.171636	-3.699124	3.945395
117	15	0	-1.189175	0.786344	-1.050891
118	8	0	-0.994859	-0.425178	-0.276172
119	8	0	-0.466538	0.827537	-2.437634
120	1	0	-0.302113	0.029337	-2.954037

Zero-point correction=	0.841933 (Hartree/Particle)
Thermal correction to Energy=	0.914779
Thermal correction to Enthalpy=	0.915723
Thermal correction to Gibbs Free Energy=	0.723188
Sum of electronic and zero-point Energies=	-5817.376368
Sum of electronic and thermal Energies=	-5817.303522
Sum of electronic and thermal Enthalpies=	-5817.302577
Sum of electronic and thermal Free Energies=	-5817.495112

M0242[open] (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.757697	7.501953	-3.912475
2	6	0	0.424196	6.761312	-3.213967
3	6	0	-0.488510	4.851806	-1.375800
4	6	0	-0.919292	6.767374	-2.779135
5	6	0	1.279003	5.812786	-2.757914
6	6	0	0.840272	4.822687	-1.841804
7	6	0	-1.362774	5.845402	-1.886773
8	1	0	-1.594308	7.505236	-3.163966
9	1	0	2.297721	5.787521	-3.092706
10	1	0	-2.381551	5.851915	-1.565633
11	6	0	1.711448	3.795924	-1.407050
12	6	0	1.277109	2.792344	-0.599762
13	6	0	-0.060226	2.841537	-0.142001
14	6	0	-0.916864	3.849860	-0.445625
15	1	0	2.729741	3.806190	-1.740276
16	6	0	-2.274286	3.884984	0.177565
17	6	0	-4.862479	3.932151	1.227863
18	6	0	-2.706226	5.025914	0.928337
19	6	0	-3.107378	2.814199	0.071085
20	6	0	-4.424832	2.813088	0.591392
21	6	0	-4.021920	5.049859	1.428031
22	1	0	-5.854262	3.953613	1.633436
23	6	0	-4.469701	6.174735	2.167443
24	6	0	-3.636050	7.212900	2.420537
25	6	0	-2.303622	7.174927	1.952790
26	6	0	-1.850911	6.118566	1.230491
27	1	0	-5.478336	6.179354	2.531815
28	1	0	-3.976032	8.057812	2.984983
29	1	0	-1.643473	7.988179	2.178857
30	1	0	-0.839181	6.095679	0.888688
31	6	0	2.176730	1.686491	-0.224757
32	6	0	2.999495	1.016721	-1.057158
33	6	0	3.840314	0.063328	-0.377792
34	6	0	3.603173	0.019216	0.958156
35	16	0	2.374173	1.133610	1.406902
36	1	0	3.016327	1.160940	-2.114547
37	6	0	-5.301228	1.630957	0.476813
38	16	0	-6.900533	1.766606	-0.185284
39	6	0	-7.264986	0.123664	0.183534
40	6	0	-6.205474	-0.484163	0.763426
41	6	0	-5.071593	0.384369	0.930794
42	1	0	-4.146818	0.065650	1.359841
43	8	0	-2.661690	1.656512	-0.567530
44	8	0	-0.518226	1.756548	0.618447
45	6	0	7.134659	0.933457	0.398342
46	6	0	6.970907	-0.388186	0.153307
47	6	0	6.092092	-0.979884	-0.850319
48	6	0	4.800249	-0.780553	-1.087475
49	6	0	7.794473	-1.222759	0.995701
50	6	0	8.544888	-0.521415	1.866013

50	6	0	8.544888	-0.521415	1.866013
51	16	0	8.279957	1.183101	1.663466
52	1	0	7.782985	-2.289554	0.935847
53	6	0	-6.221546	-1.861746	1.273154
54	6	0	-5.772147	-2.969258	0.709053
55	6	0	-5.108114	-3.126128	-0.592238
56	6	0	-5.675063	-3.692809	-1.682181
57	16	0	-4.567617	-3.729430	-3.002198
58	6	0	-3.322575	-2.964183	-2.067890
59	6	0	-3.750055	-2.700595	-0.816255
60	1	0	-3.161812	-2.189274	-0.082205
61	6	0	-5.995291	-4.151676	1.615877
62	6	0	-6.254092	-3.521608	2.976016
63	6	0	-6.815814	-2.154554	2.622974
64	6	0	4.331278	-1.652546	-2.216722
65	6	0	5.609546	-2.167246	-2.860356
66	6	0	6.640931	-2.052726	-1.749257
67	9	0	3.586434	-2.709585	-1.765338
68	9	0	3.559186	-0.980985	-3.125129
69	9	0	5.959966	-1.311191	-3.858698
70	9	0	5.488665	-3.416101	-3.355947
71	9	0	7.875921	-1.771231	-2.231935
72	9	0	6.725812	-3.249558	-1.082021
73	9	0	-6.521452	-1.217548	3.556426
74	9	0	-8.185532	-2.251499	2.552877
75	9	0	-5.062018	-3.349727	3.608052
76	9	0	-7.076103	-4.254787	3.756882
77	9	0	-7.116234	-4.864227	1.258970
78	9	0	-4.953642	-5.017592	1.636409
79	6	0	-1.996363	-2.668075	-2.639484
80	6	0	0.516616	-2.025173	-3.662338
81	6	0	-1.870191	-2.102425	-3.903690
82	6	0	-0.844212	-2.927378	-1.898290
83	6	0	0.403772	-2.603065	-2.406712
84	6	0	-0.622169	-1.785808	-4.410512
85	1	0	1.484121	-1.755413	-4.029522
86	1	0	-2.750456	-1.885752	-4.474914
87	1	0	-0.930800	-3.392064	-0.936792
88	1	0	1.288553	-2.801416	-1.839443
89	1	0	-0.542898	-1.334929	-5.379316
90	6	0	9.487169	-1.048405	2.870858
91	6	0	11.254957	-2.076749	4.757924
92	6	0	9.537344	-0.515695	4.154343
93	6	0	10.337655	-2.098323	2.541828
94	6	0	11.212592	-2.610416	3.481408
95	6	0	10.416714	-1.027153	5.090556
96	1	0	11.935721	-2.472137	5.484885
97	1	0	8.879047	0.286772	4.422706
98	1	0	10.324019	-2.497122	1.547596
99	1	0	11.865648	-3.416950	3.213537
100	1	0	10.441556	-0.611502	6.078063
101	6	0	4.243464	-0.870744	1.991046
102	1	0	4.580869	-1.791136	1.534626
103	1	0	5.101673	-0.382751	2.437685
104	1	0	3.539986	-1.116930	2.776660
105	6	0	6.484968	2.103115	-0.291552
106	1	0	7.186874	2.920121	-0.406962
107	1	0	6.139916	1.810494	-1.273353

108	1	0	5.631171	2.458734	0.274021
109	6	0	-8.606216	-0.484137	-0.140250
110	1	0	-9.398317	0.250264	-0.061211
111	1	0	-8.816503	-1.283852	0.553591
112	1	0	-8.610626	-0.881510	-1.149691
113	6	0	-7.076437	-4.227029	-1.834104
114	1	0	-7.506164	-4.416417	-0.864410
115	1	0	-7.077868	-5.156218	-2.391690
116	1	0	-7.699750	-3.514858	-2.364603
117	15	0	-1.514969	0.697902	-0.034662
118	8	0	-1.934127	-0.352000	0.881139
119	8	0	-0.811718	0.256995	-1.341347
120	1	0	-0.672839	-0.665891	-1.604941

Zero-point correction=	0.842078 (Hartree/Particle)
Thermal correction to Energy=	0.914738
Thermal correction to Enthalpy=	0.915683
Thermal correction to Gibbs Free Energy=	0.723704
Sum of electronic and zero-point Energies=	-5817.378271
Sum of electronic and thermal Energies=	-5817.305611
Sum of electronic and thermal Enthalpies=	-5817.304667
Sum of electronic and thermal Free Energies=	-5817.496645

M0107 (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.822167	6.330238	-4.880966
2	6	0	2.278992	5.759466	-4.132614
3	6	0	0.835881	4.298314	-2.177777
4	6	0	0.934391	6.087507	-3.832517
5	6	0	2.886881	4.706880	-3.485704
6	6	0	2.183848	3.942531	-2.512562
7	6	0	0.233025	5.378778	-2.879376
8	1	0	0.448184	6.903041	-4.361345
9	1	0	3.912591	4.432057	-3.720981
10	1	0	-0.798006	5.639920	-2.668315
11	6	0	2.793252	2.831746	-1.879554
12	6	0	2.107167	2.026215	-0.986242
13	6	0	0.765747	2.397730	-0.674954
14	6	0	0.142154	3.526230	-1.182427
15	1	0	3.829998	2.604443	-2.112296
16	6	0	-1.238162	3.872228	-0.729495
17	6	0	-3.910373	4.407813	0.049800
18	6	0	-1.557198	5.134040	-0.115532
19	6	0	-2.245428	2.929681	-0.839835
20	6	0	-3.600660	3.168930	-0.475764
21	6	0	-2.915916	5.397653	0.262210
22	1	0	-4.939011	4.623445	0.326740
23	6	0	-3.244274	6.643246	0.865680
24	6	0	-2.272429	7.585568	1.118957
25	6	0	-0.924526	7.312181	0.783016
26	6	0	-0.576350	6.120764	0.181375
27	1	0	-4.280523	6.831558	1.136700
28	1	0	-2.533841	8.530786	1.586967

29	1	0	-0.154624	8.046366	1.005588
30	1	0	0.462701	5.926903	-0.060444
31	6	0	2.759806	0.838028	-0.413427
32	6	0	3.666244	0.021364	-1.043356
33	6	0	4.227143	-0.994512	-0.198019
34	6	0	3.716146	-0.955788	1.089738
35	16	0	2.553802	0.323691	1.250933
36	1	0	3.926771	0.131703	-2.089824
37	6	0	-4.622585	2.110905	-0.602466
38	16	0	-5.112019	1.451896	-2.149052
39	6	0	-6.212824	0.328400	-1.412763
40	6	0	-6.193265	0.458593	-0.033566
41	6	0	-5.299759	1.493114	0.412635
42	1	0	-5.123176	1.722439	1.456391
43	8	0	-1.928019	1.661649	-1.332595
44	8	0	0.069377	1.578017	0.213613
45	6	0	7.583119	-2.449410	2.096434
46	6	0	7.070417	-1.787395	0.994828
47	6	0	6.365845	-2.395389	-0.150035
48	6	0	5.186075	-1.990904	-0.691830
49	6	0	7.316413	-0.371792	1.033075
50	6	0	8.016118	0.049761	2.134361
51	16	0	8.365169	-1.321845	3.169614
52	1	0	7.013619	0.294312	0.232857
53	6	0	-6.999346	-0.364944	0.876785
54	6	0	-7.111586	-1.722137	0.916846
55	6	0	-6.276902	-2.709552	0.213265
56	6	0	-6.719417	-3.887591	-0.369517
57	16	0	-5.386120	-4.766951	-1.054757
58	6	0	-4.215332	-3.561569	-0.555653
59	6	0	-4.852034	-2.538455	0.099261
60	1	0	-4.325418	-1.673700	0.489237
61	6	0	-8.185384	-2.125392	1.904700
62	6	0	-8.367657	-0.877957	2.809557
63	6	0	-7.905795	0.287113	1.896440
64	6	0	4.925273	-2.692755	-2.005600
65	6	0	5.928973	-3.876547	-2.025584
66	6	0	7.037940	-3.417819	-1.041730
67	9	0	3.639361	-3.127871	-2.137875
68	9	0	5.168726	-1.868254	-3.079169
69	9	0	6.393503	-4.162748	-3.259385
70	9	0	5.319531	-4.988322	-1.530336
71	9	0	8.068688	-2.845349	-1.742781
72	9	0	7.573930	-4.482927	-0.378977
73	9	0	-7.292751	1.266531	2.625776
74	9	0	-8.993566	0.875131	1.301884
75	9	0	-7.533308	-0.976597	3.878459
76	9	0	-9.628479	-0.731435	3.270240
77	9	0	-9.387683	-2.389576	1.283671
78	9	0	-7.874952	-3.232898	2.631991
79	6	0	-2.778760	-3.731834	-0.825031
80	6	0	-0.013050	-4.029407	-1.331698
81	6	0	-2.319520	-4.389110	-1.982112
82	6	0	-1.823788	-3.234251	0.082485
83	6	0	-0.456851	-3.378968	-0.172764
84	6	0	-0.954195	-4.536256	-2.232222

85	1	0	1.050229	-4.139349	-1.526144
86	1	0	-3.037400	-4.768165	-2.705205
87	1	0	-2.149788	-2.733087	0.987854
88	1	0	0.262970	-3.002218	0.550538
89	1	0	-0.625539	-5.039885	-3.137425
90	6	0	8.450862	1.411588	2.478499
91	6	0	9.270720	4.038775	3.098932
92	6	0	9.626645	1.645263	3.215251
93	6	0	7.689357	2.521592	2.065219
94	6	0	8.099865	3.819909	2.366315
95	6	0	10.029292	2.944930	3.524611
96	1	0	9.586216	5.050786	3.338281
97	1	0	10.240817	0.805475	3.530296
98	1	0	6.760618	2.362446	1.524413
99	1	0	7.495353	4.662358	2.039848
100	1	0	10.943031	3.102103	4.091970
101	6	0	3.990174	-1.862106	2.253501
102	1	0	4.252207	-2.866906	1.906684
103	1	0	4.826851	-1.493704	2.859794
104	1	0	3.115003	-1.946267	2.906286
105	6	0	7.509325	-3.897913	2.490166
106	1	0	7.388939	-4.003864	3.574010
107	1	0	6.662375	-4.392318	2.007366
108	1	0	8.415963	-4.442600	2.200528
109	6	0	-7.031621	-0.590717	-2.270717
110	1	0	-7.281447	-0.122898	-3.228876
111	1	0	-7.968363	-0.851498	-1.768370
112	1	0	-6.495767	-1.524857	-2.482047
113	6	0	-8.103257	-4.462735	-0.490714
114	1	0	-8.825632	-3.702073	-0.802222
115	1	0	-8.450954	-4.873186	0.464577
116	1	0	-8.126902	-5.271075	-1.228178
117	15	0	-1.154902	0.646162	-0.329031
118	8	0	-1.900392	0.038846	0.791264
119	8	0	-0.539738	-0.347463	-1.419122
120	1	0	-0.589920	-1.285124	-1.138085

Zero-point correction=	0.840600 (Hartree/Particle)
Thermal correction to Energy=	0.912946
Thermal correction to Enthalpy=	0.913890
Thermal correction to Gibbs Free Energy=	0.724628
Sum of electronic and zero-point Energies=	-5817.433080
Sum of electronic and thermal Energies=	-5817.360734
Sum of electronic and thermal Enthalpies=	-5817.359790
Sum of electronic and thermal Free Energies=	-5817.549053

M008 (SMD)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.836921	6.839245	3.038814
2	6	0	-3.190417	6.206173	2.437058
3	6	0	-1.475295	4.582432	0.868490
4	6	0	-1.786415	6.388721	2.477663
5	6	0	-3.728369	5.215223	1.647318
6	6	0	-2.892666	4.370482	0.863312
7	6	0	-0.952105	5.601248	1.712078
8	1	0	-1.361296	7.154543	3.121018
9	1	0	-4.803238	5.051108	1.622157
10	1	0	0.120412	5.752647	1.760988
11	6	0	-3.440007	3.318180	0.092235
12	6	0	-2.647100	2.429379	-0.616175
13	6	0	-1.240529	2.670959	-0.605379
14	6	0	-0.647594	3.739063	0.049072
15	1	0	-4.519733	3.202870	0.069806
16	6	0	0.824186	3.962195	-0.065787
17	6	0	3.637423	4.287048	-0.141805
18	6	0	1.381126	5.195932	-0.555080
19	6	0	1.696855	2.939668	0.261085
20	6	0	3.114249	3.072535	0.259404
21	6	0	2.806940	5.350689	-0.578929
22	1	0	4.715341	4.425824	-0.138033
23	6	0	3.369858	6.566644	-1.056901
24	6	0	2.566479	7.582447	-1.525005
25	6	0	1.160453	7.416657	-1.539426
26	6	0	0.583170	6.257024	-1.065484
27	1	0	4.452191	6.672616	-1.058448
28	1	0	3.007648	8.503872	-1.895313
29	1	0	0.528841	8.209013	-1.932403
30	1	0	-0.495006	6.145777	-1.092788
31	6	0	-3.264663	1.291887	-1.315422
32	6	0	-4.445581	0.679046	-0.979577
33	6	0	-4.861737	-0.366751	-1.873225
34	6	0	-3.960558	-0.536906	-2.922217
35	16	0	-2.625595	0.559940	-2.772599
36	1	0	-5.013380	0.954295	-0.100648
37	6	0	3.999514	1.952063	0.626323
38	16	0	3.930600	1.161319	2.187699
39	6	0	5.218320	0.069426	1.782542
40	6	0	5.671344	0.304914	0.494447
41	6	0	4.984603	1.394673	-0.143510
42	1	0	5.179398	1.711387	-1.160945
43	8	0	1.166155	1.689242	0.602416
44	8	0	-0.442408	1.798763	-1.347177
45	6	0	-6.901347	-0.238955	1.828164
46	6	0	-6.250311	-1.049992	0.916839
47	6	0	-6.727323	-1.350892	-0.449038
48	6	0	-6.099768	-1.123502	-1.639314
49	6	0	-5.040416	-1.620880	1.441648
50	6	0	-4.771132	-1.266286	2.738493
51	16	0	-6.019312	-0.187227	3.329781
52	1	0	-4.416297	-2.300985	0.872109
53	6	0	6.736470	-0.472580	-0.152169

54	6	0	6.848516	-1.825993	-0.264597
55	6	0	5.819028	-2.834207	0.033312
56	6	0	6.032501	-4.084513	0.595256
57	16	0	4.534743	-4.955218	0.732883
58	6	0	3.602654	-3.647956	0.028686
59	6	0	4.434111	-2.602615	-0.282429
60	1	0	4.076665	-1.678251	-0.722644
61	6	0	8.192501	-2.187096	-0.860302
62	6	0	8.678902	-0.880194	-1.541542
63	6	0	7.939263	0.225678	-0.745156
64	6	0	-6.904298	-1.739904	-2.767256
65	6	0	-8.300965	-2.020394	-2.153669
66	6	0	-7.990209	-2.157941	-0.646215
67	9	0	-7.003396	-0.940320	-3.866651
68	9	0	-6.371136	-2.935085	-3.191840
69	9	0	-8.908719	-3.101246	-2.685438
70	9	0	-9.104686	-0.939781	-2.351982
71	9	0	-7.784519	-3.480284	-0.333973
72	9	0	-9.044266	-1.749752	0.116591
73	9	0	7.615763	1.278087	-1.554464
74	9	0	8.761503	0.729869	0.230309
75	9	0	8.258118	-0.868274	-2.834200
76	9	0	10.021690	-0.741248	-1.532698
77	9	0	9.109284	-2.538642	0.107328
78	9	0	8.142628	-3.223362	-1.741034
79	6	0	2.151532	-3.766117	-0.180514
80	6	0	-0.635089	-3.981169	-0.602427
81	6	0	1.525571	-3.061485	-1.227244
82	6	0	1.352518	-4.580150	0.645159
83	6	0	-0.023203	-4.687843	0.436589
84	6	0	0.146960	-3.166400	-1.431364
85	1	0	-1.704801	-4.071049	-0.771659
86	1	0	2.113741	-2.432532	-1.887001
87	1	0	1.808036	-5.121883	1.470382
88	1	0	-0.617534	-5.319487	1.091308
89	1	0	-0.308858	-2.630531	-2.260864
90	6	0	-3.631700	-1.658593	3.583057
91	6	0	-1.431756	-2.418758	5.171177
92	6	0	-2.343534	-1.758440	3.025701
93	6	0	-3.795595	-1.936834	4.952491
94	6	0	-2.705042	-2.311366	5.738359
95	6	0	-1.256399	-2.140659	3.812273
96	1	0	-0.582765	-2.709429	5.784474
97	1	0	-2.189719	-1.501223	1.981771
98	1	0	-4.785533	-1.878405	5.397935
99	1	0	-2.852564	-2.526468	6.793653
100	1	0	-0.268186	-2.201873	3.364063
101	6	0	-3.927914	-1.501751	-4.076894
102	1	0	-4.019004	-2.538774	-3.739647
103	1	0	-4.743337	-1.312795	-4.782300
104	1	0	-2.986381	-1.408829	-4.627123
105	6	0	-8.151174	0.581758	1.675728
106	1	0	-8.036750	1.565436	2.145537
107	1	0	-8.387144	0.738255	0.619688
108	1	0	-9.016511	0.091097	2.137221
109	6	0	5.692665	-0.937383	2.788847
110	1	0	5.596341	-0.554384	3.810281

111	1	0	6.745683	-1.182609	2.618909
112	1	0	5.118895	-1.870754	2.723788
113	6	0	7.294243	-4.742099	1.080971
114	1	0	7.889756	-4.058784	1.693928
115	1	0	7.923982	-5.065741	0.244130
116	1	0	7.065953	-5.624827	1.686243
117	15	0	0.623058	0.792512	-0.636560
118	8	0	1.590640	0.259160	-1.615758
119	8	0	-0.224647	-0.292833	0.182779
120	1	0	-0.069559	-1.194641	-0.168193

Zero-point correction=	0.840634 (Hartree/Particle)
Thermal correction to Energy=	0.912963
Thermal correction to Enthalpy=	0.913907
Thermal correction to Gibbs Free Energy=	0.725340
Sum of electronic and zero-point Energies=	-5817.430051
Sum of electronic and thermal Energies=	-5817.357722
Sum of electronic and thermal Enthalpies=	-5817.356778
Sum of electronic and thermal Free Energies=	-5817.545345

M022-(SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.924914	8.735743	2.822711
2	6	0	-2.569324	7.837305	2.325489
3	6	0	-1.611782	5.513787	1.012968
4	6	0	-1.214747	7.740980	1.924288
5	6	0	-3.426663	6.784387	2.096879
6	6	0	-2.972112	5.597739	1.456309
7	6	0	-0.749306	6.612093	1.282630
8	1	0	-0.533218	8.562911	2.126893
9	1	0	-4.465053	6.837833	2.415883
10	1	0	0.292774	6.554698	0.989063
11	6	0	-3.841667	4.497539	1.259578
12	6	0	-3.410024	3.305552	0.703152
13	6	0	-2.044068	3.240104	0.291383
14	6	0	-1.169880	4.311739	0.356521
15	1	0	-4.880887	4.599459	1.561706
16	6	0	0.206296	4.191113	-0.211324
17	6	0	2.880916	3.984273	-1.088919
18	6	0	0.684932	5.091594	-1.224779
19	6	0	1.043994	3.173780	0.213326
20	6	0	2.405381	3.039878	-0.191571
21	6	0	2.050531	4.984764	-1.646766
22	1	0	3.924870	3.956802	-1.386859
23	6	0	2.549408	5.884347	-2.631177
24	6	0	1.728498	6.827247	-3.207518
25	6	0	0.367692	6.906134	-2.822301
26	6	0	-0.139510	6.064436	-1.854474
27	1	0	3.591187	5.800431	-2.931820
28	1	0	2.116990	7.501985	-3.965554

29	1	0	-0.284859	7.634316	-3.296673
30	1	0	-1.185305	6.135944	-1.577044
31	6	0	-4.320269	2.161376	0.548376
32	6	0	-4.406001	1.238807	-0.464098
33	6	0	-5.434835	0.258368	-0.266021
34	6	0	-6.152970	0.453082	0.899583
35	16	0	-5.545047	1.833701	1.761518
36	1	0	-3.749535	1.242360	-1.325175
37	6	0	3.296223	1.971424	0.285084
38	16	0	3.163138	1.200324	1.855511
39	6	0	4.584814	0.239250	1.601480
40	6	0	5.133197	0.493443	0.354689
41	6	0	4.399655	1.483400	-0.375621
42	1	0	4.672099	1.792940	-1.377124
43	8	0	0.545366	2.242188	1.129265
44	8	0	-1.584413	2.026863	-0.228515
45	6	0	-5.836550	-3.754842	1.038288
46	6	0	-5.170948	-2.810919	0.277710
47	6	0	-5.640847	-2.175004	-0.968661
48	6	0	-5.680997	-0.841321	-1.213263
49	6	0	-3.900291	-2.442934	0.835278
50	6	0	-3.588175	-3.087717	2.003201
51	16	0	-4.887034	-4.182926	2.436680
52	1	0	-3.255232	-1.702751	0.375680
53	6	0	6.361434	-0.146406	-0.140496
54	6	0	6.654755	-1.473974	-0.224649
55	6	0	5.719985	-2.599512	-0.092425
56	6	0	5.987507	-3.837899	0.472013
57	16	0	4.602671	-4.880150	0.330237
58	6	0	3.656608	-3.670285	-0.517301
59	6	0	4.393020	-2.521076	-0.643671
60	1	0	4.027261	-1.645355	-1.166944
61	6	0	8.108976	-1.659435	-0.603335
62	6	0	8.529605	-0.293979	-1.210804
63	6	0	7.540640	0.703018	-0.552829
64	6	0	-5.968677	-0.559061	-2.669316
65	6	0	-6.472271	-1.916635	-3.236465
66	6	0	-5.903641	-2.960258	-2.234260
67	9	0	-6.886061	0.429647	-2.853148
68	9	0	-4.833619	-0.171886	-3.339752
69	9	0	-6.087456	-2.139227	-4.509923
70	9	0	-7.831770	-1.944917	-3.189009
71	9	0	-4.738921	-3.490554	-2.727151
72	9	0	-6.763305	-4.008417	-2.075946
73	9	0	7.208676	1.707991	-1.419984
74	9	0	8.133139	1.309122	0.525567
75	9	0	8.321985	-0.321232	-2.554293
76	9	0	9.825980	0.011833	-0.989999
77	9	0	8.898963	-1.907168	0.498666
78	9	0	8.326039	-2.682064	-1.473854
79	6	0	2.298796	-3.946626	-1.010622
80	6	0	-0.289816	-4.435521	-2.019525
81	6	0	1.375857	-2.894707	-1.165620
82	6	0	1.894644	-5.249199	-1.359226
83	6	0	0.612514	-5.490536	-1.854034
84	6	0	0.099648	-3.137716	-1.673569
85	1	0	-1.285903	-4.622439	-2.412322
86	1	0	1.638324	-1.882905	-0.872884

87	1	0	2.594769	-6.075824	-1.265659
88	1	0	0.323249	-6.503711	-2.121691
89	1	0	-0.586658	-2.303111	-1.786083
90	6	0	-2.380684	-2.928012	2.825786
91	6	0	-0.053469	-2.542383	4.378269
92	6	0	-1.152728	-2.594711	2.215769
93	6	0	-2.412709	-3.077845	4.223879
94	6	0	-1.260441	-2.890805	4.989820
95	6	0	-0.004770	-2.397524	2.987311
96	1	0	0.841518	-2.394075	4.976296
97	1	0	-1.082653	-2.531517	1.133462
98	1	0	-3.349739	-3.321481	4.718173
99	1	0	-1.310741	-3.007477	6.069301
100	1	0	0.930758	-2.152049	2.491476
101	6	0	-7.302735	-0.335917	1.452714
102	1	0	-7.817766	-0.874184	0.651298
103	1	0	-6.963776	-1.076577	2.188229
104	1	0	-8.033812	0.314768	1.944512
105	6	0	-7.185941	-4.387245	0.845175
106	1	0	-7.678148	-4.568137	1.806907
107	1	0	-7.837120	-3.743127	0.248254
108	1	0	-7.109078	-5.348787	0.323262
109	6	0	5.052092	-0.708812	2.666234
110	1	0	4.765082	-0.361221	3.664190
111	1	0	6.142537	-0.803904	2.643352
112	1	0	4.630256	-1.712016	2.522410
113	6	0	7.220464	-4.360233	1.155545
114	1	0	7.636882	-3.622502	1.847862
115	1	0	8.004440	-4.609382	0.430349
116	1	0	6.995878	-5.267231	1.725632
117	15	0	-0.522613	1.130256	0.608141
118	8	0	-0.021261	-0.007540	-0.188729
119	8	0	-1.226589	0.769463	1.999670
120	1	0	-1.177998	-0.186857	2.205047

Zero-point correction=	0.840477 (Hartree/Particle)
Thermal correction to Energy=	0.913028
Thermal correction to Enthalpy=	0.913972
Thermal correction to Gibbs Free Energy=	0.725438
Sum of electronic and zero-point Energies=	-5817.433743
Sum of electronic and thermal Energies=	-5817.361193
Sum of electronic and thermal Enthalpies=	-5817.360249
Sum of electronic and thermal Free Energies=	-5817.548783

M0258 (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.318529	8.436731	-4.009563
2	6	0	-2.251697	7.541150	-3.397783
3	6	0	-2.112362	5.212663	-1.786577
4	6	0	-3.428102	6.959019	-2.866770
5	6	0	-1.028524	6.959890	-3.148685
6	6	0	-0.926945	5.780923	-2.358504
7	6	0	-3.360411	5.828130	-2.079812
8	1	0	-4.395095	7.404732	-3.084361
9	1	0	-0.118903	7.386543	-3.565029
10	1	0	-4.273023	5.392988	-1.688407
11	6	0	0.327055	5.160597	-2.134904
12	6	0	0.446436	3.975640	-1.430063
13	6	0	-0.753755	3.413475	-0.901365
14	6	0	-1.993332	4.023078	-0.984912
15	1	0	1.219434	5.636262	-2.533688
16	6	0	-3.167510	3.424172	-0.282420
17	6	0	-5.481355	2.278550	0.861567
18	6	0	-3.927257	4.178426	0.679250
19	6	0	-3.533346	2.110451	-0.527696
20	6	0	-4.706915	1.504154	0.015124
21	6	0	-5.112537	3.594397	1.232939
22	1	0	-6.380561	1.849303	1.295950
23	6	0	-5.882674	4.333135	2.174336
24	6	0	-5.488432	5.588308	2.580370
25	6	0	-4.296976	6.152548	2.063160
26	6	0	-3.538367	5.468060	1.136672
27	1	0	-6.784324	3.878988	2.578812
28	1	0	-6.079782	6.141086	3.305329
29	1	0	-3.973223	7.132563	2.403544
30	1	0	-2.624814	5.913832	0.759471
31	6	0	1.754294	3.335907	-1.219251
32	6	0	2.256246	2.741161	-0.090220
33	6	0	3.606310	2.271659	-0.229936
34	6	0	4.137404	2.525550	-1.483803
35	16	0	2.964868	3.324526	-2.488951
36	1	0	1.684689	2.635605	0.823726
37	6	0	-5.113265	0.128391	-0.324714
38	16	0	-6.769401	-0.207560	-0.798086
39	6	0	-6.465687	-1.909423	-0.979986
40	6	0	-5.143459	-2.199268	-0.680829
41	6	0	-4.388232	-1.032049	-0.312262
42	1	0	-3.337591	-1.071373	-0.050287
43	8	0	-2.765862	1.355681	-1.418367
44	8	0	-0.657271	2.172726	-0.260403
45	6	0	4.196235	-1.133824	-0.714478
46	6	0	5.266581	-0.500001	-0.104598
47	6	0	5.119373	0.549083	0.915187
48	6	0	4.356815	1.673955	0.883286
49	6	0	6.536797	-1.013258	-0.537967
50	6	0	6.448093	-2.004912	-1.482544
51	16	0	4.762409	-2.345763	-1.825594
52	1	0	7.482671	-0.621865	-0.183424
53	6	0	-4.491910	-3.516435	-0.752549

54	6	0	-3.547111	-4.008842	0.095835
55	6	0	-3.126768	-3.480280	1.400988
56	6	0	-4.007277	-3.198790	2.432421
57	16	0	-3.145555	-2.599547	3.817979
58	6	0	-1.591425	-2.711629	3.011441
59	6	0	-1.759084	-3.213204	1.746766
60	1	0	-0.941566	-3.324066	1.045939
61	6	0	-2.960331	-5.298240	-0.432158
62	6	0	-3.455494	-5.380589	-1.900088
63	6	0	-4.717350	-4.476539	-1.898745
64	6	0	4.340509	2.352410	2.235499
65	6	0	5.538988	1.730398	3.004147
66	6	0	5.787460	0.386723	2.263657
67	9	0	4.450339	3.707604	2.160725
68	9	0	3.173794	2.092421	2.915092
69	9	0	5.300258	1.571032	4.323776
70	9	0	6.626030	2.534321	2.862365
71	9	0	5.237105	-0.648115	2.972753
72	9	0	7.126787	0.121673	2.176410
73	9	0	-5.825152	-5.272535	-1.698846
74	9	0	-4.895916	-3.863659	-3.101732
75	9	0	-3.702060	-6.641920	-2.314157
76	9	0	-2.520694	-4.838335	-2.727069
77	9	0	-1.595573	-5.339913	-0.374735
78	9	0	-3.408853	-6.385275	0.273348
79	6	0	-0.344387	-2.290320	3.665147
80	6	0	2.078536	-1.465042	4.853123
81	6	0	0.870751	-2.924046	3.341518
82	6	0	-0.321606	-1.244515	4.605977
83	6	0	0.876668	-0.839580	5.195385
84	6	0	2.068628	-2.509599	3.923234
85	1	0	3.013396	-1.141358	5.302214
86	1	0	0.869589	-3.755805	2.642347
87	1	0	-1.243990	-0.727008	4.857633
88	1	0	0.872662	-0.022603	5.912462
89	1	0	2.996724	-3.009194	3.657240
90	6	0	7.536731	-2.734545	-2.149314
91	6	0	9.654124	-4.109117	-3.410144
92	6	0	7.388079	-3.253746	-3.448814
93	6	0	8.766923	-2.925193	-1.490916
94	6	0	9.814770	-3.598298	-2.118287
95	6	0	8.434324	-3.936668	-4.069970
96	1	0	10.469347	-4.639451	-3.895051
97	1	0	6.453406	-3.107202	-3.984403
98	1	0	8.892668	-2.562466	-0.474629
99	1	0	10.754866	-3.736389	-1.590261
100	1	0	8.297164	-4.327691	-5.074876
101	6	0	5.509672	2.236899	-2.017014
102	1	0	6.248992	2.270717	-1.210482
103	1	0	5.566530	1.239905	-2.471184
104	1	0	5.803974	2.969640	-2.775478
105	6	0	2.723269	-0.935107	-0.510510
106	1	0	2.163009	-1.850663	-0.724770
107	1	0	2.504259	-0.649056	0.522604
108	1	0	2.335122	-0.138063	-1.157630
109	6	0	-7.591830	-2.809068	-1.407478
110	1	0	-8.557984	-2.306275	-1.299726

111	1	0	-7.619360	-3.723505	-0.807132
112	1	0	-7.487019	-3.108829	-2.456974
113	6	0	-5.497382	-3.363068	2.485492
114	1	0	-5.821061	-4.157746	1.805954
115	1	0	-6.014429	-2.441111	2.188546
116	1	0	-5.833730	-3.625630	3.494280
117	15	0	-1.273606	0.876026	-1.014141
118	8	0	-1.117793	-0.358374	-0.218687
119	8	0	-0.619537	0.840183	-2.483810
120	1	0	-0.095297	0.031901	-2.612088

Zero-point correction=	0.840419 (Hartree/Particle)
Thermal correction to Energy=	0.912990
Thermal correction to Enthalpy=	0.913934
Thermal correction to Gibbs Free Energy=	0.723235
Sum of electronic and zero-point Energies=	-5817.432667
Sum of electronic and thermal Energies=	-5817.360097
Sum of electronic and thermal Enthalpies=	-5817.359153
Sum of electronic and thermal Free Energies=	-5817.549852

M0242 (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.744158	7.479192	-4.010317
2	6	0	0.414406	6.730878	-3.294642
3	6	0	-0.475017	4.801750	-1.417054
4	6	0	-0.908522	6.769830	-2.790691
5	6	0	1.272077	5.733687	-2.887662
6	6	0	0.849655	4.738911	-1.961297
7	6	0	-1.340066	5.833944	-1.873904
8	1	0	-1.592418	7.542308	-3.132280
9	1	0	2.284226	5.680501	-3.282300
10	1	0	-2.358443	5.876088	-1.504270
11	6	0	1.716847	3.688018	-1.576478
12	6	0	1.305184	2.657752	-0.746763
13	6	0	-0.021685	2.740002	-0.229726
14	6	0	-0.880816	3.798834	-0.468469
15	1	0	2.733932	3.691132	-1.958122
16	6	0	-2.197505	3.861759	0.232383
17	6	0	-4.776323	3.983421	1.377590
18	6	0	-2.564782	5.003948	1.027679
19	6	0	-3.085793	2.800182	0.151822
20	6	0	-4.400574	2.833059	0.706128
21	6	0	-3.885939	5.066044	1.577980
22	1	0	-5.770449	4.039260	1.813179
23	6	0	-4.270784	6.196465	2.352055
24	6	0	-3.381308	7.216741	2.603836
25	6	0	-2.062004	7.139522	2.094968
26	6	0	-1.665061	6.064810	1.326991
27	1	0	-5.280293	6.230634	2.755180
28	1	0	-3.682597	8.072113	3.202528

29	1	0	-1.352297	7.932383	2.316271
30	1	0	-0.647815	6.021286	0.954568
31	6	0	2.220547	1.548318	-0.438133
32	6	0	3.233395	1.078803	-1.240116
33	6	0	4.047797	0.068050	-0.629223
34	6	0	3.624970	-0.249179	0.653008
35	16	0	2.236334	0.693953	1.094007
36	1	0	3.397085	1.437632	-2.248873
37	6	0	-5.347751	1.709063	0.576548
38	16	0	-6.974778	1.999839	-0.008952
39	6	0	-7.460181	0.351890	0.270706
40	6	0	-6.403314	-0.376676	0.777437
41	6	0	-5.204297	0.395023	0.939411
42	1	0	-4.282498	-0.014276	1.337924
43	8	0	-2.720526	1.669962	-0.577637
44	8	0	-0.460859	1.687643	0.578246
45	6	0	7.110865	0.926646	0.791399
46	6	0	7.102674	-0.384752	0.345675
47	6	0	6.423398	-0.851174	-0.868629
48	6	0	5.162123	-0.602204	-1.316042
49	6	0	7.887268	-1.258255	1.175129
50	6	0	8.464966	-0.638346	2.253564
51	16	0	8.068085	1.070300	2.236286
52	1	0	7.976932	-2.322710	0.990490
53	6	0	-6.494427	-1.785225	1.225221
54	6	0	-6.031107	-2.896906	0.617445
55	6	0	-5.327259	-3.016258	-0.679407
56	6	0	-5.935894	-3.379774	-1.862680
57	16	0	-4.757079	-3.486159	-3.140104
58	6	0	-3.437019	-3.040636	-2.075061
59	6	0	-3.913316	-2.824090	-0.804317
60	1	0	-3.289378	-2.497103	0.020722
61	6	0	-6.304080	-4.132511	1.449512
62	6	0	-6.721790	-3.587867	2.845858
63	6	0	-7.149404	-2.121030	2.549985
64	6	0	4.935176	-1.241827	-2.667824
65	6	0	6.340146	-1.703587	-3.140548
66	6	0	7.157950	-1.767516	-1.822598
67	9	0	4.096571	-2.325736	-2.570452
68	9	0	4.364649	-0.402791	-3.584532
69	9	0	6.877706	-0.756159	-3.954069
70	9	0	6.315969	-2.874312	-3.812190
71	9	0	8.455965	-1.415179	-2.025545
72	9	0	7.173546	-3.064991	-1.358656
73	9	0	-6.777685	-1.282080	3.553682
74	9	0	-8.519127	-2.047274	2.465145
75	9	0	-5.642179	-3.584072	3.669044
76	9	0	-7.698235	-4.316962	3.429002
77	9	0	-7.327037	-4.878742	0.916766
78	9	0	-5.226971	-4.959088	1.539425
79	6	0	-2.053995	-2.942739	-2.559626
80	6	0	0.623040	-2.731941	-3.454854
81	6	0	-1.758032	-2.701663	-3.914393
82	6	0	-0.974286	-3.083716	-1.659904
83	6	0	0.346288	-2.972250	-2.104381
84	6	0	-0.437522	-2.603532	-4.355360
85	1	0	1.650991	-2.648303	-3.794167
86	1	0	-2.567916	-2.569379	-4.627018

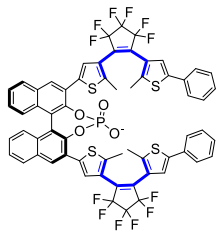
87	1	0	-1.171596	-3.307554	-0.615443
88	1	0	1.162011	-3.088448	-1.395549
89	1	0	-0.238329	-2.412071	-5.406545
90	6	0	9.307963	-1.225754	3.305478
91	6	0	10.917114	-2.393137	5.307032
92	6	0	9.329612	-0.701043	4.610962
93	6	0	10.115448	-2.343711	3.020902
94	6	0	10.904818	-2.923916	4.013317
95	6	0	10.128677	-1.276903	5.599292
96	1	0	11.537244	-2.842877	6.077829
97	1	0	8.702512	0.151375	4.860105
98	1	0	10.139058	-2.744784	2.011543
99	1	0	11.522198	-3.785213	3.771259
100	1	0	10.127380	-0.856826	6.601804
101	6	0	4.155714	-1.279074	1.607024
102	1	0	4.597773	-2.119887	1.063305
103	1	0	4.935328	-0.862795	2.257072
104	1	0	3.360047	-1.671701	2.248659
105	6	0	6.481041	2.147981	0.190221
106	1	0	7.081661	3.041903	0.389146
107	1	0	6.389833	2.037300	-0.894785
108	1	0	5.474190	2.323463	0.589376
109	6	0	-8.863500	-0.084981	-0.039218
110	1	0	-9.573933	0.274646	0.715644
111	1	0	-8.931074	-1.175855	-0.059290
112	1	0	-9.193290	0.292307	-1.014115
113	6	0	-7.379069	-3.686129	-2.139765
114	1	0	-8.001857	-3.395223	-1.289739
115	1	0	-7.537344	-4.758162	-2.311780
116	1	0	-7.740247	-3.149487	-3.024876
117	15	0	-1.568865	0.663596	-0.038469
118	8	0	-1.956755	-0.375073	0.939087
119	8	0	-0.991042	0.167758	-1.440110
120	1	0	-0.838311	-0.799729	-1.481918

Zero-point correction=	0.840379 (Hartree/Particle)
Thermal correction to Energy=	0.912969
Thermal correction to Enthalpy=	0.913913
Thermal correction to Gibbs Free Energy=	0.723824
Sum of electronic and zero-point Energies=	-5817.433601
Sum of electronic and thermal Energies=	-5817.361011
Sum of electronic and thermal Enthalpies=	-5817.360067
Sum of electronic and thermal Free Energies=	-5817.550156

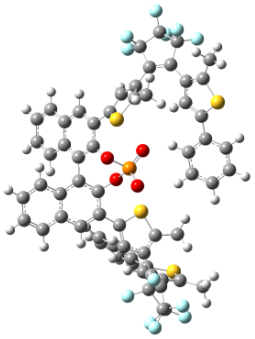
Free Energy Value for Each Optimized structure of (*S*)-DTE-BPA open-1 anion in Gas and Solvent Phase.

N.B.-Values in green color indicate gas phase free energy values. Whereas,values in blue color indicate solvent phase free energy values.

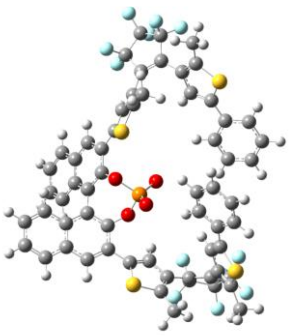
General Structure



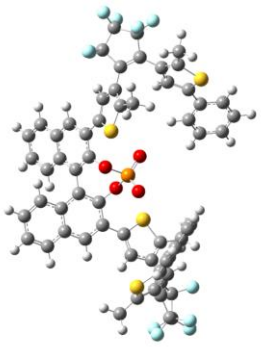
(*S*)-DTE-BPA open-**1 anion**



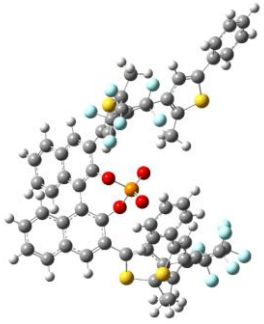
M0107- ***open isomer anion*** (Hartree/Particle)
G = -5817.017202
ZPG = 0.830194
G = -5817.120902
ZPG = 0.829059



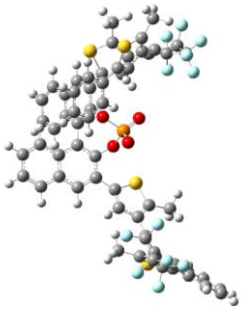
M022- ***open isomer*** (Hartree/Particle)
G = -5817.02287
ZPG = 0.830366
G = -5817.120264
ZPG =0.829168



M008- ***open isomer*** (Hartree/Particle)
G = -5817.021112
ZPG = 0.830417
G = --5817.118140
ZPG = 0.829260



M0258- ***open isomer*** (Hartree/Particle)
G = -5817.020242
ZPG = 0.829606
G = -5817.121452
ZPG = 0.828809



M0242- ***open isomer*** (Hartree/Particle)
G = -5817.019760
ZPG = 0.829798
G = -5817.122945
ZPG = 0.828642

Level of Theory Associated with Free Energy (G) values: SMD/B3LYP 6-31+G(d)//B3LYP 6-31+G(d)
[Unit of G is in Hatree. ($1E_h$= 627.50 Kcal/mol)]

open conformers	ZPG (HA)	E_{sol} (HA) (hatree)	ZPG (A^-)	E_{sol} (A^-) (hatree)
M0107	0.840600	-5818.273680	0.829059	-5817.832770
M022	**0.840477**	**-5818.274220**	**0.829168**	**- 5817.832403**
M008	0.840594	-5818.270685	0.829260	-5817.831459
M0258	0.840419	-5818.273087	0.828809	-5817.832335
M0242	0.840379	-5818.273980	0.828642	-5817.833301

M0107-openanion (gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.821050	6.329965	-4.880580
2	6	0	2.277880	5.758914	-4.132437
3	6	0	0.834778	4.297033	-2.178138
4	6	0	0.933249	6.086779	-3.832282
5	6	0	2.885804	4.706149	-3.485852
6	6	0	2.182778	3.941438	-2.512990
7	6	0	0.231887	5.377695	-2.879403
8	1	0	0.447015	6.902460	-4.360859
9	1	0	3.911539	4.431462	-3.721182
10	1	0	-0.799167	5.638708	-2.668294
11	6	0	2.792221	2.830478	-1.880327
12	6	0	2.106148	2.024612	-0.987307
13	6	0	0.764695	2.395948	-0.675947
14	6	0	0.141057	3.524580	-1.183070
15	1	0	3.828989	2.603311	-2.113105
16	6	0	-1.239296	3.870350	-0.730076
17	6	0	-3.911567	4.405524	0.049295
18	6	0	-1.558427	5.131940	-0.115708
19	6	0	-2.246504	2.927782	-0.840766
20	6	0	-3.601763	3.166833	-0.476668
21	6	0	-2.917174	5.395351	0.262070
22	1	0	-4.940228	4.621006	0.326267
23	6	0	-3.245626	6.640725	0.865940
24	6	0	-2.273844	7.583019	1.119565
25	6	0	-0.925913	7.309820	0.783585
26	6	0	-0.577646	6.118622	0.181563
27	1	0	-4.281896	6.828888	1.136983
28	1	0	-2.535328	8.528067	1.587878
29	1	0	-0.156061	8.043975	1.006429
30	1	0	0.461425	5.924900	-0.060281
31	6	0	2.758833	0.836273	-0.414861
32	6	0	3.665342	0.019869	-1.045026
33	6	0	4.226267	-0.996255	-0.200004
34	6	0	3.715219	-0.957986	1.087747
35	16	0	2.552796	0.321373	1.249321
36	1	0	3.925902	0.130569	-2.091447
37	6	0	-4.623623	2.108792	-0.603758
38	16	0	-5.112961	1.450267	-2.150581
39	6	0	-6.213730	0.326464	-1.414706
40	6	0	-6.194230	0.456202	-0.035465
41	6	0	-5.300800	1.490626	0.411112
42	1	0	-5.124270	1.719616	1.454951
43	8	0	-1.929004	1.659931	-1.333934
44	8	0	0.068338	1.575901	0.212322
45	6	0	7.582239	-2.451721	2.094095
46	6	0	7.069541	-1.789370	0.992689
47	6	0	6.365047	-2.397026	-0.152402
48	6	0	5.185274	-1.992428	-0.694108
49	6	0	7.315454	-0.373766	1.031413
50	6	0	8.015094	0.047462	2.132865
51	16	0	8.364184	-1.324466	3.167678
52	1	0	7.012653	0.292586	0.231404
53	6	0	-7.000299	-0.367682	0.874583

53	6	0	-7.000299	-0.367682	0.874583
54	6	0	-7.112463	-1.724895	0.914191
55	6	0	-6.277696	-2.712029	0.210314
56	6	0	-6.720122	-3.889901	-0.372874
57	16	0	-5.386749	-4.768958	-1.058355
58	6	0	-4.216049	-3.563674	-0.558807
59	6	0	-4.852834	-2.540813	0.096421
60	1	0	-4.326282	-1.676158	0.486703
61	6	0	-8.186276	-2.128538	1.901870
62	6	0	-8.368654	-0.881413	2.807133
63	6	0	-7.906824	0.283986	1.894419
64	6	0	4.924562	-2.693859	-2.008120
65	6	0	5.928330	-3.877588	-2.028458
66	6	0	7.037234	-3.419122	-1.044410
67	9	0	3.638680	-3.129005	-2.140588
68	9	0	5.168009	-1.868989	-3.081407
69	9	0	6.392923	-4.163354	-3.262336
70	9	0	5.318933	-4.989561	-1.533601
71	9	0	8.067976	-2.846361	-1.745233
72	9	0	7.573259	-4.484419	-0.381989
73	9	0	-7.293863	1.263197	2.624103
74	9	0	-8.994606	0.872138	1.300017
75	9	0	-7.534340	-0.980359	3.876034
76	9	0	-9.629502	-0.735115	3.267817
77	9	0	-9.388536	-2.392585	1.280708
78	9	0	-7.875808	-3.236267	2.628807
79	6	0	-2.779457	-3.733768	-0.828187
80	6	0	-0.013710	-4.031016	-1.334848
81	6	0	-2.320135	-4.390635	-1.985468
82	6	0	-1.824547	-3.236431	0.079530
83	6	0	-0.457592	-3.380986	-0.175715
84	6	0	-0.954792	-4.537620	-2.235575
85	1	0	1.049582	-4.140833	-1.529290
86	1	0	-3.037966	-4.769492	-2.708714
87	1	0	-2.150610	-2.735585	0.985052
88	1	0	0.262180	-3.004434	0.547738
89	1	0	-0.626073	-5.040931	-3.140932
90	6	0	8.449747	1.409200	2.477471
91	6	0	9.269432	4.036228	3.098804
92	6	0	9.625489	1.642698	3.214344
93	6	0	7.688194	2.519297	2.064529
94	6	0	8.098617	3.817538	2.366070
95	6	0	10.028050	2.942286	3.524150
96	1	0	9.584861	5.048178	3.338500
97	1	0	10.239697	0.802841	3.529135
98	1	0	6.759485	2.360278	1.523635
99	1	0	7.494069	4.660061	2.039859
100	1	0	10.941758	3.099323	4.091595
101	6	0	3.989254	-1.864673	2.251220
102	1	0	4.251358	-2.869344	1.904080
103	1	0	4.825887	-1.496424	2.857667
104	1	0	3.114063	-1.949100	2.903944
105	6	0	7.508512	-3.900358	2.487345
106	1	0	7.388091	-4.006675	3.571149
107	1	0	6.661609	-4.394652	2.004349
108	1	0	8.415192	-4.444898	2.197561
109	6	0	-7.032442	-0.592415	-2.272995
110	1	0	-7.282258	-0.124294	-3.231008

111	1	0	-7.969188	-0.853416	-1.770770
112	1	0	-6.496527	-1.526455	-2.484614
113	6	0	-8.103925	-4.465083	-0.494314
114	1	0	-8.826331	-3.704359	-0.805598
115	1	0	-8.451634	-4.875870	0.460828
116	1	0	-8.127496	-5.273181	-1.232046
117	15	0	-1.155867	0.644156	-0.330677
118	8	0	-1.901365	0.036427	0.789389
119	8	0	-0.540605	-0.349073	-1.421073

Zero-point correction=	0.830194 (Hartree/Particle)
Thermal correction to Energy=	0.902040
Thermal correction to Enthalpy=	0.902984
Thermal correction to Gibbs Free Energy=	0.713442
Sum of electronic and zero-point Energies=	-5816.900450
Sum of electronic and thermal Energies=	-5816.828604
Sum of electronic and thermal Enthalpies=	-5816.827660
Sum of electronic and thermal Free Energies=	-5817.017202

M022 open anion (gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.926469	8.735584	2.826134
2	6	0	-2.570955	7.837117	2.328911
3	6	0	-1.613614	5.513522	1.016378
4	6	0	-1.216458	7.740800	1.927439
5	6	0	-3.428310	6.784155	2.100561
6	6	0	-2.973856	5.597469	1.459992
7	6	0	-0.751115	6.611875	1.285775
8	1	0	-0.534911	8.562767	2.129838
9	1	0	-4.466636	6.837596	2.419774
10	1	0	0.290906	6.554488	0.991998
11	6	0	-3.843419	4.497228	1.263527
12	6	0	-3.411855	3.305210	0.707107
13	6	0	-2.045982	3.239769	0.295063
14	6	0	-1.171812	4.311435	0.359936
15	1	0	-4.882580	4.599142	1.565861
16	6	0	0.204251	4.190804	-0.208183
17	6	0	2.878696	3.983973	-1.086311
18	6	0	0.682652	5.091219	-1.221808
19	6	0	1.042066	3.173530	0.216376
20	6	0	2.403374	3.039636	-0.188790
21	6	0	2.048167	4.984396	-1.644067
22	1	0	3.922590	3.956510	-1.384464
23	6	0	2.546815	5.883915	-2.628652
24	6	0	1.725759	6.826745	-3.204899
25	6	0	0.365030	6.905622	-2.819409
26	6	0	-0.141948	6.063986	-1.851411

27	1	0	3.588535	5.800006	-2.929503
28	1	0	2.114075	7.501434	-3.963069
29	1	0	-0.287640	7.633747	-3.293705
30	1	0	-1.187688	6.135486	-1.573771
31	6	0	-4.322098	2.160994	0.552610
32	6	0	-4.408011	1.238342	-0.459773
33	6	0	-5.436775	0.257889	-0.261407
34	6	0	-6.154676	0.452674	0.904329
35	16	0	-5.546617	1.833380	1.766029
36	1	0	-3.751722	1.241846	-1.320986
37	6	0	3.294345	1.971246	0.287767
38	16	0	3.161606	1.200267	1.858282
39	6	0	4.583258	0.239215	1.604035
40	6	0	5.131377	0.493325	0.357112
41	6	0	4.397656	1.483202	-0.373126
42	1	0	4.669885	1.792670	-1.374710
43	8	0	0.543654	2.241996	1.132492
44	8	0	-1.586398	2.026500	-0.224833
45	6	0	-5.838104	-3.755229	1.043304
46	6	0	-5.172686	-2.811347	0.282514
47	6	0	-5.642860	-2.175545	-0.963811
48	6	0	-5.683100	-0.841883	-1.208511
49	6	0	-3.901925	-2.443280	0.839792
50	6	0	-3.589550	-3.087961	2.007702
51	16	0	-4.888288	-4.183174	2.441535
52	1	0	-3.256983	-1.703115	0.380002
53	6	0	6.359531	-0.146527	-0.138275
54	6	0	6.652874	-1.474093	-0.222383
55	6	0	5.718164	-2.599649	-0.089877
56	6	0	5.985839	-3.837983	0.474605
57	16	0	4.601005	-4.880286	0.333196
58	6	0	3.654732	-3.670516	-0.514243
59	6	0	4.391084	-2.521296	-0.640856
60	1	0	4.025191	-1.645627	-1.164124
61	6	0	8.107023	-1.659542	-0.601353
62	6	0	8.527486	-0.294122	-1.209017
63	6	0	7.538627	0.702899	-0.550918
64	6	0	-5.971087	-0.559747	-2.664527
65	6	0	-6.474758	-1.917381	-3.231464
66	6	0	-5.905891	-2.960908	-2.229293
67	9	0	-6.888538	0.428919	-2.848249
68	9	0	-4.836179	-0.172592	-3.335227
69	9	0	-6.090198	-2.140063	-4.504984
70	9	0	-7.834246	-1.945700	-3.183727
71	9	0	-4.741257	-3.491209	-2.722381
72	9	0	-6.765492	-4.009079	-2.070719
73	9	0	7.206455	1.707793	-1.418085
74	9	0	8.131330	1.309106	0.527308
75	9	0	8.319591	-0.321488	-2.552461
76	9	0	9.823898	0.011746	-0.988503
77	9	0	8.897244	-1.907164	0.500505
78	9	0	8.323937	-2.682234	-1.471835
79	6	0	2.296827	-3.946936	-1.007263
80	6	0	-0.291978	-4.435988	-2.015595
81	6	0	1.373825	-2.895057	-1.162155
82	6	0	1.892641	-5.249549	-1.355680
83	6	0	0.610417	-5.490963	-1.850206

84	6	0	0.097518	-3.138144	-1.669822
85	1	0	-1.288141	-4.622967	-2.408172
86	1	0	1.636322	-1.883224	-0.869554
87	1	0	2.592810	-6.076146	-1.262192
88	1	0	0.321127	-6.504168	-2.117722
89	1	0	-0.588835	-2.303568	-1.782262
90	6	0	-2.381895	-2.928155	2.830026
91	6	0	-0.054372	-2.542334	4.382000
92	6	0	-1.154074	-2.594866	2.219730
93	6	0	-2.413628	-3.077878	4.228137
94	6	0	-1.261208	-2.890743	4.993826
95	6	0	-0.005963	-2.397584	2.991020
96	1	0	0.840734	-2.393952	4.979831
97	1	0	-1.084223	-2.531756	1.137403
98	1	0	-3.350549	-3.321502	4.722643
99	1	0	-1.311282	-3.007330	6.073327
100	1	0	0.929456	-2.152121	2.494973
101	6	0	-7.304304	-0.336314	1.457759
102	1	0	-7.819484	-0.874660	0.656492
103	1	0	-6.965172	-1.076906	2.193264
104	1	0	-8.035299	0.314388	1.949656
105	6	0	-7.187516	-4.387687	0.850519
106	1	0	-7.679520	-4.568517	1.812367
107	1	0	-7.838836	-3.743636	0.253681
108	1	0	-7.110732	-5.349269	0.328667
109	6	0	5.050783	-0.708749	2.668769
110	1	0	4.763968	-0.361087	3.666756
111	1	0	6.141226	-0.803810	2.645670
112	1	0	4.628947	-1.711976	2.525111
113	6	0	7.218952	-4.360226	1.157925
114	1	0	7.635491	-3.622428	1.850097
115	1	0	8.002786	-4.609410	0.432587
116	1	0	6.994510	-5.267185	1.728130
117	15	0	-0.524399	1.129991	0.611676
118	8	0	-0.023178	-0.007853	-0.185207
119	8	0	-1.228079	0.769288	2.003378

Zero-point correction=	0.830366 (Hartree/Particle)
Thermal correction to Energy=	0.902222
Thermal correction to Enthalpy=	0.903166
Thermal correction to Gibbs Free Energy=	0.715753
Sum of electronic and zero-point Energies=	-5816.908257
Sum of electronic and thermal Energies=	-5816.836401
Sum of electronic and thermal Enthalpies=	-5816.835457
Sum of electronic and thermal Free Energies=	-5817.022870

M008-openanion (gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.837081	6.837312	3.038546
2	6	0	-3.190573	6.204245	2.436790
3	6	0	-1.475439	4.580516	0.868222
4	6	0	-1.786572	6.386803	2.477395
5	6	0	-3.728518	5.213291	1.647050
6	6	0	-2.892809	4.368556	0.863044
7	6	0	-0.952256	5.599336	1.711810
8	1	0	-1.361459	7.152628	3.120750
9	1	0	-4.803385	5.049168	1.621889
10	1	0	0.120259	5.750743	1.760720
11	6	0	-3.440142	3.316250	0.091967
12	6	0	-2.647228	2.427455	-0.616443
13	6	0	-1.240659	2.669045	-0.605647
14	6	0	-0.647732	3.737153	0.048804
15	1	0	-4.519867	3.200932	0.069538
16	6	0	0.824046	3.960296	-0.066055
17	6	0	3.637281	4.285169	-0.142073
18	6	0	1.380977	5.194037	-0.555348
19	6	0	1.696723	2.937775	0.260817
20	6	0	3.114116	3.070652	0.259136
21	6	0	2.806790	5.348804	-0.579197
22	1	0	4.715198	4.423953	-0.138301
23	6	0	3.369700	6.564763	-1.057169
24	6	0	2.566313	7.580560	-1.525273
25	6	0	1.160288	7.414760	-1.539694
26	6	0	0.583014	6.255123	-1.065752
27	1	0	4.452032	6.670743	-1.058716
28	1	0	3.007476	8.501988	-1.895581
29	1	0	0.528671	8.207112	-1.932671
30	1	0	-0.495161	6.143868	-1.093056
31	6	0	-3.264783	1.289958	-1.315690
32	6	0	-4.445697	0.677108	-0.979845
33	6	0	-4.861845	-0.368692	-1.873493
34	6	0	-3.960665	-0.538840	-2.922485
35	16	0	-2.625710	0.558016	-2.772867
36	1	0	-5.013498	0.952353	-0.100916
37	6	0	3.999389	1.950187	0.626055
38	16	0	3.930481	1.159442	2.187431
39	6	0	5.218209	0.067558	1.782274
40	6	0	5.671231	0.303050	0.494179
41	6	0	4.984482	1.392804	-0.143778
42	1	0	5.179275	1.709519	-1.161213
43	8	0	1.166032	1.687345	0.602148
44	8	0	-0.442532	1.796854	-1.347445
45	6	0	-6.901456	-0.240910	1.827896
46	6	0	-6.250414	-1.051943	0.916571
47	6	0	-6.727424	-1.352846	-0.449306
48	6	0	-6.099871	-1.125451	-1.639582
49	6	0	-5.040515	-1.622822	1.441380
50	6	0	-4.771234	-1.268226	2.738225
51	16	0	-6.019422	-0.189176	3.329513
52	1	0	-4.416391	-2.302922	0.871841
53	6	0	6.736363	-0.474437	-0.152437

54	6	0	6.848418	-1.827849	-0.264865
55	6	0	5.818938	-2.836070	0.033044
56	6	0	6.032420	-4.086375	0.594988
57	16	0	4.534668	-4.957090	0.732615
58	6	0	3.602570	-3.649835	0.028418
59	6	0	4.434019	-2.604488	-0.282697
60	1	0	4.076566	-1.680127	-0.722912
61	6	0	8.192406	-2.188942	-0.860570
62	6	0	8.678797	-0.882036	-1.541810
63	6	0	7.939150	0.223830	-0.745424
64	6	0	-6.904396	-1.741859	-2.767524
65	6	0	-8.301061	-2.022359	-2.153937
66	6	0	-7.990304	-2.159904	-0.646483
67	9	0	-7.003500	-0.942276	-3.866919
68	9	0	-6.371226	-2.937036	-3.192108
69	9	0	-8.908807	-3.103216	-2.685706
70	9	0	-9.104790	-0.941752	-2.352250
71	9	0	-7.784605	-3.482246	-0.334241
72	9	0	-9.044364	-1.751723	0.116323
73	9	0	7.615643	1.276237	-1.554732
74	9	0	8.761387	0.728027	0.230041
75	9	0	8.258013	-0.870120	-2.834468
76	9	0	10.021584	-0.743081	-1.532966
77	9	0	9.109192	-2.540481	0.107060
78	9	0	8.142540	-3.225208	-1.741302
79	6	0	2.151448	-3.768007	-0.180782
80	6	0	-0.635171	-3.983079	-0.602695
81	6	0	1.525482	-3.063379	-1.227512
82	6	0	1.352440	-4.582046	0.644891
83	6	0	-0.023280	-4.689748	0.436321
84	6	0	0.146872	-3.168304	-1.431632
85	1	0	-1.704882	-4.072967	-0.771927
86	1	0	2.113648	-2.434422	-1.887269
87	1	0	1.807962	-5.123775	1.470114
88	1	0	-0.617606	-5.321397	1.091040
89	1	0	-0.308950	-2.632439	-2.261132
90	6	0	-3.631799	-1.660525	3.582789
91	6	0	-1.431849	-2.420674	5.170909
92	6	0	-2.343632	-1.760362	3.025433
93	6	0	-3.795692	-1.938767	4.952223
94	6	0	-2.705136	-2.313291	5.738091
95	6	0	-1.256494	-2.142573	3.812005
96	1	0	-0.582856	-2.711339	5.784206
97	1	0	-2.189819	-1.503144	1.981503
98	1	0	-4.785630	-1.880345	5.397667
99	1	0	-2.852657	-2.528394	6.793385
100	1	0	-0.268281	-2.203780	3.363795
101	6	0	-3.928014	-1.503685	-4.077162
102	1	0	-4.019096	-2.540708	-3.739915
103	1	0	-4.743438	-1.314735	-4.782568
104	1	0	-2.986482	-1.410756	-4.627391
105	6	0	-8.151289	0.579794	1.675460
106	1	0	-8.036872	1.563472	2.145269
107	1	0	-8.387260	0.736289	0.619420
108	1	0	-9.016623	0.089126	2.136953
109	6	0	5.692561	-0.939247	2.788579
110	1	0	5.596234	-0.556249	3.810013

111	1	0	6.745581	-1.184465	2.618641
112	1	0	5.118798	-1.872622	2.723520
113	6	0	7.294166	-4.743951	1.080703
114	1	0	7.889675	-4.060632	1.693660
115	1	0	7.923908	-5.067589	0.243862
116	1	0	7.065883	-5.626681	1.685975
117	15	0	0.622941	0.790611	-0.636828
118	8	0	1.590527	0.257266	-1.616026
119	8	0	-0.224756	-0.294740	0.182511

Zero-point correction=	0.830417 (Hartree/Particle)
Thermal correction to Energy=	0.902100
Thermal correction to Enthalpy=	0.903044
Thermal correction to Gibbs Free Energy=	0.715833
Sum of electronic and zero-point Energies=	-5816.906528
Sum of electronic and thermal Energies=	-5816.834845
Sum of electronic and thermal Enthalpies=	-5816.833901
Sum of electronic and thermal Free Energies=	-5817.021112

M0258-openanion (gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.318676	8.436783	-4.013729
2	6	0	-2.251845	7.541202	-3.401949
3	6	0	-2.112511	5.212715	-1.790743
4	6	0	-3.428250	6.959072	-2.870936
5	6	0	-1.028672	6.959941	-3.152851
6	6	0	-0.927094	5.780974	-2.362670
7	6	0	-3.360560	5.828183	-2.083978
8	1	0	-4.395243	7.404785	-3.088527
9	1	0	-0.119051	7.386594	-3.569195
10	1	0	-4.273172	5.393041	-1.692573
11	6	0	0.326906	5.160648	-2.139070
12	6	0	0.446286	3.975691	-1.434229
13	6	0	-0.753905	3.413526	-0.905531
14	6	0	-1.993482	4.023130	-0.989078
15	1	0	1.219285	5.636312	-2.537854
16	6	0	-3.167660	3.424225	-0.286586
17	6	0	-5.481506	2.278604	0.857401
18	6	0	-3.927407	4.178479	0.675084
19	6	0	-3.533497	2.110504	-0.531862
20	6	0	-4.707066	1.504207	0.010958
21	6	0	-5.112687	3.594451	1.228773
22	1	0	-6.380712	1.849357	1.291784
23	6	0	-5.882824	4.333189	2.170170
24	6	0	-5.488581	5.588362	2.576204
25	6	0	-4.297125	6.152601	2.058994
26	6	0	-3.538516	5.468113	1.132506
27	1	0	-6.784474	3.879043	2.574646
28	1	0	-6.079931	6.141140	3.301163
29	1	0	-3.973371	7.132616	2.399378

30	1	0	-2.624963	5.913884	0.755305
31	6	0	1.754144	3.335957	-1.223417
32	6	0	2.256095	2.741211	-0.094386
33	6	0	3.606159	2.271708	-0.234102
34	6	0	4.137253	2.525599	-1.487969
35	16	0	2.964718	3.324575	-2.493117
36	1	0	1.684538	2.635655	0.819560
37	6	0	-5.113417	0.128445	-0.328880
38	16	0	-6.769553	-0.207505	-0.802252
39	6	0	-6.465840	-1.909369	-0.984152
40	6	0	-5.143612	-2.199214	-0.684995
41	6	0	-4.388385	-1.031996	-0.316428
42	1	0	-3.337744	-1.071320	-0.054453
43	8	0	-2.766013	1.355733	-1.422533
44	8	0	-0.657422	2.172777	-0.264569
45	6	0	4.196082	-1.133775	-0.718644
46	6	0	5.266429	-0.499953	-0.108764
47	6	0	5.119221	0.549131	0.911021
48	6	0	4.356664	1.674004	0.879120
49	6	0	6.536644	-1.013211	-0.542133
50	6	0	6.447940	-2.004865	-1.486710
51	16	0	4.762256	-2.345715	-1.829760
52	1	0	7.482519	-0.621818	-0.187590
53	6	0	-4.492064	-3.516382	-0.756715
54	6	0	-3.547265	-4.008789	0.091669
55	6	0	-3.126922	-3.480227	1.396822
56	6	0	-4.007431	-3.198737	2.428255
57	16	0	-3.145708	-2.599494	3.813813
58	6	0	-1.591578	-2.711577	3.007275
59	6	0	-1.759238	-3.213152	1.742600
60	1	0	-0.941720	-3.324015	1.041773
61	6	0	-2.960486	-5.298188	-0.436324
62	6	0	-3.455649	-5.380536	-1.904254
63	6	0	-4.717504	-4.476486	-1.902911
64	6	0	4.340358	2.352459	2.231333
65	6	0	5.538837	1.730446	2.999981
66	6	0	5.787308	0.386771	2.259491
67	9	0	4.450189	3.707652	2.156559
68	9	0	3.173643	2.092470	2.910926
69	9	0	5.300107	1.571080	4.319610
70	9	0	6.625879	2.534368	2.858199
71	9	0	5.236953	-0.648067	2.968587
72	9	0	7.126635	0.121720	2.172244
73	9	0	-5.825307	-5.272481	-1.703012
74	9	0	-4.896070	-3.863605	-3.105898
75	9	0	-3.702216	-6.641867	-2.318323
76	9	0	-2.520849	-4.838283	-2.731235
77	9	0	-1.595728	-5.339861	-0.378901
78	9	0	-3.409008	-6.385222	0.269182
79	6	0	-0.344540	-2.290269	3.660981
80	6	0	2.078383	-1.464992	4.848957
81	6	0	0.870597	-2.923996	3.337352
82	6	0	-0.321759	-1.244464	4.601811
83	6	0	0.876516	-0.839530	5.191219
84	6	0	2.068475	-2.509549	3.919068
85	1	0	3.013243	-1.141309	5.298048

86	1	0	0.869435	-3.755755	2.638181
87	1	0	-1.244142	-0.726956	4.853467
88	1	0	0.872510	-0.022553	5.908296
89	1	0	2.996570	-3.009145	3.653074
90	6	0	7.536578	-2.734498	-2.153480
91	6	0	9.653970	-4.109071	-3.414310
92	6	0	7.387925	-3.253699	-3.452980
93	6	0	8.766769	-2.925147	-1.495082
94	6	0	9.814616	-3.598252	-2.122453
95	6	0	8.434170	-3.936622	-4.074136
96	1	0	10.469193	-4.639406	-3.899217
97	1	0	6.453252	-3.107155	-3.988569
98	1	0	8.892515	-2.562420	-0.478795
99	1	0	10.754712	-3.736344	-1.594427
100	1	0	8.297010	-4.327645	-5.079042
101	6	0	5.509521	2.236947	-2.021180
102	1	0	6.248841	2.270765	-1.214648
103	1	0	5.566379	1.239953	-2.475350
104	1	0	5.803824	2.969688	-2.779644
105	6	0	2.723117	-0.935058	-0.514676
106	1	0	2.162856	-1.850613	-0.728936
107	1	0	2.504107	-0.649006	0.518438
108	1	0	2.334970	-0.138013	-1.161796
109	6	0	-7.591984	-2.809013	-1.411644
110	1	0	-8.558137	-2.306220	-1.303892
111	1	0	-7.619514	-3.723450	-0.811298
112	1	0	-7.487173	-3.108774	-2.461140
113	6	0	-5.497536	-3.363014	2.481326
114	1	0	-5.821215	-4.157692	1.801788
115	1	0	-6.014582	-2.441057	2.184380
116	1	0	-5.833884	-3.625576	3.490114
117	15	0	-1.273758	0.876078	-1.018307
118	8	0	-1.117945	-0.358323	-0.222853
119	8	0	-0.619689	0.840234	-2.487976

Zero-point correction=	0.829606 (Hartree/Particle)
Thermal correction to Energy=	0.901771
Thermal correction to Enthalpy=	0.902715
Thermal correction to Gibbs Free Energy=	0.712060
Sum of electronic and zero-point Energies=	-5816.902696
Sum of electronic and thermal Energies=	-5816.830532
Sum of electronic and thermal Enthalpies=	-5816.829588
Sum of electronic and thermal Free Energies=	-5817.020242

M0242 open anion (Gas phase) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.742745	7.479784	-4.009213
2	6	0	0.412977	6.731127	-3.293904
3	6	0	-0.476488	4.801098	-1.417262
4	6	0	-0.909989	6.769783	-2.790032
5	6	0	1.270668	5.733792	-2.887316

6	6	0	0.848227	4.738573	-1.961436
7	6	0	-1.341554	5.833458	-1.873704
8	1	0	-1.593899	7.542383	-3.131318
9	1	0	2.282848	5.680837	-3.281905
10	1	0	-2.359960	5.875383	-1.504125
11	6	0	1.715443	3.687547	-1.577034
12	6	0	1.303770	2.656882	-0.747819
13	6	0	-0.023140	2.738831	-0.230841
14	6	0	-0.882306	3.797729	-0.469164
15	1	0	2.732556	3.690886	-1.958602
16	6	0	-2.199050	3.860269	0.231620
17	6	0	-4.777957	3.981282	1.376694
18	6	0	-2.566441	5.002077	1.027411
19	6	0	-3.087279	2.798686	0.150510
20	6	0	-4.402102	2.831245	0.704735
21	6	0	-3.887641	5.063857	1.577643
22	1	0	-5.772118	4.036873	1.812236
23	6	0	-4.272599	6.193906	2.352206
24	6	0	-3.383192	7.214110	2.604518
25	6	0	-2.063847	7.137189	2.095711
26	6	0	-1.666795	6.062847	1.327273
27	1	0	-5.282139	6.227841	2.755273
28	1	0	-3.684567	8.069194	3.203578
29	1	0	-1.354195	7.929984	2.317428
30	1	0	-0.649519	6.019543	0.954904
31	6	0	2.219166	1.547353	-0.439628
32	6	0	3.232096	1.078254	-1.241751
33	6	0	4.046503	0.067263	-0.631260
34	6	0	3.623598	-0.250572	0.650795
35	16	0	2.234883	0.692290	1.092123
36	1	0	3.395842	1.437551	-2.250333
37	6	0	-5.349214	1.707261	0.574573
38	16	0	-6.976213	1.998224	-0.010914
39	6	0	-7.461555	0.350123	0.267957
40	6	0	-6.404689	-0.378622	0.774433
41	6	0	-5.205722	0.393063	0.936846
42	1	0	-4.283932	-0.016373	1.335240
43	8	0	-2.721903	1.668817	-0.579438
44	8	0	-0.462321	1.686082	0.576618
45	6	0	7.109425	0.925361	0.789977
46	6	0	7.101331	-0.385833	0.343654
47	6	0	6.422167	-0.851735	-0.870912
48	6	0	5.160912	-0.602623	-1.318303
49	6	0	7.885907	-1.259676	1.172767
50	6	0	8.463496	-0.640231	2.251527
51	16	0	8.066532	1.068403	2.235000
52	1	0	7.975638	-2.324042	0.987649
53	6	0	-6.495765	-1.787379	1.221567
54	6	0	-6.032346	-2.898760	0.613318
55	6	0	-5.328397	-3.017485	-0.683537
56	6	0	-5.936928	-3.380491	-1.867020
57	16	0	-4.758014	-3.486235	-3.144407
58	6	0	-3.438054	-3.041133	-2.079064
59	6	0	-3.914454	-2.825190	-0.808256
60	1	0	-3.290593	-2.498549	0.016978
61	6	0	-6.305318	-4.134758	1.444801
62	6	0	-6.723157	-3.590772	2.841365

63	6	0	-7.150822	-2.123821	2.546130
64	6	0	4.934096	-1.241640	-2.670394
65	6	0	6.339123	-1.703115	-3.143226
66	6	0	7.156834	-1.767605	-1.825245
67	9	0	4.095537	-2.325635	-2.573578
68	9	0	4.363594	-0.402214	-3.586761
69	9	0	6.876696	-0.755289	-3.956275
70	9	0	6.315053	-2.873535	-3.815404
71	9	0	8.454846	-1.415111	-2.027937
72	9	0	7.172460	-3.065291	-1.361894
73	9	0	-6.779218	-1.285311	3.550237
74	9	0	-8.520543	-2.050094	2.461223
75	9	0	-5.643607	-3.587299	3.664631
76	9	0	-7.699609	-4.320181	3.424105
77	9	0	-7.328200	-4.880796	0.911640
78	9	0	-5.228175	-4.961323	1.534415
79	6	0	-2.054999	-2.942947	-2.563483
80	6	0	0.622091	-2.731608	-3.458419
81	6	0	-1.758949	-2.701238	-3.918118
82	6	0	-0.975349	-3.084281	-1.663746
83	6	0	0.345252	-2.972547	-2.108076
84	6	0	-0.438412	-2.602840	-4.358944
85	1	0	1.650062	-2.647764	-3.797619
86	1	0	-2.568788	-2.568669	-4.630742
87	1	0	-1.172724	-3.308605	-0.619402
88	1	0	1.160929	-3.089028	-1.399237
89	1	0	-0.239151	-2.410890	-5.410027
90	6	0	9.306445	-1.228077	3.303235
91	6	0	10.915508	-2.396294	5.304373
92	6	0	9.327973	-0.703961	4.608960
93	6	0	10.114006	-2.345864	3.018208
94	6	0	10.903332	-2.926483	4.010415
95	6	0	10.126994	-1.280232	5.597085
96	1	0	11.535603	-2.846355	6.075010
97	1	0	8.700812	0.148312	4.858446
98	1	0	10.137710	-2.746475	2.008667
99	1	0	11.520773	-3.787639	3.768009
100	1	0	10.125603	-0.860613	6.599789
101	6	0	4.154323	-1.280876	1.604380
102	1	0	4.596463	-2.121419	1.060309
103	1	0	4.933869	-0.864856	2.254675
104	1	0	3.358628	-1.673836	2.245777
105	6	0	6.479584	2.146940	0.189311
106	1	0	7.080145	3.040800	0.388688
107	1	0	6.388461	2.036749	-0.895752
108	1	0	5.472695	2.322190	0.588472
109	6	0	-8.864830	-0.086675	-0.042269
110	1	0	-9.575336	0.272572	0.712705
111	1	0	-8.932348	-1.177543	-0.062844
112	1	0	-9.194567	0.291041	-1.017018
113	6	0	-7.380067	-3.686791	-2.144351
114	1	0	-8.002932	-3.396304	-1.294237
115	1	0	-7.538277	-4.758753	-2.316866
116	1	0	-7.741207	-3.149763	-3.029243
117	15	0	-1.570232	0.662261	-0.040645
118	8	0	-1.958142	-0.376873	0.936408
119	8	0	-0.992282	0.167092	-1.442470

....

Zero-point correction=	0.829798 (Hartree/Particle)
Thermal correction to Energy=	0.901982
Thermal correction to Enthalpy=	0.902926
Thermal correction to Gibbs Free Energy=	0.711775
Sum of electronic and zero-point Energies=	-5816.901738
Sum of electronic and thermal Energies=	-5816.829553
Sum of electronic and thermal Enthalpies=	-5816.828609
Sum of electronic and thermal Free Energies=	-5817.019760

M0107 open anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	2.945915	6.670554	-4.741345
2	6	0	2.423386	6.000886	-4.062344
3	6	0	1.034461	4.274461	-2.285893
4	6	0	1.072382	6.254097	-3.717038
5	6	0	3.062539	4.894647	-3.547178
6	6	0	2.389308	3.999842	-2.667867
7	6	0	0.399591	5.416131	-2.851987
8	1	0	0.558925	7.113522	-4.141875
9	1	0	4.093642	4.676473	-3.819078
10	1	0	-0.636855	5.618481	-2.603775
11	6	0	3.031793	2.843436	-2.167352
12	6	0	2.372562	1.917267	-1.374561
13	6	0	1.014235	2.197630	-1.011555
14	6	0	0.373725	3.376983	-1.383464
15	1	0	4.074628	2.686811	-2.429163
16	6	0	-0.993300	3.646135	-0.850355
17	6	0	-3.621737	4.037063	0.114368
18	6	0	-1.293121	4.815661	-0.071260
19	6	0	-1.984879	2.691306	-1.044098
20	6	0	-3.321286	2.870393	-0.565051
21	6	0	-2.634998	5.014021	0.395932
22	1	0	-4.640018	4.207610	0.455390
23	6	0	-2.949280	6.177541	1.152113
24	6	0	-1.978962	7.101924	1.472506
25	6	0	-0.643972	6.888445	1.050215
26	6	0	-0.312126	5.778483	0.300534
27	1	0	-3.975412	6.314958	1.487756
28	1	0	-2.230768	7.982843	2.058261
29	1	0	0.129251	7.602941	1.323242
30	1	0	0.717113	5.627998	-0.005790
31	6	0	3.074029	0.710505	-0.911964
32	6	0	4.250813	0.200161	-1.409596
33	6	0	4.764360	-0.920600	-0.676839
34	6	0	3.932413	-1.287284	0.374583
35	16	0	2.544512	-0.256879	0.453449
36	1	0	4.753443	0.610603	-2.276810
37	6	0	-4.358074	1.841161	-0.733209
38	16	0	-4.636075	0.973472	-2.227332
39	6	0	-5.980392	0.098550	-1.569606
40	6	0	-6.186533	0.439658	-0.239012
41	6	0	-5.268079	1.447970	0.213308
42	1	0	-5.242396	1.819604	1.229544

43	8	0	-1.683546	1.550317	-1.729945
44	8	0	0.360831	1.299480	-0.222557
45	6	0	7.538733	-2.570648	2.200022
46	6	0	7.227467	-1.687985	1.182441
47	6	0	7.032921	-2.012559	-0.245040
48	6	0	6.008171	-1.596833	-1.042956
49	6	0	7.133539	-0.328384	1.639151
50	6	0	7.381256	-0.161812	2.976706
51	16	0	7.722878	-1.718442	3.710639
52	1	0	6.916946	0.496091	0.969126
53	6	0	-7.229421	-0.138952	0.614032
54	6	0	-7.584302	-1.449441	0.782785
55	6	0	-6.864932	-2.645822	0.319863
56	6	0	-7.445472	-3.833125	-0.102942
57	16	0	-6.220812	-4.987961	-0.535266
58	6	0	-4.907239	-3.893878	-0.133854
59	6	0	-5.424182	-2.698750	0.297031
60	1	0	-4.797511	-1.872818	0.614516
61	6	0	-8.833089	-1.540844	1.629060
62	6	0	-8.916324	-0.176126	2.355234
63	6	0	-8.142405	0.770579	1.406826
64	6	0	6.326499	-1.869230	-2.498532
65	6	0	7.509841	-2.872331	-2.460645
66	6	0	8.138650	-2.628370	-1.065275
67	9	0	5.279521	-2.364732	-3.207294
68	9	0	6.734243	-0.722665	-3.146704
69	9	0	8.386949	-2.708021	-3.477173
70	9	0	7.027500	-4.143904	-2.524205
71	9	0	9.208067	-1.770543	-1.182524
72	9	0	8.654106	-3.789528	-0.553917
73	9	0	-7.492405	1.738375	2.120860
74	9	0	-9.028770	1.434245	0.590999
75	9	0	-8.270164	-0.260974	3.549582
76	9	0	-10.186564	0.225282	2.599560
77	9	0	-9.977930	-1.690070	0.867424
78	9	0	-8.831829	-2.576066	2.517075
79	6	0	-3.504418	-4.297535	-0.319522
80	6	0	-0.828536	-5.050773	-0.774855
81	6	0	-3.128859	-5.655380	-0.318856
82	6	0	-2.510553	-3.324940	-0.534766
83	6	0	-1.186200	-3.699230	-0.765953
84	6	0	-1.803379	-6.027415	-0.543728
85	1	0	0.201837	-5.341951	-0.966031
86	1	0	-3.874305	-6.424817	-0.129342
87	1	0	-2.750862	-2.266425	-0.530409
88	1	0	-0.458102	-2.917932	-0.966243
89	1	0	-1.533668	-7.081442	-0.538622
90	6	0	7.375336	1.082133	3.760105
91	6	0	7.351414	3.492400	5.227501
92	6	0	8.217518	1.257405	4.873851
93	6	0	6.514130	2.137111	3.401101
94	6	0	6.508961	3.330321	4.123032
95	6	0	8.202457	2.448391	5.600980
96	1	0	7.340199	4.420211	5.793737
97	1	0	8.901726	0.462511	5.160325
98	1	0	5.829507	2.009725	2.567459

99	1	0	5.831668	4.128628	3.830447
100	1	0	8.863564	2.562427	6.456745
101	6	0	4.041855	-2.450714	1.316238
102	1	0	4.583485	-3.279663	0.848286
103	1	0	4.578425	-2.181493	2.234917
104	1	0	3.049771	-2.815383	1.603087
105	6	0	7.664161	-4.067982	2.189166
106	1	0	7.264903	-4.500655	3.113531
107	1	0	7.110588	-4.497270	1.350101
108	1	0	8.708573	-4.388989	2.092588
109	6	0	-6.740395	-0.862462	-2.435897
110	1	0	-6.751711	-0.529197	-3.479460
111	1	0	-7.777856	-0.948965	-2.096819
112	1	0	-6.297558	-1.866219	-2.409336
113	6	0	-8.886927	-4.230655	-0.266611
114	1	0	-9.458681	-3.458251	-0.790337
115	1	0	-9.374125	-4.399531	0.700950
116	1	0	-8.967855	-5.156810	-0.845158
117	15	0	-0.865130	0.307303	-0.905357
118	8	0	-1.683615	-0.160812	0.253520
119	8	0	-0.272777	-0.568378	-1.958667

Zero-point correction=	0.829059 (Hartree/Particle)
Thermal correction to Energy=	0.901123
Thermal correction to Enthalpy=	0.902067
Thermal correction to Gibbs Free Energy=	0.711868
Sum of electronic and zero-point Energies=	-5817.003711
Sum of electronic and thermal Energies=	-5816.931647
Sum of electronic and thermal Enthalpies=	-5816.930702
Sum of electronic and thermal Free Energies=	-5817.120902

M022-open anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.717368	8.775341	2.906386
2	6	0	-2.364722	7.894620	2.374845
3	6	0	-1.416127	5.611423	0.974626
4	6	0	-0.992350	7.765338	2.048642
5	6	0	-3.243177	6.890407	2.031124
6	6	0	-2.796173	5.726091	1.345700
7	6	0	-0.533046	6.656774	1.367355
8	1	0	-0.292070	8.543970	2.341938
9	1	0	-4.296735	6.964229	2.294252
10	1	0	0.522355	6.571187	1.133640
11	6	0	-3.686206	4.667678	1.044663
12	6	0	-3.263938	3.495149	0.441279
13	6	0	-1.883057	3.398940	0.059191
14	6	0	-0.984092	4.440786	0.262759

14	6	0	-0.984092	4.440786	0.262759
15	1	0	-4.732848	4.786354	1.316382
16	6	0	0.421376	4.284939	-0.214608
17	6	0	3.140838	3.988617	-0.913079
18	6	0	1.022221	5.221467	-1.121953
19	6	0	1.159595	3.181810	0.203116
20	6	0	2.544853	3.017470	-0.124918
21	6	0	2.408997	5.071459	-1.454597
22	1	0	4.201884	3.922379	-1.138015
23	6	0	3.023360	6.008764	-2.332460
24	6	0	2.298560	7.035664	-2.896267
25	6	0	0.918011	7.161636	-2.603430
26	6	0	0.299814	6.281517	-1.739245
27	1	0	4.079697	5.886231	-2.564037
28	1	0	2.777348	7.738472	-3.574005
29	1	0	0.338031	7.955666	-3.068021
30	1	0	-0.759685	6.387430	-1.532755
31	6	0	-4.193214	2.377058	0.233761
32	6	0	-4.176230	1.367305	-0.694434
33	6	0	-5.230515	0.407523	-0.527280
34	6	0	-6.080267	0.708182	0.522297
35	16	0	-5.560689	2.159755	1.319244
36	1	0	-3.406557	1.282560	-1.448977
37	6	0	3.336672	1.872370	0.345932
38	16	0	2.958097	0.949326	1.787548
39	6	0	4.359147	-0.054396	1.618415
40	6	0	5.081619	0.290890	0.484474
41	6	0	4.496957	1.394498	-0.218356
42	1	0	4.906490	1.784229	-1.141738
43	8	0	0.570626	2.243407	1.001568
44	8	0	-1.445439	2.264740	-0.559244
45	6	0	-6.168572	-3.480056	0.980097
46	6	0	-5.286118	-2.633183	0.335512
47	6	0	-5.453012	-2.080281	-1.023978
48	6	0	-5.362591	-0.773840	-1.388867
49	6	0	-4.124272	-2.324024	1.126226
50	6	0	-4.102193	-2.935409	2.354655
51	16	0	-5.560538	-3.896795	2.558210
52	1	0	-3.326403	-1.678727	0.774127
53	6	0	6.314548	-0.383119	0.061456
54	6	0	6.544907	-1.719684	-0.103316
55	6	0	5.544190	-2.794787	-0.142010
56	6	0	5.711972	-4.098171	0.301965
57	16	0	4.278144	-5.033731	-0.007158
58	6	0	3.442295	-3.685365	-0.758919
59	6	0	4.250011	-2.579202	-0.736972
60	1	0	3.949377	-1.631275	-1.167249
61	6	0	8.012863	-1.963115	-0.363912
62	6	0	8.563300	-0.586393	-0.817050
63	6	0	7.573552	0.417371	-0.175113
64	6	0	-5.362233	-0.627325	-2.893878
65	6	0	-5.842203	-2.008071	-3.417891
66	6	0	-5.518073	-2.969477	-2.244591
67	9	0	-6.174608	0.376176	-3.335793
68	9	0	-4.110545	-0.363191	-3.387266
69	9	0	-5.263771	-2.372722	-4.583715
70	9	0	-7.191625	-1.974635	-3.612499
71	9	0	-4.313312	-3.587026	-2.472532

72	9	0	-6.443537	-3.975008	-2.170945
73	9	0	7.394602	1.505738	-0.984695
74	9	0	8.100221	0.901236	0.998537
75	9	0	8.492668	-0.499193	-2.173376
76	9	0	9.851651	-0.379635	-0.455473
77	9	0	8.692913	-2.346428	0.776753
78	9	0	8.262810	-2.926945	-1.295896
79	6	0	2.081246	-3.821381	-1.299902
80	6	0	-0.522206	-4.046091	-2.352762
81	6	0	1.211750	-2.714808	-1.306117
82	6	0	1.621813	-5.044189	-1.825928
83	6	0	0.330826	-5.154984	-2.343473
84	6	0	-0.074446	-2.827461	-1.834353
85	1	0	-1.529114	-4.132781	-2.753182
86	1	0	1.505633	-1.759684	-0.881775
87	1	0	2.284364	-5.906830	-1.847586
88	1	0	-0.006273	-6.107598	-2.746244
89	1	0	-0.711820	-1.948725	-1.815067
90	6	0	-3.076736	-2.864330	3.406933
91	6	0	-1.102706	-2.710169	5.416385
92	6	0	-2.112139	-1.837372	3.386825
93	6	0	-3.030447	-3.809959	4.449667
94	6	0	-2.056635	-3.731956	5.445657
95	6	0	-1.136096	-1.770682	4.381135
96	1	0	-0.340932	-2.649412	6.190308
97	1	0	-2.102786	-1.079383	2.607828
98	1	0	-3.750694	-4.624653	4.476667
99	1	0	-2.039934	-4.475847	6.239190
100	1	0	-0.405633	-0.967320	4.336788
101	6	0	-7.303284	-0.016457	1.000671
102	1	0	-7.739519	-0.610390	0.191282
103	1	0	-7.068064	-0.701798	1.825049
104	1	0	-8.067765	0.684829	1.354090
105	6	0	-7.512396	-4.001649	0.554660
106	1	0	-8.204724	-4.038831	1.403978
107	1	0	-7.955669	-3.360817	-0.212315
108	1	0	-7.444106	-5.013560	0.136068
109	6	0	4.631751	-1.134622	2.623604
110	1	0	4.266050	-0.852872	3.617018
111	1	0	5.706664	-1.329285	2.700828
112	1	0	4.142653	-2.076284	2.342309
113	6	0	6.870958	-4.763836	0.991443
114	1	0	7.276797	-4.134034	1.789020
115	1	0	7.689285	-4.976908	0.292958
116	1	0	6.561159	-5.713595	1.439718
117	15	0	-0.526495	1.132154	0.311384
118	8	0	0.157691	0.302847	-0.725254
119	8	0	-1.320409	0.599483	1.460989

Zero-point correction=	0.829168 (Hartree/Particle)
Thermal correction to Energy=	0.901174
Thermal correction to Enthalpy=	0.902118
Thermal correction to Gibbs Free Energy=	0.712139
Sum of electronic and zero-point Energies=	-5817.003235
Sum of electronic and thermal Energies=	-5816.931229
Sum of electronic and thermal Enthalpies=	-5816.930285
Sum of electronic and thermal Free Energies=	-5817.120264

M008-open anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-3.912575	7.268889	2.048988
2	6	0	-3.313500	6.508774	1.553174
3	6	0	-1.722515	4.544595	0.256461
4	6	0	-1.902733	6.632030	1.513850
5	6	0	-3.917351	5.412908	0.976693
6	6	0	-3.147472	4.401736	0.335803
7	6	0	-1.131313	5.678646	0.881729
8	1	0	-1.421761	7.482777	1.990862
9	1	0	-4.998375	5.293132	1.017373
10	1	0	-0.052085	5.784611	0.868437
11	6	0	-3.763277	3.252152	-0.214068
12	6	0	-3.027349	2.220227	-0.771304
13	6	0	-1.605563	2.378213	-0.849771
14	6	0	-0.959227	3.530191	-0.415186
15	1	0	-4.847586	3.183376	-0.183090
16	6	0	0.513388	3.654353	-0.619690
17	6	0	3.322467	3.864767	-0.817287
18	6	0	1.089039	4.753166	-1.343278
19	6	0	1.349738	2.654662	-0.133719
20	6	0	2.777597	2.746052	-0.208676
21	6	0	2.517131	4.859227	-1.421047
22	1	0	4.401658	3.989784	-0.844596
23	6	0	3.100913	5.957943	-2.112682
24	6	0	2.316721	6.901222	-2.739624
25	6	0	0.905975	6.776264	-2.701337
26	6	0	0.310781	5.734040	-2.020746
27	1	0	4.186310	6.028591	-2.150292
28	1	0	2.775366	7.730262	-3.273320
29	1	0	0.285411	7.505367	-3.217112
30	1	0	-0.770387	5.649678	-2.008404
31	6	0	-3.705754	1.009043	-1.253751
32	6	0	-4.915775	0.520172	-0.828947
33	6	0	-5.369743	-0.651278	-1.526004
34	6	0	-4.469634	-1.042690	-2.516149
35	16	0	-3.083601	-0.007797	-2.535145
36	1	0	-5.476082	0.971884	-0.020360
37	6	0	3.663701	1.707554	0.335299
38	16	0	3.226608	0.649487	1.662668
39	6	0	4.782303	-0.111366	1.682686
40	6	0	5.601645	0.410996	0.691032
41	6	0	4.957688	1.452241	-0.054700
42	1	0	5.431420	1.958274	-0.886420
43	8	0	0.804028	1.571276	0.491738
44	8	0	-0.875704	1.377645	-1.423455
45	6	0	-7.216479	-0.117202	2.289483
46	6	0	-6.636787	-0.964399	1.361820
47	6	0	-7.219042	-1.366027	0.065492
48	6	0	-6.626266	-1.314012	-1.166585
49	6	0	-5.358383	-1.467974	1.790384
50	6	0	-4.970484	-1.035796	3.030170
51	16	0	-6.190014	0.039023	3.689580
52	1	0	-4.759338	-2.144838	1.191299
53	6	0	6.977386	-0.035035	0.444541

54	6	0	7.447953	-1.306860	0.278334
55	6	0	6.656918	-2.525098	0.055075
56	6	0	6.971692	-3.805558	0.485327
57	16	0	5.777243	-4.942950	-0.068234
58	6	0	4.849211	-3.709379	-0.904020
59	6	0	5.448148	-2.490025	-0.727793
60	1	0	5.060374	-1.581461	-1.173211
61	6	0	8.958022	-1.299229	0.238802
62	6	0	9.333201	0.169680	-0.084873
63	6	0	8.108370	0.967015	0.428240
64	6	0	-7.495849	-2.024243	-2.182931
65	6	0	-8.881646	-2.141797	-1.501014
66	6	0	-8.527305	-2.113813	0.002276
67	9	0	-7.589830	-1.376130	-3.379986
68	9	0	-7.048989	-3.297296	-2.461473
69	9	0	-9.573597	-3.242159	-1.876875
70	9	0	-9.636212	-1.050081	-1.812434
71	9	0	-8.395798	-3.402487	0.469064
72	9	0	-9.544305	-1.562319	0.732288
73	9	0	7.873219	2.056174	-0.365280
74	9	0	8.370200	1.461662	1.683249
75	9	0	9.446344	0.317110	-1.433094
76	9	0	10.503065	0.559179	0.474115
77	9	0	9.517980	-1.629660	1.458488
78	9	0	9.497258	-2.160165	-0.671290
79	6	0	3.625253	-4.035492	-1.651991
80	6	0	1.279754	-4.626360	-3.094630
81	6	0	2.595283	-3.083604	-1.768061
82	6	0	3.457366	-5.290872	-2.267890
83	6	0	2.293596	-5.583689	-2.979569
84	6	0	1.436599	-3.376938	-2.487510
85	1	0	0.372694	-4.856501	-3.648866
86	1	0	2.660702	-2.112320	-1.287297
87	1	0	4.249364	-6.034082	-2.206402
88	1	0	2.183260	-6.558116	-3.450442
89	1	0	0.666991	-2.613046	-2.543455
90	6	0	-3.727102	-1.332141	3.761662
91	6	0	-1.334521	-1.898583	5.127417
92	6	0	-2.497955	-1.329808	3.077500
93	6	0	-3.739531	-1.611199	5.141250
94	6	0	-2.551767	-1.892286	5.817806
95	6	0	-1.313268	-1.614188	3.759030
96	1	0	-0.409004	-2.113988	5.656705
97	1	0	-2.438161	-1.064936	2.025842
98	1	0	-4.685116	-1.625973	5.678789
99	1	0	-2.578258	-2.111358	6.883049
100	1	0	-0.380160	-1.585048	3.203845
101	6	0	-4.475290	-2.214337	-3.460505
102	1	0	-4.585700	-3.163117	-2.925146
103	1	0	-5.292686	-2.146530	-4.186349
104	1	0	-3.535532	-2.255837	-4.020283
105	6	0	-8.485789	0.686157	2.221780
106	1	0	-8.343688	1.677157	2.668525
107	1	0	-8.801872	0.828160	1.184873
108	1	0	-9.310685	0.195782	2.753378
109	6	0	5.073963	-1.191922	2.682240
110	1	0	4.521478	-1.028878	3.613993

111	1	0	6.142097	-1.218959	2.922335
112	1	0	4.795065	-2.181254	2.296807
113	6	0	8.109096	-4.310638	1.329606
114	1	0	8.278833	-3.666406	2.197710
115	1	0	9.046952	-4.351030	0.762523
116	1	0	7.899640	-5.320376	1.697682
117	15	0	0.061041	0.347019	-0.436285
118	8	0	1.057132	-0.274952	-1.359638
119	8	0	-0.818621	-0.387566	0.520821

Zero-point correction=	0.829260 (Hartree/Particle)
Thermal correction to Energy=	0.901112
Thermal correction to Enthalpy=	0.902057
Thermal correction to Gibbs Free Energy=	0.713318
Sum of electronic and zero-point Energies=	-5817.002198
Sum of electronic and thermal Energies=	-5816.930346
Sum of electronic and thermal Enthalpies=	-5816.929402
Sum of electronic and thermal Free Energies=	-5817.118140

M0242-open anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.609497	8.016022	2.226598
2	6	0	-0.368925	7.118454	1.661740
3	6	0	0.284272	4.789945	0.169856
4	6	0	0.862560	7.026596	0.966771
5	6	0	-1.247635	6.058260	1.631966
6	6	0	-0.942123	4.870218	0.908795
7	6	0	1.177375	5.896538	0.240840
8	1	0	1.569921	7.851434	1.010834
9	1	0	-2.187880	6.104870	2.178369
10	1	0	2.128746	5.839609	-0.276404
11	6	0	-1.825451	3.766166	0.913049
12	6	0	-1.515570	2.568697	0.287604
13	6	0	-0.278466	2.498397	-0.434418
14	6	0	0.569569	3.594098	-0.572027
15	1	0	-2.768694	3.874481	1.440936
16	6	0	1.770323	3.485586	-1.451783
17	6	0	4.176402	3.323736	-2.928669
18	6	0	1.999949	4.402135	-2.534875
19	6	0	2.683740	2.458208	-1.232671
20	6	0	3.918154	2.375840	-1.957890

21	6	0	3.232788	4.327134	-3.263838
22	1	0	5.109155	3.274810	-3.486247
23	6	0	3.475101	5.238801	-4.328495
24	6	0	2.533766	6.178182	-4.689574
25	6	0	1.299913	6.232826	-3.996096
26	6	0	1.042381	5.371381	-2.949602
27	1	0	4.419641	5.168973	-4.864776
28	1	0	2.728181	6.864561	-5.510342
29	1	0	0.544702	6.956350	-4.294571
30	1	0	0.087960	5.421507	-2.436958
31	6	0	-2.453014	1.436523	0.353561
32	6	0	-3.551681	1.326233	1.176786
33	6	0	-4.346812	0.156057	0.948295
34	6	0	-3.813937	-0.653802	-0.047804
35	16	0	-2.359078	0.029236	-0.689822
36	1	0	-3.803544	2.061900	1.929365
37	6	0	4.907812	1.326956	-1.642397
38	16	0	6.530242	1.769134	-1.134161
39	6	0	7.006107	0.109505	-0.928650
40	6	0	5.955690	-0.730660	-1.248715
41	6	0	4.768344	-0.034413	-1.659793
42	1	0	3.828421	-0.517997	-1.912469
43	8	0	2.448788	1.555433	-0.241782
44	8	0	0.031271	1.328277	-1.060152
45	6	0	-7.169284	0.282886	-1.084312
46	6	0	-7.277073	-0.705283	-0.120770
47	6	0	-6.770701	-0.593095	1.254429
48	6	0	-5.559501	-0.160702	1.708496
49	6	0	-8.000765	-1.855442	-0.587159
50	6	0	-8.419715	-1.767643	-1.890575
51	16	0	-7.939425	-0.220168	-2.561900
52	1	0	-8.159925	-2.736086	0.024914
53	6	0	6.061222	-2.199657	-1.191730
54	6	0	6.269193	-2.987862	-0.102668
55	6	0	6.209670	-2.578026	1.309060
56	6	0	7.004777	-3.050603	2.341296
57	16	0	6.536613	-2.319397	3.848832
58	6	0	5.258200	-1.371416	3.105452
59	6	0	5.227621	-1.626681	1.759141
60	1	0	4.516759	-1.156781	1.090181
61	6	0	6.482774	-4.420971	-0.534983
62	6	0	5.917741	-4.483439	-1.979557
63	6	0	6.026770	-3.014126	-2.462742
64	6	0	-5.541503	-0.131830	3.224333
65	6	0	-7.017579	-0.356099	3.652761
66	6	0	-7.663315	-1.000795	2.399210
67	9	0	-4.756941	-1.130935	3.733229
68	9	0	-5.065737	1.038867	3.747322
69	9	0	-7.613162	0.844670	3.893192
70	9	0	-7.141524	-1.112602	4.766790
71	9	0	-8.961580	-0.605182	2.251202
72	9	0	-7.702307	-2.372460	2.558092
73	9	0	5.005791	-2.687883	-3.298822
74	9	0	7.187826	-2.855841	-3.190139
75	9	0	4.615115	-4.861627	-1.937895
76	9	0	6.582187	-5.361452	-2.770282
77	9	0	7.823980	-4.754535	-0.579304

78	9	0	6.215503	-5.249077	0.336435
79	6	0	5.554967	-0.202197	3.986262
80	6	0	4.296734	1.612299	5.744967
81	6	0	6.248143	0.335681	5.088513
82	6	0	4.216061	0.184596	3.784066
83	6	0	3.600228	1.087673	4.651710
84	6	0	5.624379	1.229205	5.960575
85	1	0	3.811859	2.312318	6.421333
86	1	0	7.288724	0.068436	5.259076
87	1	0	3.628933	-0.210908	2.960922
88	1	0	2.568110	1.367441	4.459831
89	1	0	6.180831	1.632422	6.803659
90	6	0	-9.553869	-2.708976	-2.399004
91	6	0	-11.070589	-4.607566	-3.838503
92	6	0	-9.488053	-2.772190	-3.804216
93	6	0	-10.402000	-3.614120	-1.730365
94	6	0	-11.144650	-4.556035	-2.442352
95	6	0	-10.241170	-3.708042	-4.514829
96	1	0	-11.653619	-5.338995	-4.392283
97	1	0	-8.827485	-2.098487	-4.344404
98	1	0	-10.491145	-3.564977	-0.648668
99	1	0	-11.792444	-5.244141	-1.904582
100	1	0	-10.169987	-3.739940	-5.599275
101	6	0	-4.541730	-2.060910	-0.461531
102	1	0	-5.051001	-2.592101	0.349077
103	1	0	-5.254513	-1.960635	-1.290103
104	1	0	-3.714991	-2.689914	-0.808800
105	6	0	-6.813367	1.648760	-0.790877
106	1	0	-7.339892	2.371768	-1.423037
107	1	0	-6.826589	2.023597	0.237513
108	1	0	-5.765775	1.617153	-1.114624
109	6	0	8.388842	-0.116802	-0.920409
110	1	0	9.065518	0.548528	-1.468773
111	1	0	8.651696	-1.147837	-1.176423
112	1	0	8.582446	0.021805	0.151729
113	6	0	8.845694	-3.859415	1.785887
114	1	0	9.345265	-3.694710	0.826130
115	1	0	8.475850	-4.891930	1.793330
116	1	0	9.599859	-3.772841	2.574804
117	15	0	1.115004	0.250733	-0.508979
118	8	0	1.460012	-0.668834	-1.636353
119	8	0	0.815776	-0.176703	0.891555

Zero-point correction=	0.828642 (Hartree/Particle)
Thermal correction to Energy=	0.900001
Thermal correction to Enthalpy=	0.900945
Thermal correction to Gibbs Free Energy=	0.710356
Sum of electronic and zero-point Energies=	-5817.004659
Sum of electronic and thermal Energies=	-5816.933301
Sum of electronic and thermal Enthalpies=	-5816.932356
Sum of electronic and thermal Free Energies=	-5817.122945

M0258-open anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.546435	8.322009	-4.158118
2	6	0	-2.468143	7.440514	-3.526077
3	6	0	-2.295451	5.141687	-1.863856
4	6	0	-3.638370	6.759707	-3.110065
5	6	0	-1.232878	6.966836	-3.140916
6	6	0	-1.112175	5.808007	-2.324196
7	6	0	-3.553296	5.644482	-2.301861
8	1	0	-4.613744	7.114528	-3.434958
9	1	0	-0.322995	7.464724	-3.470925
10	1	0	-4.459769	5.130677	-2.001812
11	6	0	0.158145	5.287820	-1.976320
12	6	0	0.300114	4.123899	-1.242074
13	6	0	-0.889992	3.469367	-0.781152
14	6	0	-2.159083	3.982761	-1.024670
15	1	0	1.043924	5.821173	-2.314446
16	6	0	-3.343558	3.277006	-0.454103
17	6	0	-5.661109	1.922458	0.420995
18	6	0	-4.287160	3.958594	0.388266
19	6	0	-3.524672	1.920598	-0.723056
20	6	0	-4.710005	1.225844	-0.301926
21	6	0	-5.473663	3.271969	0.806482
22	1	0	-6.560730	1.408265	0.752267
23	6	0	-6.421919	3.943506	1.627340
24	6	0	-6.206462	5.236912	2.050887
25	6	0	-5.017439	5.907151	1.671597
26	6	0	-4.087129	5.286248	0.863801
27	1	0	-7.319643	3.406129	1.927603
28	1	0	-6.935255	5.737067	2.684397
29	1	0	-4.831537	6.918505	2.025764
30	1	0	-3.177751	5.811399	0.592877
31	6	0	1.629373	3.560116	-0.969981
32	6	0	2.094843	2.877995	0.124493
33	6	0	3.459827	2.449768	0.001976
34	6	0	4.043204	2.828643	-1.195462
35	16	0	2.900993	3.694302	-2.173440
36	1	0	1.471640	2.650867	0.979804
37	6	0	-4.930297	-0.191364	-0.640794
38	16	0	-6.477168	-0.722694	-1.284899
39	6	0	-5.970038	-2.382751	-1.378075
40	6	0	-4.666804	-2.511731	-0.921920
41	6	0	-4.087145	-1.259918	-0.511824
42	1	0	-3.068023	-1.151067	-0.149703
43	8	0	-2.613665	1.252489	-1.480735
44	8	0	-0.773429	2.313278	-0.064937
45	6	0	3.920394	-0.914634	-0.789752
46	6	0	5.010883	-0.358988	-0.136552
47	6	0	4.898657	0.583818	0.987985
48	6	0	4.177469	1.734466	1.064392
49	6	0	6.268600	-0.830844	-0.644958
50	6	0	6.155633	-1.715063	-1.688826
51	16	0	4.460596	-2.000284	-2.039470
52	1	0	7.222403	-0.482316	-0.266573
53	6	0	-3.876452	-3.749000	-0.857187

54	6	0	-3.002147	-4.104018	0.125138
55	6	0	-2.827585	-3.496949	1.453307
56	6	0	-3.864566	-3.350115	2.357757
57	16	0	-3.286215	-2.631302	3.830744
58	6	0	-1.641569	-2.509656	3.228359
59	6	0	-1.571283	-3.024187	1.959880
60	1	0	-0.672629	-2.986223	1.357810
61	6	0	-2.222544	-5.338515	-0.254488
62	6	0	-2.524695	-5.545963	-1.761657
63	6	0	-3.858424	-4.777861	-1.963617
64	6	0	4.186064	2.283569	2.473099
65	6	0	5.356828	1.542046	3.176959
66	6	0	5.563186	0.271455	2.307154
67	9	0	4.363877	3.635216	2.525588
68	9	0	3.013182	2.019481	3.134246
69	9	0	5.107851	1.259276	4.476923
70	9	0	6.476747	2.315862	3.126588
71	9	0	4.996773	-0.815909	2.922077
72	9	0	6.899710	-0.020270	2.189769
73	9	0	-4.900224	-5.681134	-1.846276
74	9	0	-3.951047	-4.254031	-3.216060
75	9	0	-2.604209	-6.851840	-2.116641
76	9	0	-1.552632	-4.968131	-2.512532
77	9	0	-0.879094	-5.231403	-0.032610
78	9	0	-2.637520	-6.442046	0.456889
79	6	0	-0.569873	-1.904139	4.029251
80	6	0	1.521199	-0.725264	5.515780
81	6	0	0.768242	-2.295262	3.831205
82	6	0	-0.837398	-0.916499	4.994993
83	6	0	0.196176	-0.338112	5.732568
84	6	0	1.801108	-1.706044	4.558950
85	1	0	2.328892	-0.260552	6.075153
86	1	0	0.995798	-3.069424	3.103915
87	1	0	-1.858228	-0.574402	5.145194
88	1	0	-0.034193	0.434079	6.462803
89	1	0	2.828340	-2.010865	4.376720
90	6	0	7.228567	-2.367311	-2.451075
91	6	0	9.320308	-3.600297	-3.901086
92	6	0	7.038119	-2.792379	-3.780130
93	6	0	8.491232	-2.582485	-1.862886
94	6	0	9.524151	-3.183355	-2.581477
95	6	0	8.069472	-3.404610	-4.493264
96	1	0	10.124093	-4.075325	-4.457955
97	1	0	6.078837	-2.627712	-4.264020
98	1	0	8.654053	-2.294019	-0.828209
99	1	0	10.488282	-3.339406	-2.103030
100	1	0	7.894998	-3.722197	-5.518504
101	6	0	5.441477	2.603848	-1.691247
102	1	0	6.140238	2.517082	-0.852792
103	1	0	5.518478	1.680367	-2.279176
104	1	0	5.776171	3.433098	-2.324432
105	6	0	2.452827	-0.749222	-0.540352
106	1	0	1.927312	-1.706651	-0.620529
107	1	0	2.270597	-0.355837	0.463087
108	1	0	1.971888	-0.070453	-1.256349
109	6	0	-6.932455	-3.414687	-1.898626
110	1	0	-7.950204	-3.012839	-1.940994

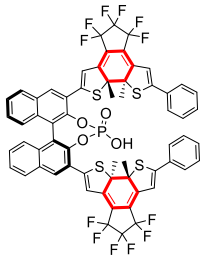
111	1	0	-6.948943	-4.304779	-1.261251
112	1	0	-6.661842	-3.742470	-2.909850
113	6	0	-5.311944	-3.716628	2.214146
114	1	0	-5.429007	-4.561847	1.528097
115	1	0	-5.897194	-2.879749	1.810563
116	1	0	-5.749935	-4.000295	3.177731
117	15	0	-1.067184	0.855933	-0.890611
118	8	0	-1.187424	-0.188736	0.175393
119	8	0	-0.182034	0.759722	-2.089364

Zero-point correction=	0.828809 (Hartree/Particle)
Thermal correction to Energy=	0.900956
Thermal correction to Enthalpy=	0.901900
Thermal correction to Gibbs Free Energy=	0.710903
Sum of electronic and zero-point Energies=	-5817.003546
Sum of electronic and thermal Energies=	-5816.931399
Sum of electronic and thermal Enthalpies=	-5816.930455
Sum of electronic and thermal Free Energies=	-5817.121452

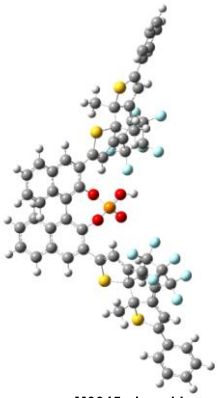
Free Energy Value for Each Optimized structure of (*S*)-DTE-BPA closed-1 in Gas and Solvent Phase.

N.B.-Values in green color indicate gas phase free energy values. Whereas,values in blue color indicate solvent phase free energy values.

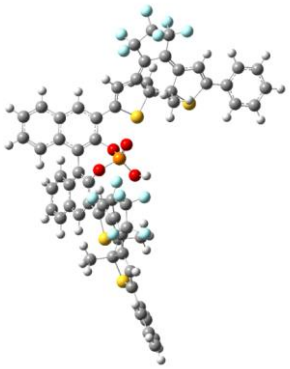
General Structure



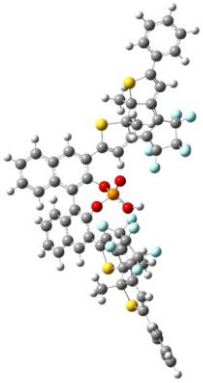
(*S*)-DTE-BPA closed-**1**



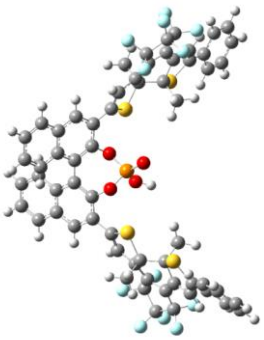
M0045-closed isomer
ZPG= 0.845580
G= -5817.444933
ZPG= 0.843753
G= -5817.502029



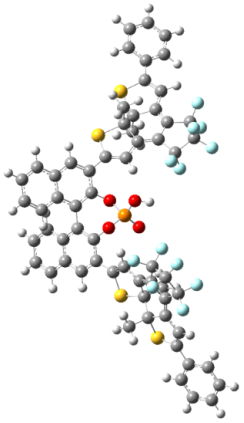
M0107-closed isomer
ZPG= 0.845502
G= -5817.443003
ZPG= 0.844046
G= -5817.499348



M0030-closed isomer
ZPG= 0.845595
G= -5817.444842
ZPG= 0.843409
G= -5817.501840



M0167-closed isomer
ZPG= 0.845364
G= -5817.443318
ZPG= 0.843772
G= -5817.499991



M0169-closed isomer
ZPG= 0.845721
G= -5817.442719
ZPG= 0.843613
G= -5817.497306

M030-closed gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.972724	-0.265857	-0.419683
2	6	0	-4.516064	0.096123	1.001156
3	6	0	-3.618069	1.229856	1.003403
4	6	0	-3.584613	1.896730	-0.149303
5	16	0	-4.652514	1.250809	-1.411788
6	6	0	-4.937282	-0.655612	2.003623
7	6	0	-5.927430	-1.706783	1.805567
8	6	0	-6.026322	-2.486908	3.065615
9	6	0	-5.641228	-1.446722	4.114448
10	6	0	-4.525739	-0.656104	3.435898
11	9	0	-4.365119	0.587721	3.968042
12	9	0	-3.355072	-1.335301	3.644016
13	9	0	-6.706508	-0.613950	4.289090
14	9	0	-7.257132	-3.028383	3.283765
15	9	0	-5.112098	-3.504351	3.142054
16	9	0	-5.284595	-1.975918	5.302492
17	6	0	-7.907069	-2.753292	-1.019627
18	6	0	-7.591164	-2.799575	0.276577
19	6	0	-6.617781	-1.810249	0.683073
20	6	0	-6.449202	-0.712319	-0.376133
21	16	0	-7.083437	-1.470410	-1.929358
22	6	0	-8.836943	-3.657335	-1.719819
23	6	0	-2.279003	7.306084	-2.757020
24	6	0	-0.909534	7.337756	-2.411947
25	6	0	-0.364577	6.361974	-1.641338
26	6	0	-1.158237	5.285881	-1.165910
27	6	0	-2.513721	5.235965	-1.544303
28	6	0	-3.058288	6.280195	-2.335508
29	6	0	-0.625821	4.229513	-0.358351
30	6	0	-1.416804	3.161084	-0.074544
31	6	0	-2.775413	3.085925	-0.465233
32	6	0	-3.301432	4.126443	-1.165352
33	6	0	0.783993	4.265763	0.134407
34	6	0	1.271929	5.342554	0.941666
35	6	0	2.631168	5.348400	1.310650
36	6	0	3.464286	4.273001	0.928733
37	6	0	2.982827	3.208225	0.231529
38	6	0	1.621388	3.238045	-0.160318
39	6	0	0.435222	6.380578	1.426390
40	6	0	0.942760	7.375084	2.198812
41	6	0	2.314222	7.399817	2.535716
42	6	0	3.134359	6.410242	2.105183
43	8	0	-0.879813	2.060578	0.603154
44	8	0	1.098702	2.119073	-0.824901
45	6	0	6.650527	-0.647214	0.280224
46	6	0	6.671839	-1.873599	-0.645561
47	6	0	7.538702	-2.914885	-0.144064
48	6	0	7.934267	-2.738652	1.119171
49	16	0	7.316496	-1.263809	1.881086
50	6	0	5.954199	-1.828417	-1.756233
51	6	0	5.018421	-0.741814	-2.016199
52	6	0	4.491788	-0.907364	-3.394963
53	6	0	4.611946	-2.415136	-3.606331

54	6	0	5.920758	-2.770017	-2.906960
55	9	0	5.991670	-4.085347	-2.555637
56	9	0	6.934322	-2.542973	-3.802539
57	9	0	3.588853	-3.014820	-2.933349
58	9	0	5.259396	-0.295064	-4.349058
59	9	0	3.212841	-0.460255	-3.552846
60	9	0	4.574214	-2.786428	-4.902895
61	6	0	3.822982	2.032810	-0.051183
62	6	0	3.774409	1.247248	-1.127574
63	6	0	4.682974	0.123994	-1.075484
64	6	0	5.206914	-0.104259	0.347904
65	16	0	5.019215	1.533697	1.166939
66	6	0	8.787017	-3.657484	1.896354
67	6	0	-8.571734	-4.086496	-3.016075
68	6	0	-9.439287	-4.951186	-3.656514
69	6	0	-10.582600	-5.392716	-3.013384
70	6	0	-10.857218	-4.963556	-1.726156
71	6	0	-9.991970	-4.099352	-1.082881
72	6	0	8.651381	-5.033329	1.739089
73	6	0	9.462412	-5.900221	2.445762
74	6	0	10.415956	-5.404741	3.318766
75	6	0	10.550294	-4.037880	3.487460
76	6	0	9.738760	-3.167328	2.784259
77	6	0	-4.002658	-1.372961	-0.910550
78	6	0	-7.408327	0.434999	0.039763
79	6	0	7.654864	0.369718	-0.321841
80	6	0	4.206586	-1.090871	1.014236
81	15	0	0.191552	1.077112	-0.025714
82	8	0	0.884531	0.230216	0.920706
83	8	0	-0.595148	0.355962	-1.169619
84	1	0	-3.055658	1.504943	1.866998
85	1	0	-7.957637	-3.535427	0.958244
86	1	0	-2.690706	8.088569	-3.362183
87	1	0	-0.295735	8.139926	-2.769844
88	1	0	0.673433	6.390189	-1.391242
89	1	0	-4.095918	6.233575	-2.602650
90	1	0	-4.330794	4.101193	-1.463408
91	1	0	4.492443	4.292202	1.231239
92	1	0	-0.604696	6.364964	1.182060
93	1	0	0.297346	8.148573	2.563873
94	1	0	2.695841	8.195922	3.142279
95	1	0	4.173552	6.404554	2.369453
96	1	0	7.801432	-3.761865	-0.739758
97	1	0	3.126392	1.407192	-1.957576
98	1	0	-7.683622	-3.756061	-3.517315
99	1	0	-9.221429	-5.280878	-4.652607
100	1	0	-11.255964	-6.061382	-3.511443
101	1	0	-11.746159	-5.293943	-1.226992
102	1	0	-10.219009	-3.750332	-0.095752
103	1	0	7.898250	-5.419499	1.082550
104	1	0	9.344210	-6.958174	2.322299
105	1	0	11.043509	-6.078102	3.867576
106	1	0	11.284358	-3.649467	4.164750
107	1	0	9.850759	-2.109774	2.914322

108	1	0	-4.092613	-2.250097	-0.283893
109	1	0	-4.218871	-1.642462	-1.933781
110	1	0	-2.990772	-0.994819	-0.854679
111	1	0	-7.410230	1.219419	-0.701998
112	1	0	-8.410949	0.041382	0.134560
113	1	0	-7.100368	0.845863	0.991827
114	1	0	8.621047	-0.105896	-0.426253
115	1	0	7.757767	1.230744	0.321985
116	1	0	7.315186	0.693942	-1.296184
117	1	0	4.473801	-1.257325	2.047135
118	1	0	3.206952	-0.679317	0.976844
119	1	0	4.223785	-2.037017	0.488939
120	1	0	-0.286878	-0.476237	-1.551228

Zero-point correction=	0.845595 (Hartree/Particle)
Thermal correction to Energy=	0.915632
Thermal correction to Enthalpy=	0.916576
Thermal correction to Gibbs Free Energy=	0.733540
Sum of electronic and zero-point Energies=	-5817.332787
Sum of electronic and thermal Energies=	-5817.262749
Sum of electronic and thermal Enthalpies=	-5817.261805
Sum of electronic and thermal Free Energies=	-5817.444842

M045-closed-gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.120134	-0.149530	0.353431
2	6	0	4.634599	0.175044	-1.065728
3	6	0	3.688915	1.272319	-1.059411
4	6	0	3.695735	1.982609	0.067798
5	16	0	4.858015	1.412867	1.289573
6	6	0	5.043342	-0.591507	-2.060786
7	6	0	6.003718	-1.668660	-1.853524
8	6	0	6.045476	-2.510884	-3.080053
9	6	0	4.757705	-2.130176	-3.805017
10	6	0	4.591844	-0.648509	-3.475700
11	9	0	5.412888	0.048785	-4.323047
12	9	0	3.323490	-0.198908	-3.670971
13	9	0	4.786272	-2.394009	-5.127357
14	9	0	7.093148	-2.188318	-3.903657
15	9	0	6.136114	-3.848651	-2.832480
16	9	0	3.727938	-2.808773	-3.225869
17	6	0	7.878861	-2.774704	1.022766
18	6	0	7.540285	-2.854970	-0.266087
19	6	0	6.679418	-1.787912	-0.722212
20	6	0	6.581088	-0.646721	0.301713
21	16	0	7.210792	-1.370777	1.873451
22	6	0	8.712036	-3.741871	1.760096
23	6	0	2.331799	7.373772	2.681085
24	6	0	0.956065	7.379712	2.360513

25	6	0	0.416088	6.393591	1.599576
26	6	0	1.222018	5.332964	1.109914
27	6	0	2.582562	5.304514	1.470621
28	6	0	3.121374	6.359328	2.251391
29	6	0	0.698454	4.269923	0.305762
30	6	0	1.501994	3.212426	0.014681
31	6	0	2.866524	3.156055	0.390605
32	6	0	3.382941	4.207483	1.082470
33	6	0	-0.713817	4.290261	-0.180679
34	6	0	-1.217561	5.361964	-0.985661
35	6	0	-2.576008	5.346851	-1.358767
36	6	0	-3.392985	4.256583	-0.983011
37	6	0	-2.895545	3.200151	-0.284944
38	6	0	-1.536674	3.250583	0.111855
39	6	0	-0.396888	6.414821	-1.466374
40	6	0	-0.918774	7.402798	-2.237536
41	6	0	-2.289432	7.406254	-2.578274
42	6	0	-3.094416	6.402521	-2.152102
43	8	0	0.971179	2.103257	-0.654837
44	8	0	-1.002449	2.140050	0.780375
45	6	0	-6.475670	-0.711295	-0.348862
46	6	0	-6.530041	-1.912238	0.607811
47	6	0	-7.487034	-2.901392	0.161465
48	6	0	-7.871476	-2.753407	-1.107950
49	16	0	-7.137560	-1.368044	-1.936876
50	6	0	-5.789649	-1.876704	1.702319
51	6	0	-4.847247	-0.794963	1.954553
52	6	0	-4.336511	-0.922192	3.345595
53	6	0	-5.350827	-1.852205	4.005544
54	6	0	-5.766280	-2.788802	2.873706
55	9	0	-4.804381	-3.761238	2.777979
56	9	0	-6.952269	-3.413574	3.114135
57	9	0	-4.867218	-2.491030	5.091162
58	9	0	-4.201682	0.263019	4.004446
59	9	0	-3.112277	-1.542091	3.396890
60	9	0	-6.438604	-1.111871	4.360357
61	6	0	-3.707456	2.001844	-0.013328
62	6	0	-3.679788	1.243553	1.083088
63	6	0	-4.526074	0.075740	1.012611
64	6	0	-5.027133	-0.180936	-0.414942
65	16	0	-4.822069	1.434374	-1.273541
66	6	0	-8.809016	-3.628777	-1.835421
67	6	0	9.834237	-4.297498	1.155174
68	6	0	10.606994	-5.220972	1.833407
69	6	0	10.269202	-5.598016	3.121666
70	6	0	9.156142	-5.045589	3.731387
71	6	0	8.383079	-4.119184	3.057685
72	6	0	-8.776543	-5.004712	-1.632812
73	6	0	-9.673684	-5.827436	-2.286524
74	6	0	-10.610579	-5.287185	-3.150645
75	6	0	-10.641880	-3.920263	-3.364292
76	6	0	-9.743890	-3.094158	-2.715147
77	6	0	4.129586	-1.212798	0.902031
78	6	0	7.578277	0.444556	-0.168574
79	6	0	-7.476078	0.332346	0.215115
80	6	0	-4.022081	-1.186241	-1.044424

81	15	0	-0.075832	1.106459	-0.005523
82	8	0	-0.750491	0.227718	-0.935929
83	8	0	0.729940	0.422423	1.148326
84	1	0	3.057255	1.474837	-1.893503
85	1	0	7.796489	-3.676872	-0.898518
86	1	0	2.740533	8.166465	3.274513
87	1	0	0.333497	8.169871	2.729777
88	1	0	-0.626941	6.401988	1.369054
89	1	0	4.163188	6.329545	2.503810
90	1	0	4.415928	4.201426	1.368804
91	1	0	-4.419353	4.256704	-1.292685
92	1	0	0.642788	6.416188	-1.221369
93	1	0	-0.285228	8.187163	-2.599981
94	1	0	-2.682406	8.196703	-3.185122
95	1	0	-4.132803	6.380685	-2.419301
96	1	0	-7.834198	-3.676686	0.808440
97	1	0	-3.092731	1.464390	1.945270
98	1	0	10.108438	-3.991223	0.165903
99	1	0	11.473171	-5.638888	1.360788
100	1	0	10.870344	-6.312678	3.647391
101	1	0	8.889267	-5.336663	4.727511
102	1	0	7.517142	-3.701615	3.531588
103	1	0	-8.038669	-5.426933	-0.981024
104	1	0	-9.637068	-6.886410	-2.127189
105	1	0	-11.306146	-5.926214	-3.656861
106	1	0	-11.364546	-3.496705	-4.032372
107	1	0	-9.774868	-2.035702	-2.878125
108	1	0	4.180666	-2.111384	0.301145
109	1	0	4.363716	-1.456317	1.927593
110	1	0	3.127448	-0.808963	0.856892
111	1	0	7.631523	1.250390	0.548146
112	1	0	8.560931	0.003927	-0.269461
113	1	0	7.269169	0.839988	-1.126349
114	1	0	-8.448817	-0.129434	0.317085
115	1	0	-7.559347	1.179245	-0.449598
116	1	0	-7.146805	0.674996	1.187003
117	1	0	-4.271676	-1.370555	-2.078926
118	1	0	-3.021915	-0.776529	-0.996354
119	1	0	-4.053151	-2.122335	-0.502464
120	1	0	0.452899	-0.420615	1.529973

Zero-point correction=	0.845580 (Hartree/Particle)
Thermal correction to Energy=	0.915628
Thermal correction to Enthalpy=	0.916572
Thermal correction to Gibbs Free Energy=	0.733394
Sum of electronic and zero-point Energies=	-5817.332746
Sum of electronic and thermal Energies=	-5817.262698
Sum of electronic and thermal Enthalpies=	-5817.261754
Sum of electronic and thermal Free Energies=	-5817.444933

M0107 closed gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.025473	0.066210	-0.395554
2	6	0	-4.474482	0.572811	0.944253
3	6	0	-3.482421	1.609735	0.747673
4	6	0	-3.493634	2.141539	-0.474188
5	16	0	-4.721375	1.454206	-1.564750
6	6	0	-4.882192	-0.017608	2.053341
7	6	0	-5.894894	-1.066019	2.035233
8	6	0	-5.927513	-1.721029	3.371225
9	6	0	-4.604096	-1.291840	3.999467
10	6	0	-4.392023	0.116548	3.449845
11	9	0	-5.166762	0.962661	4.200303
12	9	0	-3.104171	0.540001	3.549836
13	9	0	-4.601456	-1.356768	5.346675
14	9	0	-6.938496	-1.246852	4.166112
15	9	0	-6.070550	-3.076261	3.319452
16	9	0	-3.619542	-2.090921	3.500946
17	6	0	-7.937952	-2.470485	-0.586738
18	6	0	-7.544270	-2.388066	0.686707
19	6	0	-6.617806	-1.312906	0.955002
20	6	0	-6.505949	-0.336001	-0.224875
21	16	0	-7.238030	-1.239149	-1.653067
22	6	0	-8.857189	-3.478540	-1.145274
23	6	0	-1.943072	6.954298	-3.963177
24	6	0	-0.563978	6.953709	-3.658914
25	6	0	-0.054113	6.087924	-2.745830
26	6	0	-0.895567	5.160859	-2.077676
27	6	0	-2.261662	5.133308	-2.416661
28	6	0	-2.767761	6.063455	-3.360471
29	6	0	-0.404231	4.221549	-1.112965
30	6	0	-1.248175	3.263461	-0.646269
31	6	0	-2.620805	3.207599	-0.993545
32	6	0	-3.102611	4.153626	-1.843913
33	6	0	1.015599	4.262403	-0.650166
34	6	0	1.579469	5.442922	-0.068865
35	6	0	2.954009	5.454404	0.237736
36	6	0	3.724538	4.288454	0.036518
37	6	0	3.164279	3.128063	-0.405775
38	6	0	1.794232	3.154901	-0.759923
39	6	0	0.808572	6.592880	0.241208
40	6	0	1.392479	7.692877	0.781537
41	6	0	2.780133	7.718880	1.045145
42	6	0	3.538564	6.626752	0.783303
43	8	0	-0.749231	2.248763	0.181030
44	8	0	1.225010	1.966833	-1.226681
45	6	0	4.816220	-1.815652	-0.754502
46	6	0	6.063994	-2.451850	-0.121894
47	6	0	6.206697	-3.837939	-0.510788
48	6	0	5.454436	-4.190495	-1.555881
49	16	0	4.443074	-2.884448	-2.204216
50	6	0	6.775473	-1.715665	0.715684
51	6	0	6.442027	-0.317550	0.966904
52	6	0	7.182540	0.137425	2.174741
53	6	0	7.611393	-1.171315	2.833243

54	6	0	7.865037	-2.100038	1.646469
55	9	0	9.114954	-1.810371	1.163867
56	9	0	7.857796	-3.416620	1.993866
57	9	0	8.672508	-1.037642	3.655964
58	9	0	6.454514	0.935044	3.007794
59	9	0	8.322434	0.831672	1.858785
60	9	0	6.551790	-1.662623	3.534434
61	6	0	3.960841	1.886893	-0.455018
62	6	0	4.955242	1.616607	0.397083
63	6	0	5.588049	0.336560	0.196137
64	6	0	5.127207	-0.343470	-1.099052
65	16	0	3.669072	0.616867	-1.661310
66	6	0	5.417928	-5.523571	-2.186985
67	6	0	-8.646490	-4.011749	-2.412419
68	6	0	-9.502485	-4.972236	-2.917009
69	6	0	-10.582417	-5.404737	-2.167456
70	6	0	-10.804670	-4.871339	-0.909704
71	6	0	-9.948961	-3.913240	-0.400596
72	6	0	6.594531	-6.246896	-2.352791
73	6	0	6.565339	-7.506765	-2.919980
74	6	0	5.363243	-8.058018	-3.328791
75	6	0	4.189589	-7.341362	-3.172681
76	6	0	4.214959	-6.078847	-2.610530
77	6	0	-4.111268	-1.119437	-0.805616
78	6	0	-7.424779	0.866363	0.114161
79	6	0	3.685436	-1.960960	0.305133
80	6	0	6.265342	-0.180506	-2.137980
81	15	0	0.205010	1.101662	-0.355136
82	8	0	0.790962	0.251110	0.655761
83	8	0	-0.665241	0.396428	-1.450156
84	1	0	-2.815193	1.904330	1.525028
85	1	0	-7.810225	-3.097292	1.440300
86	1	0	-2.327458	7.652701	-4.678807
87	1	0	0.085382	7.642239	-4.161230
88	1	0	0.991308	6.091081	-2.527733
89	1	0	-3.813814	6.038369	-3.595015
90	1	0	-4.139635	4.149438	-2.115339
91	1	0	4.770402	4.320941	0.263928
92	1	0	-0.242282	6.579297	0.050347
93	1	0	0.796668	8.551606	1.017925
94	1	0	3.222502	8.599760	1.464341
95	1	0	4.589494	6.625137	0.996573
96	1	0	6.866164	-4.500336	0.005328
97	1	0	5.208409	2.230205	1.233500
98	1	0	-7.807844	-3.687041	-2.995371
99	1	0	-9.325417	-5.382201	-3.890948
100	1	0	-11.247954	-6.146380	-2.561366
101	1	0	-11.646545	-5.193524	-0.330427
102	1	0	-10.136047	-3.485716	0.563729
103	1	0	7.528260	-5.815250	-2.053485
104	1	0	7.478306	-8.053070	-3.047529
105	1	0	5.341738	-9.035255	-3.768186
106	1	0	3.255914	-7.764672	-3.484811
107	1	0	3.303211	-5.529979	-2.485651
108	1	0	-4.177668	-1.909288	-0.069295
109	1	0	-4.401858	-1.506489	-1.770920
110	1	0	-3.090124	-0.767614	-0.859404

111	1	0	-7.465332	1.561329	-0.711300
112	1	0	-8.423803	0.501654	0.310267
113	1	0	-7.056766	1.377753	0.992913
114	1	0	3.491925	-3.011975	0.471516
115	1	0	2.774978	-1.471487	-0.006084
116	1	0	4.001427	-1.516371	1.238496
117	1	0	5.969502	-0.587113	-3.094277
118	1	0	6.480028	0.872659	-2.261102
119	1	0	7.159409	-0.684888	-1.799792
120	1	0	-0.422016	-0.465341	-1.811325

Zero-point correction=	0.845502 (Hartree/Particle)
Thermal correction to Energy=	0.915549
Thermal correction to Enthalpy=	0.916493
Thermal correction to Gibbs Free Energy=	0.733347
Sum of electronic and zero-point Energies=	-5817.330848
Sum of electronic and thermal Energies=	-5817.260801
Sum of electronic and thermal Enthalpies=	-5817.259857
Sum of electronic and thermal Free Energies=	-5817.443003

M0167 closed gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.152538	0.101759	0.564416
2	6	0	-5.246327	0.221703	-0.961984
3	6	0	-4.450497	1.327940	-1.446753
4	6	0	-3.572935	1.800457	-0.557373
5	16	0	-3.564046	0.923835	0.991035
6	6	0	-6.055524	-0.595448	-1.612300
7	6	0	-6.777989	-1.659802	-0.927409
8	6	0	-7.804399	-2.209295	-1.853306
9	6	0	-7.926669	-1.123081	-2.918705
10	6	0	-6.506175	-0.573574	-3.027900
11	9	0	-5.797749	-1.427329	-3.831847
12	9	0	-6.459837	0.660877	-3.602707
13	9	0	-8.429966	-1.567781	-4.088529
14	9	0	-7.388602	-3.353990	-2.483691
15	9	0	-8.995406	-2.498861	-1.256592
16	9	0	-8.722811	-0.130676	-2.429626
17	6	0	-6.761355	-2.847406	2.478890
18	6	0	-7.179033	-2.902782	1.211128

19	6	0	-6.488157	-2.003889	0.317707
20	6	0	-5.238349	-1.388595	0.966006
21	16	0	-5.446023	-1.697005	2.770108
22	6	0	-7.310218	-3.626321	3.603416
23	6	0	-2.003874	7.214221	-2.990436
24	6	0	-0.669290	7.235965	-2.528854
25	6	0	-0.199169	6.256007	-1.715027
26	6	0	-1.037224	5.183728	-1.314457
27	6	0	-2.354261	5.141579	-1.811354
28	6	0	-2.822642	6.192100	-2.641154
29	6	0	-0.586078	4.121132	-0.465716
30	6	0	-1.400081	3.050792	-0.277866
31	6	0	-2.717233	2.979008	-0.787671
32	6	0	-3.181574	4.037723	-1.505580
33	6	0	0.760015	4.156738	0.178200
34	6	0	1.158911	5.245852	1.017917
35	6	0	2.478987	5.274616	1.507831
36	6	0	3.357985	4.210566	1.208295
37	6	0	2.946999	3.122132	0.500502
38	6	0	1.627064	3.128389	-0.008939
39	6	0	0.270360	6.279981	1.409709
40	6	0	0.695246	7.291955	2.208674
41	6	0	2.031350	7.341539	2.664169
42	6	0	2.898405	6.356939	2.323899
43	8	0	-0.933492	1.938149	0.428126
44	8	0	1.214937	2.003211	-0.726544
45	6	0	5.296556	-1.406220	-0.823081
46	6	0	6.549480	-2.024677	-0.184650
47	6	0	6.976320	-3.210183	-0.895712
48	6	0	6.433162	-3.342882	-2.108113
49	16	0	5.300626	-2.049847	-2.546936
50	6	0	7.021444	-1.472205	0.920000
51	6	0	6.438052	-0.255848	1.473237
52	6	0	6.977197	-0.051822	2.844955
53	6	0	7.553474	-1.420387	3.199484
54	6	0	8.064522	-1.949377	1.861143
55	9	0	9.291112	-1.378383	1.639450
56	9	0	8.238048	-3.300101	1.857514
57	9	0	8.498724	-1.371339	4.161059
58	9	0	6.054859	0.385423	3.748594
59	9	0	8.011999	0.848292	2.871622
60	9	0	6.531013	-2.223165	3.606517
61	6	0	3.856571	1.978198	0.298176
62	6	0	4.774343	1.596428	1.192060
63	6	0	5.583300	0.476420	0.778177
64	6	0	5.375552	0.131633	-0.702571
65	16	0	3.836699	1.007282	-1.188957
66	6	0	6.708355	-4.426787	-3.069354
67	6	0	-7.435774	-3.061925	4.868514
68	6	0	-7.972105	-3.795317	5.909996
69	6	0	-8.380728	-5.101159	5.703129
70	6	0	-8.253376	-5.671496	4.448367
71	6	0	-7.720004	-4.940720	3.404372
72	6	0	7.993802	-4.947838	-3.179879
73	6	0	8.257838	-5.975613	-4.064542
74	6	0	7.243636	-6.492833	-4.852208

75	6	0	5.964214	-5.975253	-4.752787
76	6	0	5.696398	-4.945759	-3.870075
77	6	0	-6.327523	0.943477	1.131050
78	6	0	-4.029482	-2.223540	0.466640
79	6	0	4.085493	-2.007202	-0.057684
80	6	0	6.569710	0.745075	-1.478033
81	15	0	0.163585	0.946795	-0.164128
82	8	0	0.647852	-0.044189	0.769068
83	8	0	-0.472620	0.409935	-1.485948
84	1	0	-4.551016	1.691548	-2.445675
85	1	0	-8.011754	-3.485924	0.883356
86	1	0	-2.357847	8.000796	-3.625650
87	1	0	-0.021418	8.034123	-2.831097
88	1	0	0.813590	6.276972	-1.376123
89	1	0	-3.832957	6.151625	-2.997999
90	1	0	-4.190775	4.036458	-1.864405
91	1	0	4.365994	4.262566	1.565366
92	1	0	-0.743579	6.246699	1.075301
93	1	0	0.010723	8.061569	2.504027
94	1	0	2.347362	8.152947	3.288064
95	1	0	3.910820	6.371570	2.677140
96	1	0	7.671016	-3.899319	-0.468290
97	1	0	4.864292	2.013126	2.171468
98	1	0	-7.129228	-2.048367	5.034304
99	1	0	-8.071850	-3.347846	6.878424
100	1	0	-8.791763	-5.670607	6.512372
101	1	0	-8.560677	-6.684664	4.284579
102	1	0	-7.601428	-5.391853	2.440060
103	1	0	8.785590	-4.533048	-2.589591
104	1	0	9.253050	-6.364822	-4.144782
105	1	0	7.450158	-7.286553	-5.542033
106	1	0	5.175787	-6.372297	-5.360142
107	1	0	4.702672	-4.552846	-3.793454
108	1	0	-7.273259	0.518792	0.821958
109	1	0	-6.287333	0.976655	2.209459
110	1	0	-6.255098	1.952877	0.749386
111	1	0	-3.118160	-1.904894	0.950759
112	1	0	-4.199593	-3.266066	0.699596
113	1	0	-3.923731	-2.115312	-0.604437
114	1	0	4.107981	-3.084257	-0.152603
115	1	0	3.152100	-1.634394	-0.450721
116	1	0	4.142878	-1.746193	0.989860
117	1	0	6.448584	0.599422	-2.541462
118	1	0	6.612231	1.806889	-1.275255
119	1	0	7.496439	0.288218	-1.160393
120	1	0	-0.520524	-0.536221	-1.668450

Zero-point correction=	0.845364 (Hartree/Particle)
Thermal correction to Energy=	0.915396
Thermal correction to Enthalpy=	0.916340
Thermal correction to Gibbs Free Energy=	0.733317
Sum of electronic and zero-point Energies=	-5817.331270
Sum of electronic and thermal Energies=	-5817.261239
Sum of electronic and thermal Enthalpies=	-5817.260294
Sum of electronic and thermal Free Energies=	-5817.443318

M0169 closed gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.544069	-0.005607	0.119832
2	6	0	4.482730	-0.049792	1.225378
3	6	0	3.917533	1.252614	1.496491
4	6	0	4.124505	2.127578	0.521865
5	16	0	5.200135	1.581506	-0.769321
6	6	0	4.143271	-1.211251	1.751503
7	6	0	4.669520	-2.474315	1.257507
8	6	0	4.194214	-3.569673	2.144237
9	6	0	3.714346	-2.836250	3.396567
10	6	0	3.221525	-1.486593	2.875289
11	9	0	1.907309	-1.636262	2.443984
12	9	0	3.192176	-0.526243	3.835433
13	9	0	2.789645	-3.516553	4.101781
14	9	0	3.106625	-4.219749	1.617467
15	9	0	5.127180	-4.522330	2.422314
16	9	0	4.798737	-2.586084	4.183321
17	6	0	6.841999	-3.294017	-1.506139
18	6	0	6.073622	-3.631356	-0.465814
19	6	0	5.360257	-2.528060	0.129512
20	6	0	5.401173	-1.271861	-0.759484
21	16	0	6.793777	-1.572264	-1.924705
22	6	0	7.702299	-4.207571	-2.278438
23	6	0	2.705254	8.042779	1.524966
24	6	0	1.383297	7.966199	1.035122
25	6	0	0.917546	6.823579	0.468714
26	6	0	1.747239	5.677633	0.357894
27	6	0	3.052341	5.744424	0.885276
28	6	0	3.515187	6.957556	1.454802
29	6	0	1.289675	4.449501	-0.225519
30	6	0	2.085006	3.352307	-0.126284
31	6	0	3.388954	3.405827	0.422742
32	6	0	3.867215	4.585290	0.882235
33	6	0	-0.028215	4.353621	-0.921268
34	6	0	-0.356695	5.213533	-2.020261
35	6	0	-1.633845	5.109637	-2.605181
36	6	0	-2.534112	4.121642	-2.146626
37	6	0	-2.191494	3.249649	-1.161389
38	6	0	-0.920530	3.397395	-0.553244
39	6	0	0.567584	6.132331	-2.581479
40	6	0	0.213492	6.922338	-3.627242
41	6	0	-1.083351	6.849129	-4.181164
42	6	0	-1.979956	5.961735	-3.685235
43	8	0	1.639100	2.104193	-0.557702
44	8	0	-0.556761	2.468743	0.430240
45	6	0	-5.830960	-0.594941	-1.024566
46	6	0	-6.153814	-1.509296	0.165958
47	6	0	-7.047977	-2.580659	-0.217157
48	6	0	-7.143615	-2.765732	-1.535643
49	16	0	-6.173749	-1.637830	-2.502278
50	6	0	-5.668731	-1.186898	1.352176
51	6	0	-4.742699	-0.074917	1.525205
52	6	0	-4.571897	0.177892	2.982453
53	6	0	-5.772079	-0.534905	3.599266

54	6	0	-5.969743	-1.747642	2.693787
55	9	0	-5.074526	-2.705270	3.092684
56	9	0	-7.215931	-2.288210	2.799443
57	9	0	-5.603496	-0.848626	4.900440
58	9	0	-4.517355	1.498040	3.316348
59	9	0	-3.440472	-0.407052	3.488882
60	9	0	-6.861957	0.272790	3.464083
61	6	0	-3.077032	2.136117	-0.780029
62	6	0	-3.303367	1.672759	0.448726
63	6	0	-4.174519	0.519848	0.489931
64	6	0	-4.376339	-0.091685	-0.903983
65	16	0	-3.925061	1.260182	-2.070118
66	6	0	-7.948035	-3.801723	-2.210195
67	6	0	8.916685	-3.772877	-2.799123
68	6	0	9.726734	-4.643334	-3.503464
69	6	0	9.331978	-5.954891	-3.700878
70	6	0	8.121490	-6.393528	-3.191969
71	6	0	7.309369	-5.526066	-2.487625
72	6	0	-8.075659	-5.065182	-1.640761
73	6	0	-8.849064	-6.032671	-2.252801
74	6	0	-9.499574	-5.753451	-3.442635
75	6	0	-9.369112	-4.502989	-4.020427
76	6	0	-8.595602	-3.532568	-3.411388
77	6	0	6.916362	0.086179	0.830751
78	6	0	4.075288	-1.299081	-1.571117
79	6	0	-6.873887	0.552935	-0.972117
80	6	0	-3.311721	-1.215284	-1.039012
81	15	0	0.438584	1.275140	0.081990
82	8	0	-0.051559	0.223841	-0.785482
83	8	0	0.902280	0.840649	1.502691
84	1	0	3.260380	1.427379	2.317317
85	1	0	6.045766	-4.609721	-0.037065
86	1	0	3.056363	8.955758	1.962092
87	1	0	0.740753	8.819539	1.119227
88	1	0	-0.087112	6.771925	0.109093
89	1	0	4.515614	6.994786	1.839881
90	1	0	4.855668	4.641032	1.293006
91	1	0	-3.493540	4.042511	-2.618297
92	1	0	1.553140	6.189206	-2.174912
93	1	0	0.926115	7.605433	-4.044203
94	1	0	-1.345620	7.486096	-5.001652
95	1	0	-2.961103	5.878356	-4.109952
96	1	0	-7.566850	-3.163010	0.512139
97	1	0	-2.892416	2.103734	1.333698
98	1	0	9.233740	-2.761108	-2.641923
99	1	0	10.662506	-4.298556	-3.895364
100	1	0	9.958899	-6.627942	-4.250518
101	1	0	7.806179	-7.405299	-3.350037
102	1	0	6.362013	-5.862357	-2.117608
103	1	0	-7.553643	-5.292347	-0.733346
104	1	0	-8.936688	-7.003403	-1.807283
105	1	0	-10.098519	-6.504905	-3.916957
106	1	0	-9.869061	-4.281763	-4.942155
107	1	0	-8.504033	-2.563632	-3.859169
108	1	0	7.101199	-0.820865	1.391677
109	1	0	7.712357	0.225982	0.114760
110	1	0	6.909063	0.926647	1.511551

111	1	0	4.058047	-0.509765	-2.306612
112	1	0	3.991902	-2.250363	-2.078601
113	1	0	3.227647	-1.180712	-0.910364
114	1	0	-7.867866	0.126710	-0.969980
115	1	0	-6.773070	1.201468	-1.829358
116	1	0	-6.739284	1.133469	-0.069465
117	1	0	-3.363373	-1.666827	-2.018783
118	1	0	-2.323414	-0.796458	-0.904487
119	1	0	-3.486277	-1.976508	-0.289944
120	1	0	1.019433	-0.088688	1.761763

Zero-point correction=	0.845721 (Hartree/Particle)
Thermal correction to Energy=	0.915668
Thermal correction to Enthalpy=	0.916612
Thermal correction to Gibbs Free Energy=	0.733823
Sum of electronic and zero-point Energies=	-5817.330822
Sum of electronic and thermal Energies=	-5817.260875
Sum of electronic and thermal Enthalpies=	-5817.259931
Sum of electronic and thermal Free Energies=	-5817.442719

M030 closed (SMD)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.621373	-0.275490	0.524189
2	6	0	4.800693	-0.282772	-0.775800
3	6	0	3.719922	0.648479	-0.759070
4	6	0	3.761898	1.559314	0.264088
5	16	0	5.167710	1.340970	1.342602
6	6	0	5.179497	-1.169533	-1.743842
7	6	0	6.394665	-1.948867	-1.627473
8	6	0	6.422329	-2.994158	-2.697976
9	6	0	5.463012	-2.427150	-3.792043
10	6	0	4.449448	-1.534036	-3.003070
11	9	0	4.056230	-0.461195	-3.754349
12	9	0	3.312652	-2.263007	-2.750922
13	9	0	6.187019	-1.635513	-4.631167
14	9	0	7.661432	-3.252355	-3.210577
15	9	0	5.926732	-4.204521	-2.261721
16	9	0	4.865005	-3.387223	-4.525965
17	6	0	9.109950	-1.974966	0.850479
18	6	0	8.517318	-2.386893	-0.314721
19	6	0	7.328784	-1.683848	-0.665763
20	6	0	7.123878	-0.409320	0.170387
21	16	0	8.244439	-0.644328	1.650577
22	6	0	10.321022	-2.530983	1.462205

23	6	0	2.113953	7.014691	2.674392
24	6	0	0.780820	7.033718	2.197562
25	6	0	0.304094	6.017714	1.394508
26	6	0	1.134301	4.923326	1.029435
27	6	0	2.470392	4.887159	1.544616
28	6	0	2.938743	5.959675	2.354748
29	6	0	0.681456	3.832728	0.207342
30	6	0	1.512456	2.738267	0.038259
31	6	0	2.859610	2.685909	0.522422
32	6	0	3.299650	3.779272	1.256145
33	6	0	-0.675111	3.843317	-0.419022
34	6	0	-1.071778	4.864859	-1.351052
35	6	0	-2.409077	4.841796	-1.866292
36	6	0	-3.292746	3.808570	-1.475526
37	6	0	-2.907730	2.780071	-0.627823
38	6	0	-1.565706	2.824383	-0.135018
39	6	0	-0.187759	5.872937	-1.822402
40	6	0	-0.613334	6.824308	-2.726810
41	6	0	-1.945971	6.822803	-3.205244
42	6	0	-2.822510	5.848191	-2.783928
43	8	0	1.024531	1.630810	-0.655509
44	8	0	-1.122272	1.778676	0.678207
45	6	0	-7.139332	-0.382922	-0.221107
46	6	0	-7.367995	-1.551419	0.751754
47	6	0	-8.491517	-2.351601	0.393808
48	6	0	-8.988433	-2.120358	-0.862448
49	16	0	-8.095015	-0.869814	-1.753030
50	6	0	-6.526224	-1.638471	1.824946
51	6	0	-5.357494	-0.790960	1.943652
52	6	0	-4.764247	-0.948899	3.309143
53	6	0	-5.297434	-2.337540	3.786625
54	6	0	-6.652140	-2.521800	3.027779
55	9	0	-6.876506	-3.841387	2.738163
56	9	0	-7.684147	-2.137268	3.853646
57	9	0	-4.426895	-3.300116	3.374218
58	9	0	-5.207673	0.017106	4.187215
59	9	0	-3.400530	-0.903929	3.348810
60	9	0	-5.423293	-2.427694	5.126793
61	6	0	-3.841588	1.703767	-0.282552
62	6	0	-3.865430	0.939292	0.852962
63	6	0	-4.923012	-0.016051	0.906148
64	6	0	-5.617672	-0.209481	-0.451996
65	16	0	-5.157034	1.322154	-1.421914
66	6	0	-10.118120	-2.805944	-1.500757
67	6	0	10.602291	-2.338218	2.829025
68	6	0	11.748311	-2.883214	3.406984
69	6	0	12.640975	-3.628390	2.632134
70	6	0	12.379136	-3.821899	1.271180
71	6	0	11.235417	-3.278771	0.691234
72	6	0	-10.540598	-4.070511	-1.040013
73	6	0	-11.617397	-4.722561	-1.635508
74	6	0	-12.296042	-4.131973	-2.707439
75	6	0	-11.883824	-2.883434	-3.179809
76	6	0	-10.805146	-2.227946	-2.586295
77	6	0	5.093520	-1.417324	1.432329
78	6	0	7.682417	0.789021	-0.641692
79	6	0	-7.826326	0.873072	0.377226
80	6	0	-4.946357	-1.417033	-1.159825

81	15	0	-0.125070	0.686062	0.003106
82	8	0	-0.671714	-0.281203	-0.964691
83	8	0	0.507345	0.072448	1.347361
84	1	0	2.963633	0.672431	-1.532252
85	1	0	8.879152	-3.230961	-0.890084
86	1	0	2.477405	7.824959	3.300435
87	1	0	0.123524	7.855025	2.470402
88	1	0	-0.722278	6.047699	1.046507
89	1	0	3.958994	5.921724	2.729224
90	1	0	4.319208	3.795937	1.631053
91	1	0	-4.306791	3.826810	-1.865787
92	1	0	0.838987	5.886758	-1.474305
93	1	0	0.083996	7.579726	-3.079091
94	1	0	-2.268737	7.581822	-3.912555
95	1	0	-3.843101	5.822829	-3.158447
96	1	0	-8.906271	-3.097340	1.062237
97	1	0	-3.166142	1.078099	1.666339
98	1	0	9.911758	-1.772394	3.448525
99	1	0	11.941933	-2.726937	4.464838
100	1	0	13.535195	-4.051170	3.082174
101	1	0	13.072963	-4.390444	0.657635
102	1	0	11.059902	-3.416859	-0.371278
103	1	0	-10.008883	-4.554624	-0.226610
104	1	0	-11.922311	-5.698904	-1.268202
105	1	0	-13.134416	-4.643808	-3.172337
106	1	0	-12.403401	-2.415517	-4.011797
107	1	0	-10.505514	-1.250731	-2.954028
108	1	0	5.269548	-2.392531	0.967393
109	1	0	5.581387	-1.402916	2.409386
110	1	0	4.017354	-1.292335	1.578342
111	1	0	7.649881	1.710973	-0.057113
112	1	0	8.720472	0.585998	-0.918219
113	1	0	7.102762	0.935470	-1.558492
114	1	0	-8.875559	0.646900	0.585617
115	1	0	-7.780152	1.715197	-0.316711
116	1	0	-7.343638	1.166117	1.314989
117	1	0	-5.335771	-1.547041	-2.171861
118	1	0	-3.867557	-1.250056	-1.218544
119	1	0	-5.124873	-2.338312	-0.595975
120	1	0	0.508730	-0.899564	1.317681

Zero-point correction=	0.843409 (Hartree/Particle)
Thermal correction to Energy=	0.913437
Thermal correction to Enthalpy=	0.914381
Thermal correction to Gibbs Free Energy=	0.732341
Sum of electronic and zero-point Energies=	-5817.390772
Sum of electronic and thermal Energies=	-5817.320745
Sum of electronic and thermal Enthalpies=	-5817.319800
Sum of electronic and thermal Free Energies=	-5817.501840

M0045 closed SMD

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.644766	-0.246117	0.502706
2	6	0	4.829274	-0.272229	-0.801293
3	6	0	3.741055	0.651534	-0.796554
4	6	0	3.776422	1.575649	0.214427
5	16	0	5.180799	1.378400	1.299303
6	6	0	5.219634	-1.165966	-1.757666
7	6	0	6.438157	-1.937914	-1.628214
8	6	0	6.512164	-2.978269	-2.703543
9	6	0	5.094565	-2.954288	-3.363104
10	6	0	4.533269	-1.532861	-3.038176
11	9	0	4.872315	-0.682647	-4.069351
12	9	0	3.173056	-1.539768	-2.974523
13	9	0	5.119622	-3.228794	-4.683171
14	9	0	7.457598	-2.677110	-3.657441
15	9	0	6.822484	-4.233381	-2.252154
16	9	0	4.308425	-3.880087	-2.747836
17	6	0	9.138149	-1.925693	0.866256
18	6	0	8.551036	-2.354866	-0.295969
19	6	0	7.364742	-1.657623	-0.662854
20	6	0	7.149713	-0.375666	0.157670
21	16	0	8.266161	-0.586840	1.644442
22	6	0	10.347783	-2.470621	1.490432
23	6	0	2.103247	7.059755	2.540906
24	6	0	0.770687	7.066382	2.062155
25	6	0	0.298987	6.036459	1.274032
26	6	0	1.133946	4.939917	0.926640
27	6	0	2.469457	4.916714	1.444009
28	6	0	2.932522	6.003195	2.238414
29	6	0	0.686472	3.835188	0.120632
30	6	0	1.522086	2.741662	-0.031016
31	6	0	2.868828	2.701923	0.455378
32	6	0	3.303492	3.807931	1.173156
33	6	0	-0.669653	3.830919	-0.506806
34	6	0	-1.069981	4.836471	-1.454514
35	6	0	-2.407013	4.800370	-1.969820
36	6	0	-3.286963	3.769991	-1.563433
37	6	0	-2.898253	2.756426	-0.699624
38	6	0	-1.556443	2.813113	-0.207464
39	6	0	-0.189666	5.840637	-1.940890
40	6	0	-0.618519	6.776312	-2.860016
41	6	0	-1.950923	6.762298	-3.338919
42	6	0	-2.823928	5.790974	-2.902939
43	8	0	1.039566	1.621978	-0.709010
44	8	0	-1.108979	1.781085	0.620680
45	6	0	-7.114083	-0.420770	-0.235712
46	6	0	-7.334209	-1.576738	0.755363
47	6	0	-8.458096	-2.384633	0.413270
48	6	0	-8.957379	-2.176102	-0.845693
49	16	0	-8.069158	-0.937131	-1.758347
50	6	0	-6.487716	-1.643323	1.825752
51	6	0	-5.324073	-0.787094	1.929942
52	6	0	-4.690999	-0.934637	3.280291
53	6	0	-5.727675	-1.766441	4.104738

54	6	0	-6.565847	-2.528598	3.029501
55	9	0	-5.986488	-3.761309	2.813264
56	9	0	-7.832792	-2.777001	3.474400
57	9	0	-5.151688	-2.584130	5.010094
58	9	0	-4.408219	0.250261	3.903617
59	9	0	-3.502173	-1.626785	3.227178
60	9	0	-6.552236	-0.909116	4.767679
61	6	0	-3.827922	1.682407	-0.336669
62	6	0	-3.848226	0.936952	0.811859
63	6	0	-4.898021	-0.024882	0.879150
64	6	0	-5.594073	-0.242320	-0.473592
65	16	0	-5.141640	1.275670	-1.468758
66	6	0	-10.085863	-2.875487	-1.471177
67	6	0	11.265261	-3.229687	0.734264
68	6	0	12.407593	-3.762553	1.326317
69	6	0	12.664883	-3.547393	2.684862
70	6	0	11.769120	-2.790901	3.445079
71	6	0	10.624617	-2.255976	2.854948
72	6	0	-10.508816	-4.130412	-0.985139
73	6	0	-11.585113	-4.794594	-1.567974
74	6	0	-12.262647	-4.226477	-2.652685
75	6	0	-11.849799	-2.988041	-3.150341
76	6	0	-10.771812	-2.320335	-2.569261
77	6	0	5.118941	-1.379028	1.422776
78	6	0	7.705064	0.815672	-0.667120
79	6	0	-7.806917	0.840688	0.343584
80	6	0	-4.917689	-1.457912	-1.163043
81	15	0	-0.107693	0.682608	-0.039344
82	8	0	-0.651905	-0.298614	-0.994365
83	8	0	0.525044	0.088400	1.313447
84	1	0	2.983025	0.657996	-1.568142
85	1	0	8.913624	-3.209904	-0.854852
86	1	0	2.462724	7.880837	3.155047
87	1	0	0.109858	7.889170	2.321677
88	1	0	-0.727061	6.057120	0.924403
89	1	0	3.952415	5.974905	2.614715
90	1	0	4.322569	3.834363	1.548821
91	1	0	-4.300981	3.778357	-1.954117
92	1	0	0.836799	5.863808	-1.592461
93	1	0	0.076016	7.528957	-3.223572
94	1	0	-2.276277	7.509109	-4.057941
95	1	0	-3.844263	5.755969	-3.277379
96	1	0	-8.872680	-3.115848	1.097290
97	1	0	-3.153029	1.096799	1.625202
98	1	0	11.093303	-3.384868	-0.326438
99	1	0	13.103788	-4.340137	0.724020
100	1	0	13.558002	-3.962260	3.144348
101	1	0	11.959220	-2.617842	4.500951
102	1	0	9.931749	-1.680964	3.463260
103	1	0	-9.978246	-4.597593	-0.161180
104	1	0	-11.890444	-5.763075	-1.180717
105	1	0	-13.100467	-4.747908	-3.107814
106	1	0	-12.368304	-2.537483	-3.992525
107	1	0	-10.471906	-1.350985	-2.957034
108	1	0	5.300679	-2.358961	0.970110
109	1	0	5.603531	-1.350915	2.401212
110	1	0	4.041822	-1.256793	1.564040

111	1	0	7.666256	1.744310	-0.093689
112	1	0	8.744852	0.614306	-0.938260
113	1	0	7.127603	0.948281	-1.587405
114	1	0	-8.854739	0.612306	0.556578
115	1	0	-7.766033	1.672145	-0.363495
116	1	0	-7.324656	1.150980	1.275999
117	1	0	-5.307923	-1.605853	-2.172255
118	1	0	-3.839786	-1.286690	-1.225714
119	1	0	-5.090949	-2.370912	-0.584293
120	1	0	0.522107	-0.883967	1.299982

Zero-point correction=	0.843753 (Hartree/Particle)
Thermal correction to Energy=	0.913753
Thermal correction to Enthalpy=	0.914698
Thermal correction to Gibbs Free Energy=	0.732136
Sum of electronic and zero-point Energies=	-5817.390412
Sum of electronic and thermal Energies=	-5817.320412
Sum of electronic and thermal Enthalpies=	-5817.319468
Sum of electronic and thermal Free Energies=	-5817.502029

M0107 closed (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.574345	-0.349969	-0.593307
2	6	0	-4.788043	-0.032364	0.690125
3	6	0	-3.697435	0.861891	0.469285
4	6	0	-3.706376	1.489585	-0.748744
5	16	0	-5.086175	1.010163	-1.776525
6	6	0	-5.202399	-0.646514	1.837590
7	6	0	-6.420063	-1.428794	1.886922
8	6	0	-6.520276	-2.154442	3.193780
9	6	0	-5.117423	-1.954938	3.855370
10	6	0	-4.545919	-0.664605	3.184765
11	9	0	-4.907309	0.423102	3.950693
12	9	0	-3.184839	-0.682181	3.155270
13	9	0	-5.172080	-1.877751	5.200262
14	9	0	-7.486119	-1.619867	4.015417
15	9	0	-6.822921	-3.484918	3.076268
16	9	0	-4.320015	-3.005852	3.518045
17	6	0	-9.065747	-2.073020	-0.582324

18	6	0	-8.505374	-2.182758	0.664083
19	6	0	-7.324538	-1.411713	0.861925
20	6	0	-7.087042	-0.387856	-0.259830
21	16	0	-8.171830	-0.982275	-1.664025
22	6	0	-10.264164	-2.763792	-1.068438
23	6	0	-1.961828	6.167349	-4.404015
24	6	0	-0.642861	6.308863	-3.908838
25	6	0	-0.194389	5.528762	-2.862536
26	6	0	-1.040199	4.559688	-2.257896
27	6	0	-2.360797	4.391225	-2.786586
28	6	0	-2.800459	5.224294	-3.853689
29	6	0	-0.617720	3.712647	-1.173952
30	6	0	-1.458671	2.694233	-0.759322
31	6	0	-2.790934	2.516986	-1.255134
32	6	0	-3.203574	3.389350	-2.253279
33	6	0	0.718738	3.884529	-0.529528
34	6	0	1.097579	5.112702	0.115199
35	6	0	2.428173	5.233951	0.635353
36	6	0	3.322672	4.143066	0.532938
37	6	0	2.942805	2.920959	-0.003333
38	6	0	1.613414	2.829737	-0.513543
39	6	0	0.203907	6.203354	0.295888
40	6	0	0.614086	7.359994	0.926116
41	6	0	1.941018	7.493192	1.403096
42	6	0	2.827048	6.449425	1.260177
43	8	0	-0.996162	1.802173	0.207528
44	8	0	1.200745	1.603618	-1.039912
45	6	0	5.671461	-1.592199	-0.711206
46	6	0	7.013329	-1.984457	-0.068844
47	6	0	7.604350	-3.125166	-0.687660
48	6	0	7.044602	-3.487463	-1.884644
49	16	0	5.704898	-2.431513	-2.382857
50	6	0	7.423552	-1.247854	1.006264
51	6	0	6.726101	-0.046160	1.415419
52	6	0	7.267993	0.448802	2.721807
53	6	0	8.189126	-0.711261	3.223651
54	6	0	8.575260	-1.495230	1.928878
55	9	0	9.757992	-0.980038	1.439461
56	9	0	8.817827	-2.810949	2.200425
57	9	0	9.258698	-0.274876	3.920871
58	9	0	6.311998	0.753875	3.651184
59	9	0	8.025794	1.589334	2.571703
60	9	0	7.462140	-1.534608	4.027253
61	6	0	3.900074	1.805903	-0.030198
62	6	0	4.897550	1.625518	0.892679
63	6	0	5.762848	0.524431	0.632287
64	6	0	5.577768	-0.047374	-0.782054
65	16	0	3.906187	0.592031	-1.327763
66	6	0	7.458491	-4.599719	-2.748169
67	6	0	-10.510363	-2.914990	-2.447254
68	6	0	-11.644441	-3.587140	-2.901527
69	6	0	-12.560120	-4.118434	-1.989440
70	6	0	-12.333353	-3.969237	-0.616691
71	6	0	-11.201480	-3.298603	-0.160063

72	6	0	8.749200	-5.156548	-2.629845
73	6	0	9.144270	-6.218868	-3.438962
74	6	0	8.264265	-6.748667	-4.389419
75	6	0	6.985621	-6.202036	-4.523887
76	6	0	6.586858	-5.137688	-3.715310
77	6	0	-5.033760	-1.683383	-1.173141
78	6	0	-7.655508	0.976373	0.212961
79	6	0	4.535073	-2.246706	0.118132
80	6	0	6.648407	0.600808	-1.700510
81	15	0	0.161098	0.717124	-0.158620
82	8	0	0.646966	0.007377	1.036915
83	8	0	-0.425379	-0.199382	-1.343497
84	1	0	-2.958860	1.073660	1.230676
85	1	0	-8.883455	-2.862396	1.419103
86	1	0	-2.303351	6.793638	-5.223588
87	1	0	0.026006	7.036907	-4.360055
88	1	0	0.821672	5.648008	-2.503804
89	1	0	-3.809789	5.090949	-4.235881
90	1	0	-4.211615	3.308877	-2.650407
91	1	0	4.339794	4.273491	0.890386
92	1	0	-0.818145	6.118332	-0.056121
93	1	0	-0.090578	8.176116	1.061816
94	1	0	2.251499	8.412811	1.891369
95	1	0	3.843030	6.530553	1.639246
96	1	0	8.440103	-3.653973	-0.244515
97	1	0	4.976633	2.227468	1.790889
98	1	0	-9.801716	-2.519008	-3.169608
99	1	0	-11.810977	-3.697305	-3.969745
100	1	0	-13.445196	-4.640061	-2.343612
101	1	0	-13.045334	-4.368970	0.100474
102	1	0	-11.053351	-3.169542	0.907712
103	1	0	9.453231	-4.741583	-1.915112
104	1	0	10.145121	-6.629238	-3.333692
105	1	0	8.575468	-7.576185	-5.021370
106	1	0	6.293613	-6.605602	-5.258347
107	1	0	5.584050	-4.733491	-3.819914
108	1	0	-5.229061	-2.511151	-0.484054
109	1	0	-5.496991	-1.913016	-2.135264
110	1	0	-3.953324	-1.600381	-1.318065
111	1	0	-7.601171	1.723105	-0.582118
112	1	0	-8.701578	0.850702	0.504767
113	1	0	-7.097369	1.345811	1.078951
114	1	0	4.712684	-3.323367	0.187140
115	1	0	3.560741	-2.079578	-0.345464
116	1	0	4.508574	-1.834583	1.131479
117	1	0	6.509541	0.300772	-2.741443
118	1	0	6.567330	1.689344	-1.636780
119	1	0	7.655537	0.311040	-1.384370
120	1	0	-0.534621	-1.117259	-1.042035

Zero-point correction=	0.844046 (Hartree/Particle)
Thermal correction to Energy=	0.913806
Thermal correction to Enthalpy=	0.914750
Thermal correction to Gibbs Free Energy=	0.735050
Sum of electronic and zero-point Energies=	-5817.390352
Sum of electronic and thermal Energies=	-5817.320592
Sum of electronic and thermal Enthalpies=	-5817.319648
Sum of electronic and thermal Free Energies=	-5817.499348

M0169 closed (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.085390	0.081841	0.410691
2	6	0	4.746971	-0.677259	0.409753
3	6	0	3.629460	0.172606	0.671598
4	6	0	3.898262	1.508308	0.597013
5	16	0	5.591469	1.871594	0.179654
6	6	0	4.799520	-2.026618	0.216555
7	6	0	6.031688	-2.698055	-0.145858
8	6	0	5.849602	-4.183830	-0.087223
9	6	0	4.457955	-4.376143	0.601524
10	6	0	3.700717	-3.036265	0.336353
11	9	0	2.975163	-3.162107	-0.826692
12	9	0	2.790599	-2.777123	1.324732
13	9	0	3.791578	-5.461241	0.158088
14	9	0	5.814502	-4.757422	-1.337475
15	9	0	6.831448	-4.845104	0.601111
16	9	0	4.645280	-4.507584	1.943778
17	6	0	9.402141	-1.459483	-0.928231
18	6	0	8.464909	-2.451391	-0.800334
19	6	0	7.143532	-1.997757	-0.521541
20	6	0	6.981775	-0.480807	-0.720251
21	16	0	8.734841	0.173638	-0.711836
22	6	0	10.833862	-1.634901	-1.192195
23	6	0	2.176453	6.956552	2.961277
24	6	0	0.852884	6.965818	2.457832
25	6	0	0.403354	5.952399	1.636675
26	6	0	1.251361	4.867881	1.280504
27	6	0	2.576943	4.842808	1.821387
28	6	0	3.018220	5.912596	2.649662
29	6	0	0.824940	3.786027	0.431563
30	6	0	1.648266	2.676844	0.307616
31	6	0	2.982405	2.638573	0.827050
32	6	0	3.421284	3.744229	1.537936
33	6	0	-0.479684	3.853289	-0.293110
34	6	0	-0.778574	4.919227	-1.214240
35	6	0	-2.078270	4.960005	-1.817270
36	6	0	-3.020175	3.946156	-1.523570
37	6	0	-2.725675	2.874421	-0.693812
38	6	0	-1.418587	2.855105	-0.113502
39	6	0	0.167608	5.909193	-1.594050
40	6	0	-0.165001	6.902853	-2.492100

41	6	0	-1.462460	6.965050	-3.055071
42	6	0	-2.396754	6.009307	-2.724604
43	8	0	1.218924	1.583803	-0.442842
44	8	0	-1.054874	1.758480	0.673293
45	6	0	-7.080744	-0.143945	-0.660810
46	6	0	-7.402953	-1.345800	0.244102
47	6	0	-8.536054	-2.083530	-0.208289
48	6	0	-8.953469	-1.780181	-1.477736
49	16	0	-7.966299	-0.528315	-2.262401
50	6	0	-6.622862	-1.511216	1.353583
51	6	0	-5.434479	-0.713163	1.573691
52	6	0	-4.885922	-0.966852	2.945196
53	6	0	-6.000361	-1.800021	3.659407
54	6	0	-6.804940	-2.461271	2.495263
55	9	0	-6.263594	-3.702700	2.236313
56	9	0	-8.104292	-2.680100	2.853767
57	9	0	-5.510566	-2.692958	4.543707
58	9	0	-4.592020	0.166207	3.653728
59	9	0	-3.724633	-1.705342	2.914159
60	9	0	-6.827102	-0.947739	4.326295
61	6	0	-3.714257	1.819721	-0.450896
62	6	0	-3.829991	1.008957	0.646741
63	6	0	-4.918801	0.090407	0.596528
64	6	0	-5.543670	-0.017022	-0.803319
65	16	0	-4.974874	1.536174	-1.676998
66	6	0	-10.070497	-2.392819	-2.206245
67	6	0	11.760797	-0.616716	-0.894607
68	6	0	13.122626	-0.797216	-1.133812
69	6	0	13.588342	-1.995994	-1.680263
70	6	0	12.678773	-3.013655	-1.988706
71	6	0	11.318146	-2.836260	-1.750608
72	6	0	-10.571951	-3.653522	-1.819980
73	6	0	-11.637856	-4.235799	-2.501145
74	6	0	-12.226504	-3.577994	-3.587076
75	6	0	-11.735183	-2.332629	-3.986430
76	6	0	-10.667324	-1.746820	-3.306708
77	6	0	6.708910	-0.051719	1.824875
78	6	0	6.409737	-0.245178	-2.143662
79	6	0	-7.755447	1.109773	-0.044556
80	6	0	-4.877523	-1.217723	-1.527767
81	15	0	-0.069257	0.679542	-0.041262
82	8	0	-0.586498	-0.105538	-1.175351
83	8	0	0.381207	-0.156941	1.256722
84	1	0	2.648182	-0.209915	0.912270
85	1	0	8.718406	-3.504867	-0.829616
86	1	0	2.518502	7.764880	3.601759
87	1	0	0.181241	7.777247	2.725315
88	1	0	-0.616412	5.974449	1.268883
89	1	0	4.031109	5.881222	3.044204
90	1	0	4.433206	3.749575	1.933160
91	1	0	-4.004818	4.014618	-1.978170
92	1	0	1.169379	5.875751	-1.181307
93	1	0	0.579702	7.642717	-2.773298
94	1	0	-1.712341	7.757296	-3.755433
95	1	0	-3.390692	6.031654	-3.165169
96	1	0	-9.017492	-2.835727	0.405615

97	1	0	-3.178514	1.091937	1.506490
98	1	0	11.416720	0.316909	-0.457913
99	1	0	13.820302	-0.000213	-0.890864
100	1	0	14.649357	-2.135528	-1.869186
101	1	0	13.029640	-3.945289	-2.424607
102	1	0	10.623134	-3.625971	-2.019040
103	1	0	-10.110564	-4.189426	-0.996225
104	1	0	-12.004544	-5.210313	-2.189690
105	1	0	-13.056378	-4.035571	-4.118967
106	1	0	-12.184338	-1.812753	-4.828524
107	1	0	-10.306034	-0.771139	-3.618903
108	1	0	6.956840	-1.095938	2.040066
109	1	0	7.617733	0.547716	1.913210
110	1	0	5.987811	0.291146	2.571876
111	1	0	6.362847	0.820205	-2.379028
112	1	0	7.052804	-0.737942	-2.877722
113	1	0	5.402927	-0.665891	-2.228495
114	1	0	-8.821904	0.914180	0.096401
115	1	0	-7.641513	1.978714	-0.696408
116	1	0	-7.315550	1.344110	0.930029
117	1	0	-5.216872	-1.290720	-2.563233
118	1	0	-3.792118	-1.087438	-1.523809
119	1	0	-5.117160	-2.154714	-1.014762
120	1	0	0.211538	-1.109405	1.148379

Zero-point correction=	0.843613 (Hartree/Particle)
Thermal correction to Energy=	0.913588
Thermal correction to Enthalpy=	0.914532
Thermal correction to Gibbs Free Energy=	0.733464
Sum of electronic and zero-point Energies=	-5817.387156
Sum of electronic and thermal Energies=	-5817.317181
Sum of electronic and thermal Enthalpies=	-5817.316237
Sum of electronic and thermal Free Energies=	-5817.497306

M0167 closed (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.399356	0.079493	0.559705
2	6	0	-5.530079	0.315110	-0.953875
3	6	0	-4.686203	1.369815	-1.411741
4	6	0	-3.735403	1.778258	-0.513112
5	16	0	-3.752721	0.850842	1.005582
6	6	0	-6.440799	-0.446455	-1.628570
7	6	0	-7.144932	-1.538171	-0.988497
8	6	0	-8.225741	-2.056458	-1.886285
9	6	0	-8.306398	-1.005509	-3.041664
10	6	0	-6.903947	-0.318202	-3.046338

11	9	0	-6.085584	-0.993876	-3.926232
12	9	0	-6.983002	0.964814	-3.507470
13	9	0	-8.637859	-1.548131	-4.231141
14	9	0	-7.917091	-3.287071	-2.420885
15	9	0	-9.442329	-2.207862	-1.276572
16	9	0	-9.243934	-0.070954	-2.722185
17	6	0	-6.909971	-3.022748	2.366154
18	6	0	-7.411270	-2.957234	1.091322
19	6	0	-6.783234	-1.997232	0.247910
20	6	0	-5.480522	-1.441847	0.845713
21	16	0	-5.582467	-1.880413	2.661684
22	6	0	-7.375494	-3.897216	3.447202
23	6	0	-1.925015	7.152318	-2.977542
24	6	0	-0.610776	7.165345	-2.449887
25	6	0	-0.183783	6.170359	-1.594888
26	6	0	-1.046590	5.102434	-1.225612
27	6	0	-2.361974	5.068251	-1.795628
28	6	0	-2.779974	6.122378	-2.656390
29	6	0	-0.648150	4.040070	-0.341350
30	6	0	-1.506719	2.967659	-0.173697
31	6	0	-2.818661	2.906156	-0.731794
32	6	0	-3.221999	3.982672	-1.508208
33	6	0	0.674552	4.045315	0.351308
34	6	0	1.058994	5.102767	1.247134
35	6	0	2.376082	5.080547	1.813299
36	6	0	3.251346	4.011815	1.509261
37	6	0	2.863181	2.938341	0.720766
38	6	0	1.548365	2.987518	0.168962
39	6	0	0.181386	6.153259	1.631139
40	6	0	0.595795	7.143611	2.497571
41	6	0	1.911241	7.142771	3.022461
42	6	0	2.780565	6.129714	2.686476
43	8	0	-1.086966	1.882694	0.595274
44	8	0	1.134987	1.908862	-0.615478
45	6	0	5.535477	-1.383952	-0.858801
46	6	0	6.837185	-1.947954	-0.263447
47	6	0	7.435754	-2.939033	-1.095713
48	6	0	6.927605	-3.009456	-2.366373
49	16	0	5.633065	-1.831400	-2.672496
50	6	0	7.208548	-1.481252	0.965808
51	6	0	6.515637	-0.379778	1.602203
52	6	0	7.003009	-0.203590	3.008100
53	6	0	7.874320	-1.473909	3.278075
54	6	0	8.308198	-1.962180	1.859105
55	9	0	9.523925	-1.387906	1.549559
56	9	0	8.510430	-3.312308	1.840628
57	9	0	8.916386	-1.236683	4.101691
58	9	0	6.009023	-0.082495	3.940192
59	9	0	7.790641	0.917670	3.149007
60	9	0	7.091606	-2.432450	3.844947
61	6	0	3.798753	1.828712	0.487145
62	6	0	4.748575	1.421260	1.387419
63	6	0	5.603035	0.378993	0.925581
64	6	0	5.473980	0.140113	-0.587050
65	16	0	3.841532	0.931552	-1.045570
66	6	0	7.362210	-3.912528	-3.438606
67	6	0	-7.080701	-3.611142	4.794765
68	6	0	-7.538989	-4.439621	5.818366

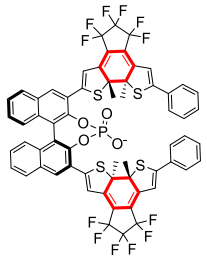
69	6	0	-8.297356	-5.574411	5.518904
70	6	0	-8.591787	-5.876080	4.184563
71	6	0	-8.135533	-5.050392	3.160202
72	6	0	8.633778	-4.521553	-3.390886
73	6	0	9.048000	-5.387072	-4.400108
74	6	0	8.206925	-5.662645	-5.484148
75	6	0	6.948002	-5.060428	-5.549306
76	6	0	6.530180	-4.192660	-4.540340
77	6	0	-6.509712	0.902297	1.266295
78	6	0	-4.299846	-2.252558	0.247484
79	6	0	4.348546	-2.173285	-0.245753
80	6	0	6.598367	0.945056	-1.292582
81	15	0	0.050072	0.872984	0.010959
82	8	0	0.480554	-0.112637	1.017395
83	8	0	-0.519700	0.287111	-1.373752
84	1	0	-4.754943	1.777210	-2.413929
85	1	0	-8.270858	-3.533356	0.768915
86	1	0	-2.249655	7.947117	-3.643451
87	1	0	0.070983	7.965944	-2.724248
88	1	0	0.828434	6.195472	-1.207274
89	1	0	-3.785199	6.088640	-3.069891
90	1	0	-4.229803	3.999478	-1.912771
91	1	0	4.259837	4.038287	1.911363
92	1	0	-0.832075	6.168133	1.246133
93	1	0	-0.096862	7.930670	2.783595
94	1	0	2.225658	7.933527	3.698019
95	1	0	3.786939	6.105287	3.097730
96	1	0	8.239610	-3.576769	-0.747008
97	1	0	4.797379	1.809140	2.398695
98	1	0	-6.501655	-2.726687	5.046003
99	1	0	-7.303673	-4.196611	6.851053
100	1	0	-8.651928	-6.221629	6.316577
101	1	0	-9.171168	-6.762591	3.940699
102	1	0	-8.351690	-5.312623	2.129082
103	1	0	9.308890	-4.299522	-2.570147
104	1	0	10.033802	-5.841357	-4.345272
105	1	0	8.533171	-6.336504	-6.271842
106	1	0	6.286276	-5.267199	-6.386259
107	1	0	5.542404	-3.744257	-4.596507
108	1	0	-7.501429	0.531414	0.987990
109	1	0	-6.409187	0.849440	2.352471
110	1	0	-6.434950	1.949018	0.959228
111	1	0	-3.353966	-1.977052	0.719140
112	1	0	-4.473414	-3.319306	0.412380
113	1	0	-4.223934	-2.078243	-0.830881
114	1	0	4.502916	-3.243031	-0.411212
115	1	0	3.400850	-1.879686	-0.701623
116	1	0	4.281245	-1.995658	0.831930
117	1	0	6.502840	0.887794	-2.379042
118	1	0	6.534944	1.994145	-0.991039
119	1	0	7.583932	0.563394	-1.007529
120	1	0	-0.746307	-0.654208	-1.287264

Zero-point correction=	0.843772 (Hartree/Particle)
Thermal correction to Energy=	0.913580
Thermal correction to Enthalpy=	0.914524
Thermal correction to Gibbs Free Energy=	0.734562
Sum of electronic and zero-point Energies=	-5817.390781
Sum of electronic and thermal Energies=	-5817.320973
Sum of electronic and thermal Enthalpies=	-5817.320029
Sum of electronic and thermal Free Energies=	-5817.499991

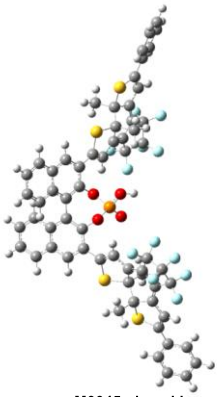
Free Energy Value for Each Optimized structure of (*S*)-DTE-BPA closed-1 anion in Gas and Solvent Phase.

N.B.-Values in green color indicate gas phase free energy values. Whereas,values in blue color indicate solvent phase free energy values.

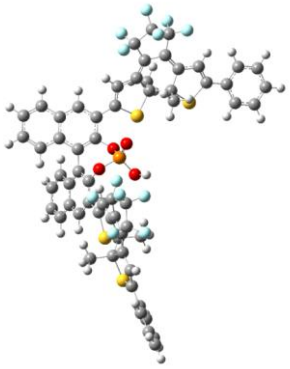
General Structure



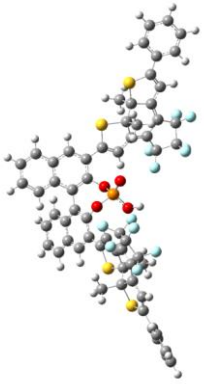
(*S*)-DTE-BPA closed-**1 anion**



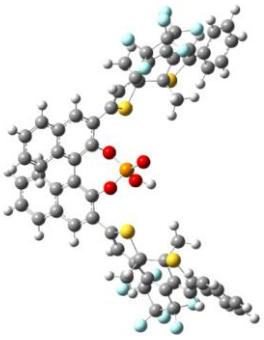
M0045-closed isomer
ZPG= 0.833223
G= -5816.969199
ZPG= 0.832342
G= -5817.073428



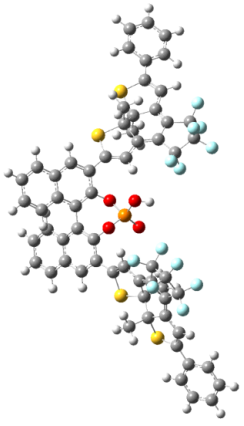
M0107-closed isomer
ZPG= 0.832973
G= -5816.970022
ZPG= 0.832292
G= -5817.073102



M0030-closed isomer
ZPG= 0.833224
G= -5816.969221
ZPG= 0.832373
G= -5817.073061



M0167-closed isomer
ZPG= 0.832741
G= -5816.971197
ZPG= 0.832207
G= -5817.073849



M0169-closed isomer
ZPG= 0.833236
G= -5816.966706
ZPG= 0.832492
G= -5817.071601

closed conformers	ZPG (HA)	E_{sol} (HA) (hatree)	ZPG (A^-)	E_{sol} (A^-) (hatree)
M0030	0.843409	-5818.234181	0.832373	-5817.691549
M0045	0.843753	-5818.234165	0.832342	-5817.691503
M0107	0.844046	-5818.234397	0.832292	-5817.692031
M0167	**0.843772**	**-5818.234553**	**0.832207**	**-5817.692516**
M0169	0.843613	5818.230769	0.832492	-5817.688994

M0030 closed anion gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.622162	-0.276826	0.526580
2	6	0	4.801521	-0.284656	-0.773430
3	6	0	3.720771	0.646627	-0.757139
4	6	0	3.762738	1.557907	0.265623
5	16	0	5.168512	1.340001	1.344274
6	6	0	5.180333	-1.171848	-1.741074
7	6	0	6.395480	-1.951159	-1.624329
8	6	0	6.423151	-2.996918	-2.694375
9	6	0	5.463880	-2.430365	-3.788718
10	6	0	4.450314	-1.536883	-3.000165
11	9	0	4.057143	-0.464360	-3.751924
12	9	0	3.313493	-2.265717	-2.747733
13	9	0	6.187931	-1.639110	-4.628165
14	9	0	7.662264	-3.255367	-3.206826
15	9	0	5.927513	-4.207079	-2.257607
16	9	0	4.865873	-3.390744	-4.522239
17	6	0	9.110690	-1.976241	0.853716
18	6	0	8.518083	-2.388662	-0.311322
19	6	0	7.329576	-1.685743	-0.662706
20	6	0	7.124675	-0.410846	0.172882
21	16	0	8.245186	-0.645234	1.653207
22	6	0	10.321730	-2.532020	1.465721
23	6	0	2.114848	7.014373	2.673499
24	6	0	0.781729	7.033224	2.196620
25	6	0	0.305004	6.016881	1.393995
26	6	0	1.135196	4.922314	1.029424
27	6	0	2.471271	4.886341	1.544661

28	6	0	2.939623	5.959199	2.354339
29	6	0	0.682350	3.831368	0.207793
30	6	0	1.513330	2.736814	0.039213
31	6	0	2.860468	2.684636	0.523439
32	6	0	3.300512	3.778309	1.256698
33	6	0	-0.674197	3.841716	-0.418616
34	6	0	-1.070813	4.862861	-1.351103
35	6	0	-2.408097	4.839604	-1.866373
36	6	0	-3.291802	3.806569	-1.475183
37	6	0	-2.906835	2.778431	-0.627020
38	6	0	-1.564825	2.822927	-0.134194
39	6	0	-0.186756	5.870712	-1.822866
40	6	0	-0.612282	6.821699	-2.727702
41	6	0	-1.944904	6.820016	-3.206175
42	6	0	-2.821479	5.845608	-2.784460
43	8	0	1.025400	1.629066	-0.654087
44	8	0	-1.121440	1.777564	0.679500
45	6	0	-7.138523	-0.384286	-0.219052
46	6	0	-7.367242	-1.552353	0.754311
47	6	0	-8.490772	-2.352665	0.396681
48	6	0	-8.987645	-2.121958	-0.859691
49	16	0	-8.094171	-0.871823	-1.750791
50	6	0	-6.525506	-1.638957	1.827567
51	6	0	-5.356759	-0.791421	1.945938
52	6	0	-4.763557	-0.948779	3.311516
53	6	0	-5.296791	-2.337199	3.789587
54	6	0	-6.651478	-2.521758	3.030781
55	9	0	-6.875866	-3.841466	2.741734
56	9	0	-7.683501	-2.136842	3.856449
57	9	0	-4.426262	-3.299975	3.377626
58	9	0	-5.206987	0.017619	4.189153
59	9	0	-3.399840	-0.903823	3.351204
60	9	0	-5.422692	-2.426766	5.129791
61	6	0	-3.840728	1.702299	-0.281308
62	6	0	-3.864622	0.938320	0.854538
63	6	0	-4.922228	-0.016975	0.908109
64	6	0	-5.616852	-0.210981	-0.449971
65	16	0	-5.156149	1.320220	-1.420543
66	6	0	-10.117329	-2.807796	-1.497735
67	6	0	10.602963	-2.338665	2.832465
68	6	0	11.748953	-2.883436	3.410696
69	6	0	12.641623	-3.628970	2.636198
70	6	0	12.379820	-3.823067	1.275320
71	6	0	11.236131	-3.280165	0.695103
72	6	0	-10.539850	-4.072152	-1.036452
73	6	0	-11.616647	-4.724437	-1.631695
74	6	0	-12.295246	-4.134300	-2.703904
75	6	0	-11.882985	-2.885977	-3.176806
76	6	0	-10.804309	-2.230256	-2.583545
77	6	0	5.094255	-1.418252	1.435202
78	6	0	7.683266	0.787128	-0.639703
79	6	0	-7.825506	0.871985	0.378713
80	6	0	-4.945544	-1.418857	-1.157253
81	15	0	-0.124243	0.684632	0.004905
82	8	0	-0.670880	-0.283042	-0.962486

83	8	0	0.508118	0.071590	1.349447
84	1	0	2.964506	0.670260	-1.530354
85	1	0	8.879915	-3.232990	-0.886306
86	1	0	2.478300	7.824906	3.299199
87	1	0	0.124444	7.854665	2.469082
88	1	0	-0.721357	6.046738	1.045950
89	1	0	3.959862	5.921387	2.728863
90	1	0	4.320059	3.795113	1.631629
91	1	0	-4.305834	3.824663	-1.865483
92	1	0	0.839980	5.884661	-1.474744
93	1	0	0.085076	7.576947	-3.080291
94	1	0	-2.267631	7.578734	-3.913827
95	1	0	-3.842059	5.820107	-3.158999
96	1	0	-8.905564	-3.098103	1.065422
97	1	0	-3.165356	1.077465	1.667876
98	1	0	9.912424	-1.772555	3.451697
99	1	0	11.942547	-2.726702	4.468487
100	1	0	13.535819	-4.051575	3.086449
101	1	0	13.073652	-4.391895	0.662044
102	1	0	11.060645	-3.418712	-0.367354
103	1	0	-10.008171	-4.555923	-0.222822
104	1	0	-11.921595	-5.700612	-1.263972
105	1	0	-13.133618	-4.646319	-3.168604
106	1	0	-12.402526	-2.418411	-4.009013
107	1	0	-10.504643	-1.253208	-2.951695
108	1	0	5.270274	-2.393666	0.970697
109	1	0	5.582093	-1.403429	2.412267
110	1	0	4.018088	-1.293174	1.581128
111	1	0	7.650734	1.709336	-0.055527
112	1	0	8.721325	0.583960	-0.916110
113	1	0	7.103642	0.933191	-1.556584
114	1	0	-8.874750	0.645928	0.587171
115	1	0	-7.779291	1.713806	-0.315590
116	1	0	-7.342839	1.165428	1.316362
117	1	0	-5.334931	-1.549297	-2.169244
118	1	0	-3.866738	-1.251931	-1.216013
119	1	0	-5.124098	-2.339886	-0.593007

Zero-point correction=	0.833224 (Hartree/Particle)
Thermal correction to Energy=	0.902608
Thermal correction to Enthalpy=	0.903552
Thermal correction to Gibbs Free Energy=	0.722327
Sum of electronic and zero-point Energies=	-5816.858325
Sum of electronic and thermal Energies=	-5816.788941
Sum of electronic and thermal Enthalpies=	-5816.787997
Sum of electronic and thermal Free Energies=	-5816.969221

M0169 closed anion gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.085724	0.080130	0.412560
2	6	0	4.747296	-0.678955	0.411848
3	6	0	3.629793	0.171007	0.673413
4	6	0	3.898611	1.506682	0.598407
5	16	0	5.591827	1.869815	0.180951
6	6	0	4.799831	-2.028375	0.219078
7	6	0	6.031995	-2.699942	-0.143110
8	6	0	5.849890	-4.185696	-0.084006
9	6	0	4.458234	-4.377774	0.604788
10	6	0	3.701015	-3.037971	0.339185
11	9	0	2.975471	-3.164173	-0.823828
12	9	0	2.790890	-2.778505	1.327472
13	9	0	3.791849	-5.463005	0.161689
14	9	0	5.814796	-4.759684	-1.334077
15	9	0	6.831721	-4.846764	0.604548
16	9	0	4.645544	-4.508792	1.947085
17	6	0	9.402470	-1.461658	-0.925840
18	6	0	8.465225	-2.453514	-0.797639
19	6	0	7.143851	-1.999776	-0.519003
20	6	0	6.982114	-0.482887	-0.718195
21	16	0	8.735188	0.171539	-0.709969
22	6	0	10.834192	-1.637177	-1.189734
23	6	0	2.176843	6.955695	2.960928
24	6	0	0.853279	6.964817	2.457467
25	6	0	0.403746	5.951143	1.636626
26	6	0	1.251743	4.866503	1.280807
27	6	0	2.577319	4.841585	1.821712
28	6	0	3.018601	5.911630	2.649652
29	6	0	0.825318	3.784385	0.432204
30	6	0	1.648632	2.675153	0.308617
31	6	0	2.982765	2.637030	0.828077
32	6	0	3.421650	3.742906	1.538617
33	6	0	-0.479298	3.851433	-0.292503
34	6	0	-0.778165	4.917083	-1.213974
35	6	0	-2.077855	4.957685	-1.817030
36	6	0	-3.019775	3.943940	-1.523019
37	6	0	-2.725296	2.872465	-0.692918
38	6	0	-1.418214	2.853317	-0.112589
39	6	0	0.168032	5.906917	-1.594088
40	6	0	-0.164556	6.900297	-2.492456
41	6	0	-1.462008	6.962331	-3.055460
42	6	0	-2.396317	6.006704	-2.724700
43	8	0	1.219285	1.581879	-0.441499
44	8	0	-1.054523	1.756937	0.674557
45	6	0	-7.080402	-0.145839	-0.659005
46	6	0	-7.402634	-1.347403	0.246284
47	6	0	-8.535739	-2.085263	-0.205885
48	6	0	-8.953138	-1.782311	-1.475432
49	16	0	-7.965945	-0.530705	-2.260483
50	6	0	-6.622557	-1.512477	1.355826
51	6	0	-5.434166	-0.714369	1.575693
52	6	0	-4.885626	-0.967630	2.947284

53	6	0	-6.000083	-1.800559	3.661747
54	6	0	-6.804658	-2.462168	2.497805
55	9	0	-6.263324	-3.703686	2.239253
56	9	0	-8.104016	-2.680868	2.856365
57	9	0	-5.510307	-2.693222	4.546335
58	9	0	-4.591718	0.165650	3.655460
59	9	0	-3.724346	-1.706143	2.916493
60	9	0	-6.826820	-0.948056	4.328357
61	6	0	-3.713893	1.817854	-0.449678
62	6	0	-3.829648	1.007439	0.648214
63	6	0	-4.918469	0.088886	0.598281
64	6	0	-5.543325	-0.018979	-0.801538
65	16	0	-4.974501	1.533933	-1.675703
66	6	0	-10.070166	-2.395166	-2.203758
67	6	0	11.761136	-0.618909	-0.892459
68	6	0	13.122965	-0.799501	-1.131593
69	6	0	13.588673	-1.998457	-1.677659
70	6	0	12.679095	-3.016205	-1.985789
71	6	0	11.318467	-2.838718	-1.747762
72	6	0	-10.571639	-3.655741	-1.817099
73	6	0	-11.637544	-4.238221	-2.498091
74	6	0	-12.226173	-3.580753	-3.584236
75	6	0	-11.734833	-2.335520	-3.983979
76	6	0	-10.666974	-1.749509	-3.304432
77	6	0	6.709228	-0.052990	1.826792
78	6	0	6.410093	-0.247702	-2.141686
79	6	0	-7.755096	1.108083	-0.043155
80	6	0	-4.877185	-1.219917	-1.525599
81	15	0	-0.068911	0.677761	-0.039646
82	8	0	-0.586150	-0.107672	-1.173491
83	8	0	0.381530	-0.158316	1.258608
84	1	0	2.648507	-0.211427	0.914196
85	1	0	8.718710	-3.507002	-0.826585
86	1	0	2.518895	7.764221	3.601158
87	1	0	0.181643	7.776339	2.724686
88	1	0	-0.616016	5.973089	1.268817
89	1	0	4.031485	5.880369	3.044215
90	1	0	4.433568	3.748365	1.933850
91	1	0	-4.004412	4.012270	-1.977650
92	1	0	1.169799	5.873594	-1.181324
93	1	0	0.580159	7.640063	-2.773880
94	1	0	-1.711873	7.754358	-3.756075
95	1	0	-3.390250	6.028923	-3.165282
96	1	0	-9.017193	-2.837260	0.408253
97	1	0	-3.178179	1.090683	1.507944
98	1	0	11.417066	0.314859	-0.456064
99	1	0	13.820648	-0.002429	-0.888890
100	1	0	14.649688	-2.138064	-1.866527
101	1	0	13.029955	-3.947981	-2.421392
102	1	0	10.623449	-3.628506	-2.015951
103	1	0	-10.110266	-4.191389	-0.993170
104	1	0	-12.004246	-5.212632	-2.186331
105	1	0	-13.056047	-4.038488	-4.115991
106	1	0	-12.183973	-1.815906	-4.826243
107	1	0	-10.305669	-0.773931	-3.616932
108	1	0	6.957143	-1.097144	2.042316
109	1	0	7.618057	0.546462	1.914947

110	1	0	5.988125	0.290120	2.573677
111	1	0	6.363219	0.817607	-2.377390
112	1	0	7.053162	-0.740706	-2.875584
113	1	0	5.403279	-0.668430	-2.226397
114	1	0	-8.821557	0.912547	0.097853
115	1	0	-7.641145	1.976816	-0.695281
116	1	0	-7.315206	1.342723	0.931360
117	1	0	-5.216524	-1.293238	-2.561046
118	1	0	-3.791778	-1.089644	-1.521671
119	1	0	-5.116838	-2.156743	-1.012300

Zero-point correction=	0.833236 (Hartree/Particle)
Thermal correction to Energy=	0.902620
Thermal correction to Enthalpy=	0.903564
Thermal correction to Gibbs Free Energy=	0.722289
Sum of electronic and zero-point Energies=	-5816.855758
Sum of electronic and thermal Energies=	-5816.786374
Sum of electronic and thermal Enthalpies=	-5816.785430
Sum of electronic and thermal Free Energies=	-5816.966706

M0045 closed anion gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.645578	-0.247447	0.505055
2	6	0	4.830124	-0.274089	-0.798958
3	6	0	3.741927	0.649702	-0.794641
4	6	0	3.777285	1.574241	0.215953
5	16	0	5.181625	1.377416	1.300954
6	6	0	5.220492	-1.168237	-1.754943
7	6	0	6.438993	-1.940159	-1.625129
8	6	0	6.513009	-2.980968	-2.700018
9	6	0	5.095430	-2.957231	-3.359632
10	6	0	4.534158	-1.535655	-3.035319
11	9	0	4.873255	-0.685882	-4.066842
12	9	0	3.173943	-1.542503	-2.971705
13	9	0	5.120521	-3.232293	-4.679583
14	9	0	7.458479	-2.680233	-3.654014
15	9	0	6.823285	-4.235897	-2.248092
16	9	0	4.309250	-3.882753	-2.743999
17	6	0	9.138910	-1.926952	0.869417
18	6	0	8.551822	-2.356600	-0.292645
19	6	0	7.365556	-1.659484	-0.659859
20	6	0	7.150532	-0.377177	0.160119
21	16	0	8.266930	-0.587751	1.647014
22	6	0	10.348512	-2.471646	1.493859
23	6	0	2.104168	7.059365	2.540073
24	6	0	0.771623	7.065822	2.061279
25	6	0	0.299923	6.035578	1.273575
26	6	0	1.134867	4.938871	0.926670
27	6	0	2.470361	4.915854	1.444089

28	6	0	2.933428	6.002658	2.238051
29	6	0	0.687391	3.833813	0.121113
30	6	0	1.522984	2.740204	-0.030049
31	6	0	2.869710	2.700638	0.456402
32	6	0	3.304378	3.806938	1.173728
33	6	0	-0.668715	3.829312	-0.506364
34	6	0	-1.068991	4.834475	-1.454507
35	6	0	-2.406008	4.798188	-1.969839
36	6	0	-3.285994	3.768001	-1.563045
37	6	0	-2.897334	2.754791	-0.698798
38	6	0	-1.555538	2.811653	-0.206621
39	6	0	-0.188637	5.838415	-1.941279
40	6	0	-0.617440	6.773714	-2.860811
41	6	0	-1.949830	6.759530	-3.339749
42	6	0	-2.822871	5.788410	-2.903387
43	8	0	1.040458	1.620246	-0.707587
44	8	0	-1.108123	1.779963	0.621971
45	6	0	-7.113253	-0.422111	-0.233677
46	6	0	-7.333436	-1.577657	0.757878
47	6	0	-8.457332	-2.385669	0.416090
48	6	0	-8.956572	-2.177656	-0.842975
49	16	0	-8.068294	-0.939090	-1.756124
50	6	0	-6.486977	-1.643811	1.828320
51	6	0	-5.323318	-0.787566	1.932185
52	6	0	-4.690288	-0.934556	3.282615
53	6	0	-5.727009	-1.765988	4.107381
54	6	0	-6.565166	-2.528578	3.032439
55	9	0	-5.985829	-3.761393	2.816738
56	9	0	-7.832130	-2.776764	3.477404
57	9	0	-5.151068	-2.583310	5.013098
58	9	0	-4.407499	0.250598	3.905451
59	9	0	-3.501477	-1.626754	3.229830
60	9	0	-6.551569	-0.908365	4.769936
61	6	0	-3.827040	1.680946	-0.335419
62	6	0	-3.847396	0.935975	0.813422
63	6	0	-4.897216	-0.025806	0.881086
64	6	0	-5.593232	-0.243797	-0.471586
65	16	0	-5.140733	1.273764	-1.467377
66	6	0	-10.085053	-2.877278	-1.468199
67	6	0	11.265995	-3.231051	0.738039
68	6	0	12.408297	-3.763695	1.330350
69	6	0	12.665551	-3.547970	2.688813
70	6	0	11.769782	-2.791137	3.448684
71	6	0	10.625310	-2.256433	2.858293
72	6	0	-10.508051	-4.131988	-0.981646
73	6	0	-11.584346	-4.796390	-1.564234
74	6	0	-12.261833	-4.228714	-2.649205
75	6	0	-11.848941	-2.990497	-3.147369
76	6	0	-10.770956	-2.322572	-2.566538
77	6	0	5.119698	-1.379959	1.425585
78	6	0	7.705936	0.813801	-0.665155
79	6	0	-7.806075	0.839607	0.345067
80	6	0	-4.916855	-1.459695	-1.160505
81	15	0	-0.106843	0.681185	-0.037561

82	8	0	-0.651049	-0.300426	-0.992185
83	8	0	0.525839	0.087531	1.315500
84	1	0	2.983921	0.655857	-1.566254
85	1	0	8.914407	-3.211882	-0.851157
86	1	0	2.463646	7.880697	3.153880
87	1	0	0.110806	7.888734	2.320435
88	1	0	-0.726114	6.056116	0.923906
89	1	0	3.953309	5.974503	2.614395
90	1	0	4.323445	3.833504	1.549413
91	1	0	-4.300000	3.776227	-1.953763
92	1	0	0.837818	5.861709	-1.592829
93	1	0	0.077123	7.526189	-3.224663
94	1	0	-2.275145	7.506046	-4.059095
95	1	0	-3.843196	5.753271	-3.277843
96	1	0	-8.871954	-3.116587	1.100405
97	1	0	-3.152220	1.096148	1.626719
98	1	0	11.094066	-3.386675	-0.322603
99	1	0	13.104497	-4.341549	0.728318
100	1	0	13.558646	-3.962664	3.148500
101	1	0	11.959854	-2.617638	4.504489
102	1	0	9.932437	-1.681149	3.466342
103	1	0	-9.977517	-4.598835	-0.157475
104	1	0	-11.889711	-5.764701	-1.176579
105	1	0	-13.099652	-4.750316	-3.104140
106	1	0	-12.367410	-2.540281	-3.989759
107	1	0	-10.471015	-1.353392	-2.954709
108	1	0	5.301427	-2.360086	0.973337
109	1	0	5.604259	-1.351445	2.404024
110	1	0	4.042578	-1.257639	1.566765
111	1	0	7.667132	1.742681	-0.092116
112	1	0	8.745727	0.612297	-0.936179
113	1	0	7.128506	0.946037	-1.585514
114	1	0	-8.853909	0.611339	0.558125
115	1	0	-7.765150	1.670765	-0.362360
116	1	0	-7.323835	1.150280	1.277366
117	1	0	-5.307062	-1.608051	-2.169666
118	1	0	-3.838946	-1.288524	-1.223215
119	1	0	-5.090154	-2.372447	-0.581376

Zero-point correction=	0.833223 (Hartree/Particle)
Thermal correction to Energy=	0.902609
Thermal correction to Enthalpy=	0.903553
Thermal correction to Gibbs Free Energy=	0.722304
Sum of electronic and zero-point Energies=	-5816.858280
Sum of electronic and thermal Energies=	-5816.788895
Sum of electronic and thermal Enthalpies=	-5816.787950
Sum of electronic and thermal Free Energies=	-5816.969199

M0107 closed anion gas phase Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.575170	-0.351705	-0.595255
2	6	0	-4.788913	-0.034574	0.688322
3	6	0	-3.698329	0.859803	0.467859
4	6	0	-3.707258	1.487972	-0.749925
5	16	0	-5.087014	1.008904	-1.777930
6	6	0	-5.203279	-0.649185	1.835536
7	6	0	-6.420918	-1.431525	1.884531
8	6	0	-6.521142	-2.157685	3.191104
9	6	0	-5.118313	-1.958392	3.852809
10	6	0	-4.546834	-0.667779	3.182722
11	9	0	-4.908281	0.419617	3.949064
12	9	0	-3.185753	-0.685298	3.153256
13	9	0	-5.173009	-1.881731	5.197729
14	9	0	-7.487025	-1.623463	4.012923
15	9	0	-6.823739	-3.488126	3.073065
16	9	0	-4.320861	-3.009148	3.515096
17	6	0	-9.066515	-2.074877	-0.585036
18	6	0	-8.506171	-2.185082	0.661343
19	6	0	-7.325366	-1.414075	0.859517
20	6	0	-7.087875	-0.389773	-0.261833
21	16	0	-8.172605	-0.983681	-1.666289
22	6	0	-10.264896	-2.765500	-1.071452
23	6	0	-1.962769	6.167218	-4.403327
24	6	0	-0.643820	6.308583	-3.908059
25	6	0	-0.195350	5.528089	-2.862049
26	6	0	-1.041144	4.558751	-2.257810
27	6	0	-2.361722	4.390450	-2.786601
28	6	0	-2.801383	5.223920	-3.853391
29	6	0	-0.618665	3.711302	-1.174184
30	6	0	-1.459593	2.692699	-0.759974
31	6	0	-2.791837	2.515600	-1.255890
32	6	0	-3.204480	3.388339	-2.253706
33	6	0	0.717770	3.882978	-0.529658
34	6	0	1.096553	5.110912	0.115558
35	6	0	2.427129	5.232003	0.635794
36	6	0	3.321667	4.141188	0.532978
37	6	0	2.941855	2.919277	-0.003779
38	6	0	1.612481	2.828210	-0.514060
39	6	0	0.202839	6.201464	0.296648
40	6	0	0.612963	7.357872	0.927337
41	6	0	1.939878	7.490928	1.404405
42	6	0	2.825946	6.447247	1.261103
43	8	0	-0.997080	1.800277	0.206541
44	8	0	1.199867	1.602282	-1.040918
45	6	0	5.670681	-1.593514	-0.713337
46	6	0	7.012545	-1.985977	-0.071093
47	6	0	7.603620	-3.126425	-0.690337
48	6	0	7.043916	-3.488274	-1.887477
49	16	0	5.704190	-2.432175	-2.385314
50	6	0	7.422714	-1.249779	1.004313
51	6	0	6.725212	-0.048268	1.413918
52	6	0	7.267053	0.446203	2.720513
53	6	0	8.188211	-0.714025	3.221930

54	6	0	8.574406	-1.497476	1.926862
55	9	0	9.757134	-0.982054	1.437677
56	9	0	8.817010	-2.813293	2.197902
57	9	0	9.257750	-0.277876	3.919348
58	9	0	6.311023	0.750882	3.649983
59	9	0	8.024820	1.586819	2.570874
60	9	0	7.461231	-1.537709	4.025191
61	6	0	3.899162	1.804264	-0.031053
62	6	0	4.896619	1.623552	0.891780
63	6	0	5.761961	0.522596	0.630983
64	6	0	5.576938	-0.048664	-0.783586
65	16	0	3.905350	0.590898	-1.329091
66	6	0	7.457866	-4.600180	-2.751424
67	6	0	-10.511053	-2.916169	-2.450333
68	6	0	-11.645096	-3.588180	-2.904898
69	6	0	-12.560782	-4.119859	-1.993043
70	6	0	-12.334056	-3.971190	-0.620230
71	6	0	-11.202218	-3.300696	-0.163310
72	6	0	8.748590	-5.157012	-2.633283
73	6	0	9.143717	-6.219003	-3.442803
74	6	0	8.263755	-6.748461	-4.393490
75	6	0	6.985097	-6.201821	-4.527779
76	6	0	6.586276	-5.137801	-3.718798
77	6	0	-5.034525	-1.684875	-1.175594
78	6	0	-7.656399	0.974253	0.211474
79	6	0	4.534292	-2.248382	0.115715
80	6	0	6.647580	0.599911	-1.701761
81	15	0	0.160226	0.715410	-0.159999
82	8	0	0.646086	0.005213	1.035272
83	8	0	-0.426189	-0.200654	-1.345249
84	1	0	-2.959781	1.071300	1.229353
85	1	0	-8.884250	-2.865027	1.416088
86	1	0	-2.304291	6.793815	-5.222665
87	1	0	0.025035	7.036825	-4.358975
88	1	0	0.820698	5.647229	-2.503244
89	1	0	-3.810699	5.090690	-4.235661
90	1	0	-4.212507	3.307987	-2.650893
91	1	0	4.338775	4.271507	0.890504
92	1	0	-0.819201	6.116545	-0.055422
93	1	0	-0.091732	8.173917	1.063337
94	1	0	2.250315	8.410367	1.893044
95	1	0	3.841915	6.528261	1.640230
96	1	0	8.439379	-3.655377	-0.247376
97	1	0	4.975658	2.225155	1.790227
98	1	0	-9.802400	-2.519882	-3.172514
99	1	0	-11.811600	-3.697934	-3.973163
100	1	0	-13.445831	-4.641378	-2.347442
101	1	0	-13.046043	-4.371226	0.096761
102	1	0	-11.054122	-3.172046	0.904519
103	1	0	9.452588	-4.742302	-1.918369
104	1	0	10.144579	-6.629381	-3.337666
105	1	0	8.575003	-7.575723	-5.025755
106	1	0	6.293122	-6.605124	-5.262415
107	1	0	5.583458	-4.733597	-3.823272

108	1	0	-5.229817	-2.512918	-0.486835
109	1	0	-5.497723	-1.914149	-2.137819
110	1	0	-3.954088	-1.601781	-1.320457
111	1	0	-7.602066	1.721296	-0.583312
112	1	0	-8.702472	0.848433	0.503203
113	1	0	-7.098295	1.343372	1.077623
114	1	0	4.711938	-3.325063	0.184308
115	1	0	3.559967	-2.081106	-0.347842
116	1	0	4.507753	-1.836654	1.129222
117	1	0	6.508752	0.300276	-2.742814
118	1	0	6.566465	1.688420	-1.637609
119	1	0	7.654711	0.310054	-1.385707

Zero-point correction=	0.832973 (Hartree/Particle)
Thermal correction to Energy=	0.902422
Thermal correction to Enthalpy=	0.903366
Thermal correction to Gibbs Free Energy=	0.722009
Sum of electronic and zero-point Energies=	-5816.859057
Sum of electronic and thermal Energies=	-5816.789609
Sum of electronic and thermal Enthalpies=	-5816.788665
Sum of electronic and thermal Free Energies=	-5816.970022

M0167 closed anion gas phase

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.400579	0.078107	0.557387
2	6	0	-5.531228	0.314180	-0.956128
3	6	0	-4.687362	1.369051	-1.413629
4	6	0	-3.736623	1.777251	-0.514825
5	16	0	-3.753992	0.849374	1.003587
6	6	0	-6.441888	-0.447210	-1.631103
7	6	0	-7.146020	-1.539143	-0.991399
8	6	0	-8.226765	-2.057192	-1.889402
9	6	0	-8.307394	-1.005894	-3.044466
10	6	0	-6.904964	-0.318541	-3.048856
11	9	0	-6.086533	-0.993922	-3.928912
12	9	0	-6.984036	0.964612	-3.509603
13	9	0	-8.638774	-1.548166	-4.234125
14	9	0	-7.918047	-3.287632	-2.424359
15	9	0	-9.443380	-2.208820	-1.279800
16	9	0	-9.244977	-0.071466	-2.724753
17	6	0	-6.911190	-3.024731	2.362814
18	6	0	-7.412424	-2.958846	1.087975
19	6	0	-6.784373	-1.998567	0.244888
20	6	0	-5.481711	-1.443322	0.842929
21	16	0	-5.583739	-1.882443	2.658761
22	6	0	-7.376743	-3.899542	3.443571
23	6	0	-1.926276	7.152117	-2.977526
24	6	0	-0.612065	7.165026	-2.449797
25	6	0	-0.185086	6.169794	-1.595078
26	6	0	-1.047878	5.101730	-1.226172

27	6	0	-2.363231	5.067678	-1.796268
28	6	0	-2.781219	6.122052	-2.656733
29	6	0	-0.649451	4.039110	-0.342211
30	6	0	-1.507995	2.966621	-0.174930
31	6	0	-2.819905	2.905245	-0.733115
32	6	0	-3.223236	3.981984	-1.509224
33	6	0	0.673213	4.044187	0.350519
34	6	0	1.057574	5.101379	1.246686
35	6	0	2.374632	5.079030	1.812915
36	6	0	3.249947	4.010418	1.508599
37	6	0	2.861858	2.937171	0.719758
38	6	0	1.547070	2.986473	0.167898
39	6	0	0.179912	6.151726	1.630964
40	6	0	0.594243	7.141829	2.497718
41	6	0	1.909661	7.140871	3.022678
42	6	0	2.779035	6.127944	2.686432
43	8	0	-1.088248	1.881436	0.593734
44	8	0	1.133768	1.908042	-0.616891
45	6	0	5.534377	-1.384557	-0.860979
46	6	0	6.836071	-1.948698	-0.265727
47	6	0	7.434717	-2.939505	-1.098262
48	6	0	6.926638	-3.009558	-2.368970
49	16	0	5.632076	-1.831451	-2.674805
50	6	0	7.207354	-1.482357	0.963689
51	6	0	6.514374	-0.381098	1.600382
52	6	0	7.001665	-0.205322	3.006358
53	6	0	7.873002	-1.475695	3.275994
54	6	0	8.306972	-1.963521	1.856899
55	9	0	9.522697	-1.389114	1.547592
56	9	0	8.509248	-3.313637	1.838023
57	9	0	8.915017	-1.238685	4.099738
58	9	0	6.007625	-0.084542	3.938434
59	9	0	7.789253	0.915921	3.147648
60	9	0	7.090289	-2.434433	3.842533
61	6	0	3.797478	1.827643	0.485850
62	6	0	4.747265	1.419948	1.386051
63	6	0	5.601783	0.377849	0.923942
64	6	0	5.472817	0.139424	-0.588769
65	16	0	3.840368	0.930950	-1.047135
66	6	0	7.361329	-3.912291	-3.441454
67	6	0	-7.082031	-3.613867	4.791237
68	6	0	-7.540347	-4.442672	5.814562
69	6	0	-8.298662	-5.577395	5.514715
70	6	0	-8.593012	-5.878668	4.180267
71	6	0	-8.136730	-5.052655	3.156181
72	6	0	8.632914	-4.521289	-3.393851
73	6	0	9.047217	-5.386488	-4.403314
74	6	0	8.206209	-5.661759	-5.487483
75	6	0	6.947270	-5.059563	-5.552525
76	6	0	6.529367	-4.192115	-4.543318
77	6	0	-6.510999	0.900661	1.264168
78	6	0	-4.300977	-2.253814	0.244517
79	6	0	4.347439	-2.174114	-0.248234
80	6	0	6.597216	0.944617	-1.293996
81	15	0	0.048853	0.871939	0.009173
82	8	0	0.479313	-0.113973	1.015333
83	8	0	-0.520826	0.286469	-1.375746

84	1	0	-4.756061	1.776748	-2.415696
85	1	0	-8.271976	-3.534897	0.765347
86	1	0	-2.250906	7.947108	-3.643211
87	1	0	0.069683	7.965730	-2.723879
88	1	0	0.827110	6.194822	-1.207402
89	1	0	-3.786421	6.088408	-3.070298
90	1	0	-4.231019	3.998880	-1.913836
91	1	0	4.258415	4.036800	1.910763
92	1	0	-0.833529	6.166685	1.245908
93	1	0	-0.098455	7.928779	2.783944
94	1	0	2.224016	7.931432	3.698493
95	1	0	3.785388	6.103425	3.097732
96	1	0	8.238574	-3.577321	-0.749708
97	1	0	4.796003	1.807522	2.397447
98	1	0	-6.503027	-2.729470	5.042774
99	1	0	-7.305094	-4.199968	6.847335
100	1	0	-8.653256	-6.224867	6.312172
101	1	0	-9.172352	-6.765124	3.936102
102	1	0	-8.352823	-5.314580	2.124970
103	1	0	9.307975	-4.299486	-2.573009
104	1	0	10.033031	-5.840759	-4.348563
105	1	0	8.532519	-6.335369	-6.275364
106	1	0	6.285596	-5.266101	-6.389576
107	1	0	5.541579	-3.743726	-4.599401
108	1	0	-7.502689	0.529831	0.985697
109	1	0	-6.410530	0.847477	2.350333
110	1	0	-6.436254	1.947478	0.957423
111	1	0	-3.355131	-1.978421	0.716307
112	1	0	-4.474520	-3.320617	0.409080
113	1	0	-4.225013	-2.079169	-0.833791
114	1	0	4.501852	-3.243804	-0.414010
115	1	0	3.399758	-1.880407	-0.704066
116	1	0	4.280074	-1.996816	0.829499
117	1	0	6.501748	0.887682	-2.380479
118	1	0	6.533743	1.993612	-0.992138
119	1	0	7.582778	0.562900	-1.009007

Zero-point correction=	0.832741 (Hartree/Particle)
Thermal correction to Energy=	0.902265
Thermal correction to Enthalpy=	0.903209
Thermal correction to Gibbs Free Energy=	0.721319
Sum of electronic and zero-point Energies=	-5816.859775
Sum of electronic and thermal Energies=	-5816.790251
Sum of electronic and thermal Enthalpies=	-5816.789307
Sum of electronic and thermal Free Energies=	-5816.971197

M0030 closed anion (SMD)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.128263	-0.237410	-0.382567
2	6	0	-4.574102	0.061307	1.019344
3	6	0	-3.658588	1.148719	1.020182
4	6	0	-3.671975	1.903727	-0.125249
5	16	0	-4.842595	1.344536	-1.334835
6	6	0	-4.972698	-0.764818	2.039011
7	6	0	-5.987579	-1.777753	1.835828
8	6	0	-6.049371	-2.668371	3.036446
9	6	0	-5.434632	-1.795524	4.173655
10	6	0	-4.451734	-0.824148	3.440580
11	9	0	-4.410630	0.388724	4.080156
12	9	0	-3.181204	-1.336850	3.522505
13	9	0	-6.436505	-1.069050	4.748659
14	9	0	-7.308201	-3.095531	3.367970
15	9	0	-5.289611	-3.809421	2.892454
16	9	0	-4.842644	-2.526194	5.143930
17	6	0	-8.114946	-2.666058	-1.027594
18	6	0	-7.693542	-2.804784	0.267024
19	6	0	-6.744532	-1.831218	0.700832
20	6	0	-6.617071	-0.649132	-0.271818
21	16	0	-7.359290	-1.289849	-1.868986
22	6	0	-9.058702	-3.533160	-1.740822
23	6	0	-2.321062	7.281294	-2.869602
24	6	0	-0.960045	7.338812	-2.479339
25	6	0	-0.421725	6.373305	-1.653998
26	6	0	-1.210699	5.291799	-1.168550
27	6	0	-2.576390	5.214122	-1.602248
28	6	0	-3.107037	6.235105	-2.440140
29	6	0	-0.691321	4.264821	-0.311761
30	6	0	-1.492252	3.171374	0.008952
31	6	0	-2.853044	3.076884	-0.439512
32	6	0	-3.362576	4.103309	-1.218517
33	6	0	0.714250	4.273326	0.188624
34	6	0	1.230183	5.322285	1.020447
35	6	0	2.596570	5.260220	1.454443
36	6	0	3.386770	4.143692	1.096268
37	6	0	2.880684	3.096880	0.342577
38	6	0	1.519129	3.175699	-0.106888
39	6	0	0.437393	6.411908	1.480807
40	6	0	0.972692	7.398946	2.282307
41	6	0	2.334314	7.356084	2.672326
42	6	0	3.123997	6.303017	2.267102
43	8	0	-0.971468	2.165987	0.759746
44	8	0	1.001571	2.151655	-0.834329
45	6	0	6.648503	-0.632487	0.272526
46	6	0	6.772205	-1.840453	-0.667329
47	6	0	7.725032	-2.800113	-0.210748
48	6	0	8.149094	-2.626015	1.078630
49	16	0	7.383911	-1.235678	1.886313
50	6	0	6.021712	-1.812917	-1.807514
51	6	0	5.007687	-0.804399	-2.036327
52	6	0	4.529670	-0.889324	-3.449420
53	6	0	4.893424	-2.346309	-3.879522

54	6	0	6.122086	-2.723928	-2.991736
55	9	0	6.114316	-4.060233	-2.682993
56	9	0	7.279848	-2.518134	-3.713270
57	9	0	3.855434	-3.169045	-3.570912
58	9	0	5.209856	-0.015483	-4.284628
59	9	0	3.207409	-0.635760	-3.634978
60	9	0	5.144479	-2.468565	-5.203765
61	6	0	3.703302	1.919005	0.056776
62	6	0	3.688521	1.133582	-1.067509
63	6	0	4.608314	0.049008	-1.040481
64	6	0	5.160969	-0.213254	0.370311
65	16	0	4.880415	1.396187	1.277244
66	6	0	9.104721	-3.464800	1.811612
67	6	0	-9.116917	-3.548183	-3.148656
68	6	0	-10.005029	-4.387278	-3.821958
69	6	0	-10.860486	-5.229406	-3.107016
70	6	0	-10.820435	-5.220622	-1.707887
71	6	0	-9.935806	-4.382523	-1.033390
72	6	0	9.387189	-4.779238	1.382633
73	6	0	10.299641	-5.576115	2.069580
74	6	0	10.950764	-5.087318	3.208301
75	6	0	10.674310	-3.791737	3.651607
76	6	0	9.761702	-2.990462	2.964423
77	6	0	-4.207563	-1.316149	-1.017733
78	6	0	-7.539574	0.489195	0.238470
79	6	0	7.574651	0.487631	-0.270120
80	6	0	4.236224	-1.270456	1.035200
81	15	0	0.017048	1.001191	-0.024490
82	8	0	0.810985	0.349923	1.057453
83	8	0	-0.774761	0.323739	-1.091844
84	1	0	-3.009669	1.378410	1.855333
85	1	0	-7.998179	-3.631566	0.898518
86	1	0	-2.734696	8.050824	-3.516765
87	1	0	-0.330221	8.148963	-2.839377
88	1	0	0.624875	6.428840	-1.375603
89	1	0	-4.147739	6.162076	-2.749750
90	1	0	-4.395419	4.059603	-1.556795
91	1	0	4.420000	4.112006	1.434748
92	1	0	-0.609718	6.456630	1.202336
93	1	0	0.340021	8.214957	2.623628
94	1	0	2.745558	8.142465	3.300477
95	1	0	4.165281	6.241483	2.577260
96	1	0	8.069196	-3.613718	-0.839415
97	1	0	3.033320	1.335608	-1.904559
98	1	0	-8.450106	-2.909628	-3.721402
99	1	0	-10.024627	-4.383801	-4.908945
100	1	0	-11.553538	-5.882087	-3.631765
101	1	0	-11.487815	-5.863479	-1.139064
102	1	0	-9.935540	-4.371692	0.052393
103	1	0	8.871595	-5.185438	0.517771
104	1	0	10.495232	-6.587345	1.721304
105	1	0	11.658944	-5.712700	3.745966
106	1	0	11.170448	-3.399589	4.536016
107	1	0	9.567602	-1.980393	3.313632
108	1	0	-4.266644	-2.248581	-0.446158

109	1	0	-4.501381	-1.519939	-2.049978
110	1	0	-3.171581	-0.963977	-1.009006
111	1	0	-7.570747	1.321132	-0.468486
112	1	0	-8.553588	0.100906	0.370150
113	1	0	-7.183623	0.864973	1.203259
114	1	0	8.586816	0.091601	-0.393131
115	1	0	7.609841	1.337815	0.414641
116	1	0	7.219358	0.839327	-1.244220
117	1	0	4.528334	-1.446336	2.073037
118	1	0	3.201386	-0.915273	1.015821
119	1	0	4.292681	-2.218782	0.490098

Zero-point correction=	0.832373 (Hartree/Particle)
Thermal correction to Energy=	0.901764
Thermal correction to Enthalpy=	0.902708
Thermal correction to Gibbs Free Energy=	0.722361
Sum of electronic and zero-point Energies=	-5816.963049
Sum of electronic and thermal Energies=	-5816.893658
Sum of electronic and thermal Enthalpies=	-5816.892714
Sum of electronic and thermal Free Energies=	-5817.073061

M0045 closed anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.166877	-0.204249	0.364092
2	6	0	4.614678	0.070945	-1.044388
3	6	0	3.693065	1.154091	-1.061887
4	6	0	3.703962	1.927528	0.070781
5	16	0	4.878825	1.393828	1.288478
6	6	0	5.017299	-0.772238	-2.047652
7	6	0	6.032142	-1.781339	-1.826186
8	6	0	6.133447	-2.683694	-3.016893
9	6	0	4.906871	-2.297979	-3.904214
10	6	0	4.542602	-0.844631	-3.462508
11	9	0	5.225310	0.036118	-4.288435
12	9	0	3.220945	-0.588763	-3.649046
13	9	0	5.160995	-2.408870	-5.228915
14	9	0	7.293082	-2.473671	-3.734846
15	9	0	6.123827	-4.022153	-2.718698
16	9	0	3.867922	-3.122886	-3.605148
17	6	0	8.152540	-2.618809	1.057584
18	6	0	7.729862	-2.782490	-0.234079
19	6	0	6.785682	-1.814172	-0.687633
20	6	0	6.656553	-0.615389	0.262941
21	16	0	7.399540	-1.225235	1.871605
22	6	0	9.094964	-3.473210	1.787579
23	6	0	2.320158	7.334319	2.740576
24	6	0	0.958592	7.377668	2.350438
25	6	0	0.426157	6.397506	1.538650
26	6	0	1.221943	5.314725	1.067436
27	6	0	2.588325	5.251781	1.501309

28	6	0	3.112732	6.287528	2.324865
29	6	0	0.708980	4.272886	0.224842
30	6	0	1.516843	3.180463	-0.081516
31	6	0	2.878373	3.100561	0.367712
32	6	0	3.381522	4.140939	1.132213
33	6	0	-0.696636	4.265541	-0.275432
34	6	0	-1.219159	5.299758	-1.121482
35	6	0	-2.584930	5.222959	-1.555096
36	6	0	-3.368033	4.106356	-1.182043
37	6	0	-2.855366	3.073305	-0.413912
38	6	0	-1.494491	3.166768	0.034629
39	6	0	-0.433297	6.388218	-1.596309
40	6	0	-0.974636	7.360691	-2.411425
41	6	0	-2.335749	7.303621	-2.801437
42	6	0	-3.118744	6.251076	-2.382187
43	8	0	1.002209	2.162309	-0.819311
44	8	0	-0.970612	2.155396	0.775088
45	6	0	-6.609357	-0.666177	-0.279442
46	6	0	-6.730743	-1.858384	0.681815
47	6	0	-7.688591	-2.823059	0.244740
48	6	0	-8.112888	-2.672788	-1.047337
49	16	0	-7.345337	-1.298865	-1.881537
50	6	0	-5.975997	-1.810712	1.818187
51	6	0	-4.961961	-0.798157	2.028418
52	6	0	-4.436906	-0.870536	3.427864
53	6	0	-5.418659	-1.847242	4.155188
54	6	0	-6.036523	-2.710294	3.012307
55	9	0	-5.278030	-3.851014	2.857436
56	9	0	-7.294870	-3.139034	3.342760
57	9	0	-4.824948	-2.586310	5.118062
58	9	0	-4.392207	0.336372	4.078135
59	9	0	-3.166759	-1.385766	3.501307
60	9	0	-6.418679	-1.124849	4.738310
61	6	0	-3.671216	1.895142	-0.110636
62	6	0	-3.653370	1.127650	1.026365
63	6	0	-4.567167	0.038797	1.016138
64	6	0	-5.122782	-0.246449	-0.387988
65	16	0	-4.845080	1.347464	-1.322598
66	6	0	-9.070790	-3.522854	-1.764159
67	6	0	9.963009	-4.345848	1.097459
68	6	0	10.846485	-5.171646	1.788375
69	6	0	10.894353	-5.144817	3.187017
70	6	0	10.047815	-4.279606	3.884799
71	6	0	9.161006	-3.452635	3.195048
72	6	0	-9.364042	-4.824936	-1.305558
73	6	0	-10.279032	-5.631802	-1.977240
74	6	0	-10.921952	-5.166115	-3.130245
75	6	0	-10.634766	-3.883352	-3.602936
76	6	0	-9.719787	-3.071988	-2.930873
77	6	0	4.246933	-1.272506	1.017344

78	6	0	7.577672	0.514440	-0.268620
79	6	0	-7.536161	0.462404	0.243936
80	6	0	-4.197881	-1.314169	-1.036084
81	15	0	0.020881	1.001145	-0.021246
82	8	0	-0.769573	0.332580	-1.095152
83	8	0	0.816416	0.340965	1.054116
84	1	0	3.038770	1.363442	-1.897852
85	1	0	8.027801	-3.625584	-0.847262
86	1	0	2.729121	8.115250	3.376964
87	1	0	0.323670	8.188482	2.699873
88	1	0	-0.620965	6.442367	1.260262
89	1	0	4.154047	6.225505	2.634810
90	1	0	4.414697	4.108426	1.470776
91	1	0	-4.400990	4.063488	-1.520075
92	1	0	0.613326	6.443635	-1.317962
93	1	0	-0.347144	8.176116	-2.763537
94	1	0	-2.751776	8.078641	-3.440463
95	1	0	-4.159452	6.178523	-2.691887
96	1	0	-8.037897	-3.620065	0.891147
97	1	0	-3.003018	1.349638	1.862455
98	1	0	9.956632	-4.363438	0.011829
99	1	0	11.506679	-5.833015	1.232561
100	1	0	11.586478	-5.788033	3.724516
101	1	0	10.073489	-4.248425	4.971209
102	1	0	8.501475	-2.795476	3.754993
103	1	0	-8.855429	-5.213892	-0.428744
104	1	0	-10.483058	-6.633037	-1.605676
105	1	0	-11.631963	-5.799459	-3.656038
106	1	0	-11.124292	-3.509064	-4.498700
107	1	0	-9.517523	-2.071906	-3.303385
108	1	0	4.307288	-2.214758	0.462243
109	1	0	4.540304	-1.458049	2.053197
110	1	0	3.210573	-0.921572	1.002052
111	1	0	7.607463	1.359505	0.422619
112	1	0	8.592225	0.125156	-0.392908
113	1	0	7.221593	0.871455	-1.240447
114	1	0	-8.547709	0.067451	0.375138
115	1	0	-7.573255	1.300133	-0.455938
116	1	0	-7.179988	0.832098	1.211035
117	1	0	-4.491106	-1.507773	-2.070401
118	1	0	-3.163380	-0.957803	-1.023736
119	1	0	-4.252844	-2.253135	-0.474885

Zero-point correction=	0.832342 (Hartree/Particle)
Thermal correction to Energy=	0.901749
Thermal correction to Enthalpy=	0.902693
Thermal correction to Gibbs Free Energy=	0.721968
Sum of electronic and zero-point Energies=	-5816.963055
Sum of electronic and thermal Energies=	-5816.893648
Sum of electronic and thermal Enthalpies=	-5816.892704
Sum of electronic and thermal Free Energies=	-5817.073428

M0107 closed anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.141217	-0.117353	-0.439097
2	6	0	-4.639569	0.520785	0.867007
3	6	0	-3.670251	1.535988	0.635469
4	6	0	-3.595767	1.963970	-0.665346
5	16	0	-4.739935	1.150762	-1.751186
6	6	0	-5.124576	0.003114	2.039986
7	6	0	-6.173905	-0.994960	2.049867
8	6	0	-6.369353	-1.526881	3.436091
9	6	0	-5.165650	-0.950804	4.248199
10	6	0	-4.716138	0.310858	3.444224
11	9	0	-5.393901	1.407023	3.956300
12	9	0	-3.393862	0.566003	3.624715
13	9	0	-5.481196	-0.682458	5.536372
14	9	0	-7.547777	-1.086756	4.003052
15	9	0	-6.410081	-2.895001	3.519477
16	9	0	-4.154098	-1.859668	4.243226
17	6	0	-8.199969	-2.534456	-0.602920
18	6	0	-7.843471	-2.345169	0.705034
19	6	0	-6.876944	-1.319214	0.924897
20	6	0	-6.651143	-0.437014	-0.311159
21	16	0	-7.348590	-1.446908	-1.727406
22	6	0	-9.146789	-3.528377	-1.119369
23	6	0	-1.853987	6.365618	-4.648015
24	6	0	-0.508916	6.470078	-4.215216
25	6	0	-0.055526	5.737346	-3.137757
26	6	0	-0.918695	4.855846	-2.426713
27	6	0	-2.267668	4.720169	-2.897070
28	6	0	-2.710038	5.502550	-4.000784
29	6	0	-0.490516	4.073182	-1.301828
30	6	0	-1.361502	3.138938	-0.749058
31	6	0	-2.704981	2.980442	-1.230225
32	6	0	-3.126530	3.782677	-2.278188
33	6	0	0.893744	4.159526	-0.752421
34	6	0	1.437147	5.378187	-0.227889
35	6	0	2.803824	5.400786	0.209496
36	6	0	3.568862	4.214498	0.154882
37	6	0	3.026139	3.007256	-0.262597
38	6	0	1.662314	2.998179	-0.708846
39	6	0	0.674610	6.572265	-0.085554
40	6	0	1.238113	7.724724	0.421185
41	6	0	2.600320	7.754371	0.812368
42	6	0	3.362092	6.612225	0.708447
43	8	0	-0.926971	2.356854	0.272915
44	8	0	1.127620	1.824701	-1.131301
45	6	0	5.026197	-1.879549	-0.506705
46	6	0	6.387425	-2.382265	0.004108
47	6	0	6.698148	-3.696974	-0.457899
48	6	0	5.898609	-4.155863	-1.469906

49	16	0	4.660425	-2.984211	-1.976365
50	6	0	7.078904	-1.550719	0.838539
51	6	0	6.641760	-0.195621	1.107336
52	6	0	7.464030	0.412720	2.192298
53	6	0	8.299560	-0.779286	2.761946
54	6	0	8.330493	-1.827921	1.606499
55	9	0	9.471238	-1.616901	0.853308
56	9	0	8.439556	-3.100179	2.097303
57	9	0	9.533531	-0.414222	3.181521
58	9	0	6.748031	1.024352	3.188841
59	9	0	8.335980	1.380397	1.724642
60	9	0	7.640790	-1.320609	3.823923
61	6	0	3.850366	1.794375	-0.246954
62	6	0	4.959856	1.617365	0.553803
63	6	0	5.633089	0.384572	0.377490
64	6	0	5.143535	-0.376175	-0.862788
65	16	0	3.515772	0.423651	-1.306041
66	6	0	5.993437	-5.457889	-2.141911
67	6	0	-9.144540	-3.903458	-2.477682
68	6	0	-10.036371	-4.861765	-2.959712
69	6	0	-10.955996	-5.466590	-2.099107
70	6	0	-10.976316	-5.099233	-0.748626
71	6	0	-10.087897	-4.141615	-0.265328
72	6	0	7.188598	-6.206664	-2.097819
73	6	0	7.279762	-7.447290	-2.724338
74	6	0	6.183410	-7.972122	-3.418604
75	6	0	4.996197	-7.238228	-3.479484
76	6	0	4.901468	-5.995592	-2.851865
77	6	0	-4.243056	-1.353693	-0.719866
78	6	0	-7.542646	0.824342	-0.164293
79	6	0	3.955008	-2.172986	0.577127
80	6	0	6.140434	-0.083655	-2.017564
81	15	0	0.028668	0.984155	-0.097243
82	8	0	0.723441	0.625038	1.170051
83	8	0	-0.737314	0.074138	-0.998357
84	1	0	-3.044657	1.948559	1.416043
85	1	0	-8.206834	-2.974343	1.509818
86	1	0	-2.200454	6.952252	-5.495303
87	1	0	0.176629	7.130141	-4.741494
88	1	0	0.980470	5.823924	-2.829933
89	1	0	-3.739810	5.391284	-4.334582
90	1	0	-4.145055	3.691684	-2.648929
91	1	0	4.612478	4.262551	0.452599
92	1	0	-0.371818	6.566017	-0.370692
93	1	0	0.628095	8.618705	0.527355
94	1	0	3.033494	8.670695	1.205619
95	1	0	4.403236	6.611323	1.024947
96	1	0	7.510622	-4.279320	-0.038203
97	1	0	5.238350	2.325158	1.325474
98	1	0	-8.428109	-3.452836	-3.158923
99	1	0	-10.008947	-5.137408	-4.011000
100	1	0	-11.652116	-6.211995	-2.475195
101	1	0	-11.693640	-5.554564	-0.070189
102	1	0	-10.134317	-3.851930	0.780079
103	1	0	8.056790	-5.803916	-1.584827
104	1	0	8.213225	-8.003064	-2.678377

105	1	0	6.257152	-8.939281	-3.909495
106	1	0	4.136238	-7.633443	-4.014451
107	1	0	3.966407	-5.444563	-2.893786
108	1	0	-4.371224	-2.101981	0.069613
109	1	0	-4.498193	-1.810596	-1.678881
110	1	0	-3.193535	-1.044915	-0.744057
111	1	0	-7.503483	1.444074	-1.062734
112	1	0	-8.578305	0.516984	0.006665
113	1	0	-7.214150	1.426357	0.689146
114	1	0	3.971613	-3.239174	0.820514
115	1	0	2.953429	-1.902463	0.236532
116	1	0	4.166291	-1.606375	1.489300
117	1	0	5.798184	-0.531232	-2.953537
118	1	0	6.221427	0.998096	-2.156333
119	1	0	7.134486	-0.478561	-1.783556

Zero-point correction=	0.832292 (Hartree/Particle)
Thermal correction to Energy=	0.901657
Thermal correction to Enthalpy=	0.902601
Thermal correction to Gibbs Free Energy=	0.722597
Sum of electronic and zero-point Energies=	-5816.963407
Sum of electronic and thermal Energies=	-5816.894042
Sum of electronic and thermal Enthalpies=	-5816.893098
Sum of electronic and thermal Free Energies=	-5817.073102

M0167 closed anion (SMD) Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.206652	0.054434	0.729157
2	6	0	-5.559611	0.447081	-0.713207
3	6	0	-4.798256	1.549849	-1.172177
4	6	0	-3.735834	1.898822	-0.365471
5	16	0	-3.559946	0.871807	1.058964
6	6	0	-6.553590	-0.272519	-1.328231
7	6	0	-7.101808	-1.468764	-0.722584
8	6	0	-8.297220	-1.933972	-1.492203
9	6	0	-8.596396	-0.766815	-2.487556
10	6	0	-7.240356	-0.004522	-2.623362
11	9	0	-6.563554	-0.513674	-3.716306
12	9	0	-7.450075	1.319726	-2.902238
13	9	0	-9.094704	-1.194010	-3.670341
14	9	0	-8.052992	-3.084663	-2.210994
15	9	0	-9.399581	-2.210837	-0.721221
16	9	0	-9.515578	0.069803	-1.926240
17	6	0	-6.271264	-3.335623	2.331989
18	6	0	-6.968595	-3.148534	1.167643
19	6	0	-6.523668	-2.055027	0.368746
20	6	0	-5.168572	-1.491713	0.826554
21	16	0	-4.970198	-2.146947	2.572216
22	6	0	-6.520193	-4.365423	3.346699
23	6	0	-2.070162	7.285313	-2.898001
24	6	0	-0.734198	7.301319	-2.424834
25	6	0	-0.268441	6.305084	-1.592165

26	6	0	-1.108332	5.229901	-1.184758
27	6	0	-2.446753	5.194494	-1.701802
28	6	0	-2.904078	6.249102	-2.542416
29	6	0	-0.668877	4.175061	-0.317268
30	6	0	-1.505717	3.084224	-0.098123
31	6	0	-2.840459	3.031844	-0.621386
32	6	0	-3.285200	4.102796	-1.383306
33	6	0	0.681324	4.178149	0.316562
34	6	0	1.111929	5.229084	1.193099
35	6	0	2.451050	5.201193	1.708787
36	6	0	3.299100	4.120122	1.379801
37	6	0	2.863581	3.052000	0.608572
38	6	0	1.527719	3.096828	0.087136
39	6	0	0.262678	6.292983	1.610615
40	6	0	0.720066	7.285843	2.451887
41	6	0	2.056463	7.277619	2.924066
42	6	0	2.899463	6.252266	2.558596
43	8	0	-1.068254	2.050805	0.664511
44	8	0	1.098736	2.066574	-0.684379
45	6	0	5.217877	-1.446037	-0.867570
46	6	0	6.577760	-2.005394	-0.415640
47	6	0	7.010163	-3.110600	-1.209299
48	6	0	6.309521	-3.294555	-2.370954
49	16	0	5.023665	-2.091256	-2.616662
50	6	0	7.154619	-1.419527	0.675142
51	6	0	6.605533	-0.225397	1.285457
52	6	0	7.312655	0.080614	2.562161
53	6	0	8.194117	-1.182084	2.830826
54	6	0	8.372467	-1.845107	1.429283
55	9	0	9.540064	-1.366390	0.863212
56	9	0	8.541459	-3.198060	1.541186
57	9	0	9.369816	-0.893731	3.436090
58	9	0	6.493303	0.337621	3.631168
59	9	0	8.140295	1.185338	2.464569
60	9	0	7.510268	-2.042198	3.635666
61	6	0	3.768667	1.929292	0.341943
62	6	0	4.837709	1.584643	1.142534
63	6	0	5.605449	0.490663	0.674677
64	6	0	5.247437	0.099795	-0.766171
65	16	0	3.595289	0.908711	-1.086735
66	6	0	6.538961	-4.337235	-3.378989
67	6	0	-5.975883	-4.260245	4.642295
68	6	0	-6.225931	-5.235077	5.608283
69	6	0	-7.023046	-6.341538	5.304699
70	6	0	-7.564991	-6.465025	4.020018
71	6	0	-7.315190	-5.493971	3.053524
72	6	0	7.779677	-5.004774	-3.456178
73	6	0	7.998203	-6.002183	-4.403498
74	6	0	6.987430	-6.356173	-5.304861
75	6	0	5.756690	-5.697595	-5.247228
76	6	0	5.534398	-4.698763	-4.298586
77	6	0	-6.253432	0.713385	1.668159
78	6	0	-4.051064	-2.134665	-0.037689
79	6	0	4.106438	-2.097883	-0.002712
80	6	0	6.287902	0.767540	-1.706559

81	15	0	0.020186	0.901075	-0.015359
82	8	0	0.666503	0.240199	1.152843
83	8	0	-0.620265	0.245848	-1.190042
84	1	0	-4.982702	2.025324	-2.128056
85	1	0	-7.837476	-3.739513	0.900490
86	1	0	-2.426311	8.079598	-3.549313
87	1	0	-0.066077	8.104736	-2.726018
88	1	0	0.759878	6.330115	-1.248817
89	1	0	-3.925879	6.208980	-2.914537
90	1	0	-4.306946	4.114535	-1.752317
91	1	0	4.320973	4.138065	1.748116
92	1	0	-0.766030	6.311845	1.268025
93	1	0	0.044989	8.080521	2.760665
94	1	0	2.405888	8.069193	3.582280
95	1	0	3.921850	6.218049	2.929672
96	1	0	7.835267	-3.747467	-0.911084
97	1	0	5.018739	2.052517	2.102970
98	1	0	-5.358224	-3.404243	4.899036
99	1	0	-5.794499	-5.127936	6.600343
100	1	0	-7.214772	-7.103103	6.056326
101	1	0	-8.176751	-7.327422	3.766593
102	1	0	-7.724010	-5.620572	2.055762
103	1	0	8.583325	-4.725911	-2.781256
104	1	0	8.964466	-6.499141	-4.444693
105	1	0	7.160656	-7.132738	-6.045617
106	1	0	4.962192	-5.962268	-5.940462
107	1	0	4.566618	-4.207579	-4.255304
108	1	0	-7.254961	0.314821	1.475857
109	1	0	-6.003374	0.538599	2.717211
110	1	0	-6.269171	1.791871	1.487681
111	1	0	-3.057811	-1.825749	0.294222
112	1	0	-4.124983	-3.223740	0.030064
113	1	0	-4.163068	-1.844054	-1.086821
114	1	0	4.186960	-3.186360	-0.073704
115	1	0	3.110709	-1.793713	-0.331739
116	1	0	4.218372	-1.809954	1.047200
117	1	0	6.034863	0.596598	-2.755454
118	1	0	6.299880	1.845219	-1.520985
119	1	0	7.291783	0.372372	-1.519677

Zero-point correction=	0.832207 (Hartree/Particle)
Thermal correction to Energy=	0.901597
Thermal correction to Enthalpy=	0.902541
Thermal correction to Gibbs Free Energy=	0.722162
Sum of electronic and zero-point Energies=	-5816.963804
Sum of electronic and thermal Energies=	-5816.894414
Sum of electronic and thermal Enthalpies=	-5816.893470
Sum of electronic and thermal Free Energies=	-5817.073849

M0169 closed anion (SMD) Standard orientation:

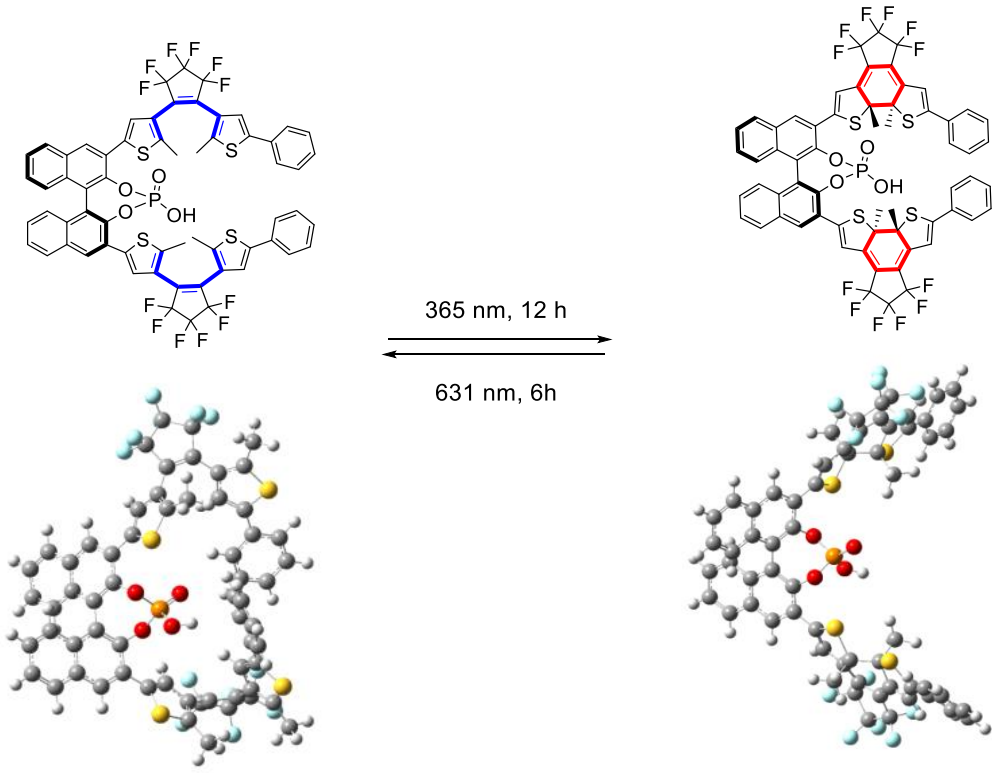
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.918513	0.027781	0.439676
2	6	0	4.551248	-0.682357	0.529520
3	6	0	3.465420	0.222109	0.727838
4	6	0	3.793135	1.539886	0.545653
5	16	0	5.494554	1.804851	0.089664
6	6	0	4.574663	-2.051666	0.468411
7	6	0	5.785835	-2.771706	0.129245
8	6	0	5.588618	-4.243308	0.329884
9	6	0	4.228081	-4.350798	1.086199
10	6	0	3.469256	-3.031598	0.726820
11	9	0	2.711563	-3.272815	-0.398565
12	9	0	2.611199	-2.680279	1.715633
13	9	0	3.540862	-5.471910	0.776048
14	9	0	5.502771	-4.928744	-0.861977
15	9	0	6.595437	-4.855319	1.035150
16	9	0	4.474813	-4.365340	2.427059
17	6	0	9.157909	-1.708071	-0.873225
18	6	0	8.200236	-2.655018	-0.629144
19	6	0	6.899981	-2.140969	-0.345092
20	6	0	6.766714	-0.645286	-0.665700
21	16	0	8.539015	-0.039824	-0.756528
22	6	0	10.573130	-1.945802	-1.174433
23	6	0	2.409253	7.251688	2.464062
24	6	0	1.086482	7.297542	1.957388
25	6	0	0.575167	6.246140	1.225303
26	6	0	1.353692	5.083575	0.959185
27	6	0	2.678407	5.027647	1.503496
28	6	0	3.183687	6.134591	2.241587
29	6	0	0.860384	3.966957	0.205694
30	6	0	1.610330	2.791049	0.146599
31	6	0	2.943706	2.734625	0.682311
32	6	0	3.453065	3.860936	1.309770
33	6	0	-0.454971	4.016251	-0.496401
34	6	0	-0.740037	4.982161	-1.520490
35	6	0	-2.032687	4.975151	-2.143743
36	6	0	-2.976150	3.988688	-1.773809
37	6	0	-2.689341	3.016361	-0.829742
38	6	0	-1.402020	3.043968	-0.195843
39	6	0	0.214959	5.928901	-1.988319
40	6	0	-0.101597	6.837694	-2.976983
41	6	0	-1.393436	6.855200	-3.558378
42	6	0	-2.334319	5.936596	-3.149008
43	8	0	1.117893	1.711602	-0.511434
44	8	0	-1.090050	2.087933	0.719344
45	6	0	-6.804133	-0.325223	-0.851804
46	6	0	-7.185820	-1.370427	0.207417
47	6	0	-8.170653	-2.293231	-0.259197
48	6	0	-8.390977	-2.270732	-1.609360
49	16	0	-7.371658	-1.087488	-2.465957
50	6	0	-6.597537	-1.246615	1.432832
51	6	0	-5.519904	-0.311041	1.679722
52	6	0	-5.208616	-0.250010	3.142415

53	6	0	-6.382064	-1.034658	3.816690
54	6	0	-6.921990	-1.977583	2.697580
55	9	0	-6.276838	-3.191991	2.789914
56	9	0	-8.253296	-2.245508	2.877825
57	9	0	-6.012559	-1.694999	4.935921
58	9	0	-5.129211	1.022099	3.649780
59	9	0	-4.023939	-0.860804	3.467821
60	9	0	-7.371070	-0.157309	4.154816
61	6	0	-3.660255	1.962871	-0.525189
62	6	0	-3.882357	1.344750	0.679106
63	6	0	-4.898908	0.351106	0.651909
64	6	0	-5.280694	-0.056788	-0.779725
65	16	0	-4.706929	1.376967	-1.831954
66	6	0	-9.324282	-3.115941	-2.363438
67	6	0	11.527564	-0.914808	-1.063619
68	6	0	12.875340	-1.150016	-1.336442
69	6	0	13.304710	-2.419618	-1.730839
70	6	0	12.368237	-3.452843	-1.853221
71	6	0	11.022088	-3.220004	-1.583042
72	6	0	-9.815989	-4.318180	-1.811553
73	6	0	-10.708881	-5.118798	-2.519470
74	6	0	-11.130883	-4.747369	-3.801498
75	6	0	-10.645174	-3.565495	-4.365998
76	6	0	-9.751833	-2.760397	-3.658227
77	6	0	6.570400	-0.028919	1.847281
78	6	0	6.157148	-0.506793	-2.085590
79	6	0	-7.669716	0.938350	-0.605584
80	6	0	-4.393878	-1.275515	-1.158765
81	15	0	-0.142539	0.772704	0.177790
82	8	0	-0.830405	0.109528	-0.966991
83	8	0	0.379221	0.117545	1.413535
84	1	0	2.456972	-0.087255	0.997801
85	1	0	8.419835	-3.715790	-0.584854
86	1	0	2.801907	8.088465	3.036589
87	1	0	0.464388	8.167654	2.153829
88	1	0	-0.443404	6.294221	0.855576
89	1	0	4.194547	6.073846	2.640076
90	1	0	4.462518	3.835697	1.711991
91	1	0	-3.950423	3.998181	-2.257284
92	1	0	1.212816	5.925610	-1.564477
93	1	0	0.652070	7.543881	-3.317480
94	1	0	-1.632129	7.579662	-4.333179
95	1	0	-3.323880	5.919449	-3.601462
96	1	0	-8.690346	-2.967488	0.411901
97	1	0	-3.334216	1.609298	1.574085
98	1	0	11.214208	0.077009	-0.749810
99	1	0	13.590831	-0.337263	-1.238843
100	1	0	14.354423	-2.602414	-1.946037
101	1	0	12.686724	-4.442993	-2.169883
102	1	0	10.308076	-4.028404	-1.706895
103	1	0	-9.479358	-4.636822	-0.829766
104	1	0	-11.068460	-6.042773	-2.073235
105	1	0	-11.823940	-5.376336	-4.354472

106	1	0	-10.961932	-3.265428	-5.361872
107	1	0	-9.393863	-1.837579	-4.105545
108	1	0	6.776576	-1.064039	2.137247
109	1	0	7.506699	0.533843	1.869978
110	1	0	5.881173	0.402215	2.578378
111	1	0	6.128063	0.537554	-2.403549
112	1	0	6.764910	-1.074364	-2.795856
113	1	0	5.137572	-0.904144	-2.105631
114	1	0	-8.725828	0.654330	-0.585420
115	1	0	-7.519617	1.680091	-1.393130
116	1	0	-7.414909	1.395170	0.356289
117	1	0	-4.561481	-1.571827	-2.196714
118	1	0	-3.339060	-1.013075	-1.033868
119	1	0	-4.623491	-2.127376	-0.509771

Zero-point correction=	0.832492 (Hartree/Particle)
Thermal correction to Energy=	0.901818
Thermal correction to Enthalpy=	0.902762
Thermal correction to Gibbs Free Energy=	0.722381
Sum of electronic and zero-point Energies=	-5816.961490
Sum of electronic and thermal Energies=	-5816.892164
Sum of electronic and thermal Enthalpies=	-5816.891220
Sum of electronic and thermal Free Energies=	-5817.071601

10. Calculation of difference in pK_a values between (*S*)-DTE-BPA 1 under the photocyclization



(*S*)-DTE-BPA open-**1**

(*S*)-DTE-BPA closed-**1**

To understand the trend in the acidities of photoresponsive DTE-BPA **1** using computational methods, the proton-exchange method[11] was utilized with respect to the experimental value of (*S*)-1,1'-binaphthyl-2,2'-diyl hydrogen phosphate (**8**) as a reference acid ($pK_{a\ (DMSO,\ experimental)} = 3.37$). The exchanged free energy in DMSO was determined[12] using the following equation:

$$\Delta G^*_{exchange} = \Delta G^*_{gas,exchange} + \Delta G^*_{solv((S)\text{-DTE-BPA }\mathbf{1}\text{ (anion))}} + \Delta G^*_{solv(\mathbf{8})} - \Delta G^*_{solv((S)\text{-DTE-BPA }\mathbf{1})} - \Delta G^*_{solv(\mathbf{8'})}$$

The ΔpK_a was then calculated using $\Delta pK_a = (\Delta G^*_{exchange,\ close} - \Delta G^*_{exchange,\ open})/RT\ln 10$, where R is the universal gas constant and T = 298.15 K.

$$\Delta G^*_{exchange,\ open} = \Delta G^*_{gas,\ exchange} + \Delta G^*_{solv((S)\text{-DTE-BPA open-}\mathbf{1}\text{ (anion))}} + \Delta G^*_{solv(\mathbf{8})} - \Delta G^*_{solv((S)\text{-DTE-BPA open-}\mathbf{1})} - \Delta G^*_{solv(\mathbf{8'})}$$

G sol $(A)^-$ (hatree)	**G sol (HA) (hatree)**	**Δ*Gas exchange (kcal/mol)**	**Δ*$G_{sol}(A)^-$ (kcal/mol)**	**Δ*G_{sol} (HA) (kcal/mol)**	**Δ*G exchange (kcal/mol)**
−5817.120264	−5817.548783	−13.8113	−61.1147	−33.2180	−1.5016

Similarly,

$$\Delta G^*_{exchange,\ closed} = \Delta G^*_{gas,\ exchange} + \Delta G^*_{solv((S)\text{-DTE-BPA closed-}\mathbf{1}\text{ (anion))}} + \Delta G^*_{solv(\mathbf{8})} - \Delta G^*_{solv((S)\text{-DTE-BPA closed-}\mathbf{1})} - \Delta G^*_{solv(\mathbf{8'})}$$

G sol $(A)^-$ (hatree)	**G sol (HA) (hatree)**	**Δ*Gas exchange (kcal/mol)**	**Δ*$G_{sol}(A)^-$ (kcal/mol)**	**Δ*G_{sol} (HA) (kcal/mol)**	**Δ*G exchange (kcal/mol)**

−5817.073849	−5817.499991	−14.3478	−64.4141	−35.5623	−2.9934

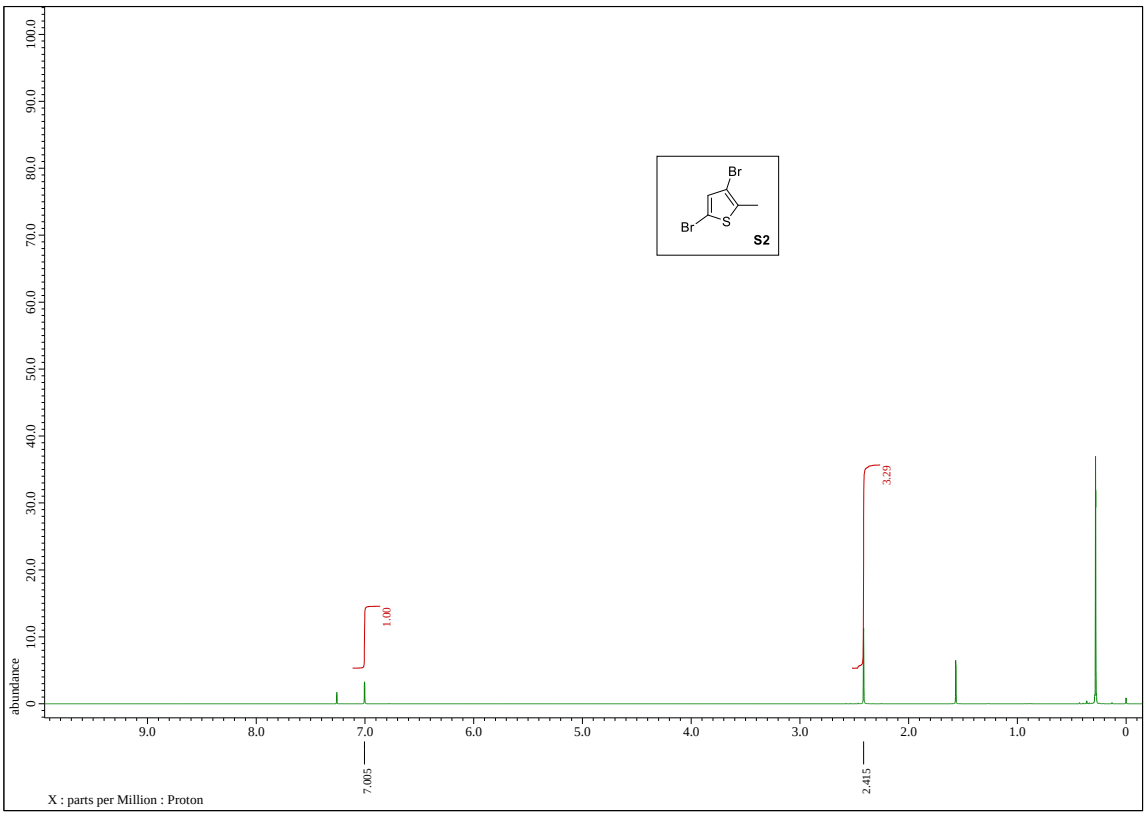
$[\Delta G^{*}_{exchange,\ closed} - \Delta G^{*}_{exchange,\ open}] = -1.4918$

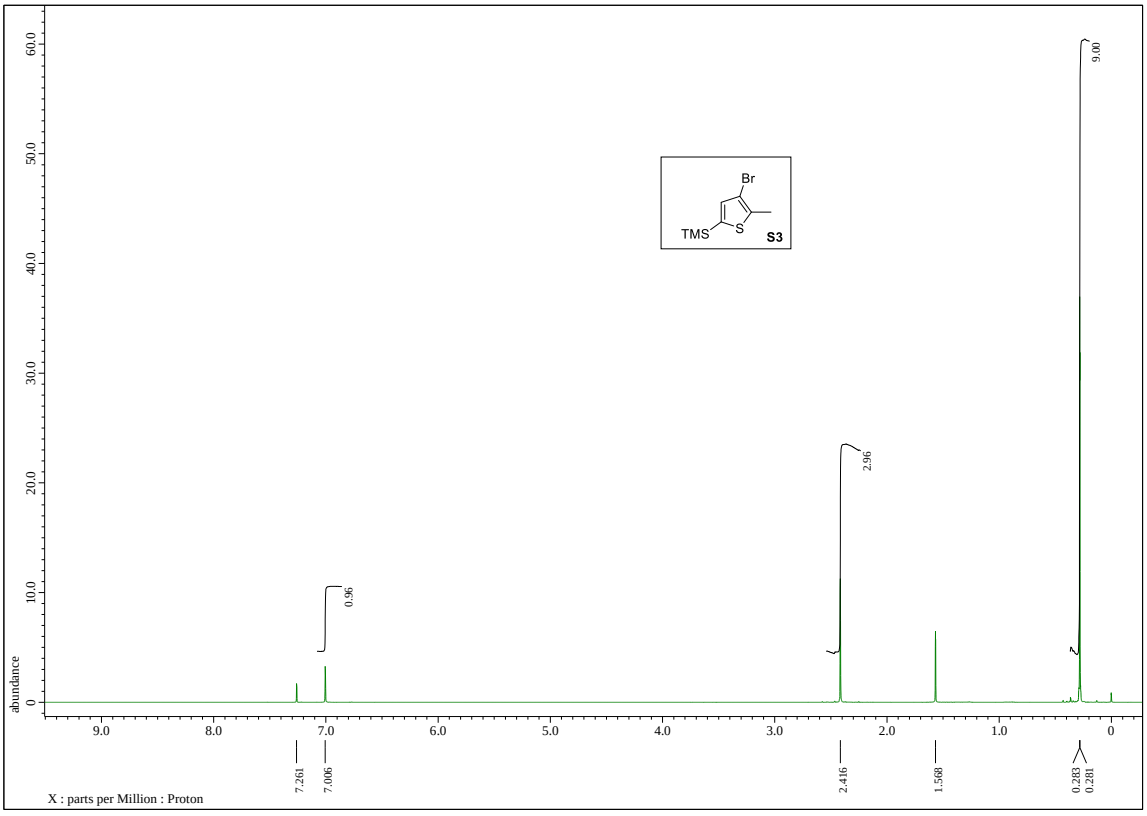
$\Delta pK_a = [\Delta G^{*}_{exchange,\ closed}/RT\ \ln(\mathbf{8}) - \Delta G^{*}_{exchange,\ open}/RT\ \ln(\mathbf{8})] + pK_a\ (\mathbf{8})$

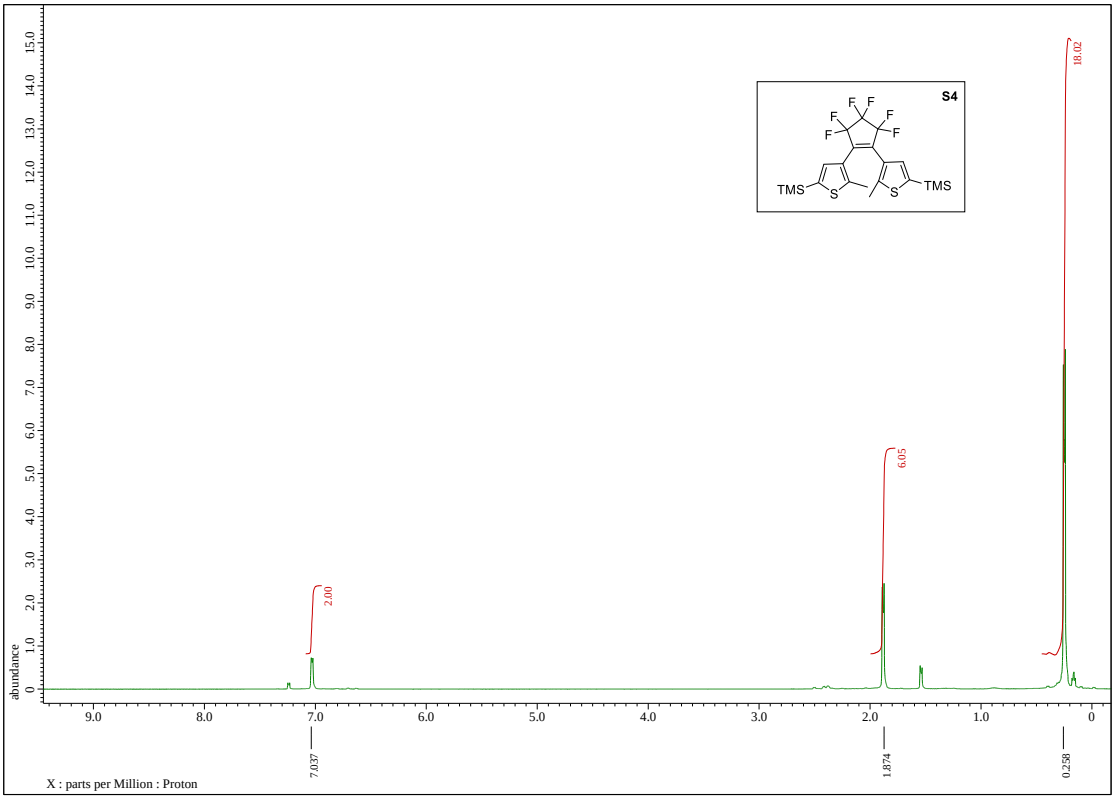
$= [[-2.99/1.34]+3.37]-[[-1.50/1.34]+3.37]$

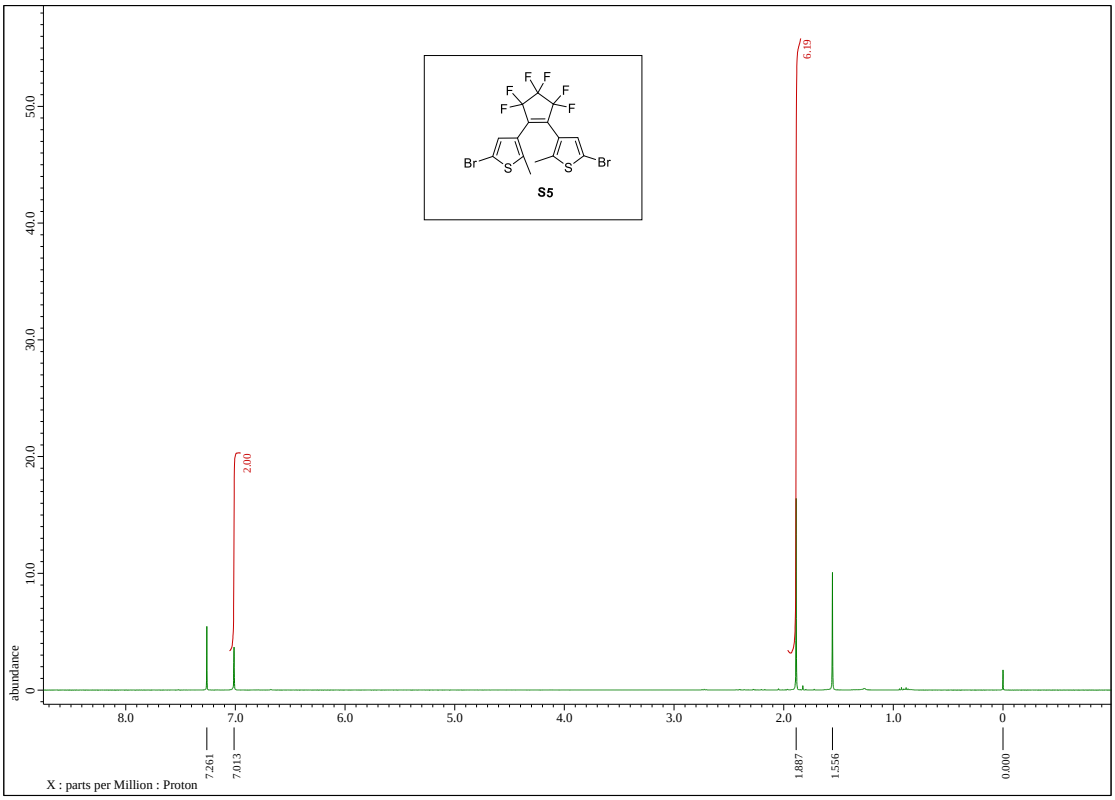
= 1.1 units (298.15K).

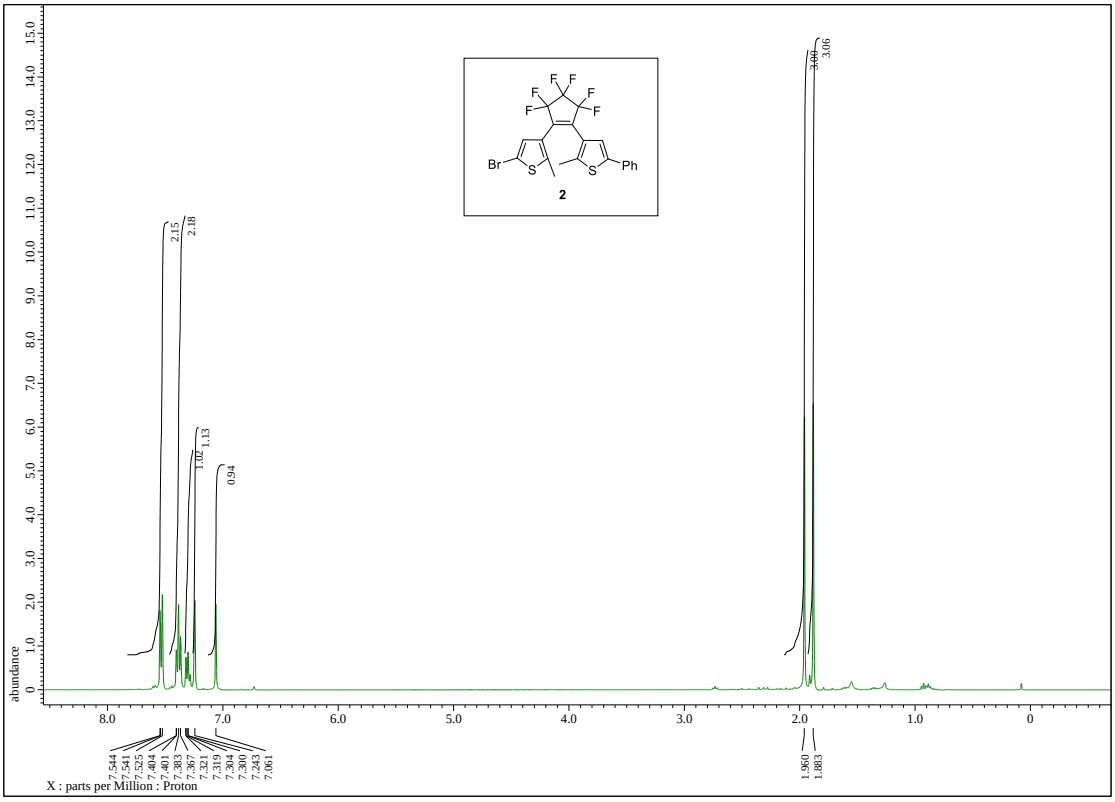
11. NMR charts

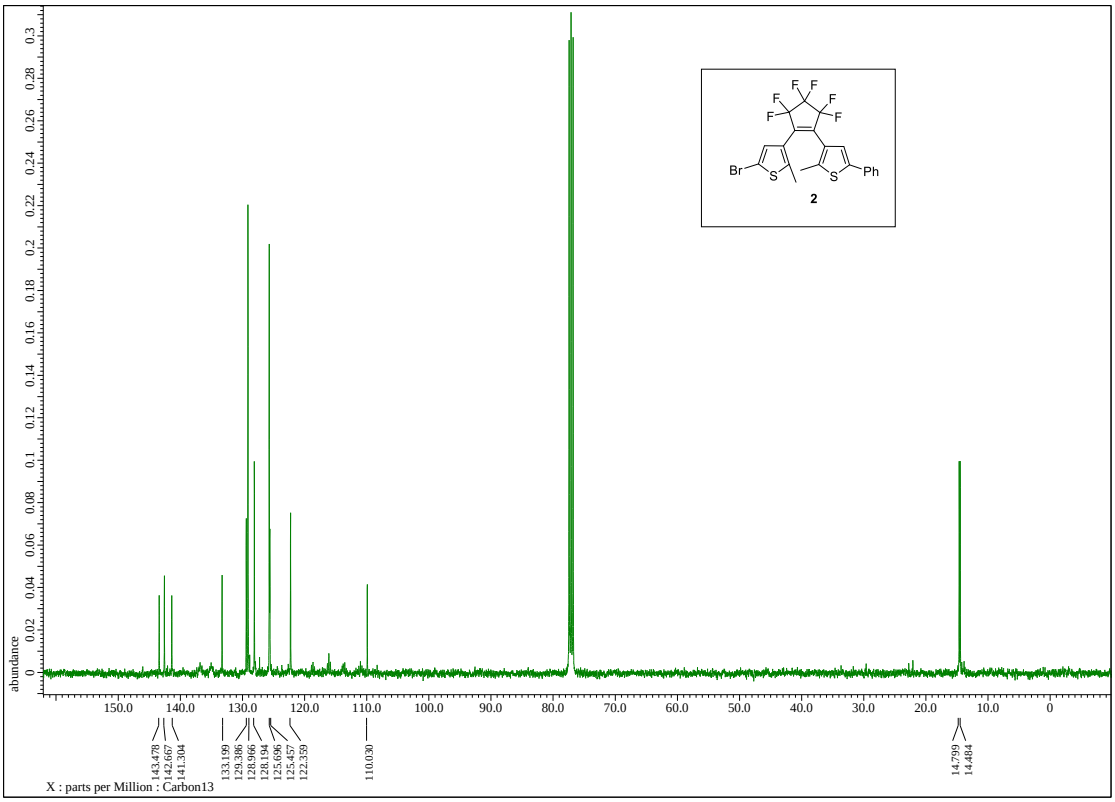


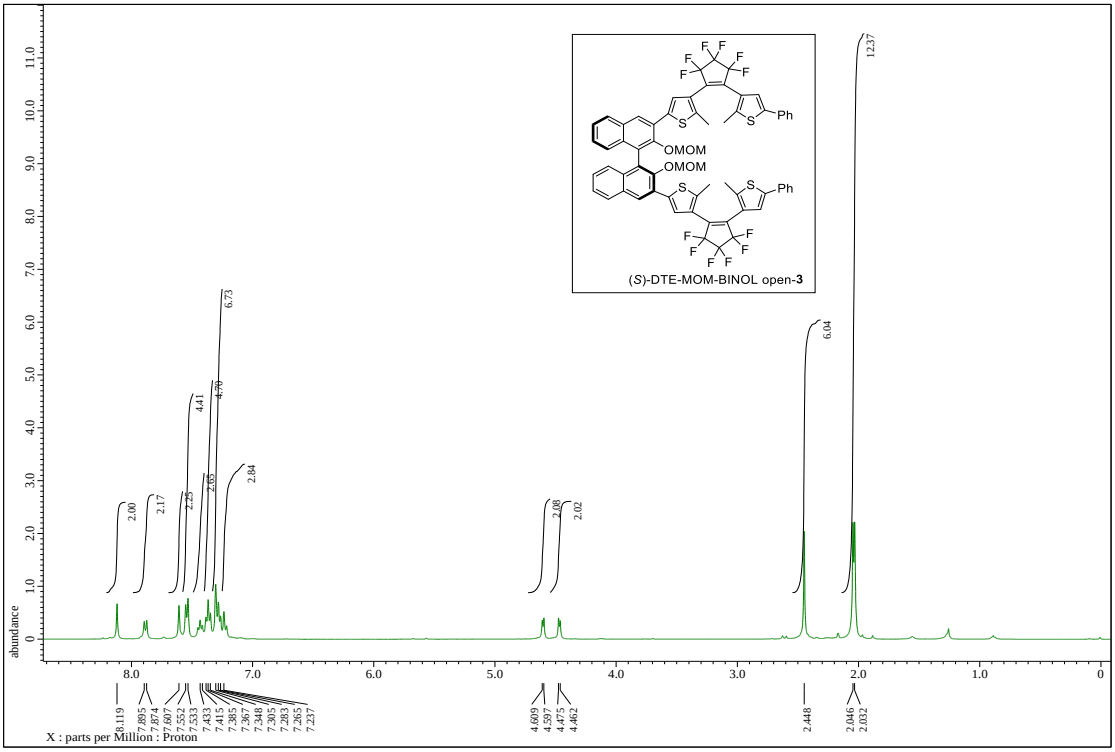


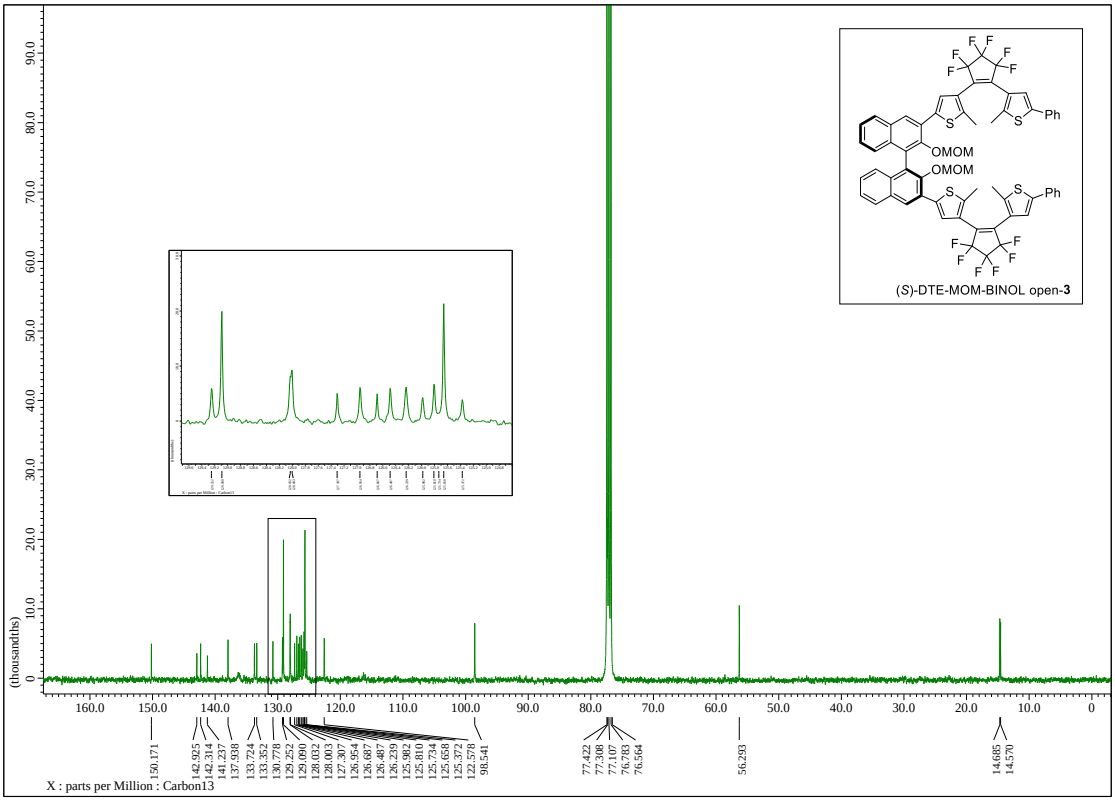

S4
TMS
TMS
F
F
F
F
F
F
S
S
abundance
2.00
6.05
18.02
7.037
1.874
0.258
X : parts per Million : Proton

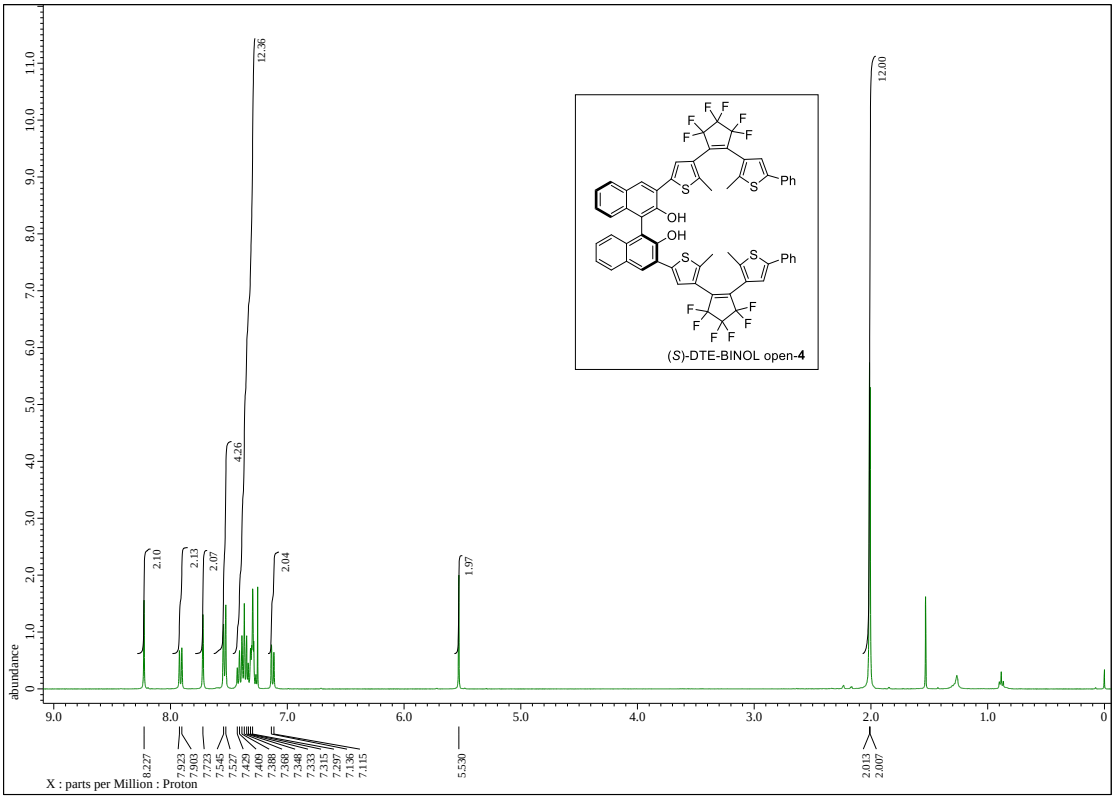

S5
Br
Br
F
F
F
F
F
F
S
S
abundance
2.00
6.19
7.261
7.013
1.887
1.556
0.000
X : parts per Million : Proton

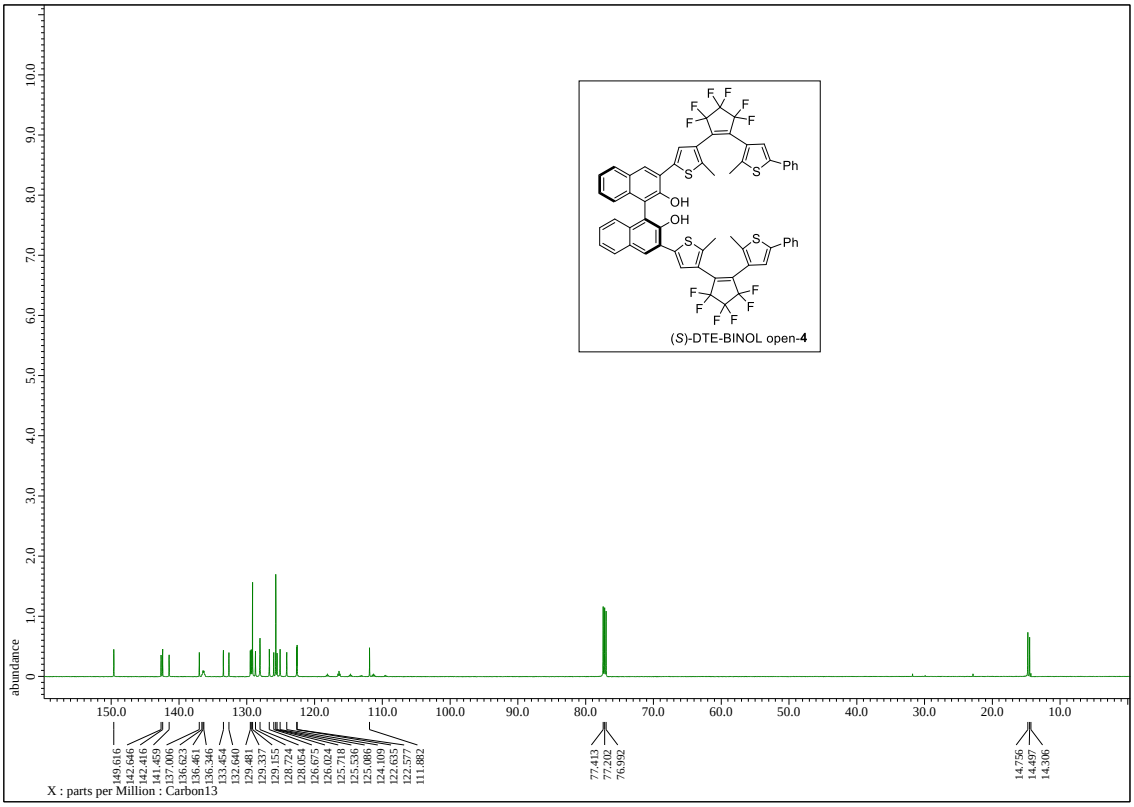

abundance
2.15
2.18
1.13
1.02
0.94
3.06
3.00
7.544
7.541
7.525
7.404
7.401
7.369
7.365
7.321
7.319
7.304
7.300
7.243
7.061
1.960
1.883
X : parts per Million : Proton
Br
S
S
Ph
F
2

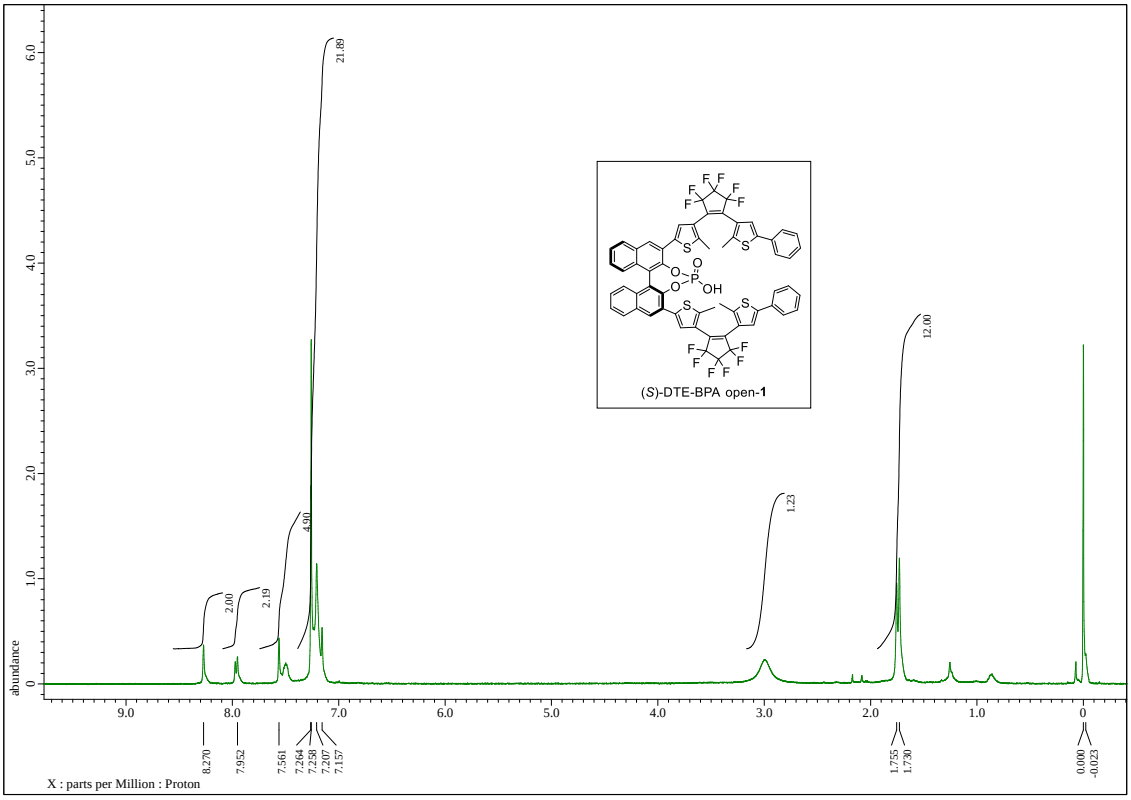

abundance
143.478
142.667
141.304
133.199
129.386
128.966
128.194
125.696
125.457
122.359
110.030
14.799
14.484
X : parts per Million : Carbon13
Br
S
S
Ph
F
2

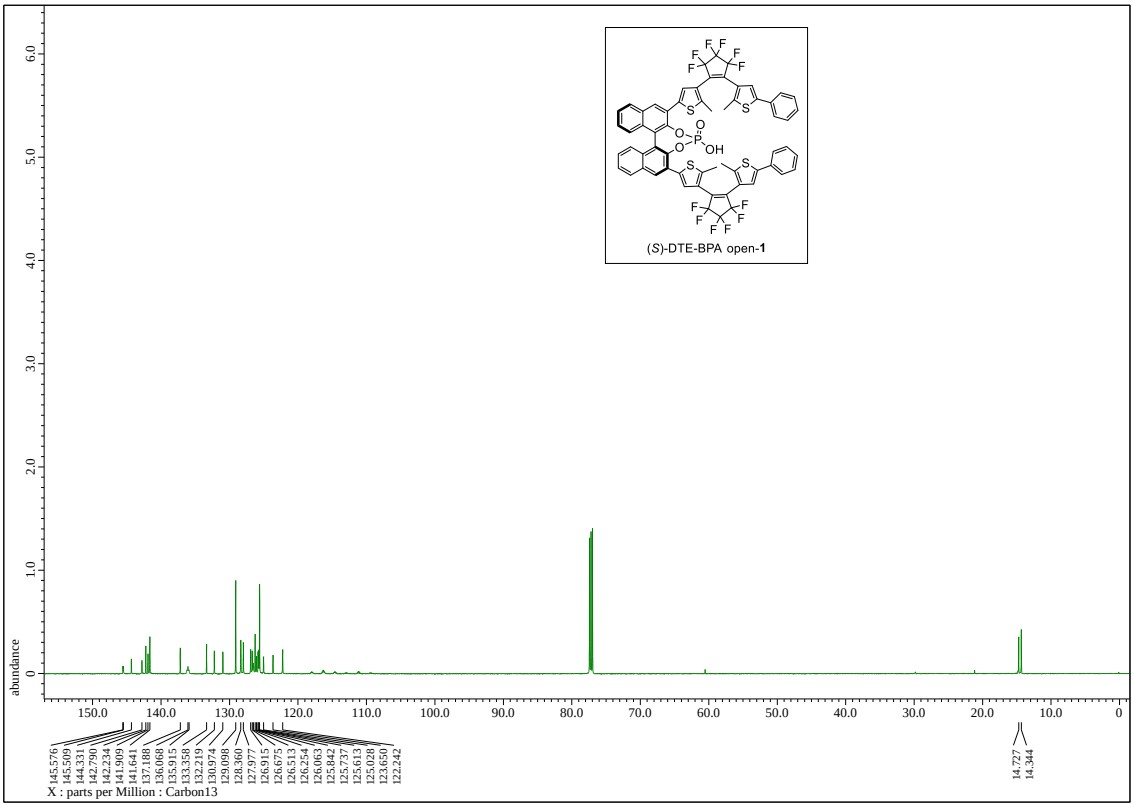

(S)-DTE-MOM-BINOL open-3
OMOM
OMOM
Ph
abundance
X : parts per Million : Proton


(S)-DTE-MOM-BINOL open-3
OMOM
OMOM
Ph
(thousandths)
X : parts per Million : Carbon13

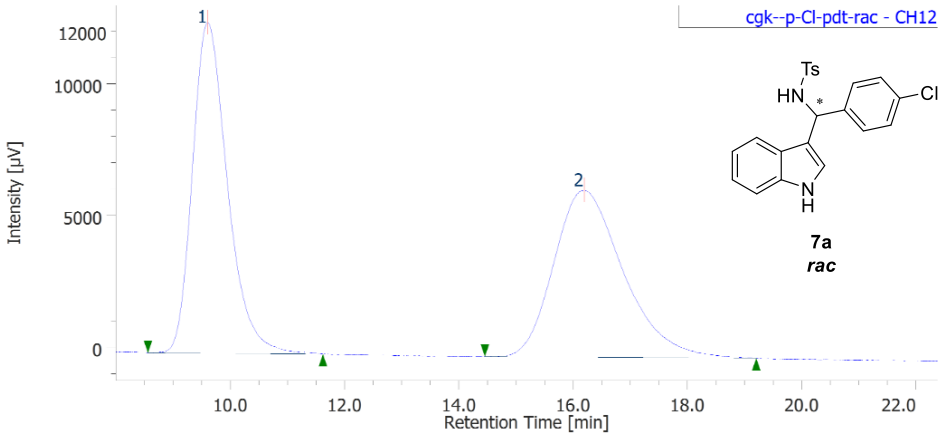

abundance
12.36
12.00
4.26
2.10
2.13
2.07
2.04
1.97
(S)-DTE-BINOL open-4
8.227
7.923
7.903
7.723
7.545
7.527
7.429
7.409
7.388
7.368
7.348
7.333
7.315
7.297
7.136
7.115
5.530
2.013
2.007
X : parts per Million : Proton


abundance
(S)-DTE-BINOL open-4
149.616
142.646
142.416
141.459
137.006
136.623
136.461
136.346
133.464
132.640
129.481
129.337
129.155
128.724
128.054
126.675
126.024
125.718
125.536
125.086
124.109
122.635
122.577
111.882
77.413
77.202
76.992
14.756
14.497
14.306
X : parts per Million : Carbon13


21.89
4.00
2.19
2.00
1.23
12.00
abundance
(S)-DTE-BPA open-1
8.270
7.952
7.561
7.264
7.238
7.207
7.157
1.755
1.730
0.000
-0.023
X : parts per Million : Proton

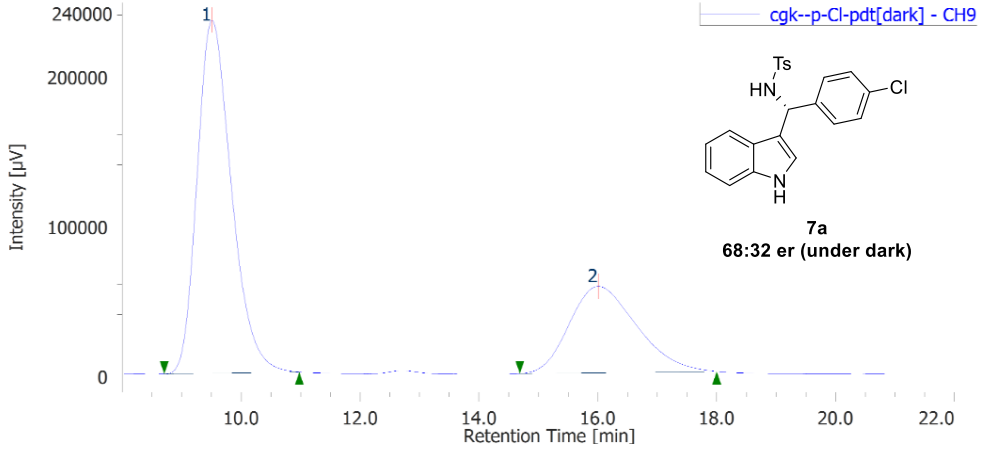

abundance
(S)-DTE-BPA open-1
145.576
145.509
144.331
142.790
142.234
141.909
141.641
137.188
136.068
135.915
133.358
132.219
130.974
129.098
128.360
127.977
127.515
126.675
126.513
126.254
126.063
125.842
125.737
125.613
125.028
123.650
122.242
14.727
14.344
X : parts per Million : Carbon13

12. HPLC charts



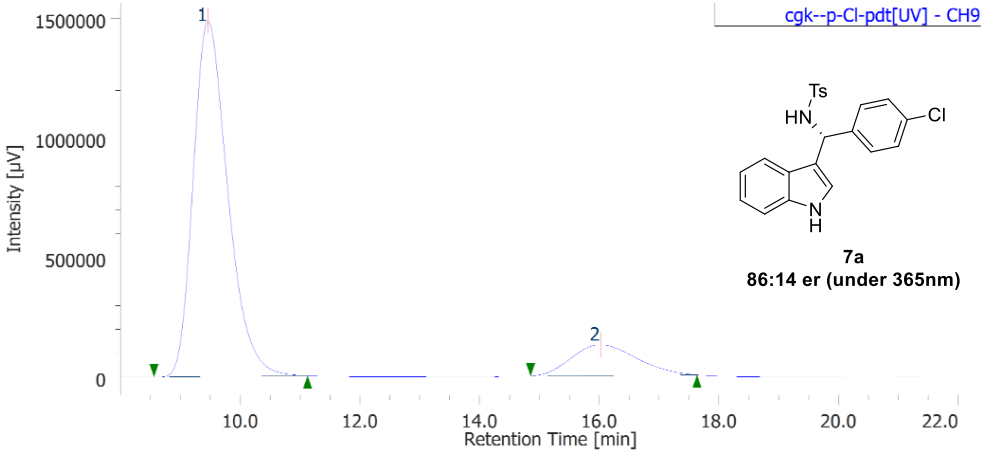
Chromatogram Name cgk--p-Cl-pdt-rac-CH12
Sample Name
Channel Name 270.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	12	9.600	534325	12542	49.996	66.447	N/A	1240	4.044	1.317	
2	Unknown	12	16.187	534411	6333	50.004	33.553	N/A	885	N/A	1.312	



Chromatogram Name cgk--p-Cl-pdt[dark]-CH9
Sample Name
Channel Name 240.0nm

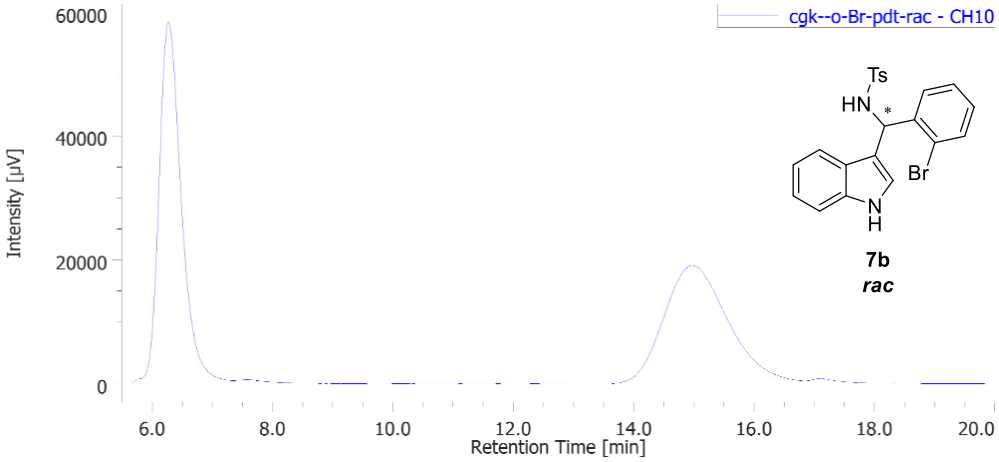
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.510	9441557	235645	67.635	80.345	N/A	1332	4.161	1.293	
2	Unknown	9	16.003	4518011	57648	32.365	19.655	N/A	941	N/A	1.280	



7a
86:14 er (under 365nm)

Chromatogram Name cgk--p-Cl-pdt[UV]-CH9
Sample Name
Channel Name 220.0nm

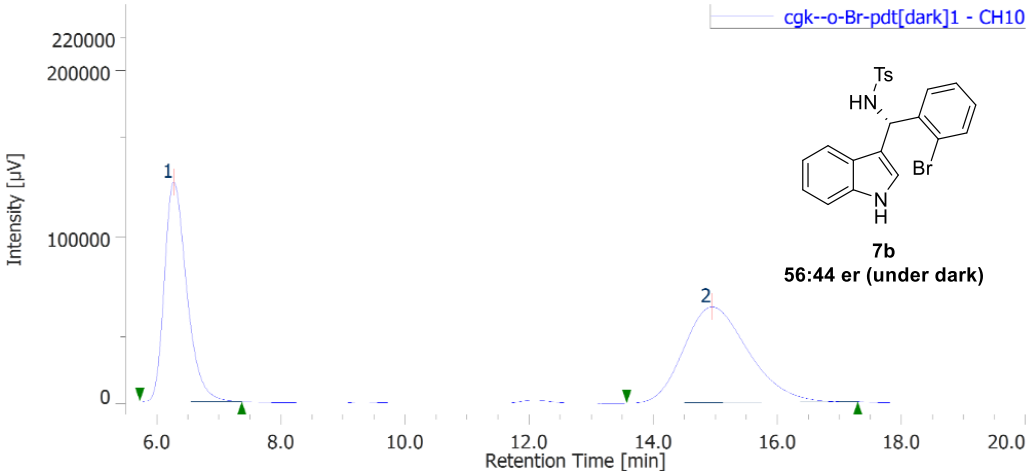
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.460	59617958	1487888	85.983	92.009	N/A	1323	4.278	1.327	
2	Unknown	9	16.020	9719107	129229	14.017	7.991	N/A	992	N/A	1.205	



7b
rac

Chromatogram Name cgk--o-Br-pdt-rac-CH9
Sample Name
Channel Name 240.0nm

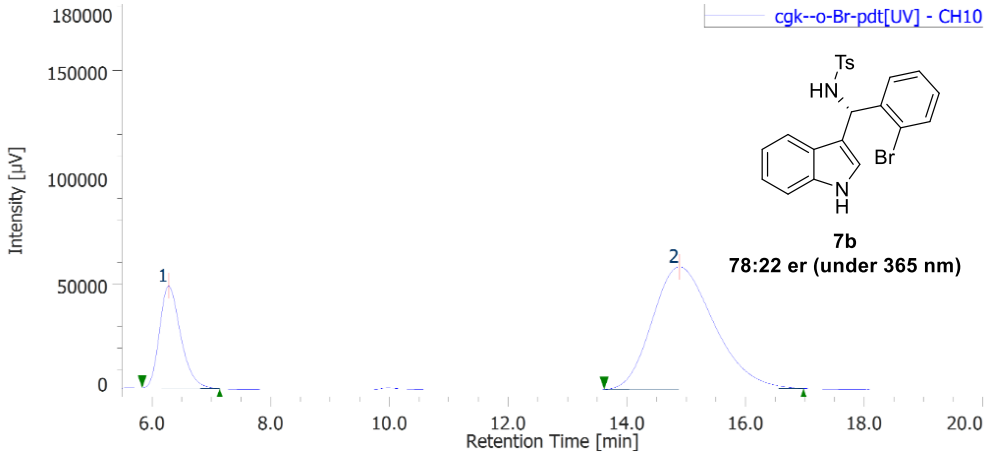
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	6.270	1402098	56888	50.773	75.153	N/A	1527	6.814	1.349	
2	Unknown	9	14.977	1359428	18809	49.227	24.847	N/A	973	N/A	1.207	



7b
56:44 er (under dark)

Chromatogram Name	cgk--o-Br-pdt[dark]1-CH10
Sample Name	
Channel Name	240.0nm

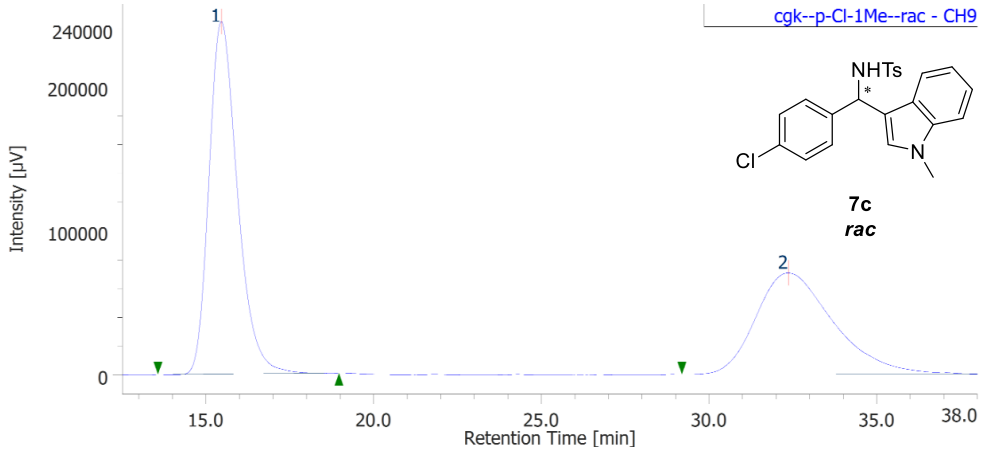
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	6.273	3289245	131844	44.178	69.636	N/A	1528	6.833	1.362	
2	Unknown	10	14.947	4156108	57490	55.822	30.364	N/A	987	N/A	1.248	



7b
78:22 er (under 365 nm)

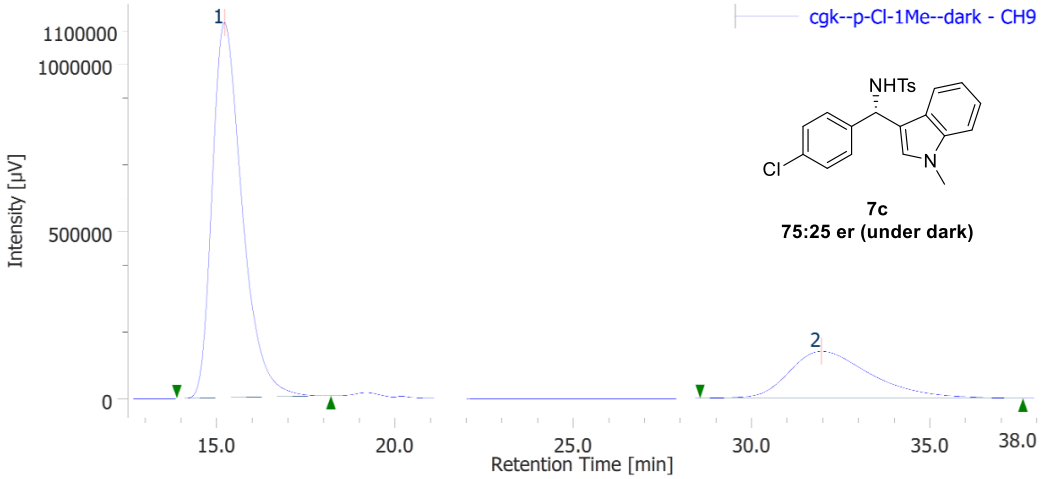
Chromatogram Name	cgk--o-Br-pdt[UV]-CH10
Sample Name	
Channel Name	240.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	10	6.280	1185290	47749	22.283	45.483	N/A	1521	6.779	1.311	
2	Unknown	10	14.887	4134083	57233	77.717	54.517	N/A	980	N/A	1.257	



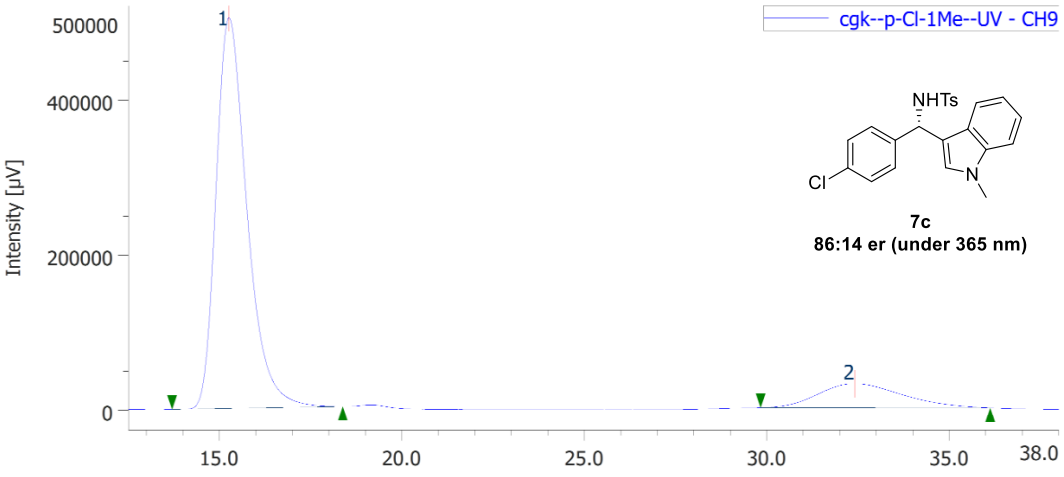
Chromatogram Name cgk--p-Cl-1Me--rac-CH9
Sample Name
Channel Name 220.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	15.460	14410196	244601	55.902	77.636	N/A	1659	5.991	1.304	
2	Unknown	9	32.367	11367413	70462	44.098	22.364	N/A	978	N/A	1.375	



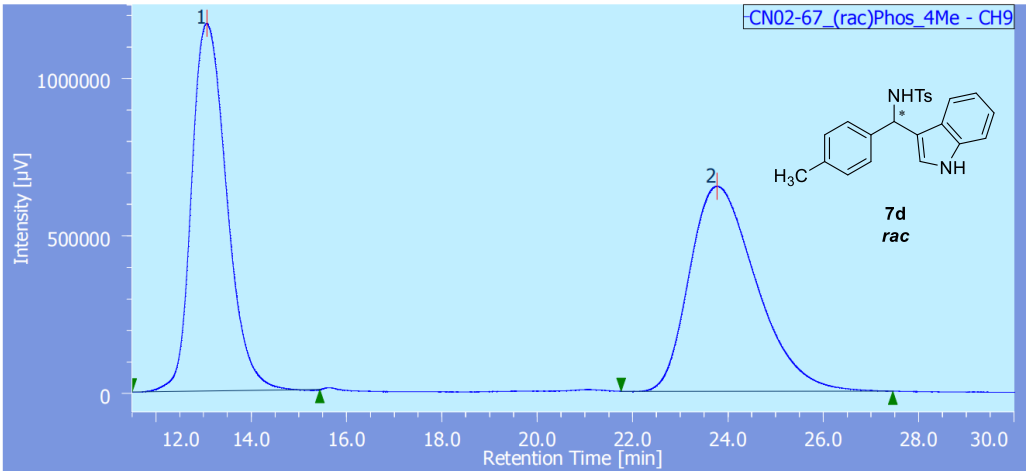
Chromatogram Name cgk--p-Cl-1Me--dark-CH9
Sample Name
Channel Name 220.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	15.223	65387532	1120514	74.430	88.876	N/A	1665	6.022	1.433	
2	Unknown	9	31.960	22463548	140246	25.570	11.124	N/A	981	N/A	1.437	



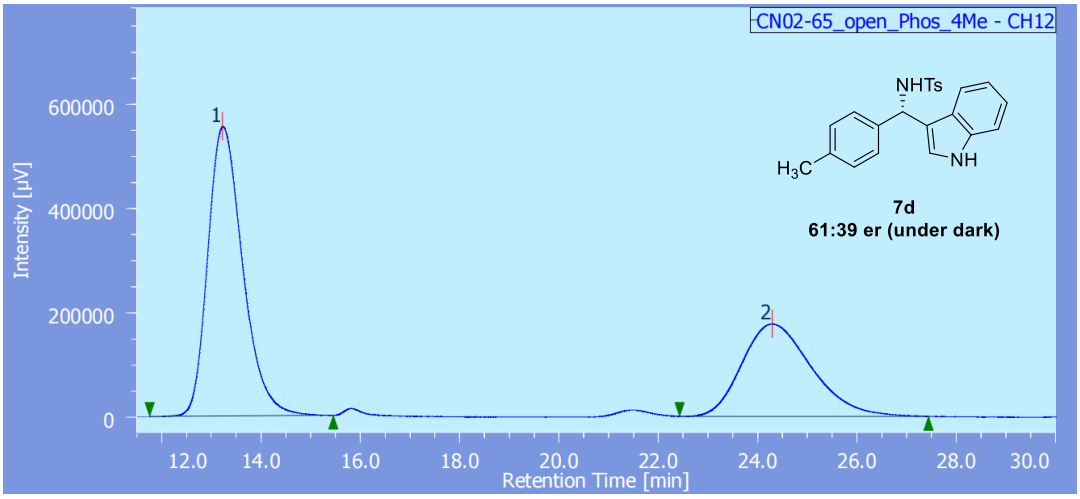
Chromatogram Name cgk--p-Cl-1Me--UV-CH9
Sample Name
Channel Name 220.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	15.267	29642310	503618	85.683	94.173	N/A	1652	5.991	1.391	
2	Unknown	9	32.413	4952819	31162	14.317	5.827	N/A	937	N/A	1.246	



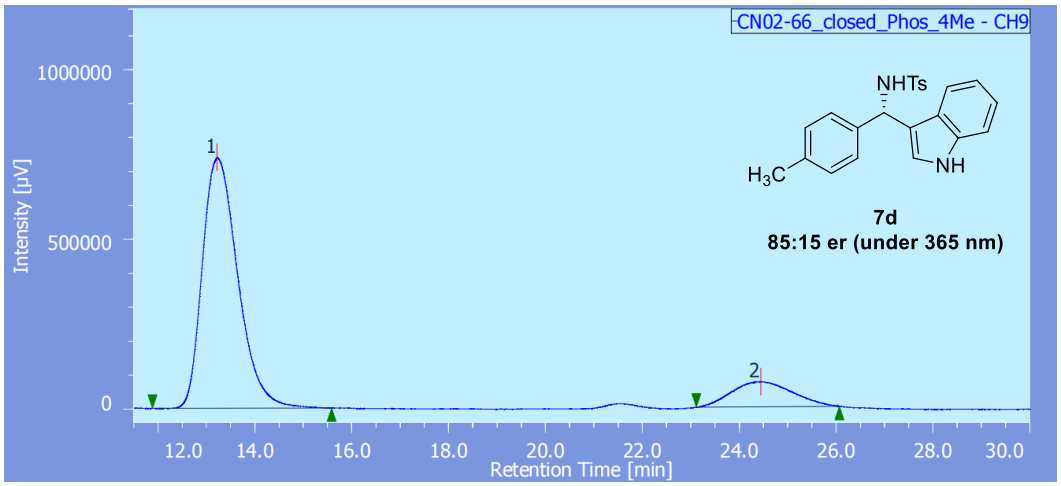
Chromatogram Name CN02-67_(rac)Phos_4Me-CH9
Sample Name
Channel Name 220.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	13.073	59764217	1167438	48.521	64.218	N/A	1536	5.505	1.258	
2	Unknown	9	23.768	63408520	650488	51.479	35.782	N/A	1377	N/A	1.377	



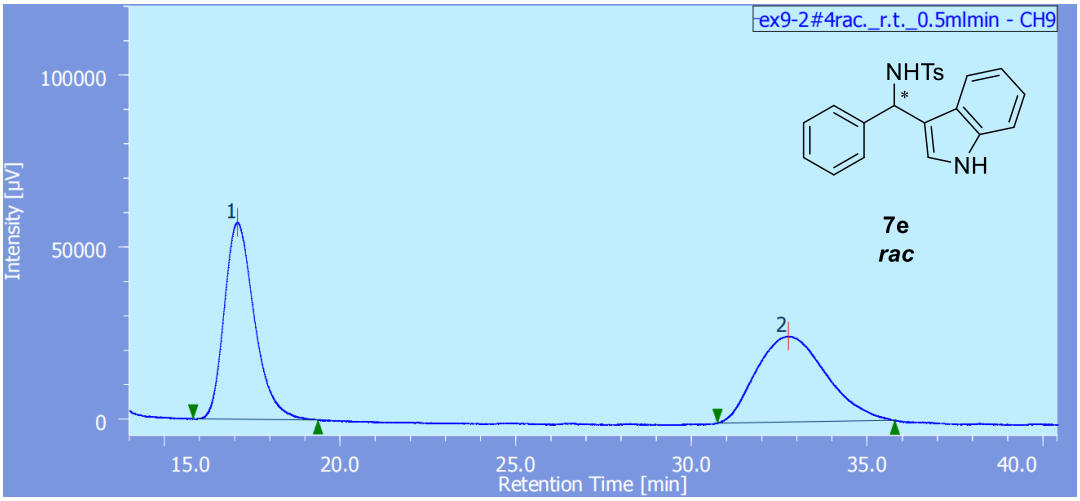
Chromatogram Name CN02-65_open_Phos_4Me-CH12
Sample Name
Channel Name 220.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	12	13.227	27106717	555056	61.085	75.800	N/A	1755	5.813	1.310	
2	Unknown	12	24.290	17268771	177204	38.915	24.200	N/A	1447	N/A	1.274	



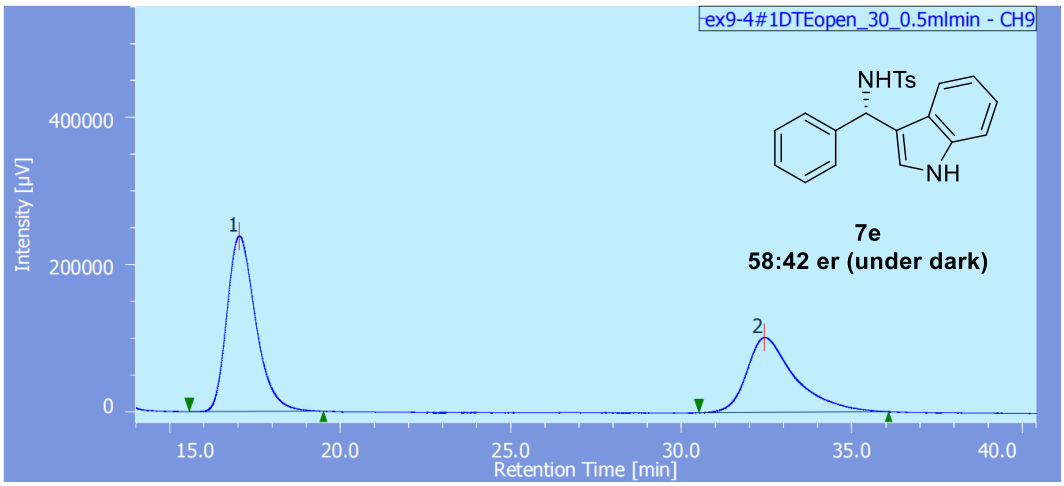
Chromatogram Name CN02-66_closed_Phos_4Me-CH9
Sample Name
Channel Name 210.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	13.218	37473754	738900	85.210	90.878	N/A	1582	6.002	1.359	
2	Unknown	9	24.442	6504177	74167	14.790	9.122	N/A	1632	N/A	1.110	



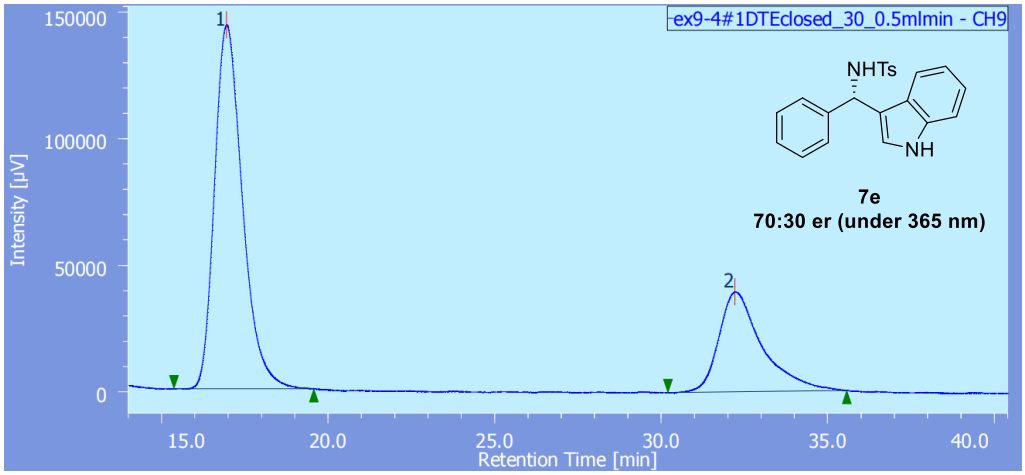
Chromatogram Name ex9-2#4rac._r.t._0.5mlmin-CH9
Sample Name
Channel Name 230.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	17.085	3388501	57113	49.635	69.584	N/A	2009	5.940	1.297	
2	Unknown	9	32.752	3438357	24964	50.365	30.416	N/A	1211	N/A	1.230	



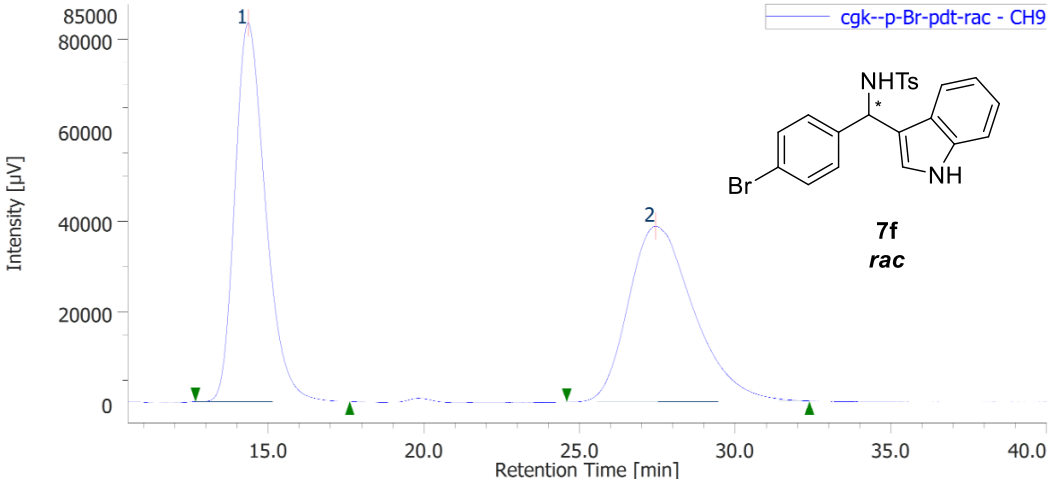
Chromatogram Name ex9-4#1DTEopen_30_0.5mlmin-CH9
Sample Name
Channel Name 230.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	17.035	13899393	238197	57.959	70.027	N/A	2059	8.003	1.323	
2	Unknown	9	32.432	10082174	101952	42.041	29.973	N/A	3032	N/A	1.573	



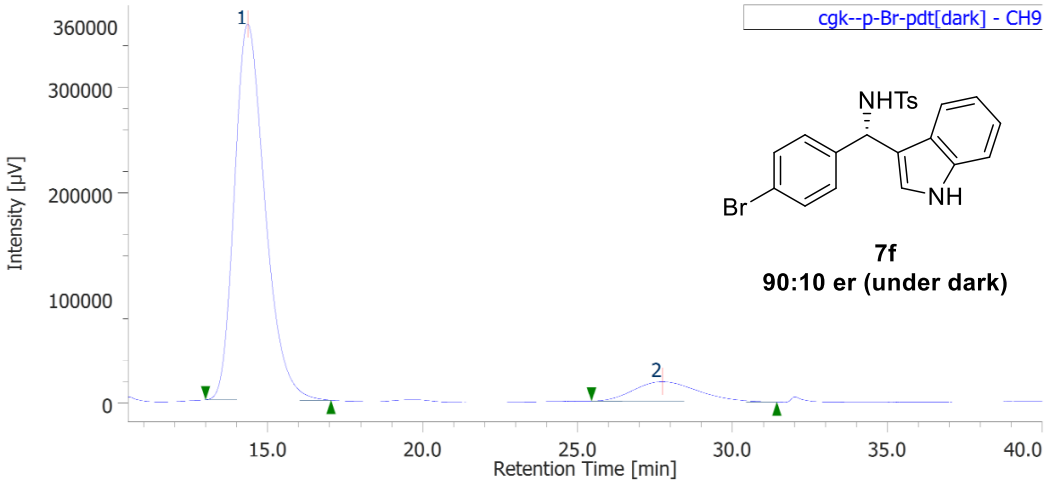
Chromatogram Name ex9-4#1DTEclosed_30_0.5mlmin-CH9
Sample Name
Channel Name 230.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	16.948	8330820	143729	70.073	78.436	N/A	2068	8.473	1.324	
2	Unknown	9	32.205	3557968	39516	29.927	21.564	N/A	3692	N/A	1.601	



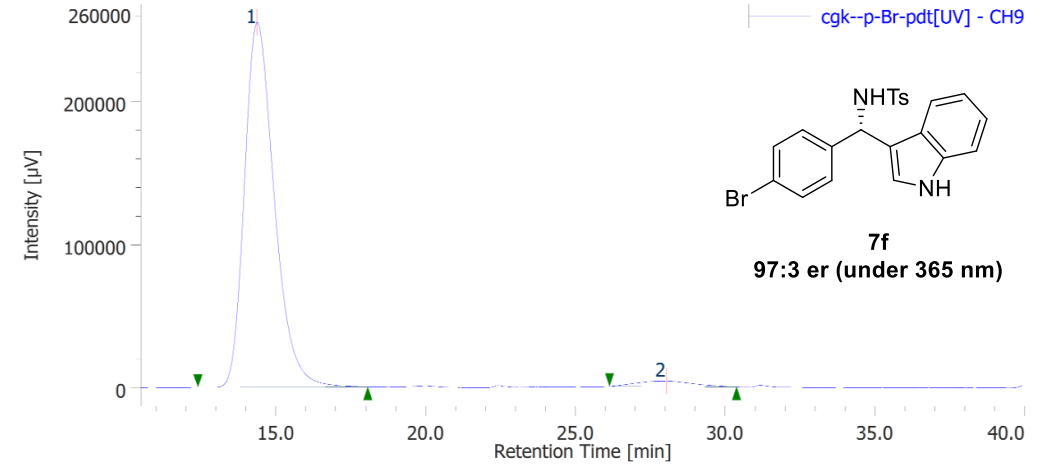
Chromatogram Name cgk--p-Br-pdt-rac-CH9
Sample Name
Channel Name 245.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	14.353	5662151	83138	50.191	68.318	N/A	1062	4.731	1.301	
2	Unknown	9	27.443	5619031	38554	49.809	31.682	N/A	840	N/A	1.345	



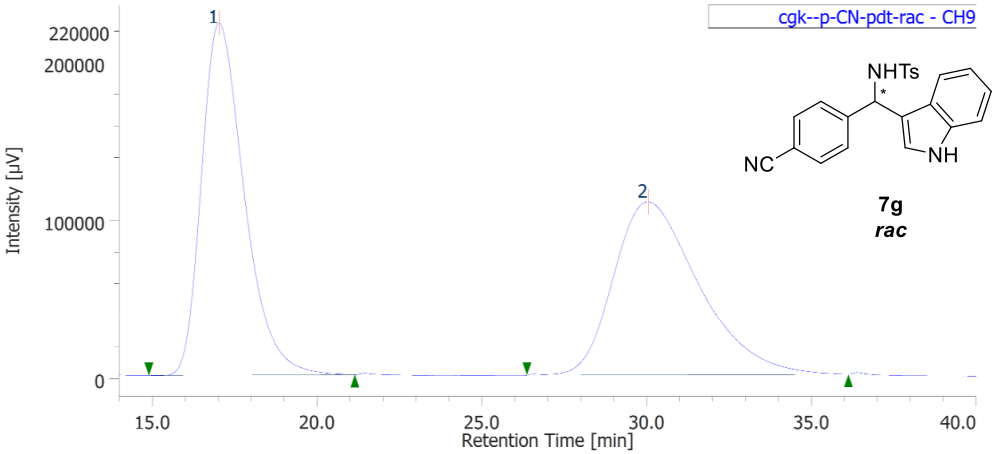
Chromatogram Name cgk--p-Br-pdt[dark]-CH9
Sample Name
Channel Name 220.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	14.353	24482954	357675	90.029	94.996	N/A	1046	4.774	1.295	
2	Unknown	9	27.733	2711453	18842	9.971	5.004	N/A	832	N/A	1.233	



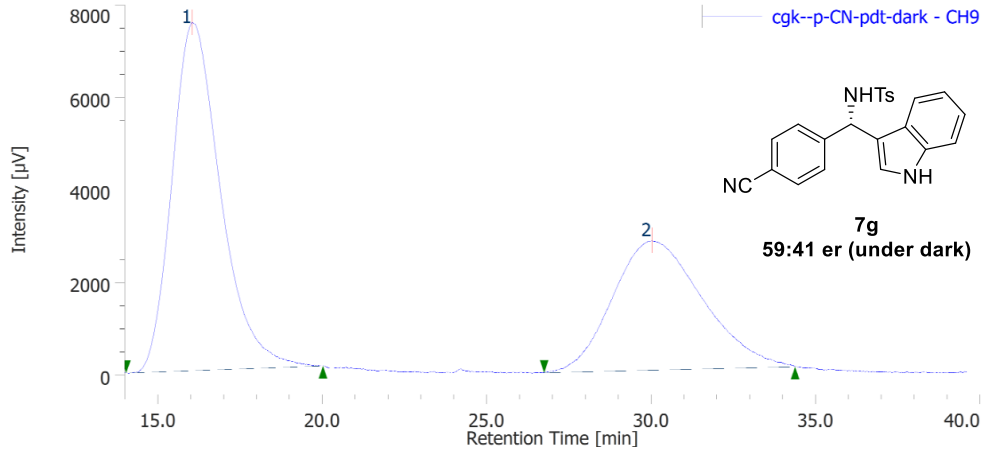
Chromatogram Name cgk--p-Br-pdt[UV]-CH9
Sample Name
Channel Name 230.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	14.377	17627535	254698	97.146	98.466	N/A	1041	5.110	1.322	
2	Unknown	9	28.030	517842	3968	2.854	1.534	N/A	983	N/A	1.094	



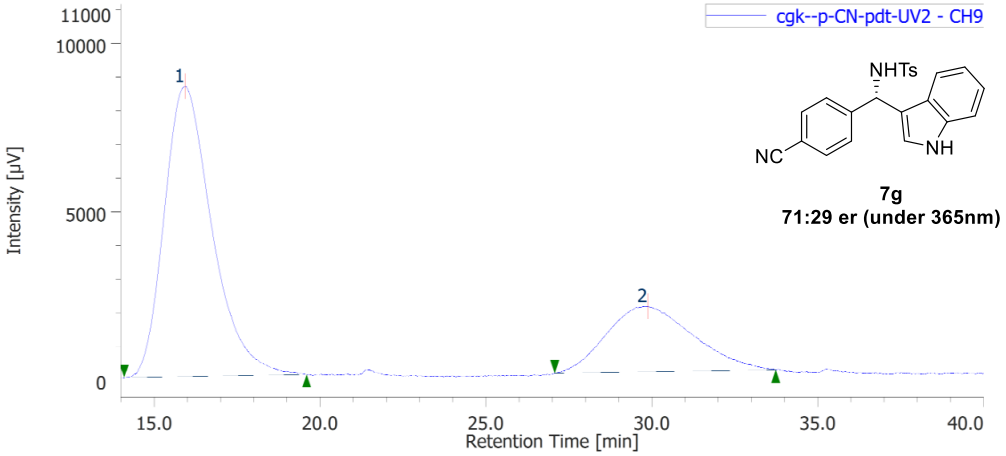
Chromatogram Name cgk--p-CN-pdt-rac-CH9
Sample Name
Channel Name 240.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	17.023	20109580	223204	50.449	67.065	N/A	861	3.740	1.404	
2	Unknown	9	30.043	19751973	109614	49.551	32.935	N/A	665	N/A	1.423	



Chromatogram Name cgk--p-CN-pdt-dark-CH9
Sample Name
Channel Name 270.0nm

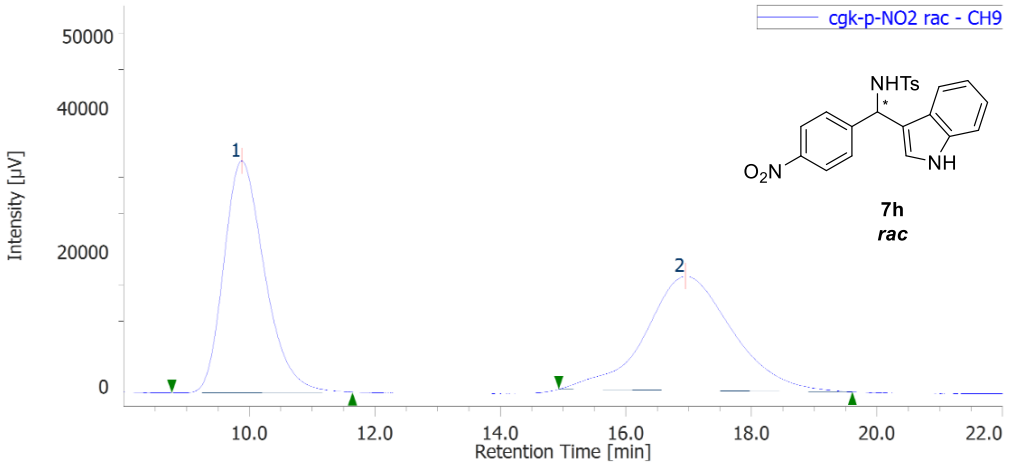
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	16.050	769923	7520	59.220	72.874	N/A	602	3.660	1.361	
2	Unknown	9	30.023	530189	2799	40.780	27.126	N/A	568	N/A	1.227	



7g
71:29 er (under 365nm)

Chromatogram Name cgk--p-CN-pdt-UV2-CH9
Sample Name
Channel Name 260.0nm

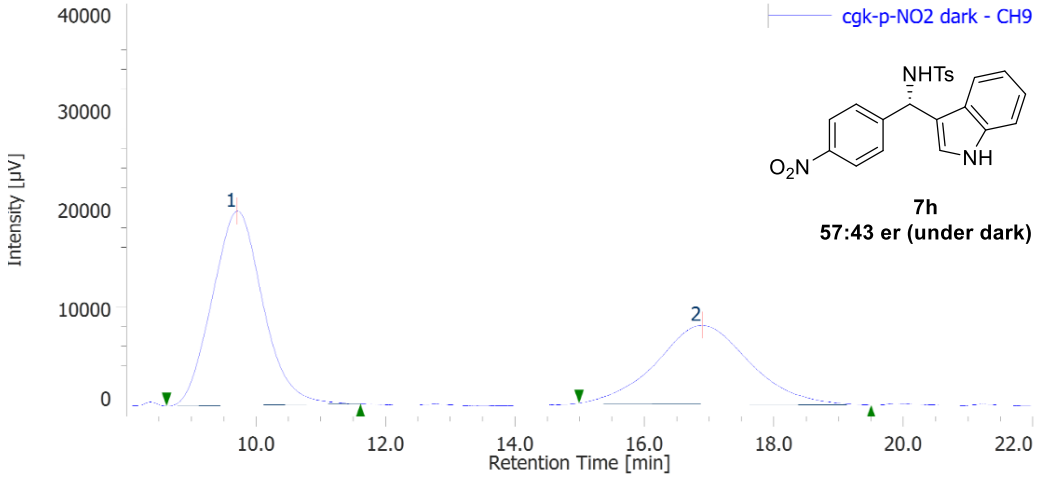
#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	15.933	861859	8625	71.060	81.630	N/A	619	3.743	1.344	
2	Unknown	9	29.877	351008	1941	28.940	18.370	N/A	593	N/A	1.180	



7h
rac

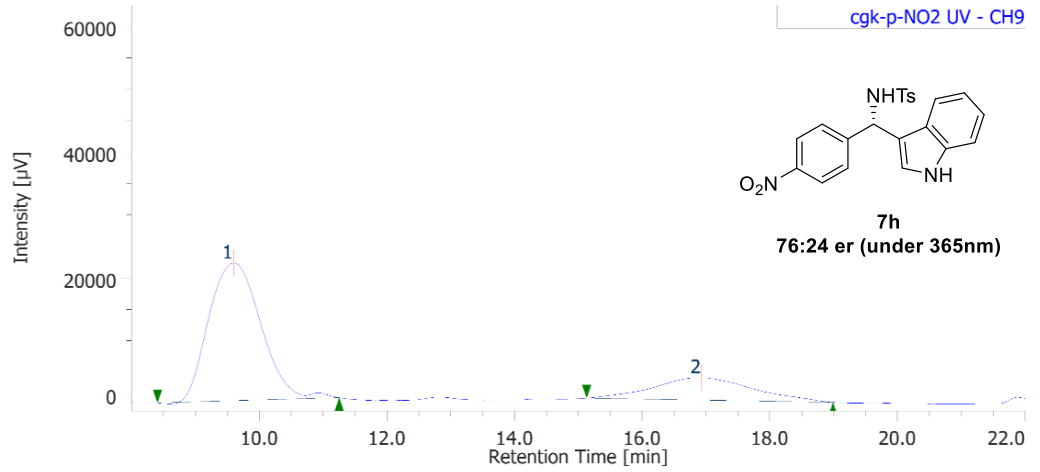
Chromatogram Name cgk-p-NO2 rac-CH9
Sample Name
Channel Name 280.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.877	1455384	32207	48.828	66.996	N/A	1139	3.966	1.290	
2	Unknown	9	16.943	1525231	15866	51.172	33.004	N/A	796	N/A	1.030	



Chromatogram Name cgk-p-NO2 dark-CH9
Sample Name
Channel Name 230.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.710	1063615	19641	57.207	71.143	N/A	753	3.623	1.114	
2	Unknown	9	16.887	795618	7967	42.793	28.857	N/A	698	N/A	1.060	



Chromatogram Name cgk-p-NO2 UV-CH9
Sample Name
Channel Name 234.0nm

#	Peak Name	CH	tR [min]	Area [μV·sec]	Height [μV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	Unknown	9	9.597	1239063	21874	76.305	85.964	N/A	627	3.401	1.154	
2	Unknown	9	16.927	384756	3571	23.695	14.036	N/A	589	N/A	1.065	

13. References

1. R. Liu Y. Yang, Q. Cui, W. Xu, R. Peng, L. Li, *Chem. Eur. J*. **2018**, *24*,17756.
2. N. Sun, C. Wang, H. Wang, X. Gao, J. Jiang, *ACS Appl. Mater. Interfaces* **2020**, *12*, 56491.
3. S. Morales, F. G. Guijarro, J. L. G. Ruano, M. B. Cid, *J. Am. Chem. Soc*. **2014**, *136*, 1082.
4. D. G. Stark, T. J. O'Riordan,, A. D. Smith, *Org. Lett.* **2014**, 16, 6496.
5. M. Barbarotto, J. Geist, S. Choppin, F. Colobert, *Tetrahedron: Asymmetry* **2009**, *20*, 2780.
6. F. Xu, D. Huang, C. Han, W. Shen, X. Lin, Y. Wang, *J. Org. Chem.* **2010**, *75*, 8677.
7. E. Xie, S. Huang, X. Lin, *Org. Lett.* **2019**, *21*, 3682.
8. S. Takizawa, F. A. Arteaga, Y. Yoshida, J. Kodera, Y. Nagata, H. Sasai, *Dalton Trans*. **2013**, *42***,** 11787.
9. K. Wu, Y.-J. Jiang, Y.-S. Fan, D. Sha, S. Zhang, *Chem. Eur. J*. **2013**, *19*, 474.
10. L. Liu, Q. Zhao, F. Du, H. Chen, Z. Qin, B. Fu, *Tetrahedron: Asymmetry* **2011**, *22*, 1874.
11. C. Yang, X. Xue, J. Jin, X. Li and J. Cheng, *J. Org. Chem*., **2013**, *78*, 7076−7085.
12. B. M. Neilson, C. W. Bielawski, *Organometallics,* **2013**, *32*, 3121.