Electronic Supplementary Information

DFT Calculation-Aided Optimisation of Chiral Phosphoric Acid Catalyst: Case Study of Kinetic Resolution of Racemic Secondary Alcohols through Lactonisation

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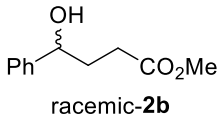
1. General Information

All reactions were carried out under nitrogen atmosphere in flame-dried glassware. Dichloromethane (CH_2Cl_2) and toluene were supplied from KANTO Chemical Co., Inc. as "Dehydrated solvent system". Other solvents and reagents were purchased from commercial suppliers and used without further purification. Purification of reaction products was carried out by flash column chromatography using silica gel 60 N ((Merck 40-63 μm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 GF 254, 0.25 mm). ^{1}H NMR spectra were recorded on a JEOL ECA-600 (600 MHz) spectrometer. Chemical shifts are reported in ppm from tetramethylsilane or solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm, TMS: 0.00 ppm). ^{13}C NMR spectra were recorded on a JEOL ECA-600 (151 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 77.0 ppm). Infrared spectra were recorded on a JASCO FT/IR-4100 spectrometer. Melting point (mp) was measured by METTLER TOLEDO MP70. Chiral stationary phase HPLC analysis was performed on a Jasco LC-2000 Plus Series system with DAICEL chiral analytical column (4.6 mmΦ* 250 mm length). Optical rotations were measured on a Jasco P-1020 digital polarimeter with a sodium lamp and reported as follows; $[\alpha]^{T\ ^\circ C}_D$ (c = g/100 mL, solvent, % ee). High resolution mass spectra analysis was performed on a Bruker Daltonics solariX 9.4T FT-ICR-MS spectrometer and a JEOL JMST100GCV Time-of-Flight Mass Spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University

2. Preparation of Substrates

The substrate methyl 4-hydroxy-4-phenylbutyrate was prepared according to the literature, and spectral data in agreement with the information reported in the literature.[1]

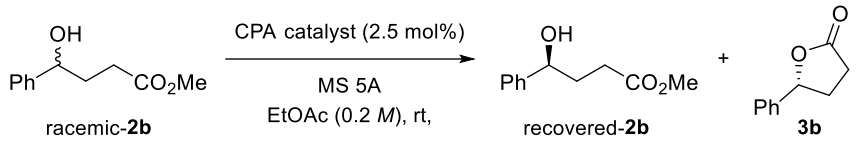
Methyl 4-hydroxy-4-phenylbutanoate (2b)



racemic-**2b**

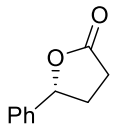
colorless oil**;**
^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.35-7.34 (m, 4H), 7.30-7.27 (m, 1H), 4.75 (t, *J* = 8.0 Hz, 1H), 3.66 (s, 3H), 2.44 (t, *J* = 8.0 Hz, 2H), 2.31 (br, 1H), 2.09-2.06 (m, 2H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 174.4, 144.1, 128.6, 127.8, 125.8, 73.6, 51.8, 33.9, 30.5; HPLC analysis Chiralpak IC-3 (Hexane/IPA = 92/8, 1.2 mL/min, 220 nm, 40 °C) (*S*)-**2b**:11.6 min, (*R*)-**2b**: 16.0 min.

3. General Procedure of Kinetic Resolution and Determination of Absolute Configuration



To a dried test tube was added racemic ester **2b** (38.8 mg, 0.2 mmol), MS 5A (25 mg), and anhydrous EtOAc (1 mL). To the mixture was added CPA catalyst **1** (0.005 mmol) and stirred at room temperature. The reaction was monitored by HPLC. The mixture was passed through flash column chromatography (Hex/EtOAc = 4/1). After purification, enantioenriched ester **2b** was recovered as a colorless oil and enantioenriched lactone **3b** was obtained as a colorless oil. The enantiomeric excess was determined by chiral stationary phase HPLC analysis.

(*R*)-5-Phenyldihydrofuran-2(3*H*)-one (3b)[2]



(*R*)-**3b**

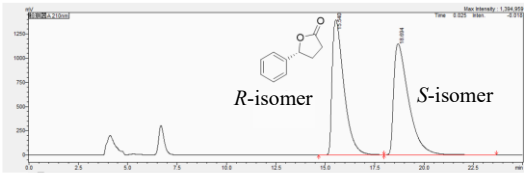
Colorless oil;

^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.40-7.37 (m, 2H), 7.35-7.32 (m, 3H), 5.52-5.50 (m, 1H), 2.68-2.62 (m, 3H), 2.23-2.15 (m, 1H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 177.2, 139.4, 128.9 (2C), 128.6, 125.4 (2C), 81.4, 31.1, 29.1; HPLC analysis Chiralpak AS-H (Hexane/IPA = 80/20, 1.0 mL/min, 220 nm, 30 °C) 13.9 min (major), 17.0 min (minor).

In the kinetic resolution, the absolute configuration of product **3b** was assigned to be the *R* configuration by comparing with the HPLC spectra information reported in the literature.[2]

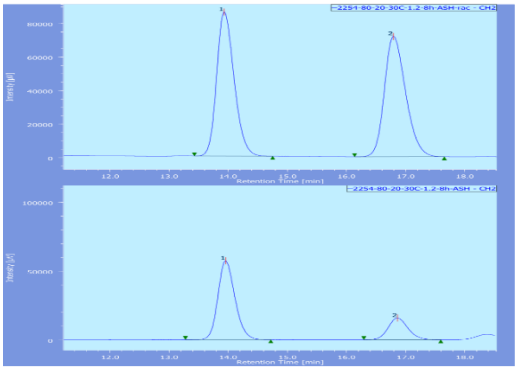
HPLC analysis in the literature: Chiralpak AS-H (Hexane/IPA = 75/25, 0.8 mL/min, 210 nm) 14.8 min (major, *R*-isomer), 17.7 min (minor, *S*-isomer);

Literature[2]



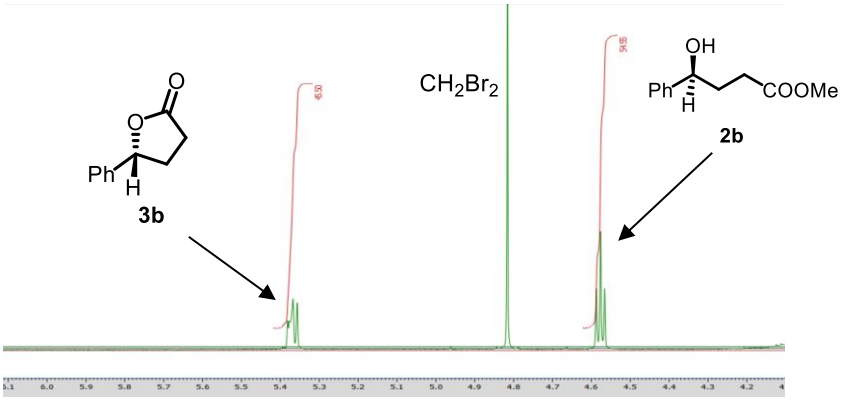
	Retention Time (min)	Area (%)	
Peak 1	14.816	91.765	**84% ee**
Peak 2	17.684	8.235	

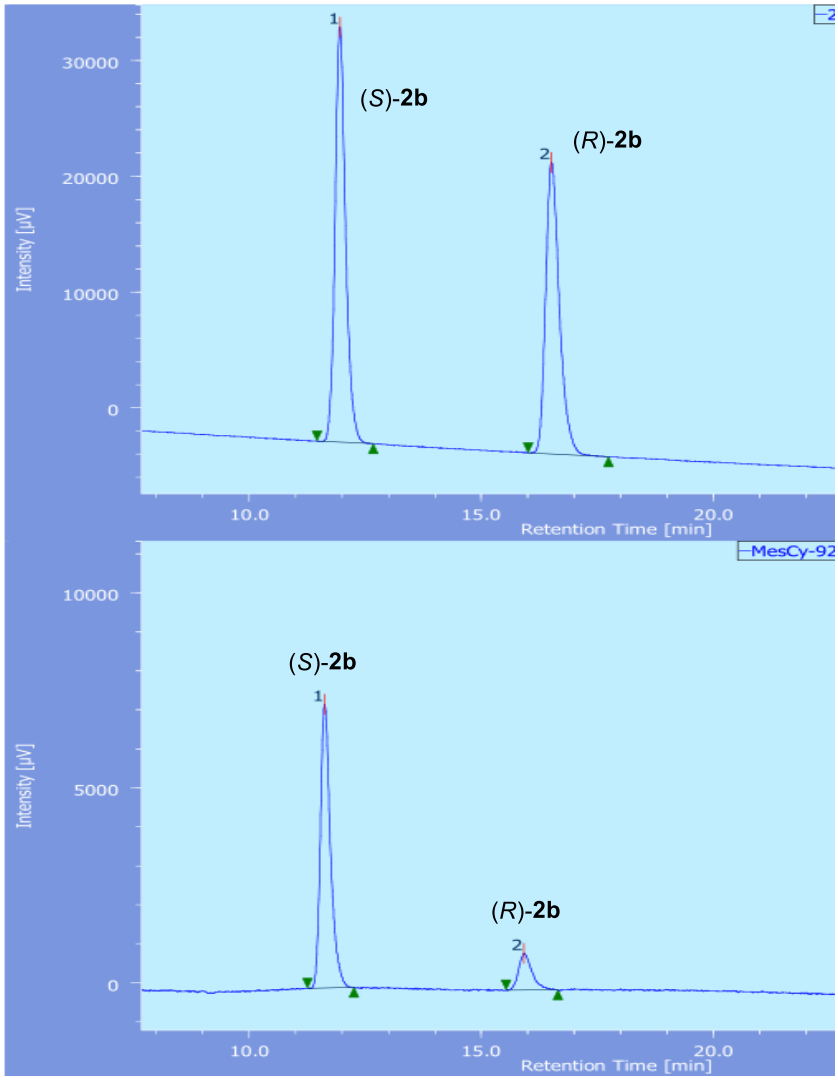
One of our samples (51.4% ee)



	Retention Time (min)	Area (%)	
Peak 1	14.0	75.7	**51.4% ee**
Peak 2	16.8	24.3	

Crude NMR chart and HPLC chart of 2b (71% ee)

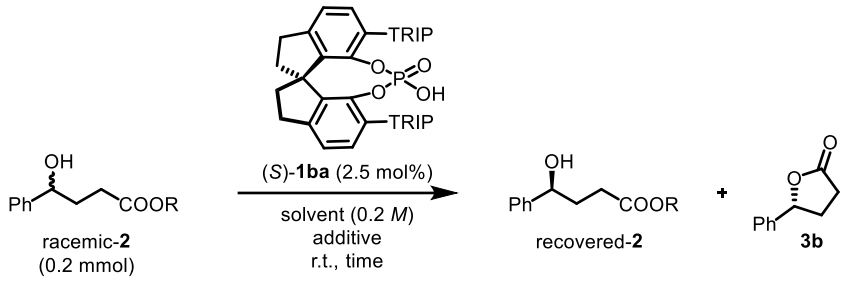




	peak 1	area 1	peak	area 2
(*rac*)-**2b**	11.9 min	50.9%	16.4 min	49.1%
(*S*)-**2b**	11.6 min	85.3%	16.0 min	14.7%

Screening of reaction conditions using SPINOL-derived CPA (*S*)-1ba

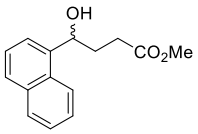
Table S1[a]



Entry	**2** (R)	solvent	additive	time	conversion (%)[b]	ee of recovered-**2** (ee %)	*s*-factor[c]
1	**2b** (Me)	CPME[d]	-	5 h	36	33	5.2
2[e]	R = *i*Pr	CPME[d]	-	5.5 h	46	22	2.1
3[e]	R = *t*Bu	CPME[d]	-	50 h	32	9	1.6
4	**2b** (Me)	CH_2Cl_2	-	35 min	63	72	4.9
5	**2b** (Me)	toluene	-	45 min	70	73	3.7
6	**2b** (Me)	THF	-	24 h	32	31	6.9
7	**2b** (Me)	EtOAc	-	5.5 h	57	71	7.0
8	**2b** (Me)	MeCN	-	2.5 h	52	65	7.6
9	R = Et	MeCN	-	4.5 h	51	49	4.3
10	**2b** (Me)	MeCN	MeOH[f]	4.5 h	49	49	5.6
11	**2b** (Me)	EtOAc	MS 5A[g]	4.5 h	59	79	7.8
12[h]	**2b** (Me)	EtOAc	-	26 h	42	22	6.6

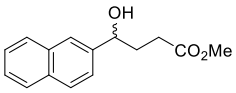
[a] Unless otherwise noted, all reactions were conducted using 0.2 mmol of **2**, and 0.005 mmol (2.5 mol%) of (*S*)-**1ba** at room temperature in the indicated solvent (1 mL). [b] The conversion is determined by ^{1}H NMR analysis of the crude reaction mixture using CH_2Br_2 as the internal standard. [c] The *s*-factor was calculated according to the conversion and ee value of recovered **2**, $s = \ln[(1 - \text{Conv.})(1 - \text{ee}_{\text{substrate}})] / \ln[(1 - \text{Conv.})(1 + \text{ee}_{\text{substrate}})]$. [d] CPME: cyclopentyl methyl ether. [e] At 50 °C. [f] 2.0 equiv. of MeOH was added. [g] 25 mg of MS 5A was added. [h] At 0 °C.

Methyl 4-hydroxy-4-(naphthalen-1-yl)butanoate (2c)



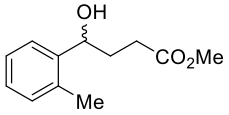
(290 mg, 12% yield) colorless oil**;** ^{1}H-NMR (600 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.6 Hz, 1H), 7.87 (d, *J* = 8.6 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 1H), 7.68 (d, *J* = 6.9 Hz, 1H), 7.55-7.47 (m, 3H), 5.60-5.57 (m, 1H), 3.70 (s, 3H), 2.62 (dt, *J* = 16.8, 7.5 Hz, 1H), 2.52 (dt, *J* = 16.7, 6.7 Hz, 1H), 2.36-2.30 (m, 2H), 2.17-2.11 (m, 1H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 174.6, 139.9, 133.9, 130.3, 129.0, 128.2, 126.3, 125.7, 125.5, 123.1, 122.8, 70.2, 51.8, 32.9, 30.5; IR (ATR) 3434, 2952, 2923, 1731, 1437, 1233, 1219, 1171, 1086, 778, 771 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{15}H_{16}O_3$ 244.10994, found: 244.10990.

Methyl 4-hydroxy-4-(naphthalen-2-yl)butanoate (2d)



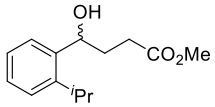
(512 mg, 21% yield) colorless oil; ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.83-7.78 (m, 4H), 7.49-7.44 (m, 3H), 4.92-4.89 (m, 1H), 3.65 (s, 3H), 2.54-2.44 (m, 3H), 2.15 (q, *J* = 7.0 Hz, 2H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 174.5, 141.5, 133.3, 133.1, 128.5, 128.0, 127.8, 126.3, 126.0, 124.6, 124.0, 73.7, 51.8, 33.7, 30.4; IR (ATR) 3434, 2951, 1732, 1437, 1236, 1168, 1084, 893, 858, 821, 769, 754 cm^{-1};HRMS (FD+) m/z: [M] Calcd for $C_{15}H_{16}O_3$ 244.10994, found: 244.10987.

Methyl 4-hydroxy-4-(o-tolyl)butanoate (2e)



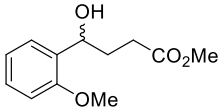
(210 mg, 10% yield) colorless oil; ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.18 (td, *J* = 7.4, 1.4 Hz, 1H), 7.14 (d, *J* = 7.0 Hz, 1H), 5.02-4.99 (m, 1H), 3.68 (s, 3H), 2.57-2.46 (m, 2H), 2.34 (s, 3H), 2.09-1.96 (m, 3H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 174.5, 142.3, 134.5, 130.5, 127.4, 126.4, 125.1, 69.9, 51.8, 32.6, 30.5, 19.0; IR (ATR) 3434, 2953, 1736, 1461, 1437, 1377, 1236, 1194, 1163, 1084, 922, 889, 757 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{12}H_{16}O_3$ 208.10994, found: 208.10987.

Methyl 4-hydroxy-4-(2-isopropylphenyl)butanoate (2f)



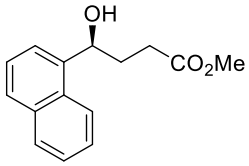
(186 mg, 8% yield) colorless oil;^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.29-7.22 (m, 2H), 7.21 (td, *J* = 7.3, 1.5 Hz, 1H), 5.13-5.09 (m, 1H), 3.68 (s, 3H), 3.21 (sept, *J* = 6.5 Hz, 1H), 2.57-2.47 (m, 2H), 2.05-2.00 (m, 3H), 1.24 (d, *J* = 6.5, 3H), 1.23 (d, *J* = 6.5, 3H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 174.4, 145.5, 140.8, 127.9, 126.1, 125.5, 125.4, 69.2, 51.8, 33.6, 30.7, 28.1, 24.7, 23.9; IR (ATR): 3467, 2964, 2927, 1736, 1437, 1235, 1088, 880 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{14}H_{20}O_3$ 236.14124, found: 236.14117.

Methyl 4-hydroxy-4-(2-methoxyphenyl)butanoate (2g)



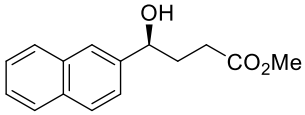
(125 mg, 6% yield) colorless oil; ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.32 (dd, J = 7.4, 1.5 Hz, 1H), 7.26-7.23 (m, 1H), 6.96 (td, J = 7.5, 0.9 Hz, 1H), 6.87 (d, J = 8.2 Hz, 1H), 4.92-4.89 (m, 1H), 3.85 (s, 3H), 3.66 (s, 3H), 2.84 (d, J = 5.8 Hz, 1H), 2.52-2.40 (m, 2H), 2.17-2.06 (m, 2H);^{13}C-NMR (151 MHz, $CDCl_3$) δ 174.6, 156.5, 131.7, 128.6, 127.0, 120.9, 110.5, 70.4, 55.3, 51.7, 32.1, 30.8; IR (ATR) 3444, 2922, 1735, 1491, 1438, 1238, 1086, 884, 756 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{12}H_{16}O_4$ 224.10486, found: 224.10482.

(*S*)-Methyl 4-hydroxy-4-(naphthalen-1-yl)butanoate ((*S*)-2c)



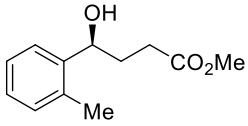
(22.5 mg, 46% recovered <51% conversion>, s = 15.3) colorless oil**;** $[\alpha]^{24.1}_{D}$ = -52.6 (c = 1.1 in $CHCl_3$, ee: 77%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 92/8, 1.2 mL/min, 254 nm, 30 °C) 11.6 mi n (major-*S*), 24.9 min (minor-*R*).

(*S*)-Methyl 4-hydroxy-4-(naphthalen-2-yl)butanoate ((*S*)-2d)



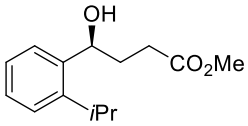
(20.5 mg, 42% recovered <56% conversion>, s = 9.2) colorless oil**;** $[\alpha]^{22.6}_{D}$ = -31.4 (c = 1.19 in $CHCl_3$, ee: 77%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 92/8, 1.2 mL/min, 220 nm, 30 °C) 14.6 min (major-*S*), 18.6 min (minor-*R*).

(*S*)-Methyl 4-hydroxy-4-(*o*-tolyl)butanoate ((*S*)-2e)



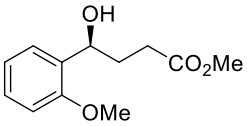
(18.7 mg, 45% recovered <53% conversion>, s = 14.1) colorless oil**;** $[\alpha]^{22.5}_{D}$ = -61.4 (c = 0.93 in $CHCl_3$, ee: 80%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 92/8, 1.2 mL/min, 220 nm, 30 °C) 10.0 min (major-*S*), 15.7 min (minor-*R*).

(*S*)-Methyl 4-hydroxy-4-(2-isopropylphenyl)butanoate ((*S*)-2f)



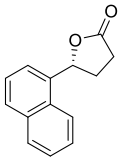
(18.2 mg, 38% recovered <57% conversion>, s = 20.2) colorless oil**;** $[\alpha]^{22.5}_{D}$ = -62.1 (c = 0.90 in $CHCl_3$, ee: 94%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 80/20, 1.0 mL/min, 220 nm, 30 °C) 5.6 min (major-*S*), 10.4 min (minor-*R*).

(*S*)-Methyl 4-hydroxy-4-(2-methoxyphenyl)butanoate ((*S*)-2g)



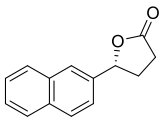
(14.6 mg, 35% recovered <62% conversion>, s = 15.5) colorless oil**;** $[\alpha]^{22.5}_{D}$ = -65.9 (c = 0.85 in $CHCl_3$, ee: 97%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 80/20, 1.0 mL/min, 220 nm, 30 °C) 11.9 min (major-*S*), 14.6 min (minor-*R*).

(*R*)-5-(Naphthalen-1-yl)dihydrofuran-2(3*H*)-one ((*R*)-3c)



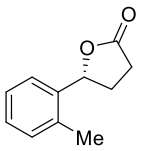
(14.0 mg, 33% isolated yield) colorless oil; $[\alpha]^{24.1}_{D}$ = 99.3 (c = 0.71 in $CHCl_3$, ee: 71%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 92/8, 0.9 mL/min, 254 nm, 40 °C) 12.0 min (major-*R*), 12.7 min (minor-*S*); ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.92-7.91 (m, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.58-7.52 (m, 3H), 7.49 (t, *J* = 7.7 Hz, 1H), 6.27 (t, *J* = 7.0 Hz, 1H), 2.93-2.87 (m, 1H), 2.74-2.63 (m, 2H), 2.33-2.27 (m, 1H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 177.2, 135.1, 133.9, 129.6, 129.3, 128.9, 126.7, 126.1, 125.5, 122.6, 121.7, 78.7, 30.1, 28.4; IR (ATR) 2924, 1774, 1219, 1184, 1162, 1054, 987, 930 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{14}H_{12}O_2$ 212.08373, found: 212.08373.

(*R*)-5-(Naphthalen-2-yl)dihydrofuran-2(3*H*)-one ((*R*)-3d)



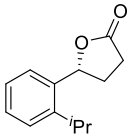
(19.9 mg, 47% isolated yield) white solid; $[\alpha]^{22.8}_{D}$ = 9.8 (c = 1.05 in $CHCl_3$, ee: 60%); HPLC analysis Chiralpak AS-H (Hexane/IPA = 92/8, 1.2 mL/min, 220 nm, 40 °C) 21.2 min (major-*R*), 28.9 min (minor-*S*); ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.6 Hz, 1H), 7.87-7.83 (m, 2H), 7.82 (s, 1H), 7.54-7.50 (m, 2H), 7.41 (dd, *J* = 8.4, 1.9 Hz, 1H), 5.70 (t, *J* = 7.2 Hz, 1H), 2.78-2.69 (m, 3H), 2.32-2.26 (m, 1H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 177.1, 136.8, 133.2, 133.1, 128.9, 128.1, 127.8, 126.7, 126.6, 124.3, 122.9, 81.4, 31.0, 29.0; IR (ATR) 2923, 1767, 1190, 1087, 1017, 934, 905, 758 cm^{-1};HRMS (FD+) m/z: [M] Calcd for $C_{14}H_{12}O_2$ 212.08373, found: 212.08369; m.p.:120.5 °C.

(*R*)-5-(*o*-Tolyl)dihydrofuran-2(3*H*)-one ((*R*)-3e)



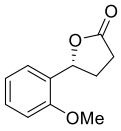
(17.8 mg, 50% isolated yield) white solid; $[\alpha]^{24.1}_{D}$ = 25.6 (c = 0.94 in $CHCl_3$, ee: 71%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 92/8, 1.2 mL/min, 220 nm, 40 °C) 22.3 min (major-*R*), 26.3 min (minor-*S*); ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.18 (td, *J* = 7.4, 1.4 Hz, 1H), 7.14 (d, *J* = 7.0 Hz, 1H), 5.02-4.99 (m, 1H), 3.64-3.72 (3H), 2.57-2.46 (m, 2H), 2.34 (s, 3H), 2.09-1.96 (m, 3H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 177.2, 137.6, 134.3, 130.8, 128.3, 126.5, 124.3, 79.0, 29.7, 28.8, 19.1; IR (ATR) 2921, 1772, 1493, 1464, 1245, 1143, 1087, 1028, 935, 890, 756 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{11}H_{12}O_2$ 176.08373, found: 176.08365; m.p.:61.0 °C.

(*R*)-5-(2-Isopropylphenyl)dihydrofuran-2(3*H*)-one ((*R*)-3f)



(25.2 mg, 62% isolated yield) colorless oil; $[\alpha]^{24.1}_{D}$ = 24.2 (c = 1.21 in $CHCl_3$, ee: 65.5%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 80/20, 1.0 mL/min, 220 nm, 30 °C) 12.6 min (major-*R*), 15.2 min (minor-*S*);^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.36-7.30 (m, 3H), 7.25-7.21 (m, 1H), 5.84 (t, *J* = 7.0 Hz, 1H), 3.06 (sept, *J* = 6.8 Hz, 1H), 2.70-2.63 (m, 3H), 2.08-2.21 (m, 1H), 1.27 (d, *J* = 6.8 Hz, 3H), 1.26 (d, *J* = 6.8 Hz, 3H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 177.2, 145.4, 136.1, 128.6, 126.3, 125.8, 124.5, 78.5, 31.0, 29.0, 28.7, 24.3, 24.0; IR (ATR): 2965, 1779, 1177, 1087, 1022, 934, 886, 766, 753 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{13}H_{16}O_2$ 204.11503, found: 204.11493.

(*R*)-5-(2-Methoxyphenyl)dihydrofuran-2(3*H*)-one ((*R*)-3g)



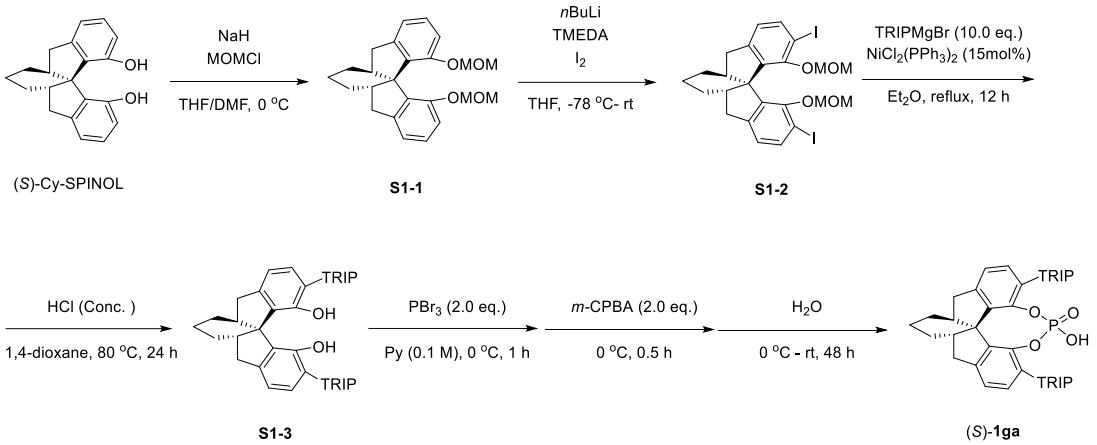
(18.2 mg, 48% isolated yield) colorless oil; $[\alpha]^{24.1}_{D}$ = 45.1 (c = 0.71 in $CHCl_3$, ee: 60%); HPLC analysis Chiralpak IC-3 (Hexane/IPA = 80/20, 1.0 mL/min, 220 nm, 30 °C) 19.9 min (major-*R*), 22.3 min (minor-*S*); ^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.35-7.29 (m, 2H), 6.98 (td,

J = 7.6, 1.0 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 5.76 (t, *J* = 7.2 Hz, 1H), 3.85 (s, 3H), 2.73-2.68 (m, 1H), 2.65-2.60 (m, 2H), 2.15-2.09 (m, 1H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 177.7, 156.1, 129.4, 128.1, 125.7, 120.7, 110.6, 78.0, 55.5, 29.4, 28.7; IR (ATR) 2955, 2923, 1775, 1461, 1216, 1189, 1175, 1143, 1023, 935, 756 cm^{-1}; HRMS (FD+) m/z: [M] Calcd for $C_{11}H_{12}O_3$ 192.07864, found: 192.07859.

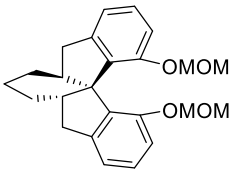
4. Preparation of CPA Catalysts

The catalyst (*S*)-**1ga** was prepared according to the literature.[3]

Synthesis of Cy-SPINOL-derived CPA (*S*)-1ga



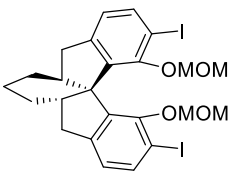
(5a*S*,8a*S*)-1,13-bis(methoxymethoxy)-5a,6,7,8,8a,9-hexahydro-5*H*-indeno[2,1-d]fluorene (S1-1)



Starting material (*S*)-Cy-SPINOL was prepared according to the literature, and spectral data was reported.[4]

To a cooled (0 °C, ice/water bath) (*S*)-Cy-SPINOL (1.46 g, 5.0 mmol, 1.0 equiv.) in THF/DMF (30 mL/10 mL) was added NaH (60% w/w dispersion in mineral oils, 600 mg, 15 mmol, 3.0 equiv.). The resultant mixture was stirred at ambient temperature for 2 h. The mixture was then cooled back to 0 °C, and MOMCl (1.13 mL, 15.0 mmol, 3.0 equiv.) was added dropwise via syringe. The resultant mixture was stirred at ambient temperature for 6 h. Upon completion, the mixture was quenched with water (10 mL) and extracted with ethyl acetate (20 mL * 3). The combined organic extracts were dried over anhydrous Na_2SO_4, filtered, and liberated of solvents in vacuo. The crude residue was purified by flash chromatography on silica gel (*n*-hexane/EtOAc 10:1), and **S1-1** was obtained as colorless oil in 85% yield (1.61 g). ^{1}H-NMR (600 MHz, $CDCl_3$); δ 7.07 (t, *J* = 7.7 Hz, 2H), 6.90 (d, *J* = 7.7 Hz, 2H), 6.74 (d, *J* = 7.7 Hz, 2H), 4.74 (d, *J* = 6.5 Hz, 2H), 4.69 (d, *J* = 6.5 Hz, 2H), 3.12 (dd, *J* = 15.3, 7.2 Hz, 2H), 3.07 (s, 6H), 3.02-2.98 (m, 2H), 2.76 (dd, *J* = 14.9, 6.7 Hz, 2H), 1.62-1.53 (m, 4H), 1.49-1.45 (m, 2H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 154.4 (2C), 147.1 (2C), 136.3 (2C), 127.6 (2C), 118.5 (2C), 112.6 (2C), 93.9 (2C), 61.8 (2C), 55.6 (2C), 43.1, 38.1 (2C), 27.0 (2C), 18.4; IR (ATR) 2922 1586, 1473, 1250, 1151, 1086, 1051, 955, 922, 871, 773 cm^{-1}; $[\alpha]_D^{22.4}$ = 90.1 (c=3.2 in $CHCl_3$, ee >99%).

(5a*S*,8a*S*)-2,12-diiodo-1,13-bis(methoxymethoxy)-5a,6,7,8,8a,9-hexahydro-5*H*-indeno[2,1-d]fluorene (S1-2)



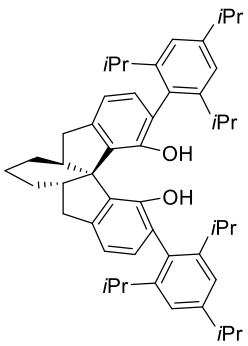
To a cooled (0 °C) solution of **S1-1** (1.52 g, 4.0 mmol, 1.0 equiv.) and freshly distilled TMEDA (1.49 mL, 10.0 mmol, 2.5 equiv.) in anhydrous Et_2O (20 mL) was added *n*-BuLi (1.55 M solution in hexanes, 7.75 mL, 15.0 mmol, 3.0 equiv.) dropwise via syringe. The resultant mixture was stirred at ambient temperature for 12 h, and then was cooled down to -78 °C (dry ice/acetone bath) . A solution of I_2 (3.15 g, 12.4 mmol, 3.1 equiv.) in anhydrous THF (4 mL) was slowly added. The reaction was allowed to slowly warm to ambient temperature and stirred for overnight. Upon completion, the solution was cooled down to 0 °C and the saturated aqueous $Na_2S_2O_3$ was added to quench the reaction. The

layers were separated, and the aqueous layer was extracted with ethyl acetate (20 mL*3). The combined organic layers were dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The crude residue was purified by flash chromatography on silica gel (hexane/ethyl acetate from 100:0 to 90:10) and **S1-2** was obtained as yellow powder in 81% yield (2.05 g).

^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.7 Hz, 2H), 6.82 (d, *J* = 7.7 Hz, 2H), 4.66 (d, *J* = 4.8 Hz, 2H), 4.00 (d, *J* = 4.8 Hz, 2H), 3.22-3.17 (m, 8H), 3.01-2.97 (m, 2H), 2.70 (dd, *J* = 15.5, 6.9 Hz, 2H), 1.54-1.46 (m, 4H), 1.38-1.34 (m, 2H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 153.7 (2C), 148.1 (2C), 142.2 (2C), 139.0 (2C), 123.6 (2C), 99.6 (2C), 90.0 (2C), 63.4 (2C), 58.0 (2C), 43.6, 37.4 (2C), 26.7 (2C), 18.0; HRMS (FD+) m/z: [M] Calcd for $C_{24}H_{26}I_2O_4$ 631.99205, found: 631.99195; IR (ATR) 3481, 2924, 2848, 1561, 1434, 1388, 1218, 1159, 1087, 1049, 1017, 993, 919, 827, 671 cm^{-1}; $[\alpha]^{21.9}_D$ = -57.6 (c=1.9 in $CHCl_3$, ee >99%); m.p.: 114 °C.

(5aS,8aS)-2,12-bis(2,4,6-triisopropylphenyl)-5a,6,7,8,8a,9-hexahydro-5H-indeno[2,1-d]fluorene-1,13-diol (S1-3)

The Grignard solution (TRIPMgBr (0.60 M in Et_2O)) was prepared followed by above procedure.[4]

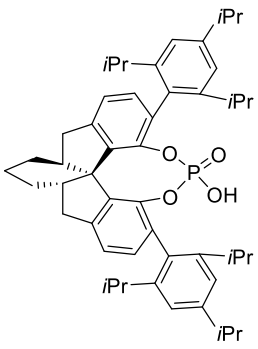


To the solution of **S1-2** (948 mg, 1.5 mmol, 1.0 equiv.) and $NiCl_2(PPh_3)_2$ (148 mg, 0.225 mmol, 15 mol%) in anhydrous Et_2O (7.5 mL) was slowly added the TRIPMgBr solution (*ca.* 25 mL, 15 mmol, 10.0 equiv.). The solution was heated at reflux for 24 h, and cooled to 0 °C, quenched with saturated aqueous NH_4Cl. The aqueous layer was extracted with ethyl acetate (30 mL*3), and the combined organic extracts were dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo. The crude product was used for next step without further purification.

To a solution of the above crude product in 1,4-dioxane (10 mL) was slowly added an aqueous solution of HCl (12.0 *N*, 2 mL). The mixture was stirred at 80 °C for 12 h before it was cooled to room temperature. Water was added, and the resulting mixture was extracted with dichloromethane (30 mL * 3). the combined organic extracts were dried over anhydrous Na_2SO_4, filtered and concentrated in vacuo. The residue was purified by silica gel flash chromatography (hexanes/ethyl acetate = 50:1). The desired product **S1-3** was obtained as white solid in 37% yield (390 mg).

^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.07 (d, *J* = 1.7 Hz, 2H), 7.04 (d, *J* = 1.7 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 6.85 (d, *J* = 7.6 Hz, 2H), 4.72 (s, 2H), 3.16-3.10 (m, 4H), 2.94-2.87 (m, 2H), 2.82-2.77 (m, 2H), 2.66-2.55 (m, 4H), 1.57-1.53 (m, 4H), 1.26 (d, *J* = 6.4 Hz, 12H), 1.13 (d, *J* = 6.9 Hz, 6H), 1.06 (d, J = 6.9 Hz, 6H), 1.03 (d, *J* = 6.9 Hz, 6H), 0.96 (d, *J* = 6.9 Hz, 6H); ^{13}C-NMR (151 MHz, $CDCl_3$) δ 151.1 (2C), 148.8 (2C), 148.2 (2C), 148.1 (2C), 145.4 (2C), 131.2 (2C), 130.6 (2C), 129.8 (2C), 125.2 (2C), 121.3 (2C), 121.1 (2C), 117.2 (2C), 61.6 (2C), 43.9, 37.3 (2C), 34.4 (2C), 30.6 (2C), 30.5 (2C), 27.2 (2C), 24.5 (2C), 24.4 (2C), 24.1 (2C), 24.1 (2C), 24.1 (2C), 23.9 (2C), 18.8; HRMS (FD+) m/z: [M] Calcd for $C_{50}H_{64}O_2$ 696.49063, found: 696.49046; IR (ATR) 3509, 2959, 2927, 2867, 1767, 1698, 1606, 1573, 1460, 1439, 1382, 1362, 1320, 1282, 1218, 1103, 1060, 1045, 984, 936, 877, 809, 666 cm^{-1}; $[\alpha]_{21.7}{}^D$=(c = 1.90 in $CHCl_3$, ee>99%); m.p.: 144 °C.

(5*S*,8a*S*)-14-hydroxy-1,12-bis(2,4,6-triisopropylphenyl)-5,6,7,8,8a,9-hexahydro-4,5-methanobenzo[g]fluoreno[4,4b-de][1,3,2]dioxaphosphocine 14-oxide ((*S*)-1ga)



To a stir solution of **S1-3** (300 mg, 0.43 mmol) in pyridine (4.3 mL) was added dropwise PBr_3 (81.7 μL, 0.86 mmol, 2.0 equiv.). After stirring it for 1 h at room temperature, *m*-CPBA (229 mg, 0.86mmol, >65% wt) was added at 0 °C. The color of solution changed immediately. After stirring it for 1 h at room temperature, water (1.5 mL) was added to the solution at 0 °C. After stirring it for 24 h at 80 °C, the reaction was quenched with HCl (aq. 6 *N*, 20.0 ml) and extracted with dichloromethane. The combined organic layers were washed with 6 *N* HCl, $NaHCO_3$ (aq. Saturated, 10 mL*3), and HCl (aq. 6 *N*, 10 mL*2), then concentrated. After purification by flash column chromatography on silica gel (n-hexane/EtOAc = 10:1 to 4:1 as eluent), the obtained product was dissolved in dichloromethane, washed with HCl (aq. 6 *N*, 10 mL), concentrated under reduced pressure and recrystallization with MeCN Then the product was dried over at 60 °C under vacuum to give the pure product (*S*)-**1ga** (89 mg) in 27% yield as a white solid.

^{1}H-NMR (600 MHz, $CDCl_3$) δ 7.13 (s, 4H), 7.04 (d, *J* = 1.7 Hz, 2H), 6.96 (d, *J* = 1.7 Hz, 2H), 3.22 (dd, *J* = 17.2 Hz, 8.6 Hz, 2H), 3.04 (dd, *J* = 17.2, 10.3 Hz, 2H), 2.89 (sept, *J* = 6.8 Hz, 4H), 2.73 (sept, *J* = 6.8 Hz, 2H), 2.52-2.48 (m, 2H), 1.99-1.94 (m, 2H), 1.68-1.57 (m, 4H), 1.26(4) (d, *J* = 6.8 Hz, 6H), 1.26(3) (d, *J* = 6.8 Hz, 6H), 1.22 (d, *J* = 7.2 Hz, 6H), 1.20 (d, *J* = 6.8 Hz, 6H) 1.11 (d, *J* = 6.5 Hz, 6H), 0.81 (d, *J* = 6.9 Hz, 6H); ^{31}P-NMR (243 MHz, $CDCl_3$) δ -8.2; ^{13}C-NMR (151 MHz, $CDCl_3$) δ 148.2 (2C), 147.9 (2C), 147.2 (2C), 144.1 (2C), 143.9 (2C), 140.0 (2C), 132.4 (2C), 131.4 (2C), 131.4 (2C), 121.6 (2C), 121.3 (2C), 120.3 (2C), 63.2 (2C), 58.7 (2C), 46.3, 36.1 (2C), 34.2 (2C), 30.8 (2C), 27.0 (2C), 24.8 (2C), 24.1 (2C), 23.9 (2C), 23.5 (2C), 19.1 (2C), 17.7 (2C), 15.1; HRMS (FD+) m/z: [M] Calcd for $C_{50}H_{63}PO_4$ 758.44640, found: 758.44618; IR (ATR) 2961, 2924, 2869, 1465, 1236, 1091, 1036, 997, 877, 755 cm^{-1}; $[\alpha]^{22.1}_D$ = -194.2° (c = 1.0 in $CHCl_3$, ee > 99%); m.p.:183 °C.

5. References

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M. Venugopal, S. Elango, A. Parthiban and Eni, *Tetrahedron: Asymmetry* **2004**, *15*, 3427–3431.

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Main text, Ref. 11

Gaussian 09: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox.

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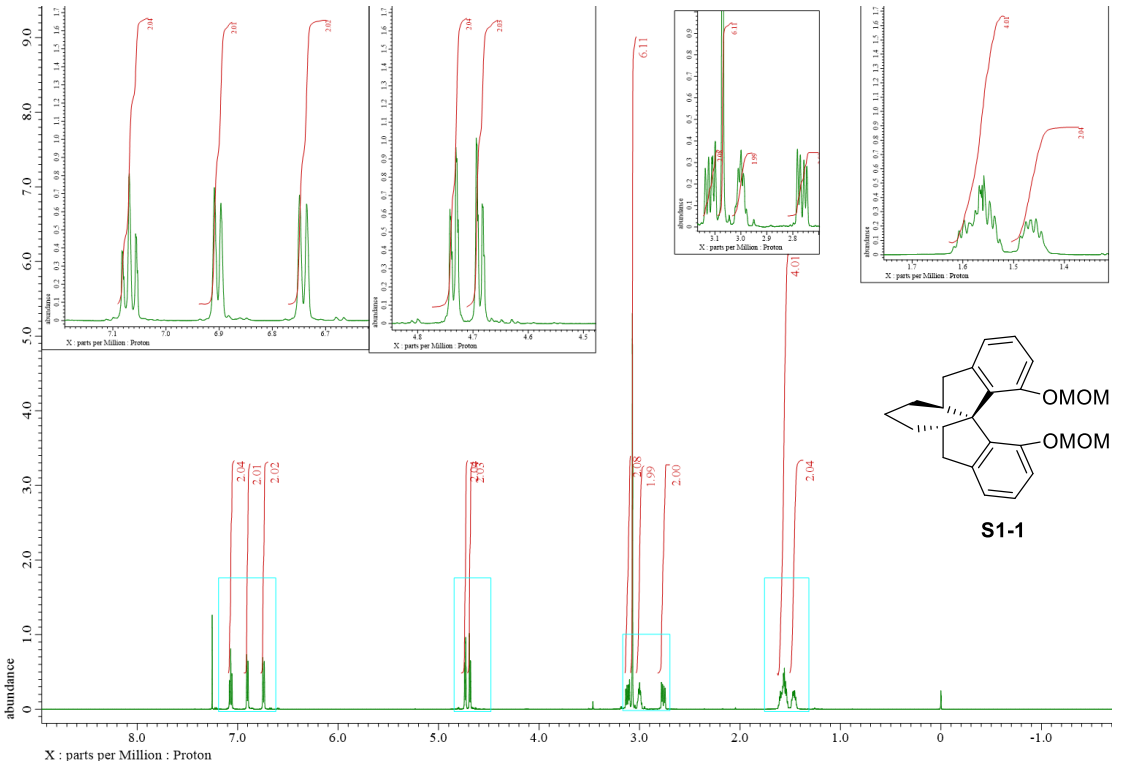
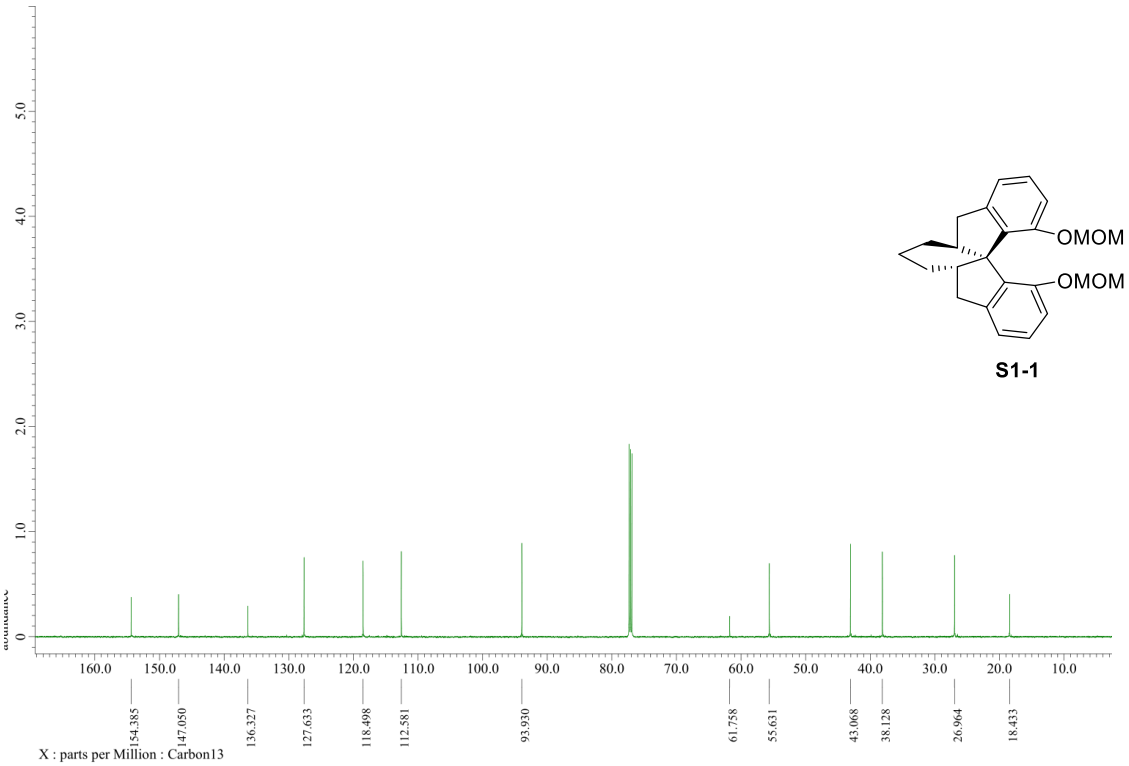
6. NMR Charts


OMOM
OMOM
S1-1
abundance
X : parts per Million : Proton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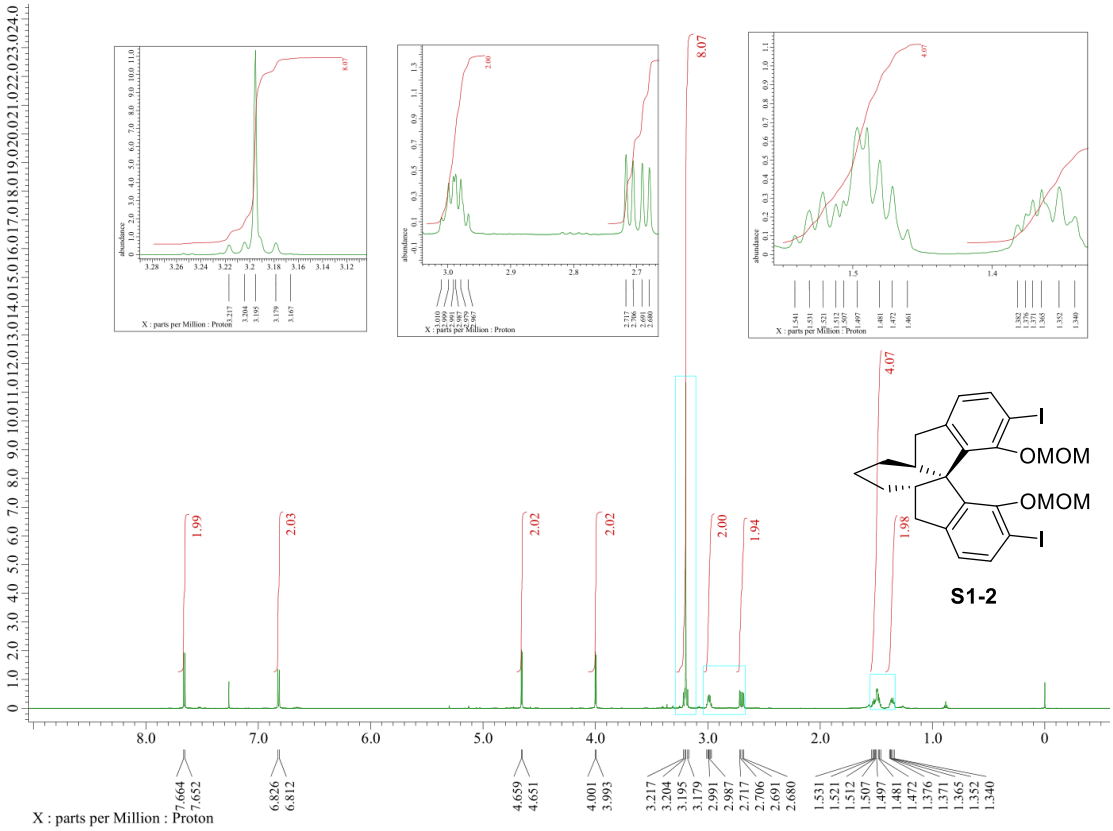
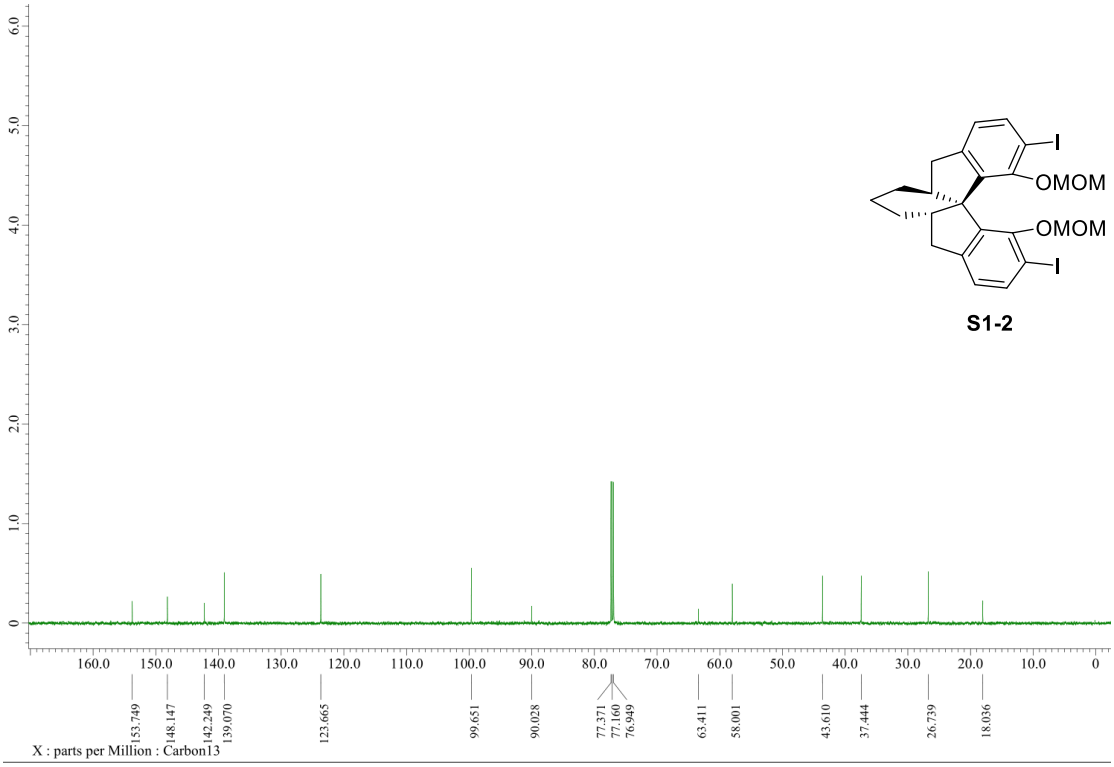
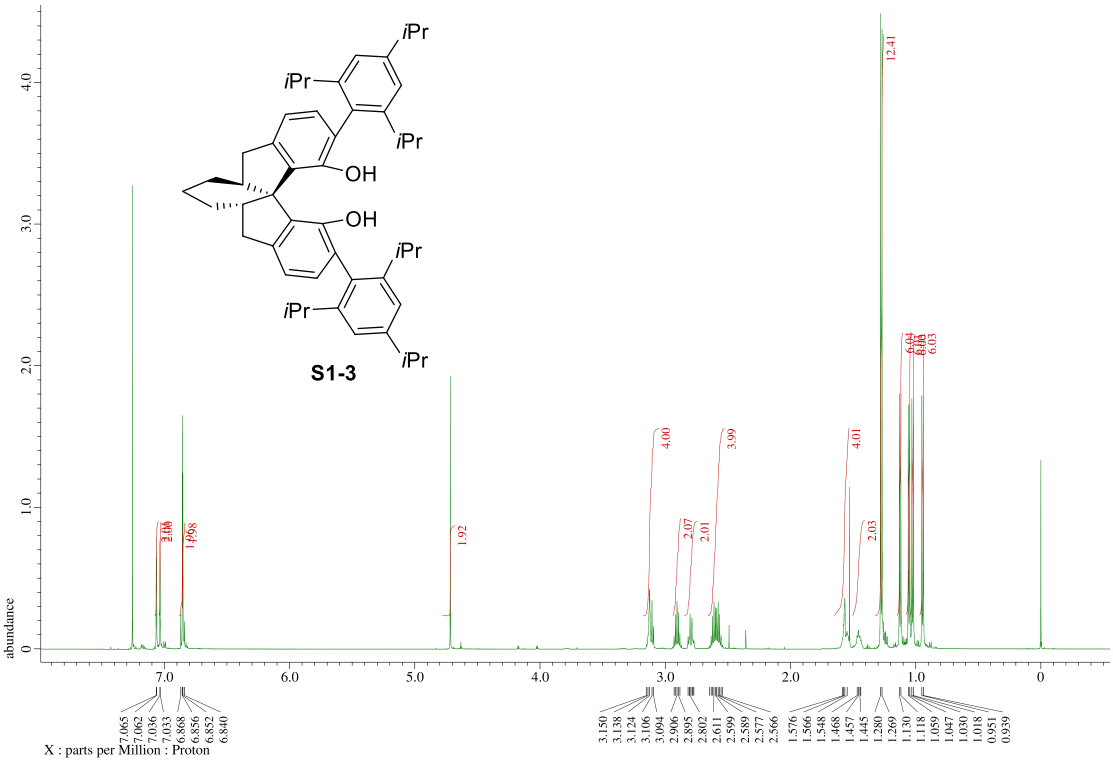
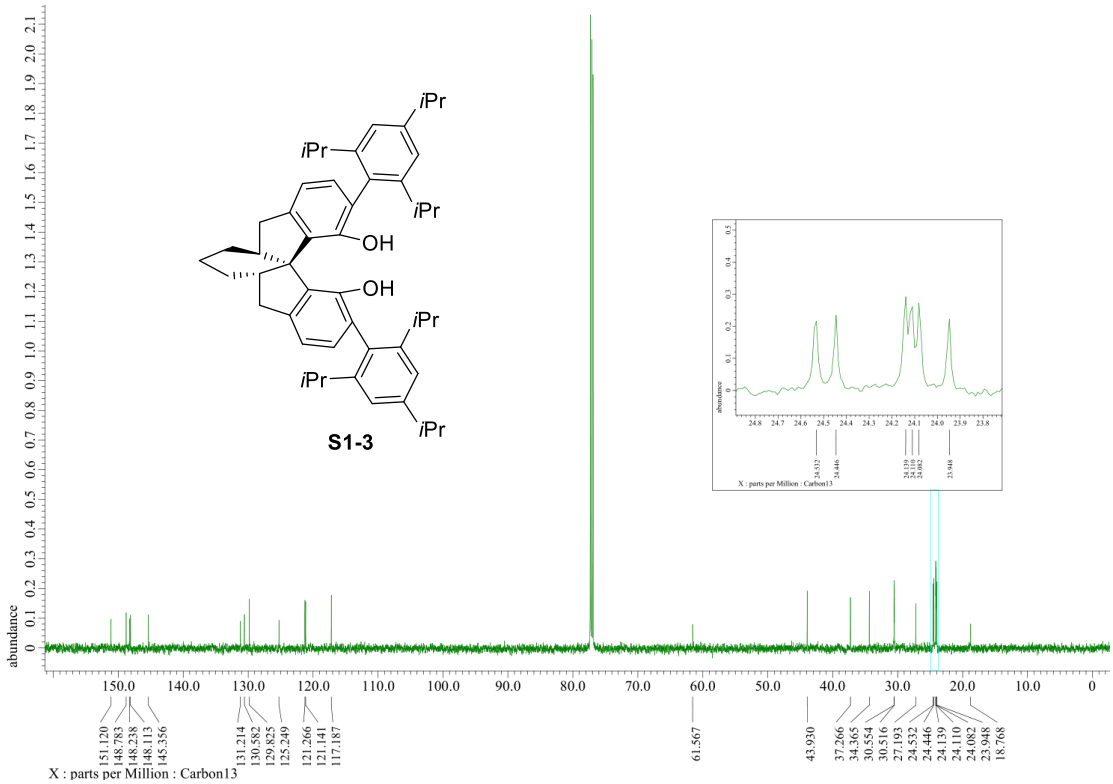
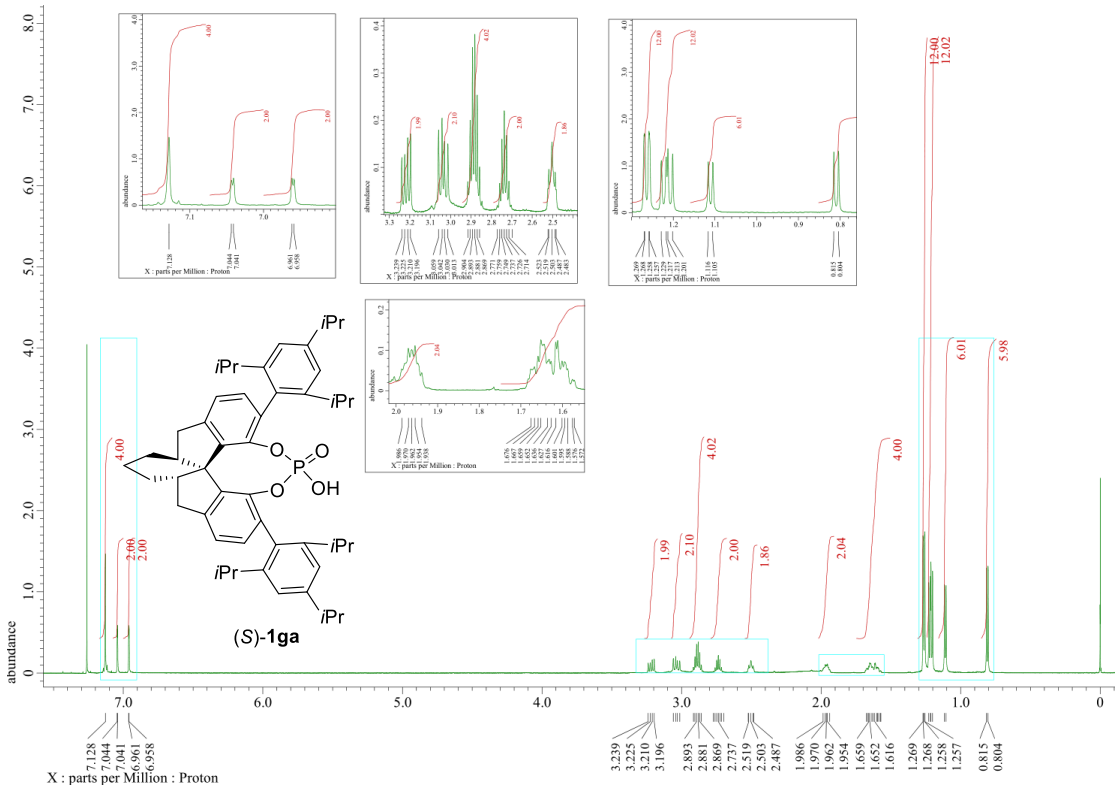
OMOM
S1-1
X : parts per Million : Carbon13

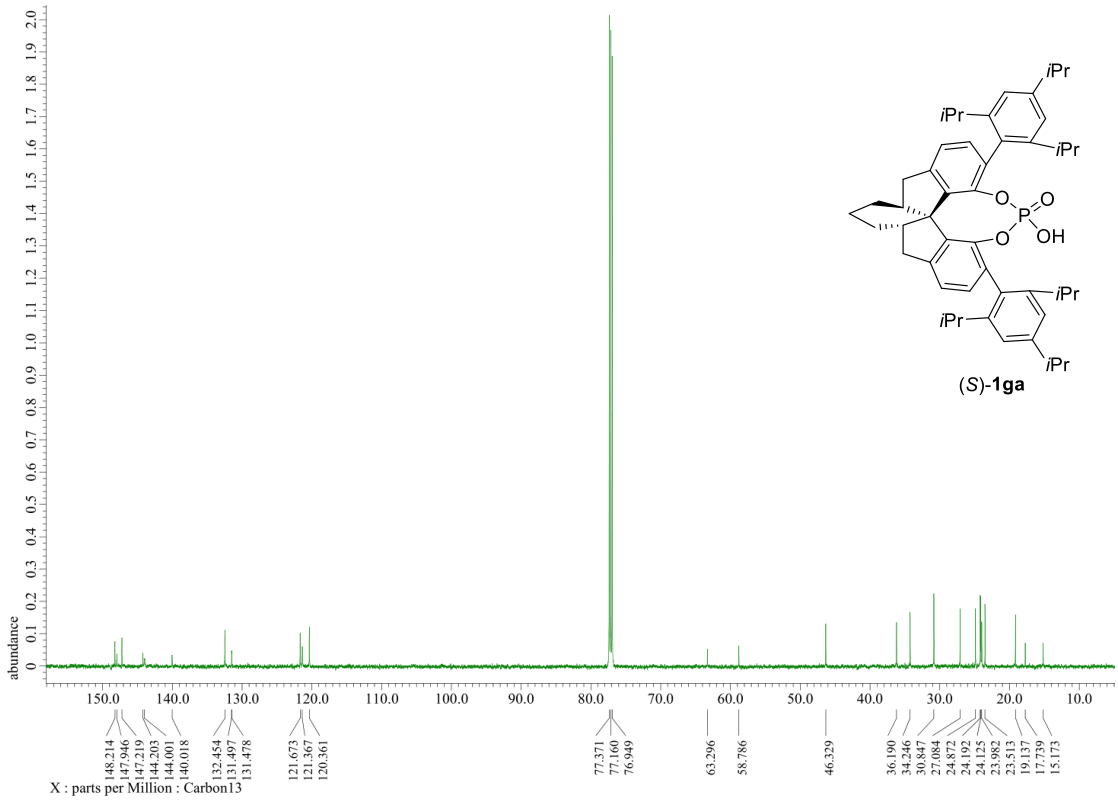

8.07
4.07
2.00
1.99
2.03
2.02
2.02
1.94
1.98
I
OMOM
OMOM
I
S1-2
X : parts per Million : Proton


I
OMOM
OMOM
I
S1-2
X : parts per Million : Carbon13

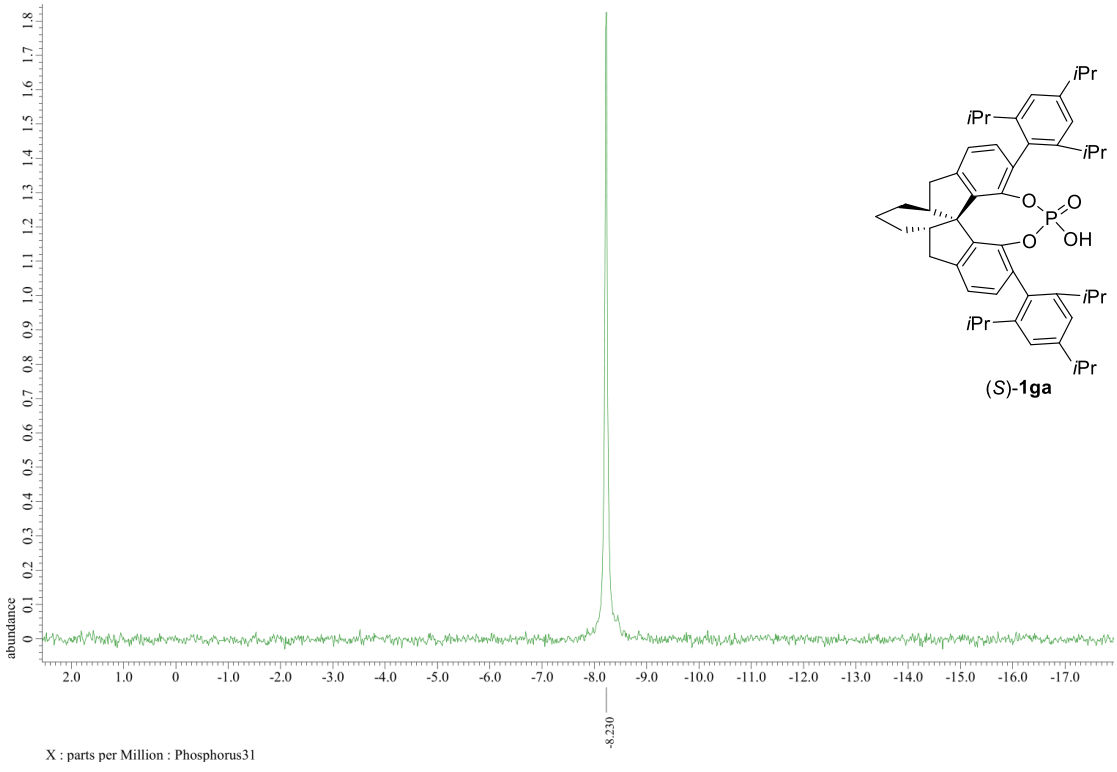

iPr
iPr
iPr
OH
OH
iPr
iPr
iPr
S1-3
abundance
X : parts per Million : Proton


iPr
iPr
iPr
OH
OH
iPr
iPr
iPr
S1-3
abundance
X : parts per Million : Carbon13

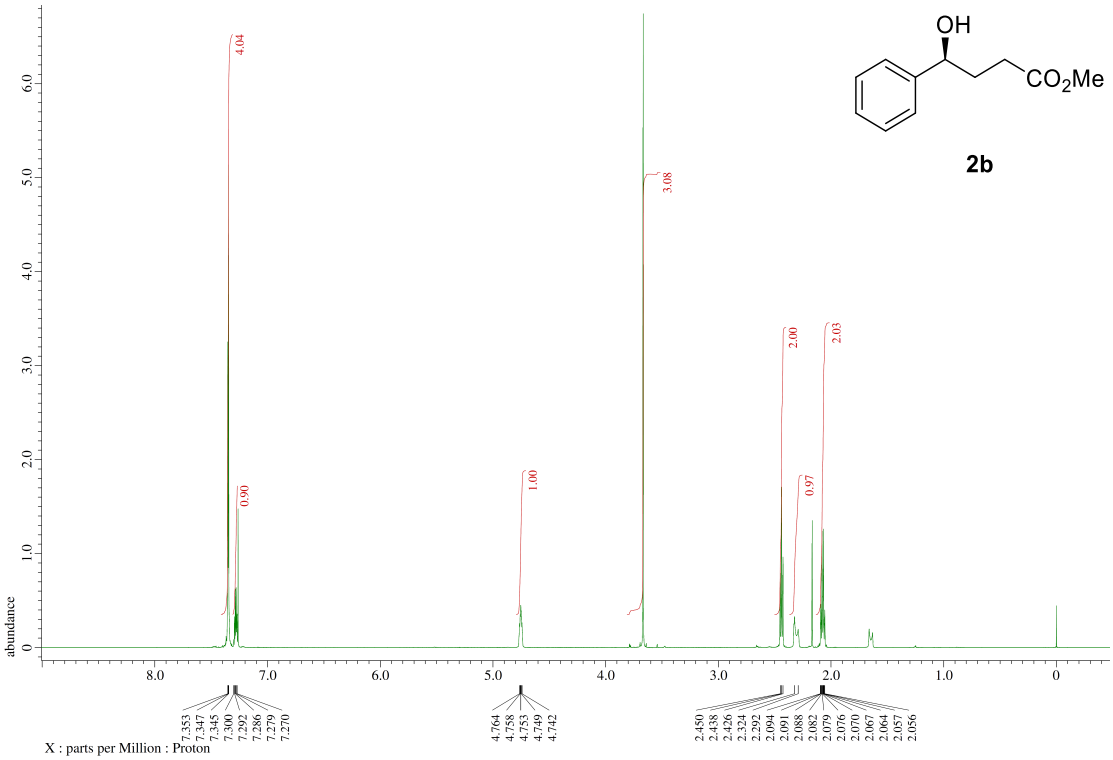

iPr
iPr
iPr
O
P
O
OH
O
iPr
iPr
iPr
(S)-1ga
abundance
X : parts per Million : Proton
4.00
2.00
2.00
1.99
2.10
2.00
1.86
4.02
2.04
4.00
12.00
12.02
6.01
5.98

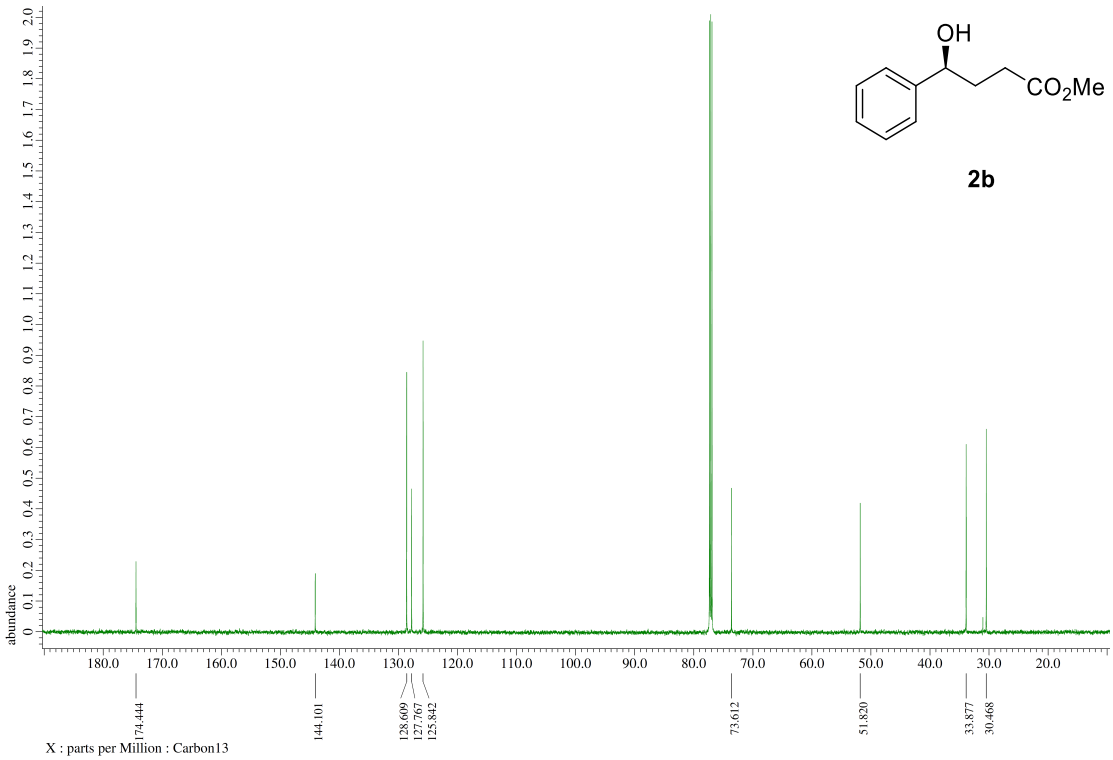

iPr
iPr
iPr
O
P
O
OH
O
iPr
iPr
iPr
(S)-1ga
abundance
X : parts per Million : Carbon13

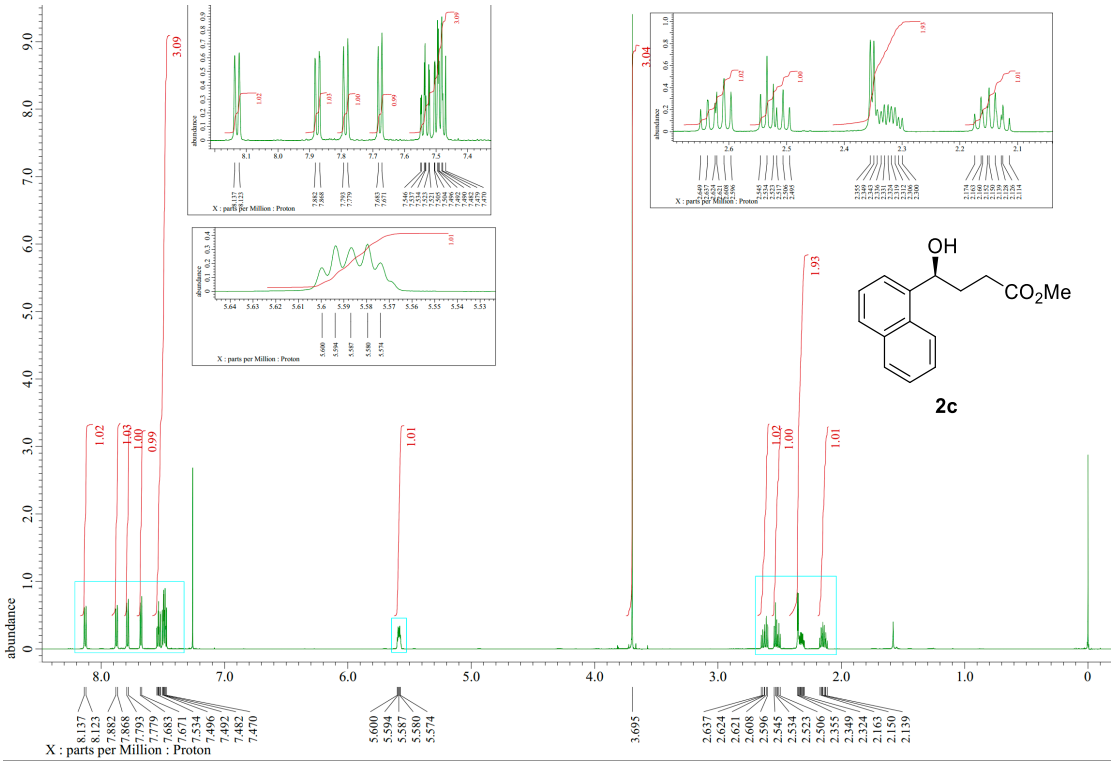
^{31}P NMR

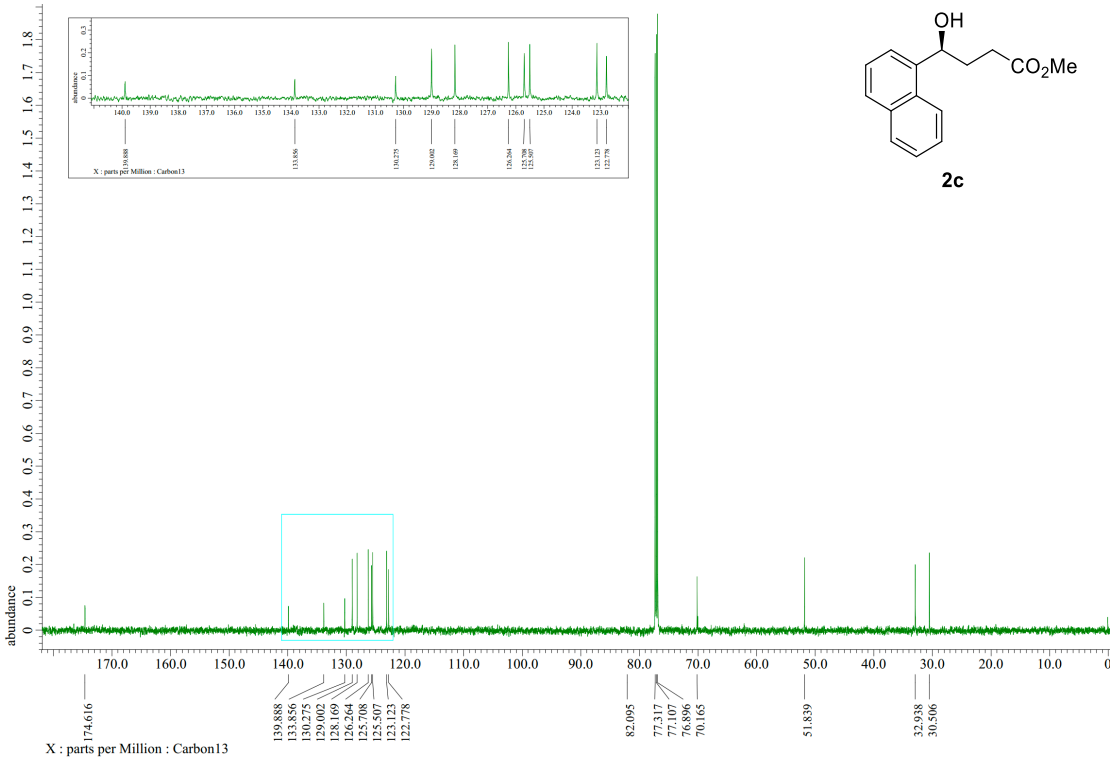

abundance
2.0
1.0
0
-1.0
-2.0
-3.0
-4.0
-5.0
-6.0
-7.0
-8.0
-9.0
-10.0
-11.0
-12.0
-13.0
-14.0
-15.0
-16.0
-17.0
-8.230
X : parts per Million : Phosphorus31
iPr
iPr
iPr
O
P
O
O
OH
iPr
iPr
iPr

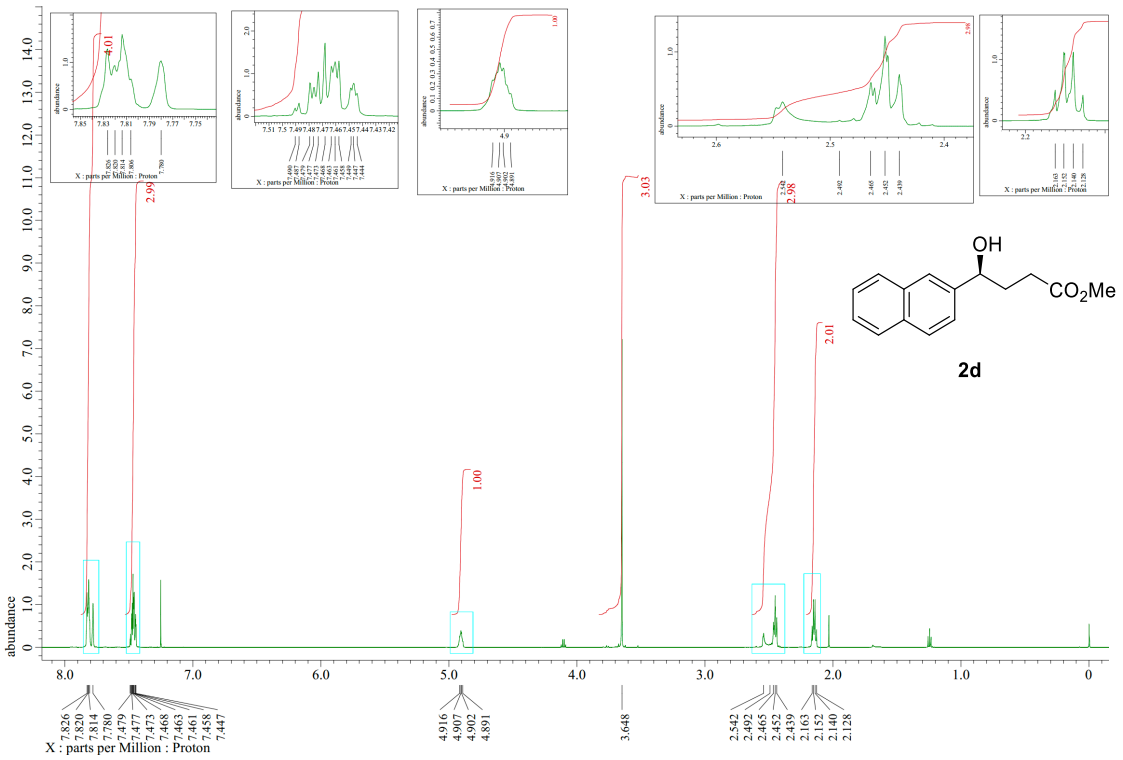
(*S*)-**1ga**

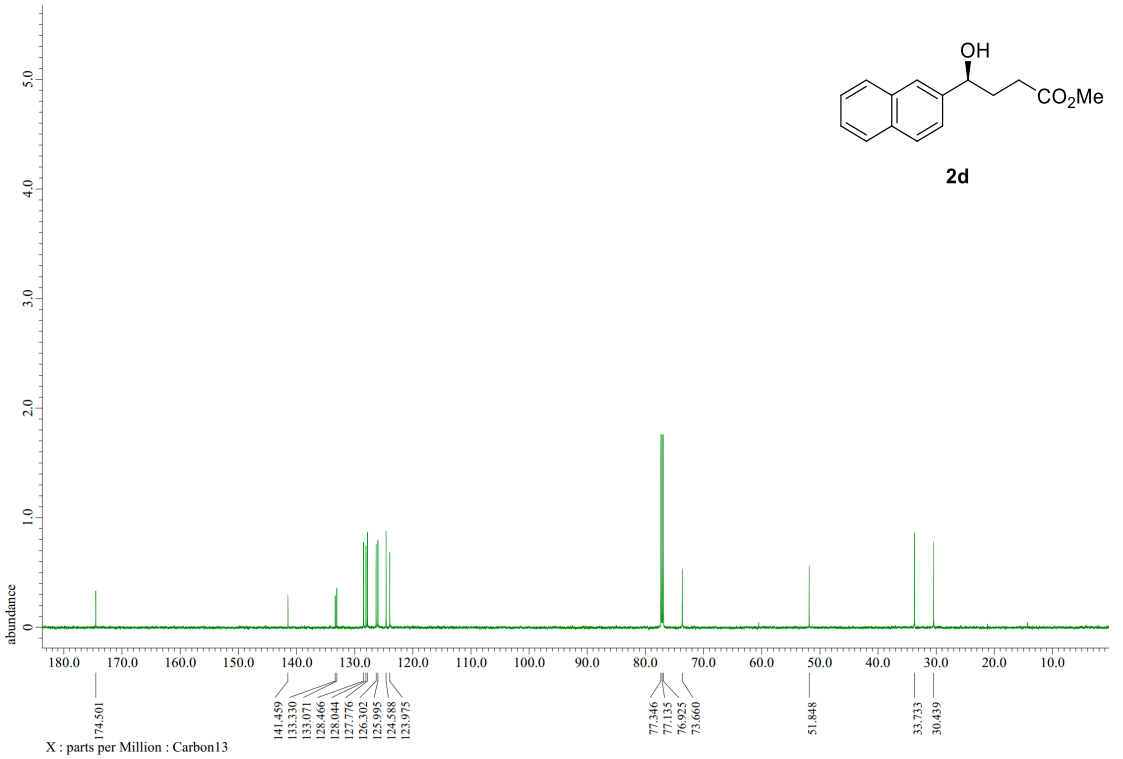

OH
CO2Me
2b
4.04
3.08
2.00
2.03
1.00
0.97
0.90
abundance
X : parts per Million : Proton

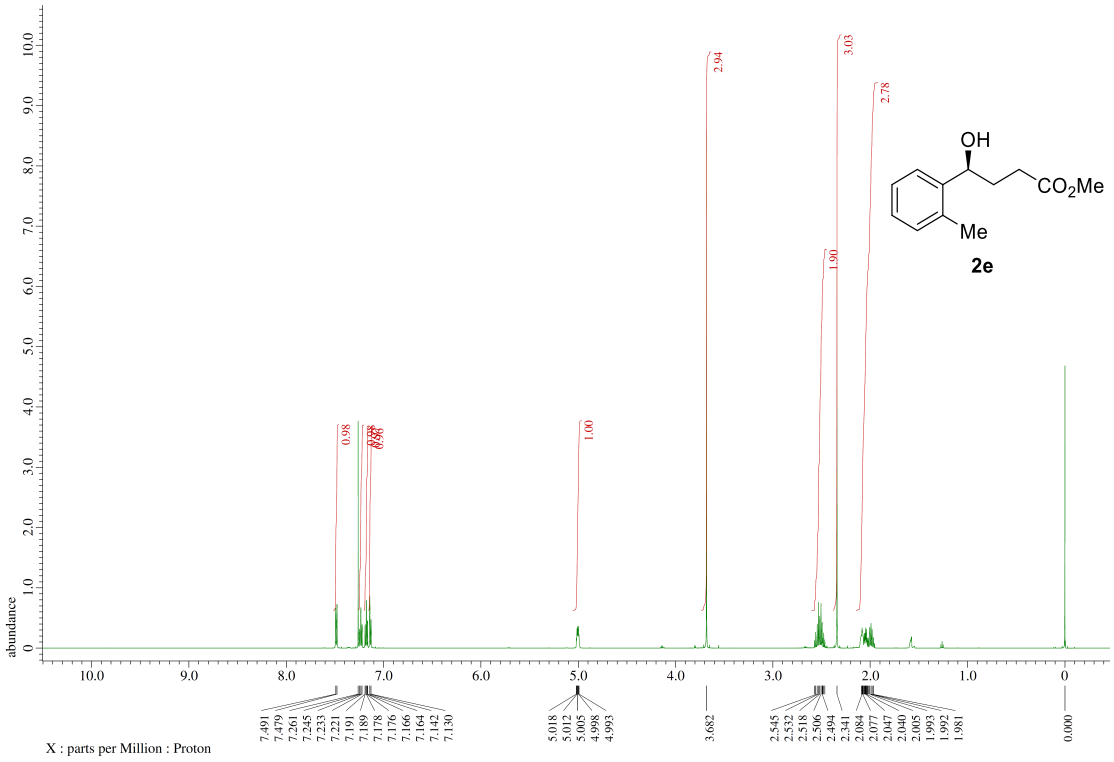

OH
CO2Me
2b
abundance
174.444
144.101
128.609
127.767
125.842
73.612
51.820
33.877
30.468
X : parts per Million : Carbon13

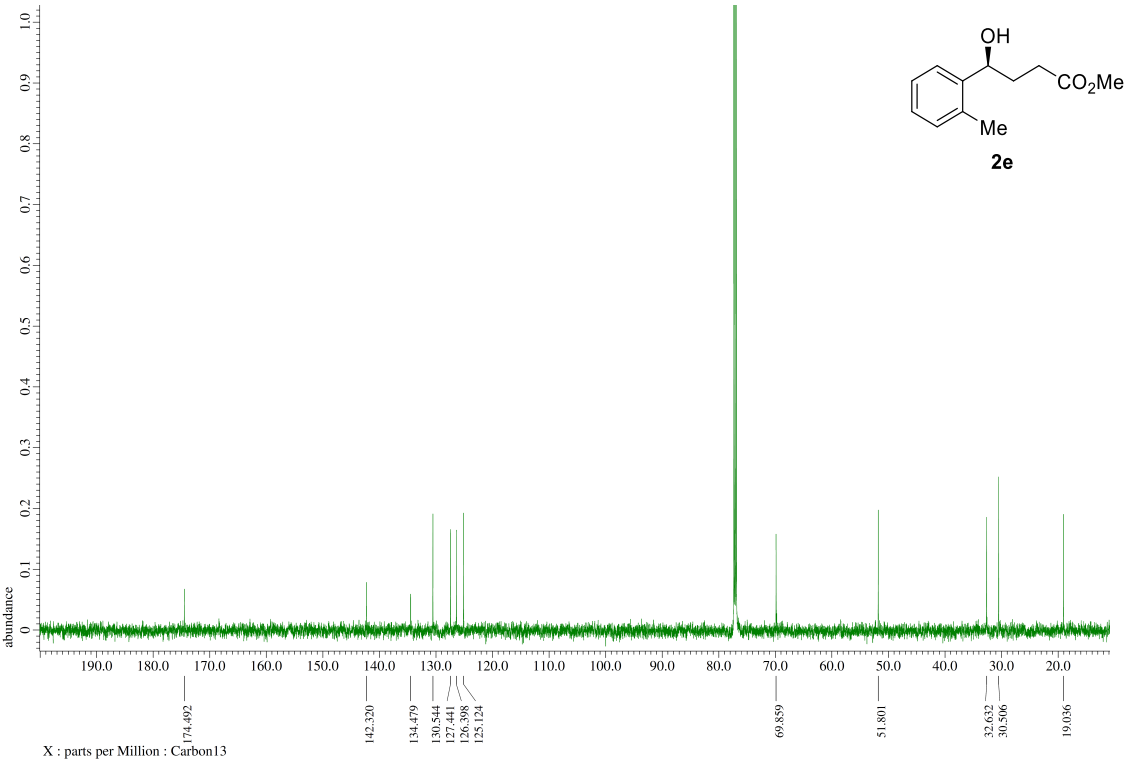

OH
CO2Me
2c
X : parts per Million : Proton

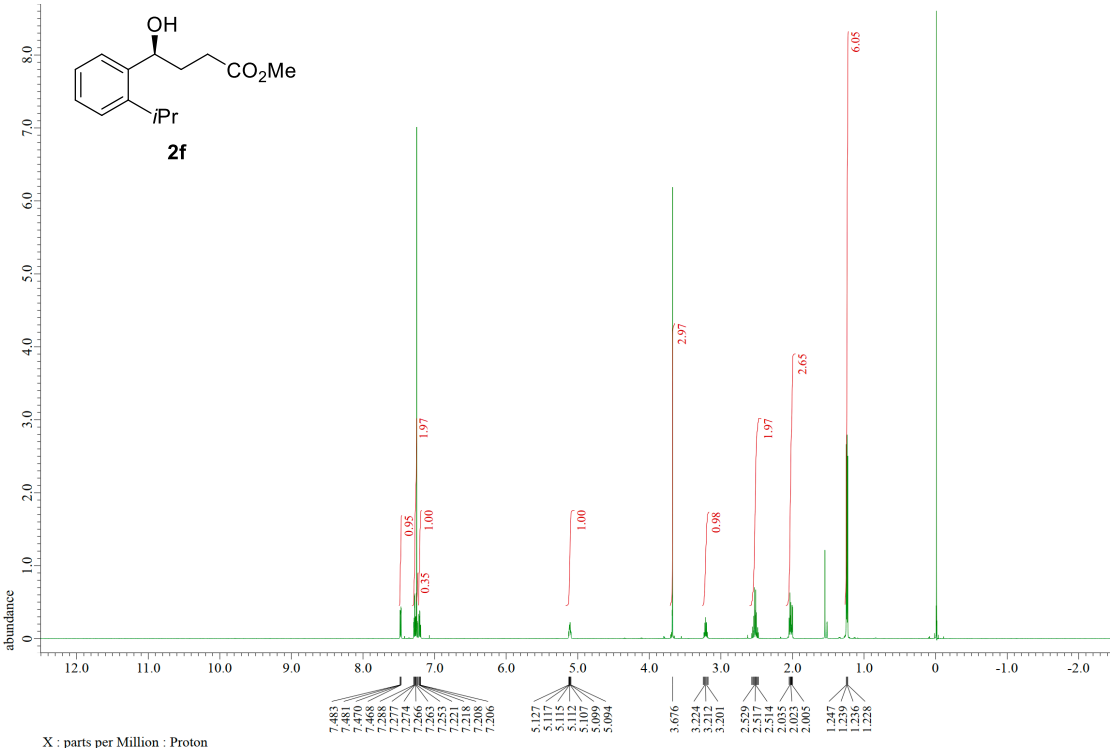

OH
CO2Me
2c
X : parts per Million : Carbon13

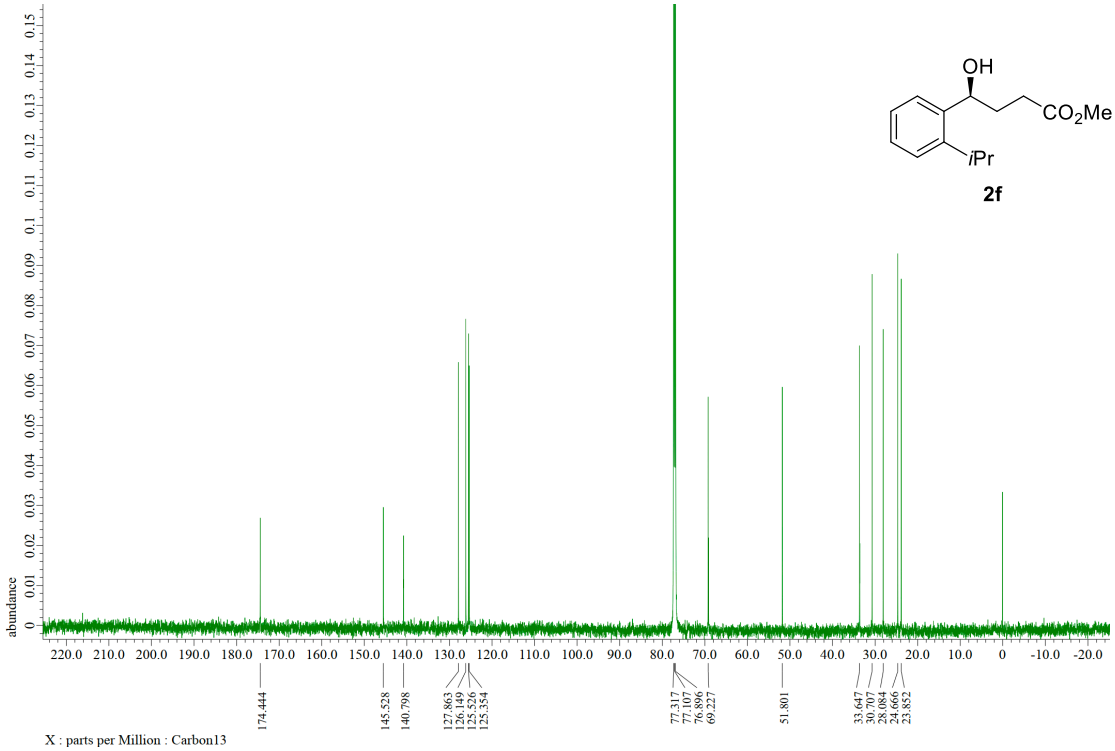

OH
CO2Me
2d
X : parts per Million : Proton

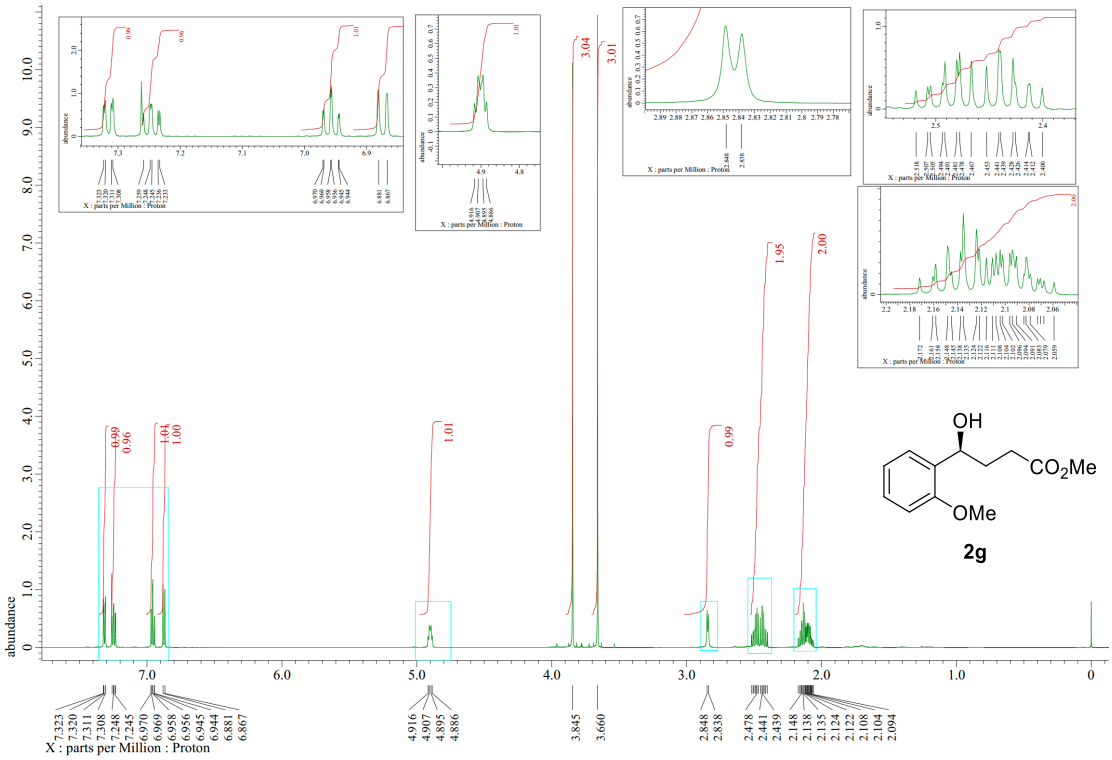

OH
CO2Me
2d
X : parts per Million : Carbon13

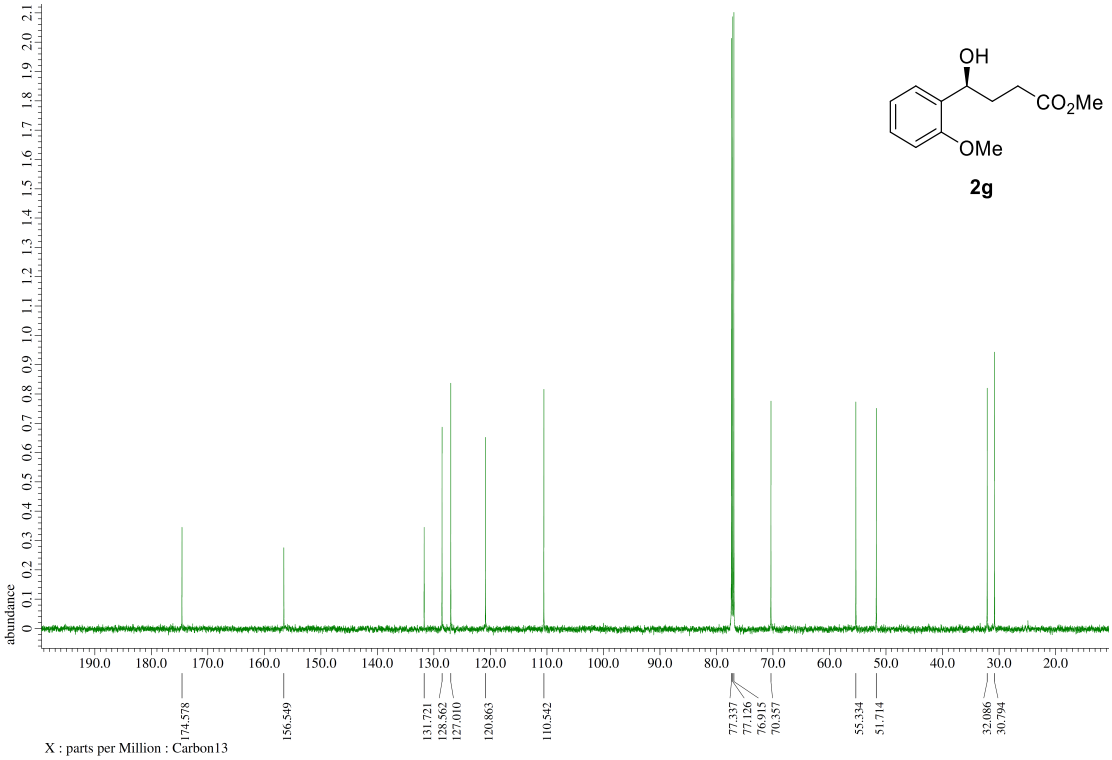

OH
CO2Me
Me
2e
abundance
X : parts per Million : Proton

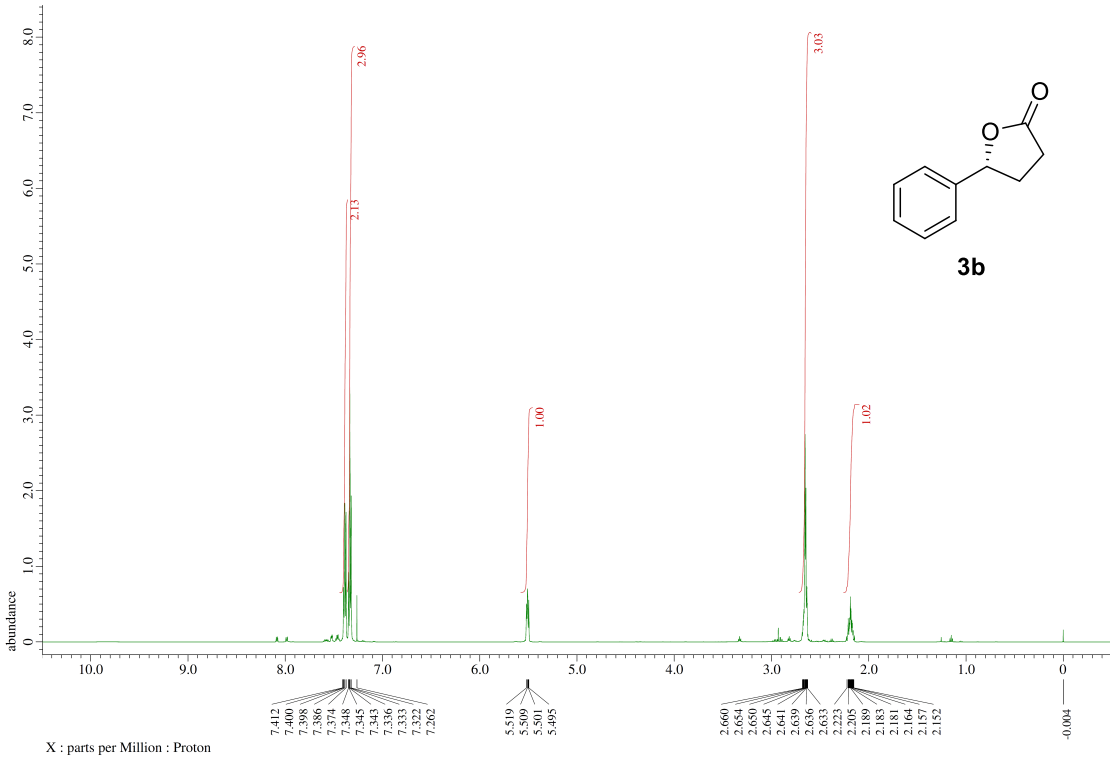

OH
CO2Me
Me
2e
abundance
X : parts per Million : Carbon13


OH
CO2Me
iPr
2f
abundance
X : parts per Million : Proton

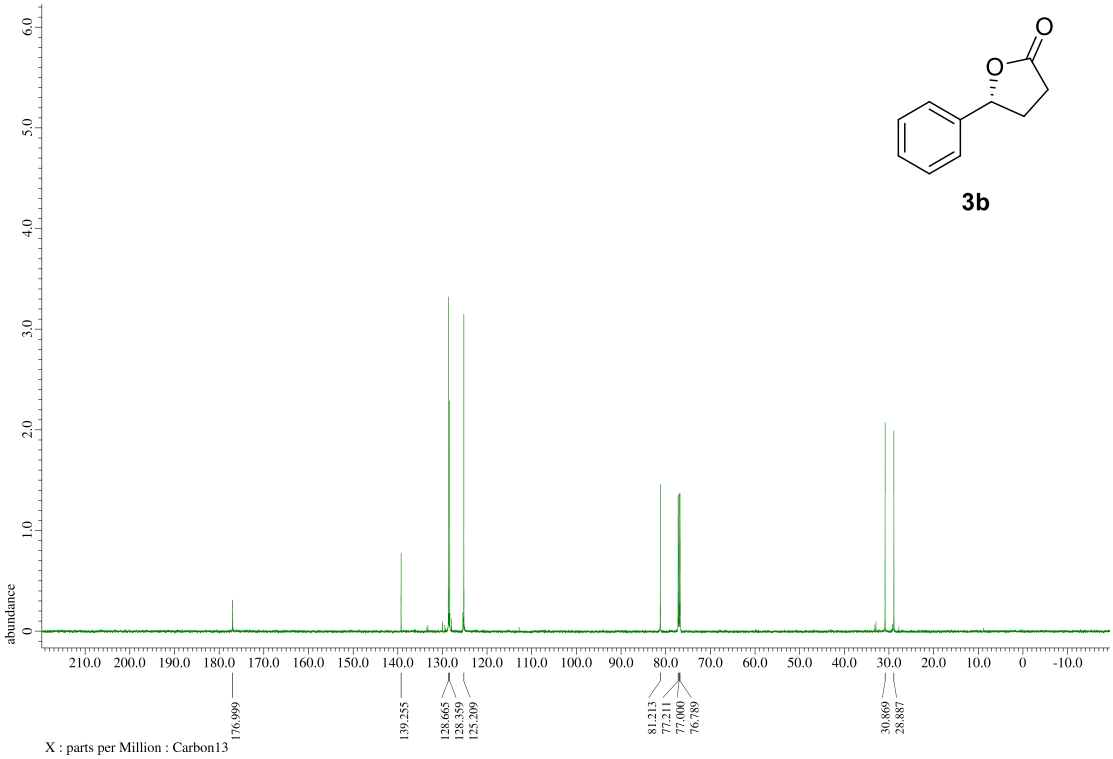

OH
CO2Me
iPr
2f
abundance
X : parts per Million : Carbon13


OH
CO2Me
OMe
2g
X : parts per Million : Proton

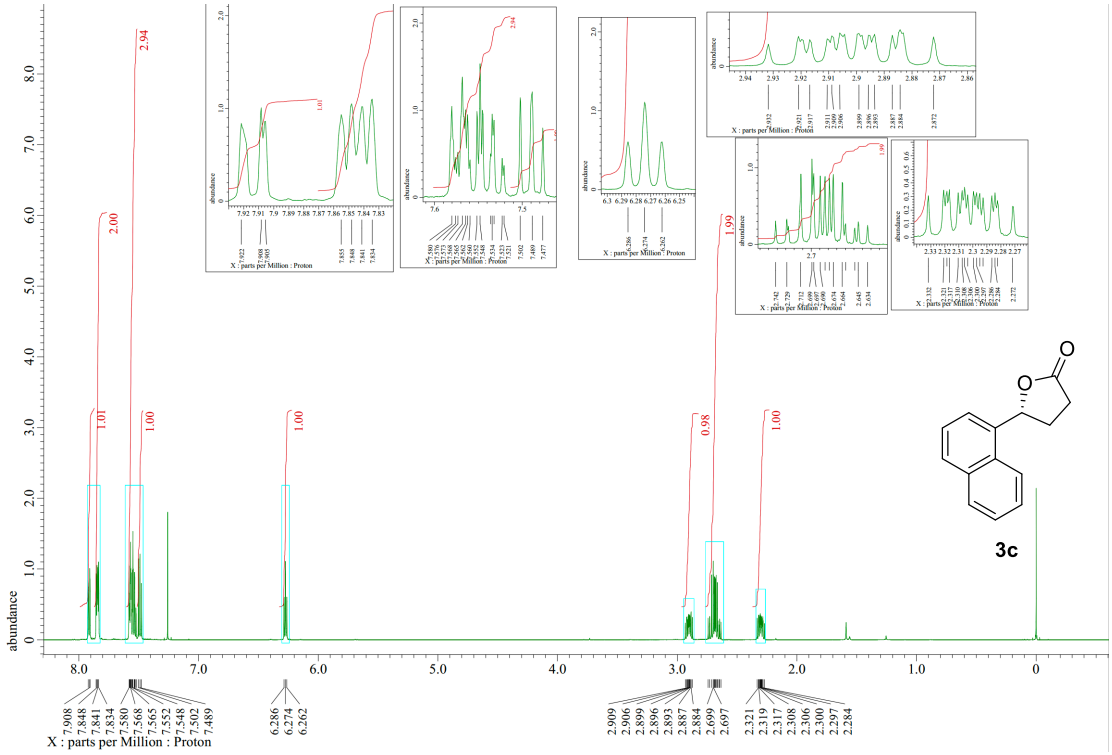

OH
CO2Me
OMe
2g
X : parts per Million : Carbon13

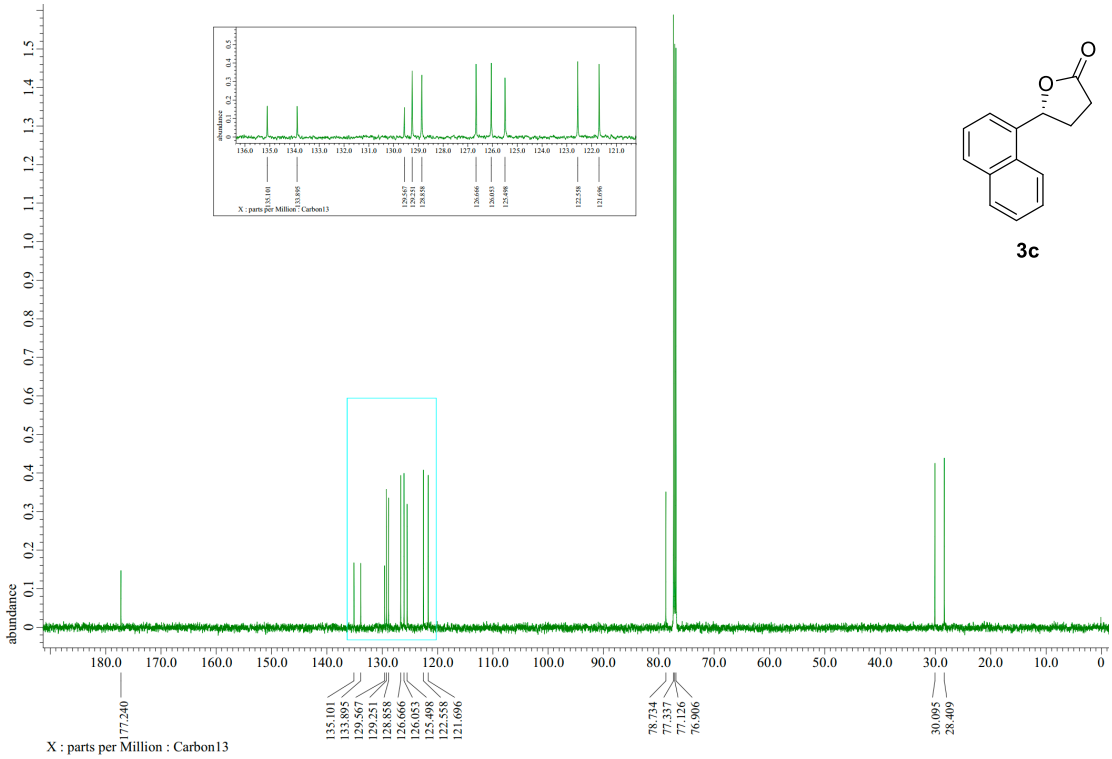

2.96
2.13
1.00
3.03
1.02
abundance
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
7.412 7.400 7.398 7.386 7.374 7.348 7.345 7.343 7.336 7.333 7.322 7.262
5.519 5.509 5.501 5.495
2.660 2.654 2.650 2.645 2.641 2.639 2.636 2.633 2.223 2.205 2.189 2.183 2.181 2.164 2.157 2.152
-0.004
X : parts per Million : Proton

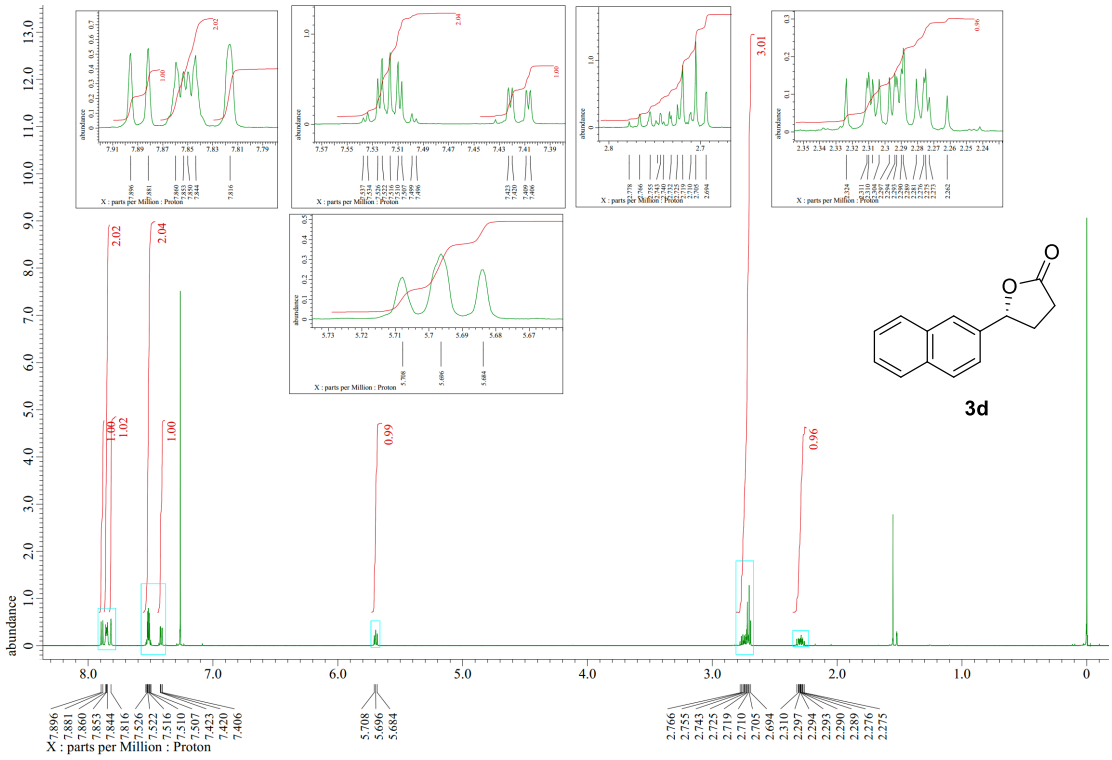
3b

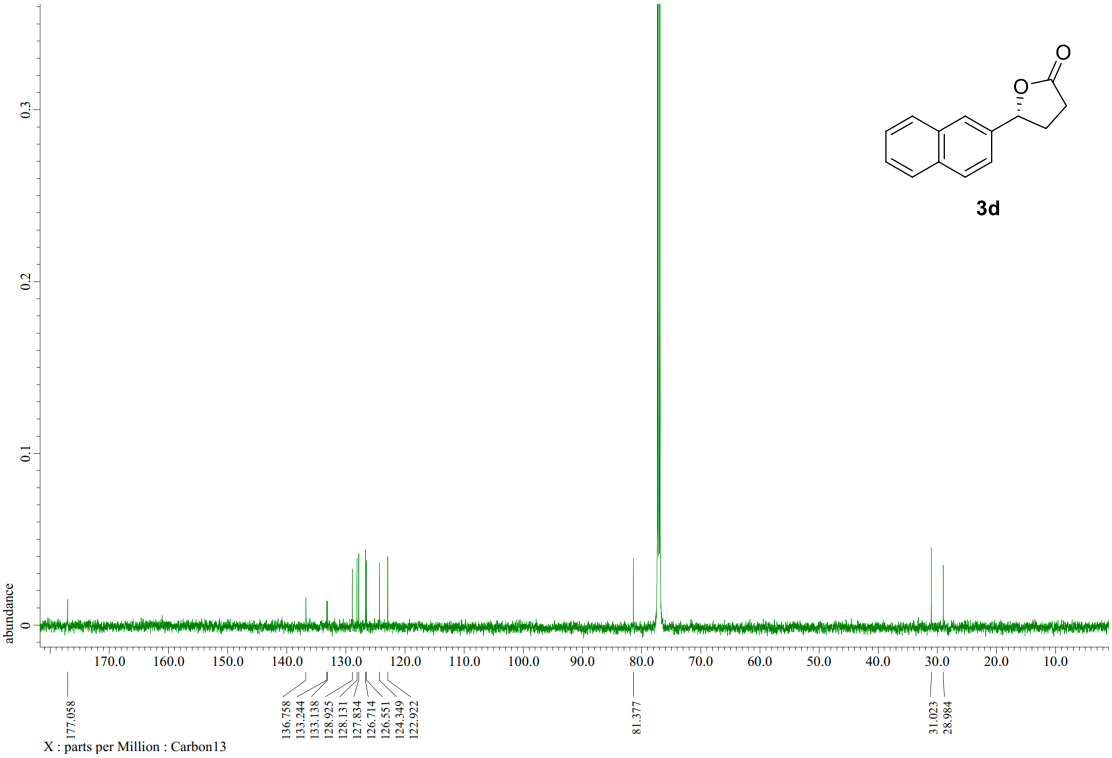

abundance
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
176.999
139.255
128.665
128.359
125.209
81.213
77.211
77.000
76.789
30.869
28.887
X : parts per Million : Carbon13

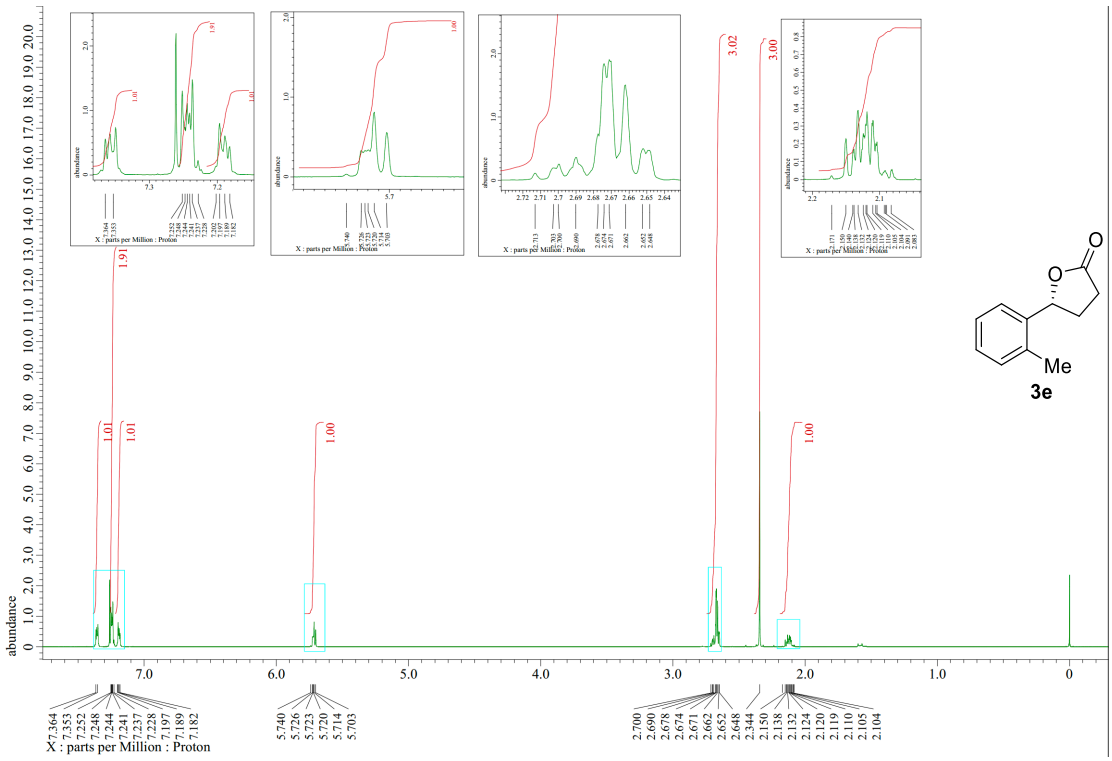
3b

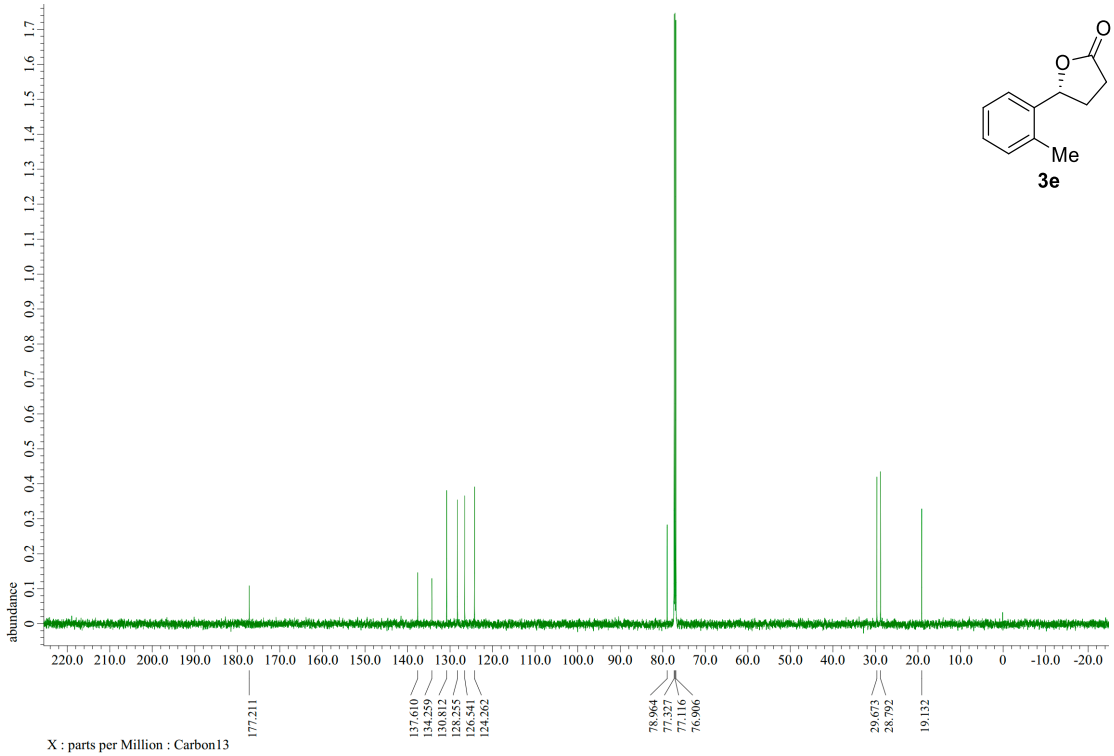

3c
X : parts per Million : Proton

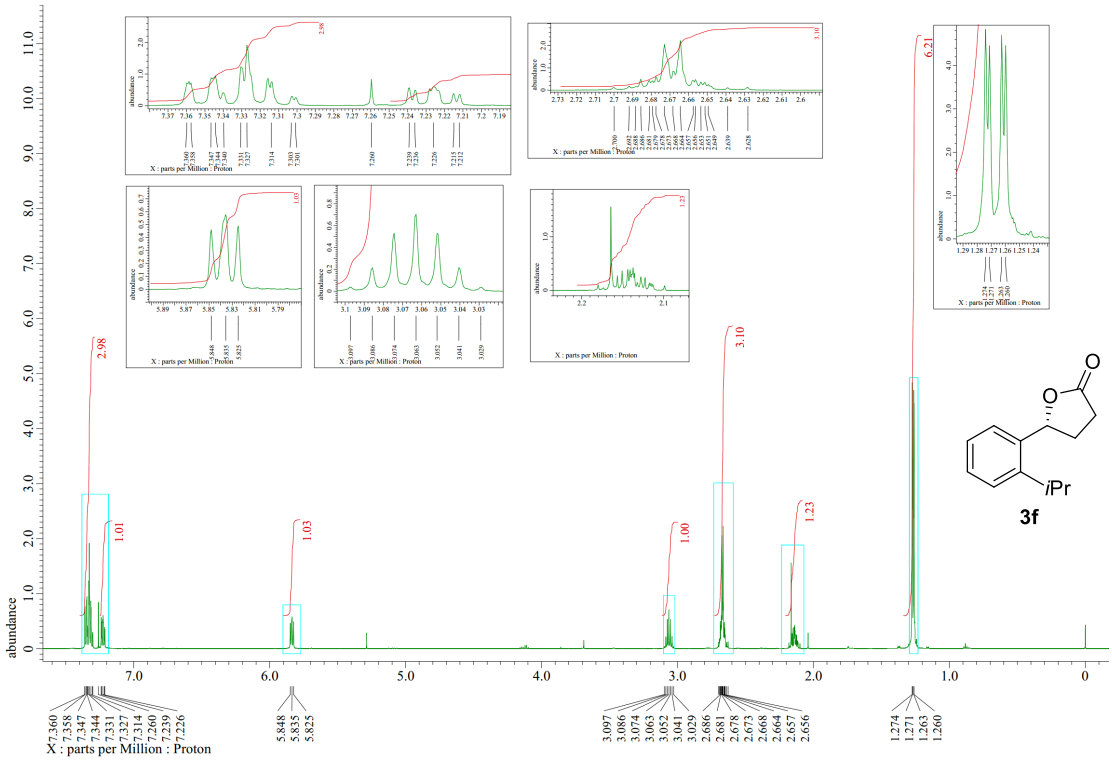

3c
X : parts per Million : Carbon13

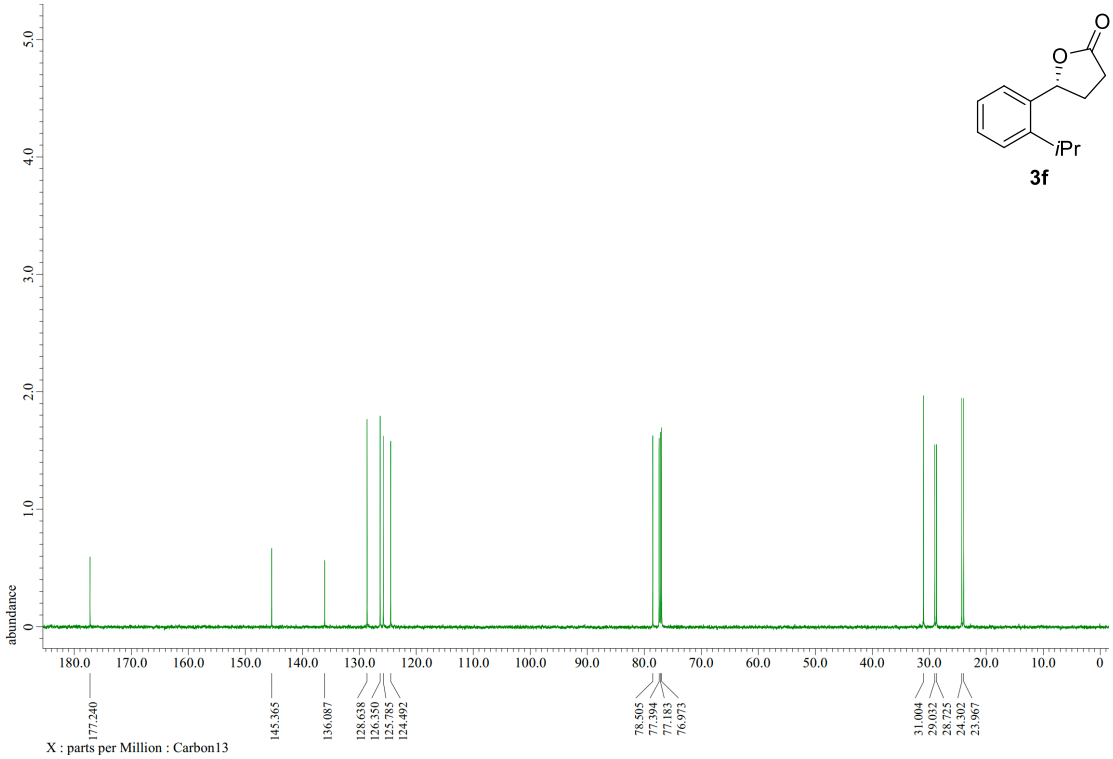

3d
X : parts per Million : Proton

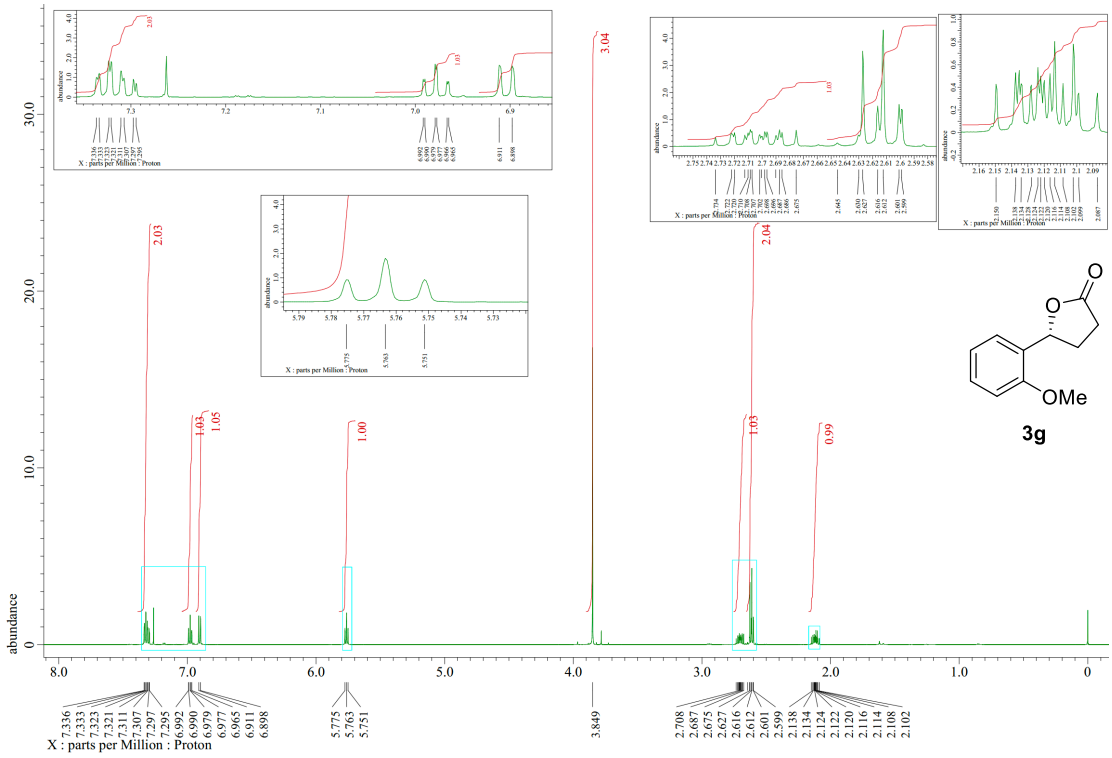

3d
X : parts per Million : Carbon13

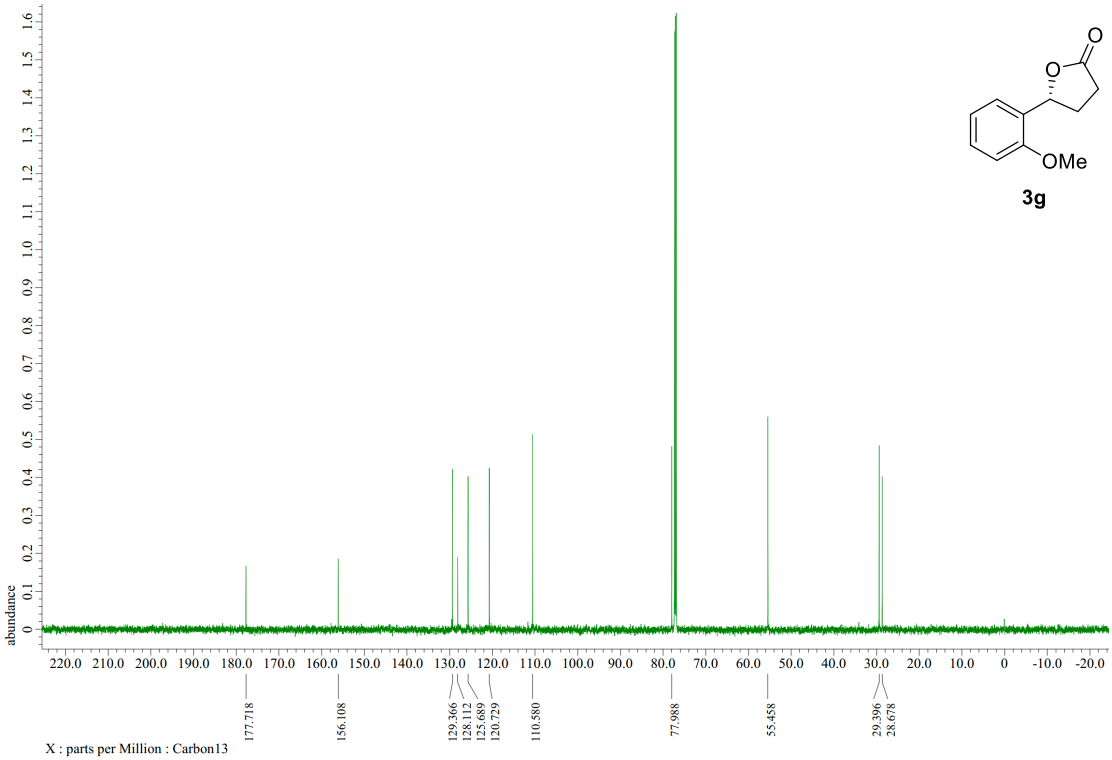

abundance
X : parts per Million : Proton
1.91
1.01
1.01
1.00
3.02
3.00
1.00
Me
3e


abundance
X : parts per Million : Carbon13
177.211
137.610
134.259
130.812
128.255
126.541
124.262
78.964
77.327
77.116
76.906
29.673
28.792
19.132
Me
3e

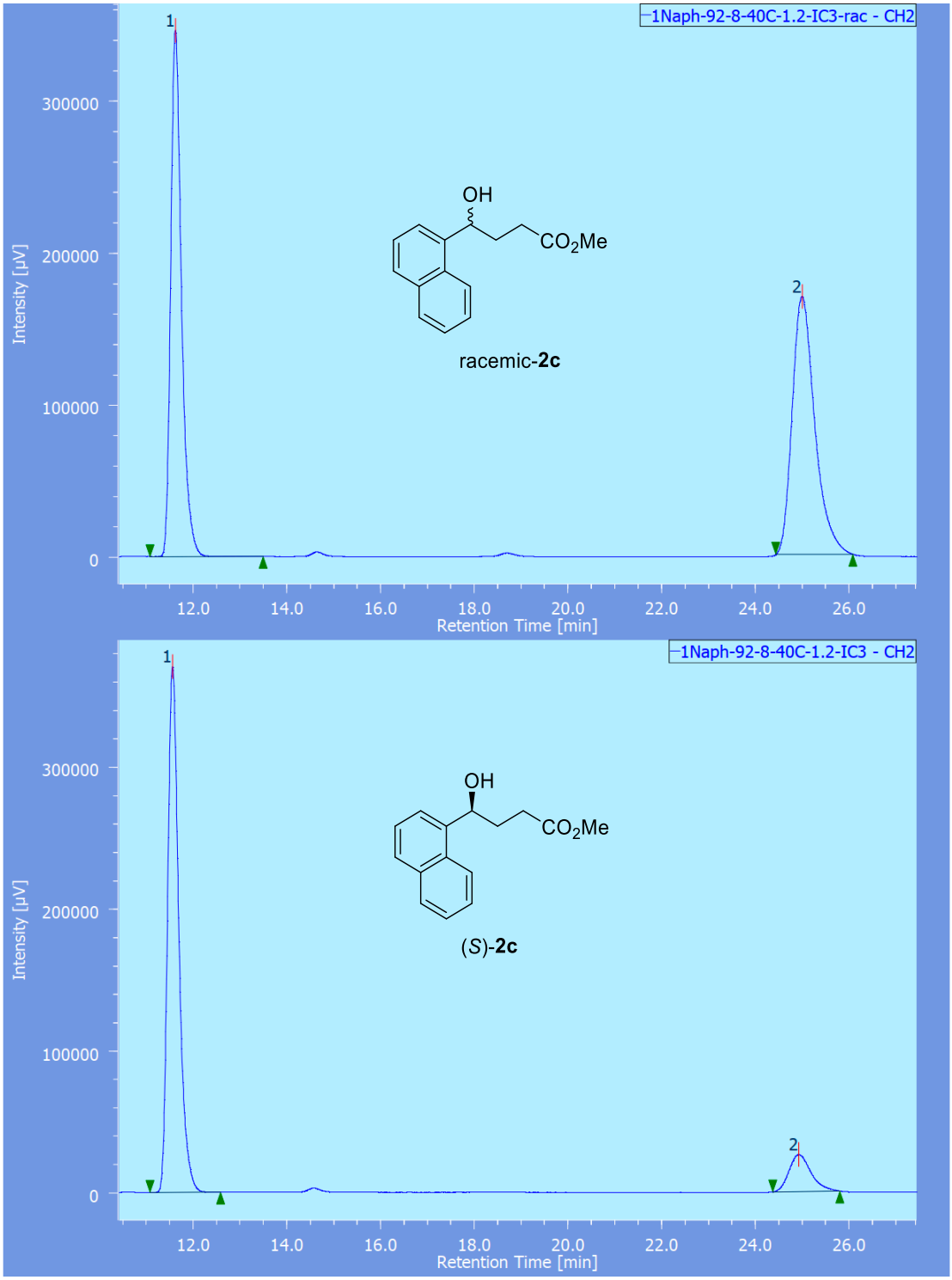

2.98
1.01
1.03
1.00
3.10
1.23
6.21
iPr
3f
abundance
X : parts per Million : Proton


iPr
3f
abundance
X : parts per Million : Carbon13

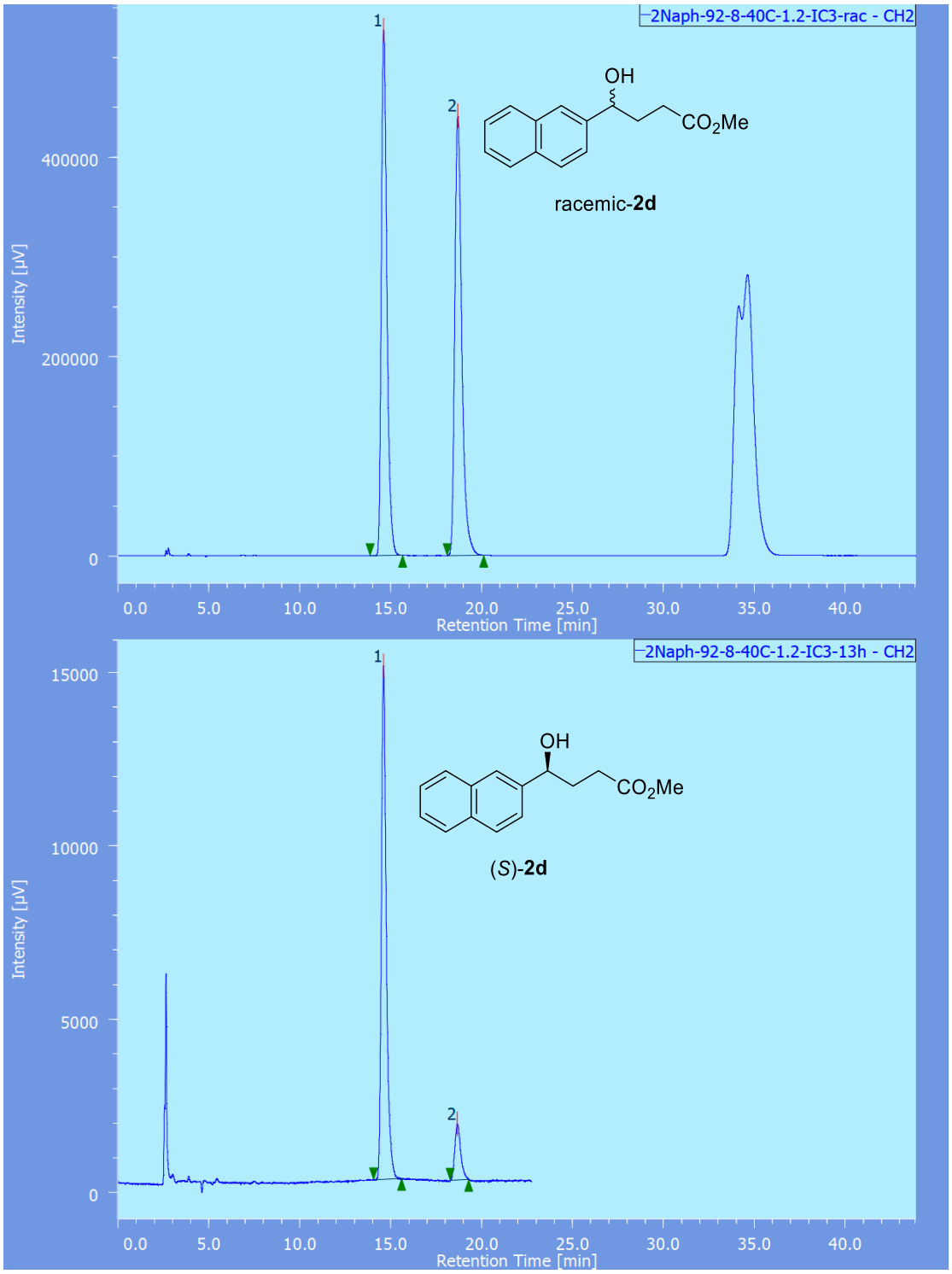

abundance
X : parts per Million : Proton
2.03
1.03
1.05
1.00
3.04
2.04
1.03
0.99
OMe
3g


abundance
X : parts per Million : Carbon13
177.718
156.108
129.366
128.112
125.689
120.729
110.580
77.988
55.458
29.396
28.678
OMe
3g

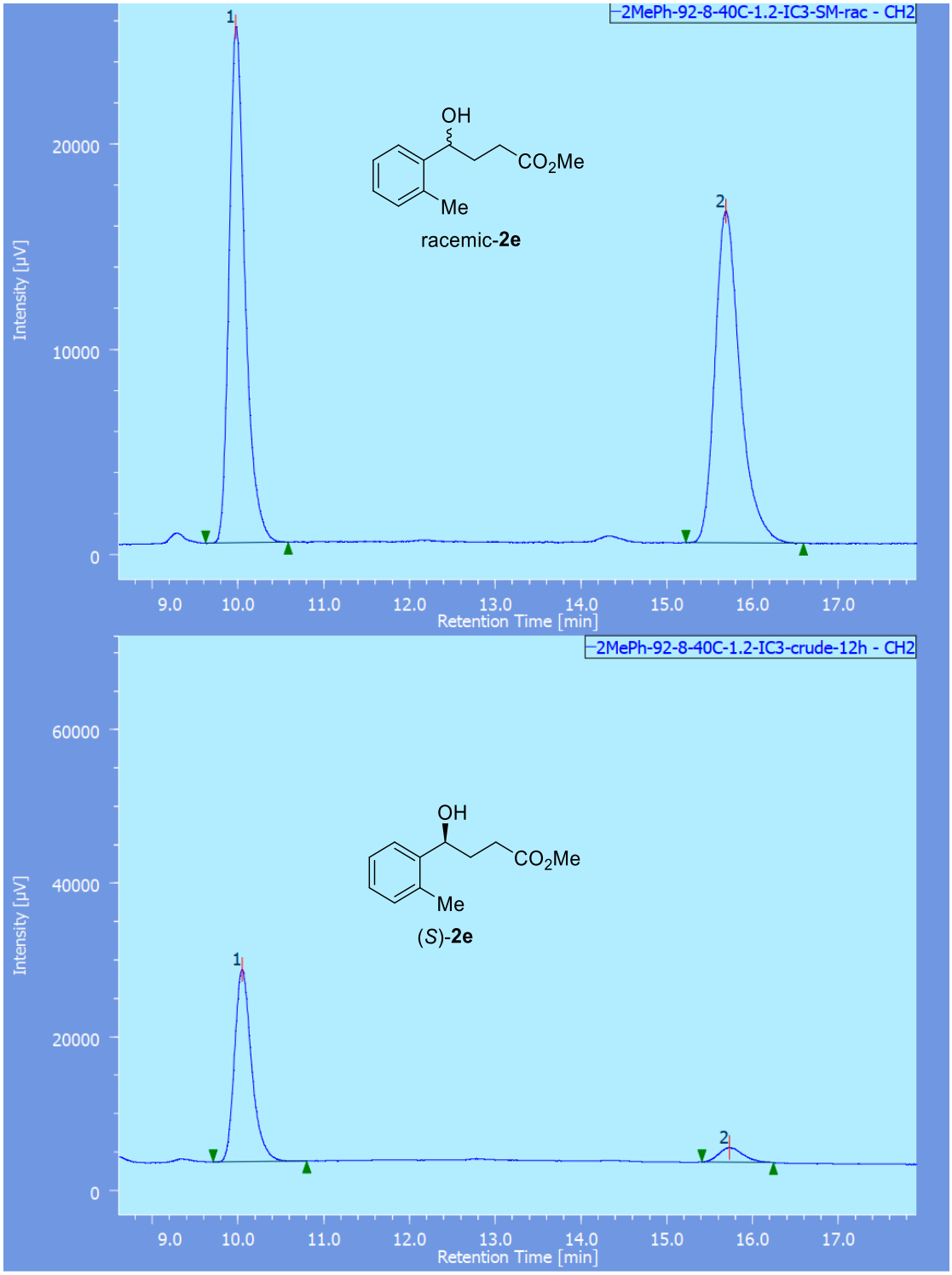
7. HPLC Charts



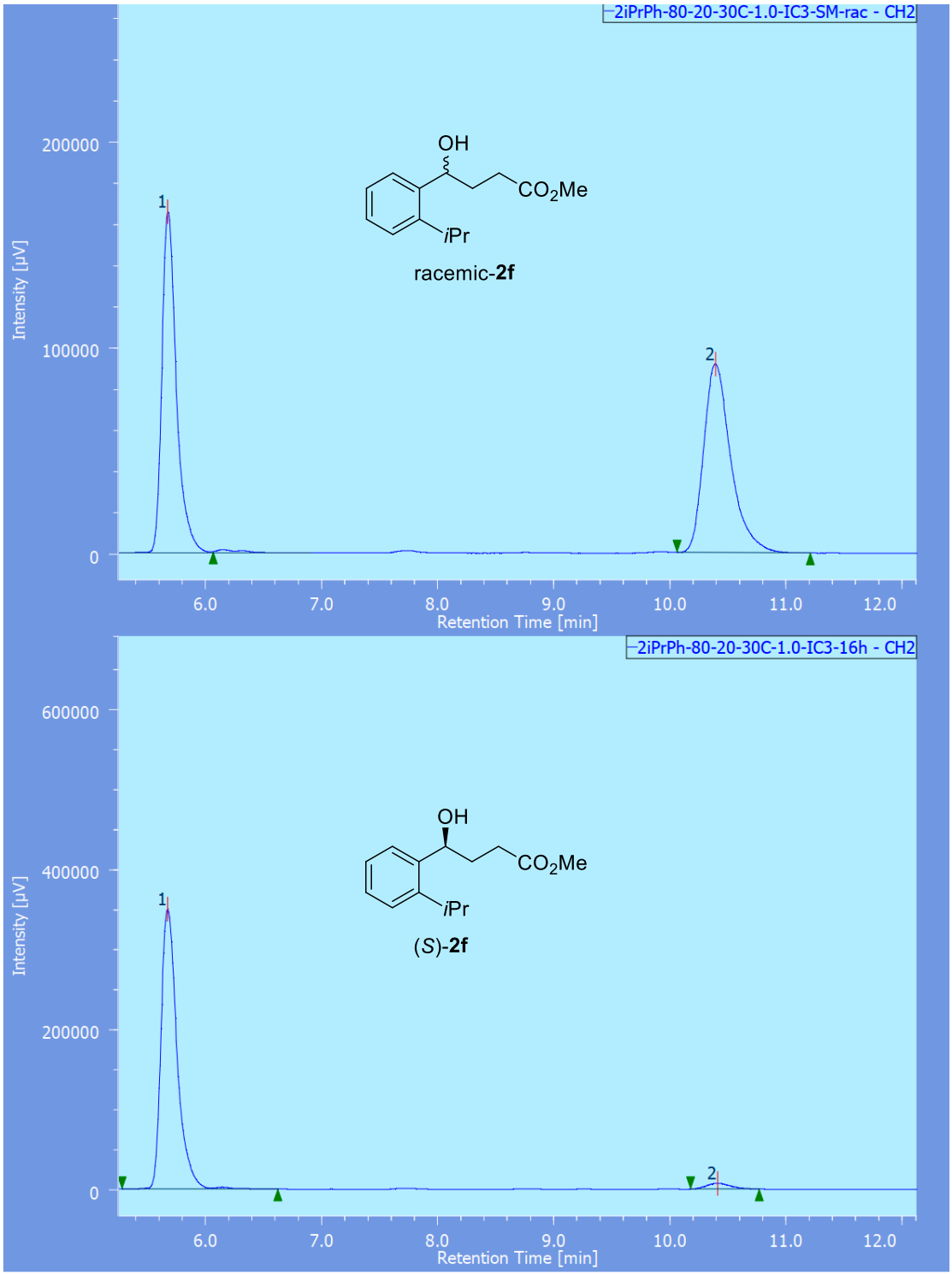
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-2c	11.6	24.9	49.4	50.6
recovered-2c	11.5	24.9	87.9	12.1



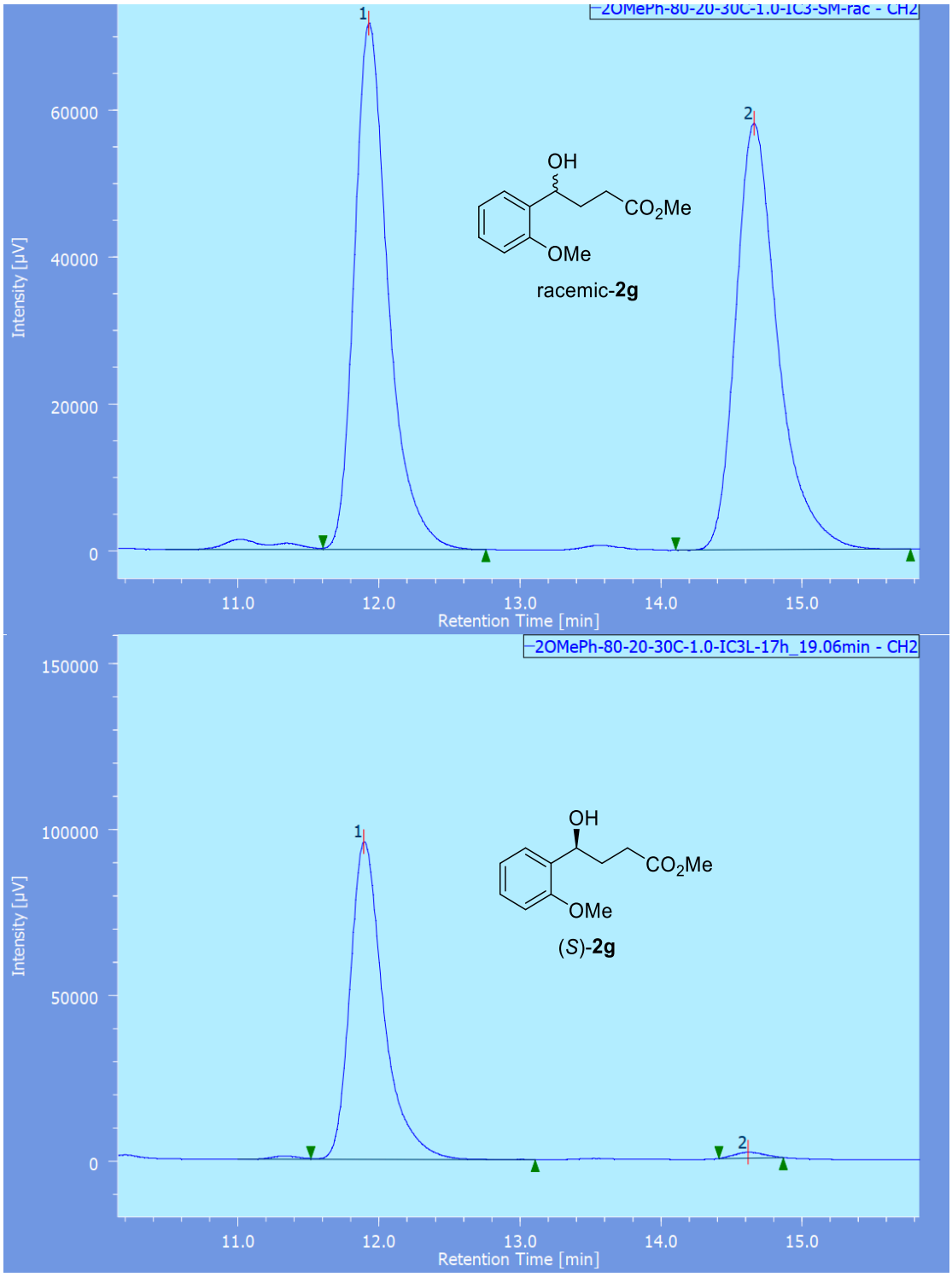
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-2d	**14.6**	**18.6**	**49.8**	**50.2**
recovered-2d	**14.6**	**18.6**	**88.6**	**11.4**



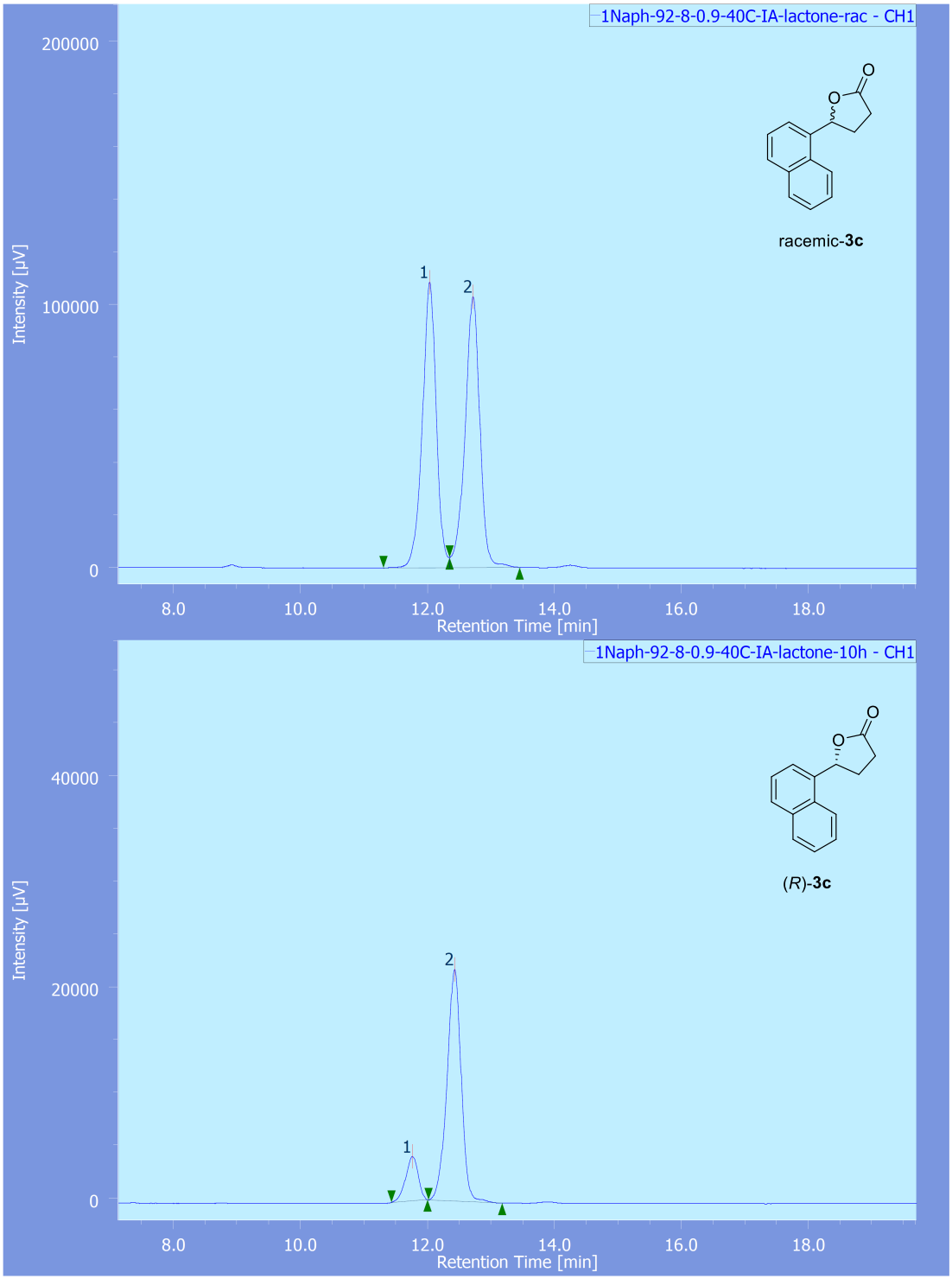
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-2e	**9.9**	**15.6**	**50.0**	**50.0**
recovered-2e	**10.0**	**15.7**	**90.2**	**9.8**



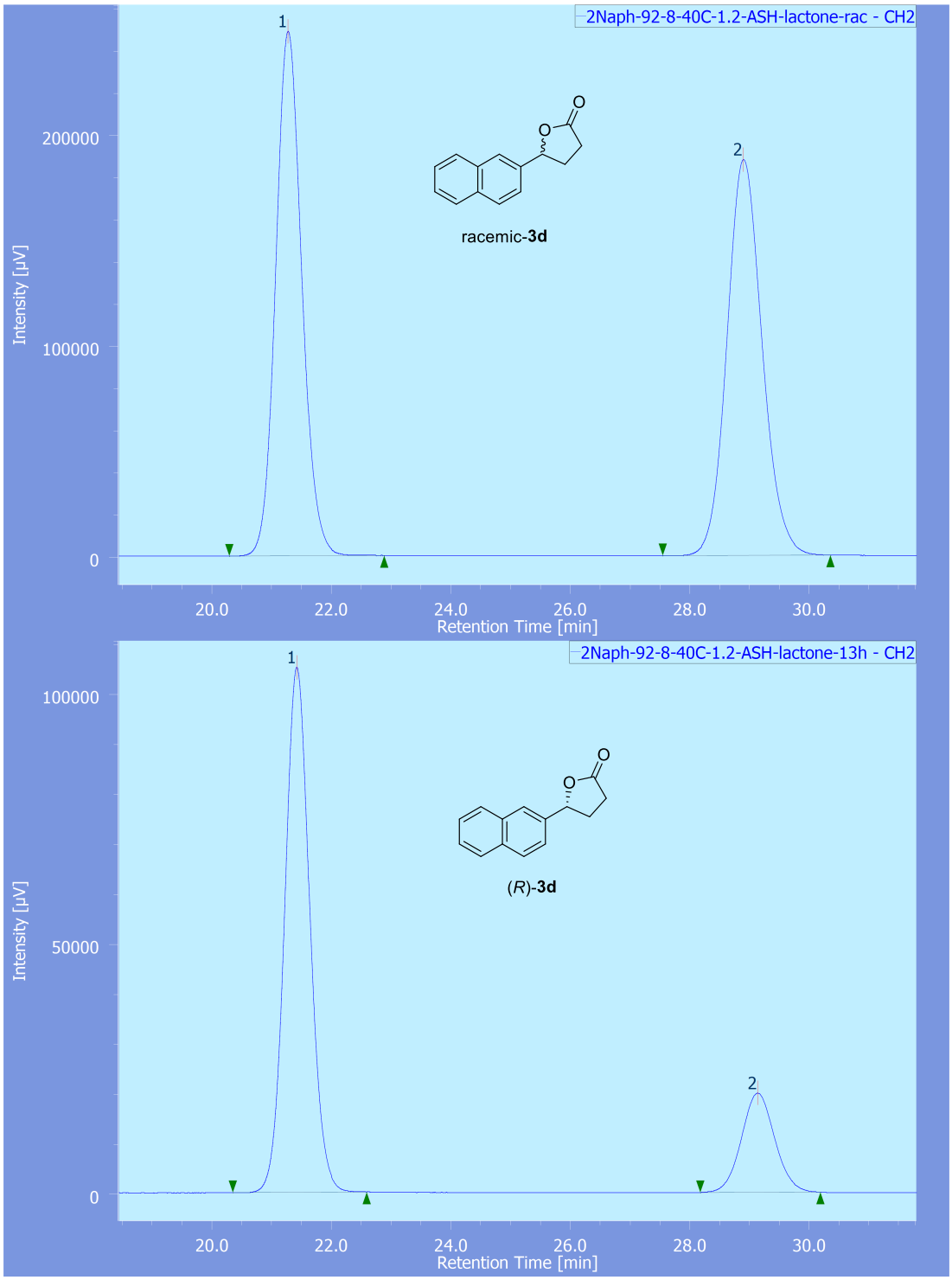
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-2f	**5.6**	**10.4**	**49.2**	**50.8**
recovered-2f	**5.6**	**10.4**	**97.0**	**3.0**



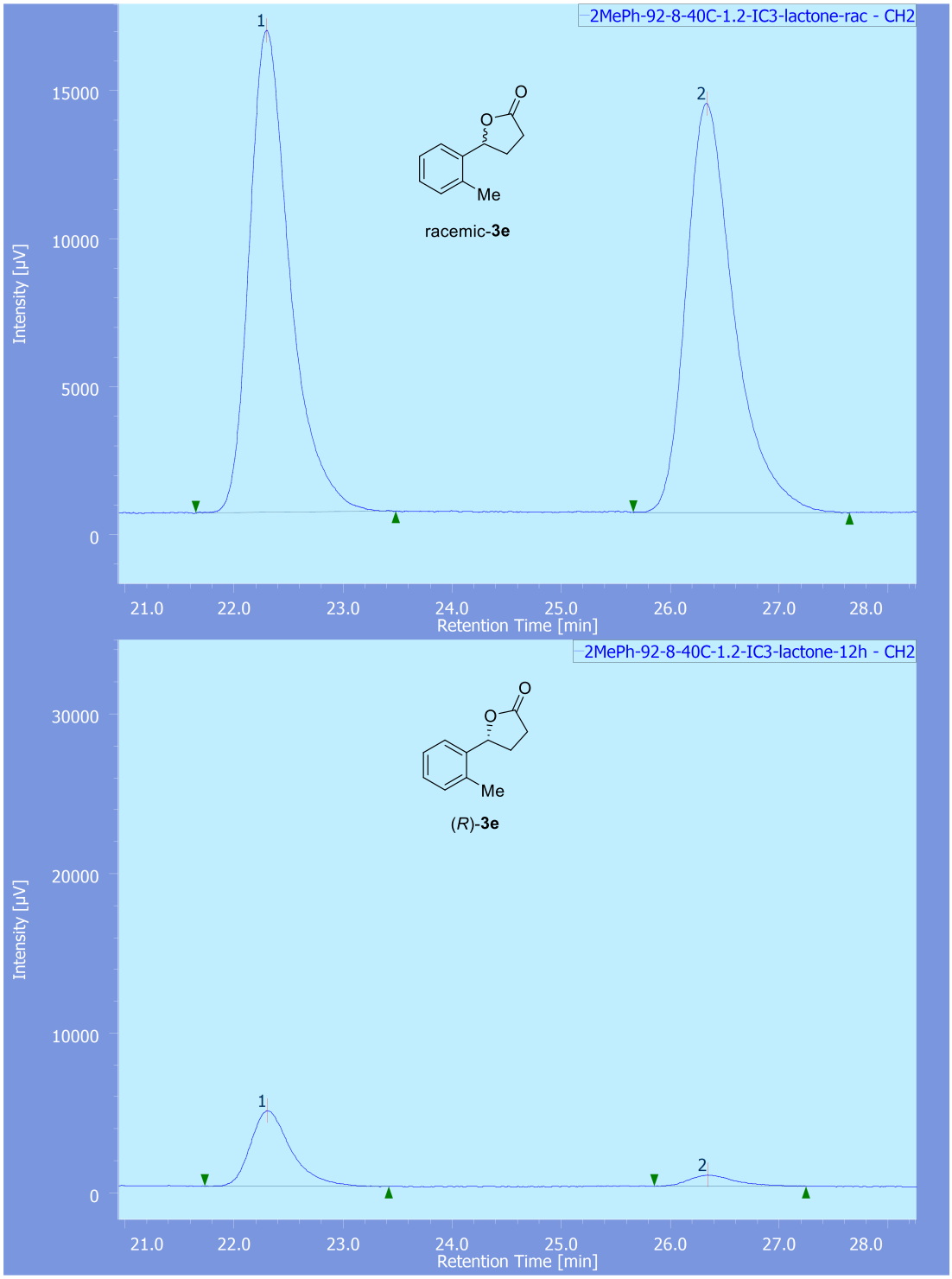
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-2g	**11.9**	**14.6**	**49.9**	**50.1**
recoverd-2g	**11.9**	**14.6**	**98.5**	**1.5**



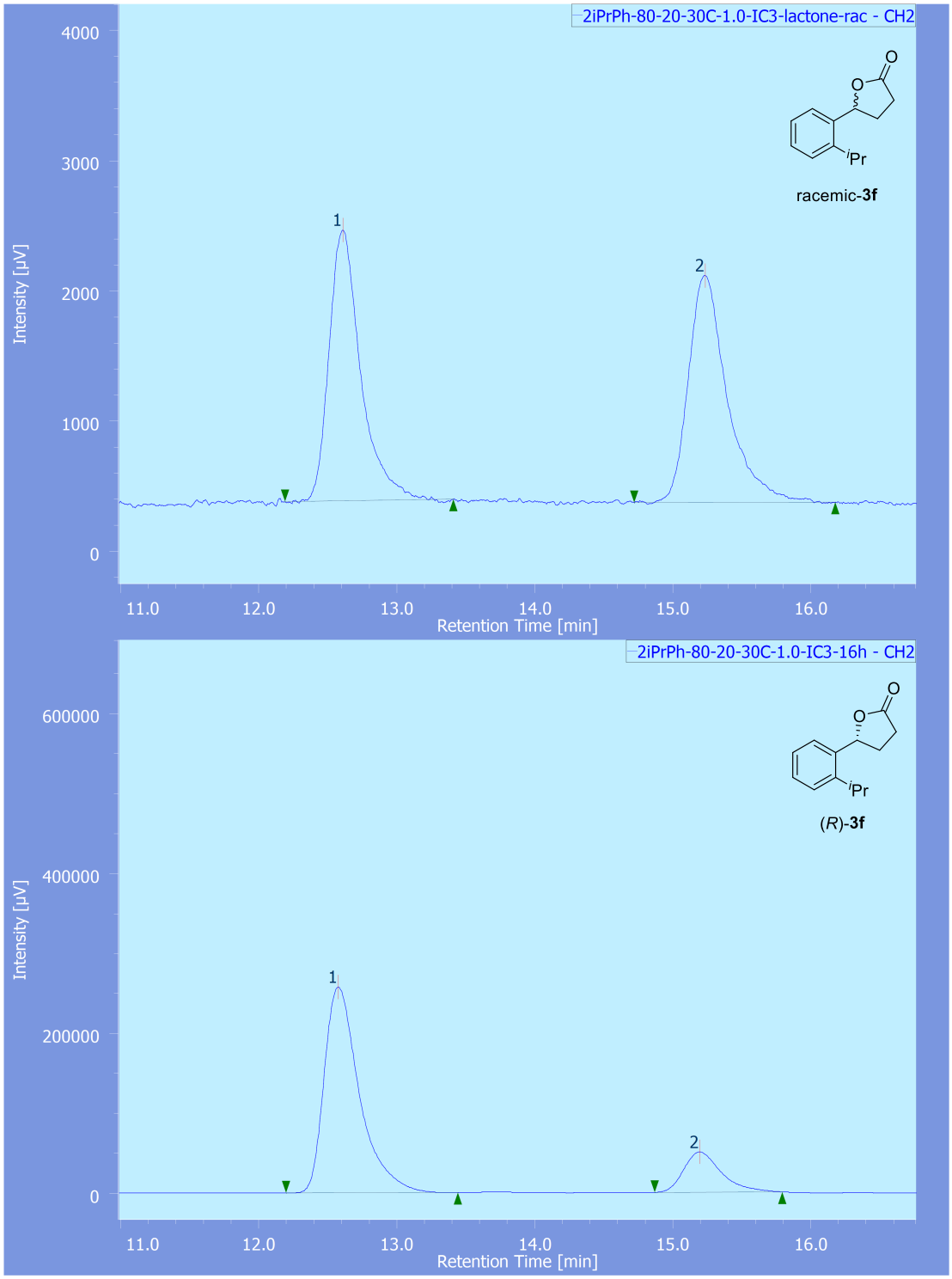
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-3c	**12.0**	**12.7**	**49.7**	**50.3**
lactone-3c	**11.8**	**12.4**	**14.4**	**85.6**



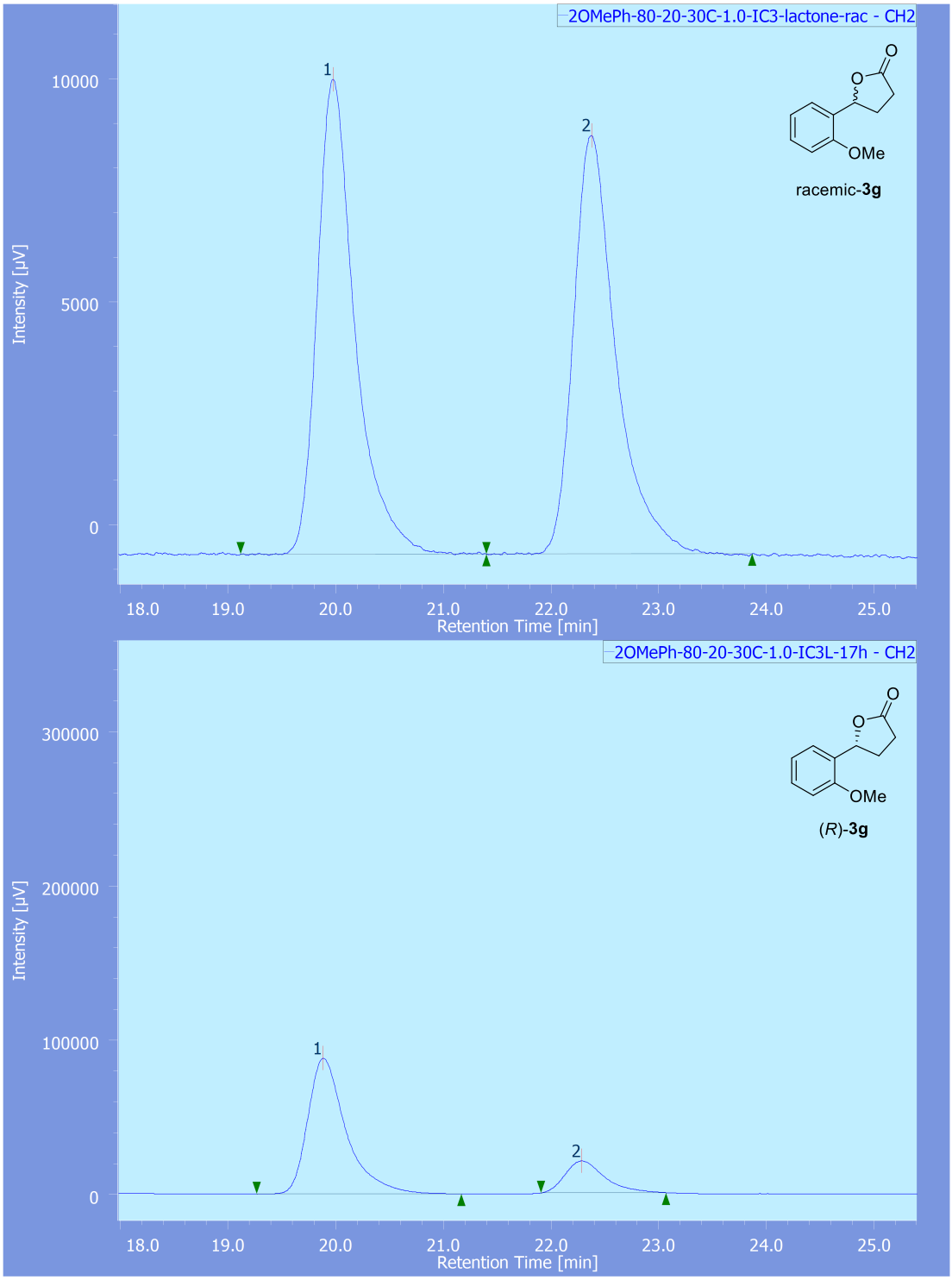
	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-3d	**21.3**	**28.9**	**49.5**	**50.5**
lactone-3d	**21.4**	**29.1**	**79.8**	**20.2**



	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-3e	**22.3**	**26.3**	**50.0**	**50.0**
lactone-3e	**22.3**	**26.3**	**85.5**	**14.5**

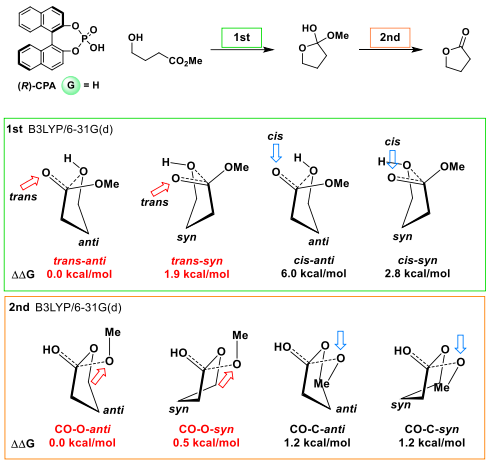


	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-3f	**12.6**	**15.2**	**49.3**	**50.7**
lactone-3f	**12.6**	**15.2**	**82.7**	**17.3**

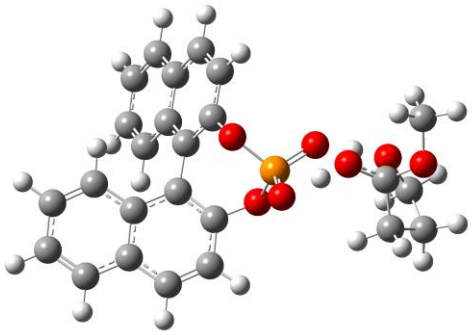


	Retention Time 1 (min)	Retention Time 2 (min)	Area 1 (%)	Area 2 (%)
racemic-3f	**20.0**	**22.4**	**50.3**	**49.7**
lactone-3f	**19.9**	**22.3**	**80.3**	**19.7**

8. DFT Calculation of Transition States of Model System



TS-1st-*trans-anti*



B3LYP/6-31G(d); E(B3LYP) = -1834.537960 hartree

Zero-point Energy Correction = 0.436800 hartree

Thermal Correction to Energy = 0.463820 hartree

Thermal correction to Enthalpy = 0.464764 hartree

Thermal correction to Gibbs Free Energy= 0.378190 hartree

Sum of electronic and Zero-point Energies = -1834.101159 hartree

Sum of electronic and thermal Energies = -1834.074139 hartree

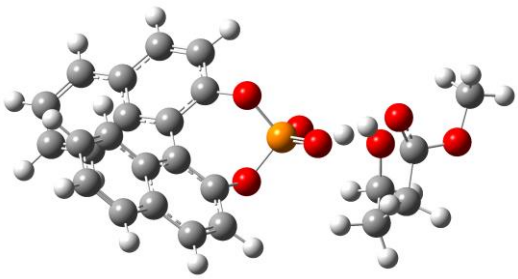
Sum of electronic and thermal Enthalpies = -1834.073195 hartree

Sum of electronic and thermal Free Energies= -1834.159770 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.148308	-0.344640	-0.399759
2	8	0	-4.465961	0.871495	0.604649
3	1	0	-3.474228	-0.798651	-1.271946
4	6	0	-4.668086	0.485180	1.983107
5	6	0	-5.500373	-0.808901	1.960914
6	6	0	-5.143597	-1.466661	0.626029
7	1	0	-3.682995	0.326973	2.433911
8	1	0	-6.569660	-0.579563	1.988009
9	1	0	-5.268008	-1.448304	2.817378
10	1	0	-5.861352	-2.233170	0.321150
11	1	0	-4.142159	-1.906851	0.644826
12	8	0	-4.388898	-0.399077	-1.480669
13	8	0	-6.398529	0.100732	-0.626483
14	6	0	-6.543646	1.144040	-1.605318
15	1	0	-7.599347	1.416671	-1.580331
16	1	0	-6.266612	0.784521	-2.598544
17	1	0	-5.924905	2.003632	-1.332670
18	1	0	-3.343640	1.000352	0.431392
19	6	0	4.960865	2.125856	1.545515
20	6	0	3.998479	1.234455	1.125392
21	6	0	2.942994	1.640504	0.261889
22	6	0	2.888096	3.021753	-0.125125
23	6	0	3.906359	3.910548	0.312768
24	6	0	4.926467	3.476248	1.126704
25	1	0	5.751135	1.788479	2.210802
26	1	0	4.034548	0.206489	1.466434
27	6	0	1.917842	0.737060	-0.192913
28	6	0	1.800946	3.483814	-0.913254
29	1	0	3.853992	4.950843	-0.000078
30	1	0	5.695541	4.167778	1.459680
31	6	0	0.785755	2.633717	-1.271834
32	6	0	0.849618	1.276013	-0.894157
33	1	0	1.769608	4.530485	-1.205005
34	6	0	1.936536	-0.722924	0.106593
35	6	0	3.031577	-1.581799	-0.264337
36	6	0	0.839398	-1.307753	0.721297
37	6	0	4.134456	-1.130007	-1.041685
38	6	0	3.004043	-2.965118	0.118107
39	6	0	0.802984	-2.668159	1.092984
40	6	0	5.163573	-1.979495	-1.383025
41	1	0	4.154452	-0.100704	-1.379940
42	6	0	4.090131	-3.809656	-0.236410
43	6	0	1.877888	-3.474550	0.816970
44	6	0	5.152540	-3.331182	-0.967108
45	1	0	5.989101	-1.607960	-1.984167
46	1	0	4.056370	-4.852054	0.071932
47	1	0	1.866685	-4.522676	1.104939
48	1	0	5.973672	-3.989240	-1.237739
49	8	0	-0.201792	0.457804	-1.297203
50	15	0	-1.266099	-0.064884	-0.173985
51	8	0	-0.274648	-0.535470	1.039300
52	8	0	-2.065109	1.107988	0.394163
53	8	0	-2.046264	-1.211545	-0.761971
54	1	0	-0.074024	2.970264	-1.840910
55	1	0	-0.084636	-3.042905	1.591093
56	1	0	-5.171665	1.303367	2.505198

TS-1st-*trans-syn*



B3LYP/6-31G(d); E(B3LYP) = -1834.535833 hartree

Zero-point Energy Correction = 0.437361 hartree

Thermal Correction to Energy = 0.464305 hartree

Thermal correction to Enthalpy = 0.465250 hartree

Thermal correction to Gibbs Free Energy= 0.379105 hartree

Sum of electronic and Zero-point Energies = -1834.098472 hartree

Sum of electronic and thermal Energies = -1834.071528 hartree

Sum of electronic and thermal Enthalpies = -1834.070584 hartree

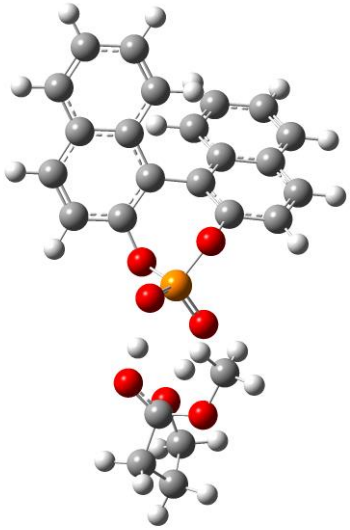
Sum of electronic and thermal Free Energies= -1834.156729 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-3.559042	-0.791615	-1.295271
2	6	0	4.902646	2.096559	1.580809
3	6	0	3.940394	1.215855	1.138353
4	6	0	2.918716	1.629824	0.238696
5	6	0	2.897292	3.008031	-0.162197
6	6	0	3.914706	3.885495	0.299930
7	6	0	4.901926	3.443450	1.149491
8	1	0	5.666687	1.753443	2.273260
9	1	0	3.950404	0.190493	1.488852
10	6	0	1.894199	0.737946	-0.239595
11	6	0	1.842961	3.479027	-0.988700
12	1	0	3.888198	4.923516	-0.023563
13	1	0	5.670652	4.126391	1.500537
14	6	0	0.826734	2.640961	-1.371961
15	6	0	0.857551	1.286233	-0.979763
16	1	0	1.837065	4.523256	-1.290652
17	6	0	1.879225	-0.718956	0.074917
18	6	0	2.971050	-1.598877	-0.253540
19	6	0	0.754218	-1.279224	0.662070
20	6	0	4.104561	-1.172641	-1.000750
21	6	0	2.909911	-2.977381	0.142083
22	6	0	0.685273	-2.635163	1.045790
23	6	0	5.130452	-2.041436	-1.300613
24	1	0	4.151382	-0.147454	-1.348709
25	6	0	3.993081	-3.842352	-0.169438
26	6	0	1.754826	-3.461469	0.811007
27	6	0	5.085264	-3.388190	-0.871184
28	1	0	5.980119	-1.689122	-1.879275
29	1	0	3.933314	-4.880708	0.148463
30	1	0	1.717853	-4.506174	1.109112
31	1	0	5.904072	-4.061648	-1.108977
32	8	0	-0.193734	0.479828	-1.406287
33	15	0	-1.302644	-0.001192	-0.308209
34	8	0	-0.355290	-0.486037	0.939183
35	8	0	-2.084803	1.194318	0.228642
36	8	0	-2.089247	-1.141372	-0.900698
37	1	0	-0.009531	2.984950	-1.970825
38	1	0	-0.222686	-2.990970	1.520675
39	6	0	-5.143680	-0.380439	-0.256057
40	8	0	-4.494131	1.008860	0.516292
41	6	0	-4.638512	0.741716	1.924546
42	6	0	-4.907088	-1.431418	0.842670
43	1	0	-5.875730	-1.888711	1.058698
44	1	0	-4.237717	-2.198832	0.449989
45	8	0	-4.517592	-0.461265	-1.417587
46	8	0	-6.453893	-0.078650	-0.353282
47	6	0	-6.827026	0.828986	-1.405815
48	1	0	-7.892539	1.011778	-1.261985
49	1	0	-6.646156	0.379587	-2.384432
50	1	0	-6.266264	1.763208	-1.314416
51	1	0	-3.392911	1.104762	0.305974
52	1	0	-5.672867	0.972948	2.195116
53	6	0	-4.311050	-0.743669	2.089448
54	1	0	-4.715402	-1.150987	3.021025
55	1	0	-3.224953	-0.875922	2.109163
56	1	0	-3.960539	1.403019	2.469091

TS-1st-*cis-anti*



B3LYP/6-31G(d); E(B3LYP) = -1834.52837806 hartree

Zero-point Energy Correction = 0.436960 hartree

Thermal Correction to Energy = 0.464116 hartree

Thermal correction to Enthalpy = 0.465060 hartree

Thermal correction to Gibbs Free Energy= 0.378169 hartree

Sum of electronic and Zero-point Energies = -1834.091418 hartree

Sum of electronic and thermal Energies = -1834.064262hartree

Sum of electronic and thermal Enthalpies = -1834.063318 hartree

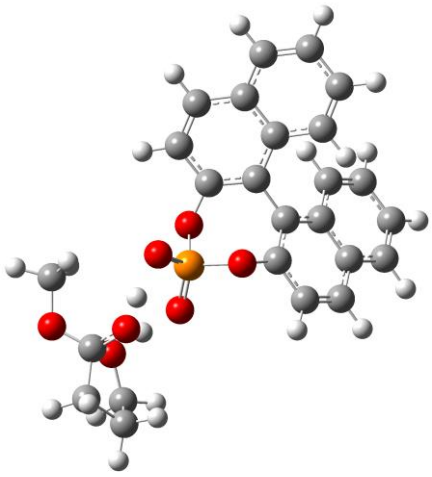
Sum of electronic and thermal Free Energies= -1834.150209 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.175402	-0.626373	0.199925
2	8	0	4.329858	0.331360	-1.041939
3	1	0	3.455516	-1.543657	0.566402
4	6	0	5.285895	1.198784	-1.669766
5	6	0	6.673603	0.693853	-1.209109
6	6	0	6.443920	-0.708853	-0.624430
7	1	0	5.155817	1.105893	-2.752844
8	1	0	7.079970	1.350264	-0.434841
9	1	0	7.387079	0.671130	-2.037588
10	1	0	7.274150	-1.029650	0.011197
11	1	0	6.284755	-1.457411	-1.404172
12	8	0	4.451720	-1.708126	0.319295
13	8	0	5.343592	0.215210	1.237803
14	6	0	4.342477	0.319648	2.269187
15	1	0	4.850019	0.797945	3.107594
16	1	0	3.973912	-0.665251	2.560557
17	1	0	3.517729	0.942103	1.917718
18	1	0	3.397073	0.757168	-0.719205
19	6	0	-4.905907	2.202511	-1.539569
20	6	0	-3.953108	1.291206	-1.140828
21	6	0	-2.917689	1.654209	-0.234676
22	6	0	-2.872474	3.015276	0.219184
23	6	0	-3.880518	3.925051	-0.198754
24	6	0	-4.881573	3.531283	-1.055820
25	1	0	-5.680588	1.898039	-2.238245
26	1	0	-3.981265	0.280782	-1.531295
27	6	0	-1.903384	0.728446	0.199325
28	6	0	-1.803808	3.437936	1.053120
29	1	0	-3.835405	4.949122	0.164758
30	1	0	-5.642939	4.238635	-1.372986
31	6	0	-0.797731	2.569864	1.393659
32	6	0	-0.851180	1.231069	0.950809

33	1	0	-1.778883	4.469510	1.395140
34	6	0	-1.914492	-0.714288	-0.174711
35	6	0	-3.015839	-1.591751	0.125927
36	6	0	-0.802194	-1.264000	-0.794949
37	6	0	-4.137595	-1.181934	0.899547
38	6	0	-2.976095	-2.953320	-0.327053
39	6	0	-0.754307	-2.603233	-1.236461
40	6	0	-5.172254	-2.049156	1.172889
41	1	0	-4.168084	-0.171177	1.289191
42	6	0	-4.067748	-3.816451	-0.041060
43	6	0	-1.833232	-3.424040	-1.026244
44	6	0	-5.147986	-3.377745	0.688621
45	1	0	-6.012689	-1.710016	1.772606
46	1	0	-4.024167	-4.841611	-0.401604
47	1	0	-1.813035	-4.455892	-1.367643
48	1	0	-5.973402	-4.050055	0.906101
49	8	0	0.189857	0.396096	1.341949
50	15	0	1.282082	-0.082194	0.221094
51	8	0	0.314103	-0.472395	-1.042777
52	8	0	2.128012	1.096428	-0.237541
53	8	0	1.994271	-1.283267	0.795041
54	1	0	0.048346	2.878389	1.998168
55	1	0	0.145249	-2.950207	-1.733298
56	1	0	5.105209	2.238458	-1.379365

TS-1st-*cis*-*syn*



B3LYP/6-31G(d); E(B3LYP) = -1834.532908 hartree

Zero-point Energy Correction = 0.436561 hartree

Thermal Correction to Energy = 0.463636 hartree

Thermal correction to Enthalpy = 0.464580 hartree

Thermal correction to Gibbs Free Energy= 0.377642 hartree

Sum of electronic and Zero-point Energies = -1834.096348 hartree

Sum of electronic and thermal Energies = -1834.069273 hartree

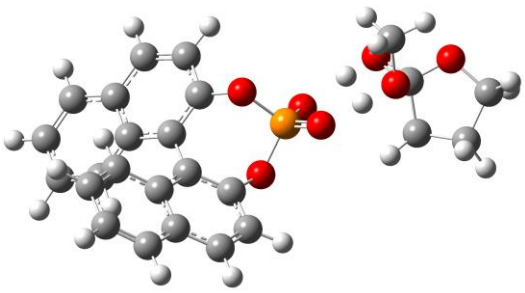
Sum of electronic and thermal Enthalpies = -1834.068329 hartree

Sum of electronic and thermal Free Energies= -1834.155267 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.476292	-1.011652	0.979160
2	6	0	-4.938859	2.254119	-1.418093
3	6	0	-3.986865	1.326915	-1.055835
4	6	0	-2.877882	1.687574	-0.240468
5	6	0	-2.758962	3.061370	0.158407
6	6	0	-3.767715	3.987972	-0.218668
7	6	0	-4.840087	3.597188	-0.986164
8	1	0	-5.770925	1.950961	-2.047949
9	1	0	-4.072810	0.305208	-1.406626
10	6	0	-1.862656	0.745437	0.154251
11	6	0	-1.620087	3.477918	0.897259
12	1	0	-3.665979	5.021946	0.102908
13	1	0	-5.601424	4.317276	-1.273235
14	6	0	-0.617234	2.590754	1.195472
15	6	0	-0.742930	1.240249	0.806546
16	1	0	-1.540554	4.519079	1.199580
17	6	0	-1.947247	-0.709692	-0.156509
18	6	0	-3.051943	-1.534200	0.260699
19	6	0	-0.902415	-1.325194	-0.829492
20	6	0	-4.098058	-1.053359	1.096795
21	6	0	-3.091721	-2.913414	-0.135189
22	6	0	-0.932734	-2.681691	-1.216192
23	6	0	-5.137277	-1.871002	1.482587
24	1	0	-4.065400	-0.027711	1.445026
25	6	0	-4.187103	-3.724222	0.266368
26	6	0	-2.020399	-3.453398	-0.894817
27	6	0	-5.194017	-3.217747	1.054580
28	1	0	-5.918142	-1.478058	2.128187
29	1	0	-4.204964	-4.763796	-0.052686
30	1	0	-2.060806	-4.497754	-1.193731
31	1	0	-6.022701	-3.850296	1.360752
32	8	0	0.298338	0.384818	1.150685
33	15	0	1.288508	-0.169619	-0.027496
34	8	0	0.220519	-0.588602	-1.193370
35	8	0	2.119529	0.966626	-0.614190
36	8	0	2.040563	-1.357072	0.518842
37	1	0	-0.084827	-3.080406	-1.762504
38	1	0	0.279023	2.891723	1.727084
39	6	0	5.265329	-0.450861	0.294488
40	8	0	4.384190	-0.628046	1.265993
41	8	0	5.652648	-1.490228	-0.466044
42	6	0	4.704955	-2.532126	-0.754381
43	1	0	5.267623	-3.278140	-1.316078
44	1	0	4.310352	-2.970582	0.165364
45	1	0	3.880338	-2.146827	-1.358645
46	8	0	4.519396	0.637180	-0.848113
47	1	0	3.412816	0.735966	-0.726700
48	6	0	5.901668	1.881127	0.632976
49	1	0	5.230081	2.061189	1.478524
50	1	0	6.706007	2.622147	0.666883
51	6	0	6.427873	0.444130	0.685230
52	1	0	7.241188	0.288956	-0.029753
53	1	0	6.771683	0.153265	1.681364
54	6	0	5.125747	1.937054	-0.685004
55	1	0	4.335164	2.692364	-0.695780
56	1	0	5.792595	2.102605	-1.538227

TS-2nd-CO-O-*anti*



B3LYP/6-31G(d); E(B3LYP) = -1834.534054 hartree

Zero-point Energy Correction = 0.437237 hartree

Thermal Correction to Energy = 0.464550 hartree

Thermal correction to Enthalpy = 0.465494 hartree

Thermal correction to Gibbs Free Energy= 0.377908 hartree

Sum of electronic and Zero-point Energies = -1834.096817 hartree

Sum of electronic and thermal Energies = -1834.069504 hartree

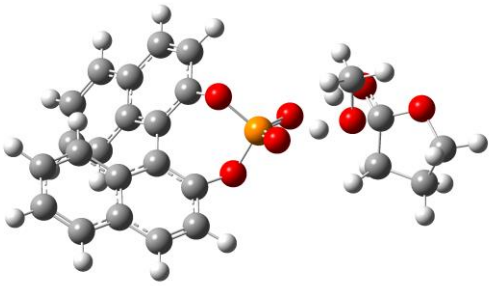
Sum of electronic and thermal Enthalpies = -1834.068560 hartree

Sum of electronic and thermal Free Energies= -1834.156146 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.040109	-0.563826	-0.071115
2	8	0	-6.344523	-0.653852	0.272648
3	8	0	-4.448190	0.680937	0.967404
4	6	0	-7.142746	0.265124	-0.517926
5	6	0	-6.157706	1.048423	-1.405034
6	6	0	-4.923161	0.137187	-1.417745
7	1	0	-7.842065	-0.345542	-1.097988
8	1	0	-5.911369	2.010319	-0.948723
9	1	0	-6.563225	1.233177	-2.403144
10	1	0	-3.974824	0.659515	-1.541599
11	1	0	-4.990998	-0.640062	-2.187360
12	8	0	-4.370185	-1.654577	0.227059
13	1	0	-3.413585	-1.591074	-0.139118
14	6	0	-4.565056	0.351099	2.363810
15	1	0	-5.624520	0.332072	2.622816
16	1	0	-4.050486	1.132016	2.927783
17	1	0	-4.113780	-0.623857	2.569379
18	1	0	-3.384093	0.839558	0.738443
19	6	0	4.998076	2.207437	1.422407
20	6	0	4.037444	1.293752	1.048812
21	6	0	2.948969	1.667340	0.211828
22	6	0	2.859613	3.040491	-0.196918
23	6	0	3.876605	3.952849	0.192683
24	6	0	4.928864	3.549332	0.981132
25	1	0	5.814009	1.894484	2.068386
26	1	0	4.100443	0.272902	1.406821
27	6	0	1.925723	0.739120	-0.195000
28	6	0	1.740616	3.470921	-0.957741
29	1	0	3.797437	4.986423	-0.136487
30	1	0	5.696769	4.258683	1.277344
31	6	0	0.729396	2.597884	-1.269039
32	6	0	0.826465	1.247503	-0.871401
33	1	0	1.682500	4.511661	-1.266317
34	6	0	1.979332	-0.714184	0.131045
35	6	0	3.075511	-1.563048	-0.257935
36	6	0	0.911417	-1.302130	0.792589
37	6	0	4.145774	-1.110451	-1.079150
38	6	0	3.081567	-2.938700	0.152169
39	6	0	0.908213	-2.655280	1.192047
40	6	0	5.176349	-1.951243	-1.437341
41	1	0	4.138800	-0.087859	-1.437852
42	6	0	4.168551	-3.773910	-0.221221
43	6	0	1.986379	-3.450630	0.897147
44	6	0	5.199420	-3.294460	-0.995278
45	1	0	5.976408	-1.579556	-2.071964
46	1	0	4.160733	-4.810419	0.108059
47	1	0	2.000687	-4.492922	1.205479
48	1	0	6.021396	-3.945646	-1.279721
49	8	0	-0.221795	0.407755	-1.232515
50	15	0	-1.242897	-0.127581	-0.072809
51	8	0	-0.202389	-0.538341	1.126101
52	8	0	-2.071863	1.022594	0.486952
53	8	0	-1.979652	-1.311875	-0.642110
54	1	0	0.042786	-3.033529	1.725372
55	1	0	-0.152742	2.910803	-1.817102
56	1	0	-7.711089	0.897843	0.168386

TS-2nd-CO-O-*syn*



B3LYP/6-31G(d); E(B3LYP) = -1834.533221 hartree

Zero-point Energy Correction = 0.437501 hartree

Thermal Correction to Energy = 0.464799 hartree

Thermal correction to Enthalpy = 0.465743 hartree

Thermal correction to Gibbs Free Energy= 0.377925 hartree

Sum of electronic and Zero-point Energies = -1834.095720 hartree

Sum of electronic and thermal Energies = -1834.068422 hartree

Sum of electronic and thermal Enthalpies = -1834.067478 hartree

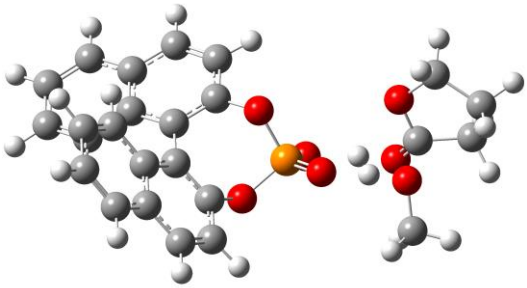
Sum of electronic and thermal Free Energies= -1834.155296 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.930900	3.574339	0.878472
2	6	0	5.025793	2.235137	1.323152
3	6	0	4.058429	1.313030	0.989767
4	6	0	2.937137	1.674987	0.191873
5	6	0	2.823014	3.045532	-0.219426
6	6	0	3.847300	3.966756	0.127781
7	6	0	1.906330	0.737778	-0.173034
8	6	0	0.779032	1.235141	-0.810534
9	6	0	0.657914	2.583113	-1.210018
10	6	0	1.673634	3.464669	-0.940154
11	6	0	1.982778	-0.713885	0.155538
12	6	0	3.070171	-1.555882	-0.271172
13	6	0	3.101835	-2.930143	0.142336
14	6	0	2.038968	-3.447723	0.929046
15	6	0	0.966378	-2.659490	1.261077
16	6	0	0.944332	-1.307696	0.857522
17	6	0	4.105678	-1.097967	-1.132967
18	6	0	5.128346	-1.932324	-1.527115
19	6	0	5.177945	-3.273950	-1.082410
20	6	0	4.180319	-3.758553	-0.268989
21	8	0	-0.274949	0.386199	-1.129588
22	8	0	-0.162262	-0.551631	1.229634
23	15	0	-1.249647	-0.151853	0.070125
24	8	0	-1.991497	-1.346604	-0.473346
25	8	0	-2.065883	0.991721	0.657461
26	1	0	5.704266	4.290353	1.142732
27	1	0	5.867258	1.931009	1.939938
28	1	0	4.142018	0.294420	1.349970
29	1	0	3.748630	4.998125	-0.203037
30	1	0	1.596737	4.503544	-1.250924
31	1	0	2.072704	-4.488785	1.240016
32	1	0	4.077838	-0.076583	-1.494045
33	1	0	5.901431	-1.556755	-2.192171
34	1	0	5.993596	-3.919931	-1.395504
35	1	0	4.192506	-4.794061	0.063300
36	1	0	-3.407783	0.852311	0.847921
37	1	0	0.124156	-3.042216	1.827323
38	1	0	-0.245941	2.887432	-1.726667
39	6	0	-5.018178	-0.515757	-0.070726
40	8	0	-6.348696	-0.551332	0.167647
41	8	0	-4.479673	0.725554	1.014311

42	1	0	-3.437367	-1.600073	-0.013384
43	6	0	-6.155733	0.551021	-1.904014
44	6	0	-4.741849	0.156480	-1.425710
45	1	0	-6.535017	-0.179241	-2.625384
46	1	0	-6.189610	1.538679	-2.371043
47	1	0	-4.243967	-0.557990	-2.084223
48	1	0	-4.082110	1.016954	-1.307275
49	8	0	-4.415490	-1.620989	0.300836
50	6	0	-4.684382	0.388622	2.399238
51	1	0	-4.179427	1.148935	2.999051
52	1	0	-5.756909	0.399985	2.597553
53	1	0	-4.274835	-0.601320	2.619191
54	6	0	-6.979400	0.490957	-0.611976
55	1	0	-8.020689	0.193984	-0.746505
56	1	0	-6.935337	1.430511	-0.049696

TS-2nd-CO-C-*anti*



B3LYP/6-31G(d); E(B3LYP) = -1834.531644 hartree

Zero-point Energy Correction = 0.436530 hartree

Thermal Correction to Energy = 0.463764 hartree

Thermal correction to Enthalpy = 0.464708 hartree

Thermal correction to Gibbs Free Energy= 0.377466 hartree

Sum of electronic and Zero-point Energies = -1834.095115 hartree

Sum of electronic and thermal Energies = -1834.067880 hartree

Sum of electronic and thermal Enthalpies = -1834.066936 hartree

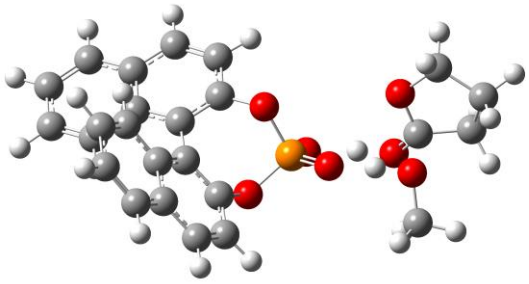
Sum of electronic and thermal Free Energies= -1834.154179 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.976709	0.522597	-0.134649
2	8	0	4.360959	0.843116	1.025314
3	8	0	4.530045	-1.187800	-0.234388
4	6	0	5.222500	0.545382	2.156118
5	6	0	6.532284	-0.018964	1.567854
6	6	0	6.470203	0.434944	0.102514
7	1	0	5.366596	1.487970	2.692716
8	1	0	6.534925	-1.109901	1.624343
9	1	0	7.413104	0.357278	2.094227
10	1	0	6.972772	-0.229768	-0.601470
11	1	0	6.872883	1.445203	-0.035909
12	8	0	4.528916	1.082569	-1.222141
13	1	0	3.484610	1.154427	-1.205349
14	6	0	4.759217	-1.815139	-1.505010
15	1	0	4.101564	-2.685199	-1.573217
16	1	0	5.801782	-2.140446	-1.557836
17	1	0	4.540200	-1.120912	-2.322284
18	1	0	3.441574	-1.192135	-0.064376
19	6	0	-4.840566	-1.968238	1.843625
20	6	0	-3.888979	-1.122694	1.317463
21	6	0	-2.932427	-1.585240	0.370797
22	6	0	-2.963845	-2.974844	0.012306
23	6	0	-3.968600	-3.815673	0.561813
24	6	0	-4.893442	-3.327070	1.454989
25	1	0	-5.554134	-1.587773	2.569671
26	1	0	-3.856923	-0.087422	1.636012
27	6	0	-1.921925	-0.730113	-0.195805
28	6	0	-1.972402	-3.492624	-0.862384
29	1	0	-3.982720	-4.863173	0.269380
30	1	0	-5.653156	-3.982114	1.872661
31	6	0	-0.966097	-2.687668	-1.332651
32	6	0	-0.942956	-1.320754	-0.981962
33	1	0	-2.006025	-4.545183	-1.132234
34	6	0	-1.856907	0.734038	0.074177
35	6	0	-2.946318	1.631243	-0.211417
36	6	0	-0.683209	1.280796	0.572056
37	6	0	-4.136063	1.212423	-0.870191
38	6	0	-2.825733	3.019125	0.134771
39	6	0	-0.556259	2.645806	0.906687
40	6	0	-5.157806	2.098296	-1.131943
41	1	0	-4.230437	0.178365	-1.180215
42	6	0	-3.905269	3.902387	-0.135317
43	6	0	-1.618093	3.492478	0.712807
44	6	0	-5.051594	3.456066	-0.750648
45	1	0	-6.051825	1.750786	-1.642828
46	1	0	-3.799529	4.948212	0.143980
47	1	0	-1.536365	4.544793	0.973067
48	1	0	-5.867246	4.143532	-0.957473
49	8	0	0.093971	-0.554072	-1.498746
50	15	0	1.283693	-0.052446	-0.489499
51	8	0	0.418321	0.465373	0.802531
52	8	0	2.096117	-1.237070	0.013264
53	8	0	2.002687	1.069913	-1.193205
54	1	0	0.389600	2.990617	1.310286
55	1	0	-0.176856	-3.067122	-1.972660
56	1	0	4.697542	-0.158954	2.804944

TS-2nd-CO-C-*syn**

*Originally, an initial structure corresponding to **CO-C-*syn*** TS was generated, however the optimized structure was similar to that of **CO-C-*anti*** TS and hence the TS energy was almost the same as that of **CO-C-*anti***.



B3LYP/6-31G(d); E(B3LYP) = -1834.531644 hartree

Zero-point Energy Correction = 0.436531 hartree

Thermal Correction to Energy = 0.463765 hartree

Thermal correction to Enthalpy = 0.464710 hartree

Thermal correction to Gibbs Free Energy= 0.377466 hartree

Sum of electronic and Zero-point Energies = -1834.095113 hartree

Sum of electronic and thermal Energies = -1834.067879 hartree

Sum of electronic and thermal Enthalpies = -1834.066935 hartree

Sum of electronic and thermal Free Energies= -1834.154178 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.051611	3.456078	-0.750634
2	6	0	-5.157833	2.098307	-1.131922
3	6	0	-4.136091	1.212431	-0.870179
4	6	0	-2.946336	1.631248	-0.211423
5	6	0	-2.825740	3.019131	0.134758

6	6	0	-3.905276	3.902397	-0.135319
7	6	0	-1.856925	0.734040	0.074161
8	6	0	-0.683218	1.280795	0.572021
9	6	0	-0.556257	2.645806	0.906645
10	6	0	-1.618091	3.492482	0.712776
11	6	0	-1.921953	-0.730112	-0.195810
12	6	0	-2.932449	-1.585232	0.370813
13	6	0	-2.963876	-2.974838	0.012335
14	6	0	-1.972447	-3.492628	-0.862365
15	6	0	-0.966148	-2.687679	-1.332654
16	6	0	-0.942998	-1.320762	-0.981978
17	6	0	-3.888986	-1.122674	1.317488
18	6	0	-4.840569	-1.968210	1.843671
19	6	0	-4.893454	-3.327046	1.455048
20	6	0	-3.968626	-3.815659	0.561863
21	8	0	0.418310	0.465366	0.802481
22	8	0	0.093924	-0.554089	-1.498785
23	15	0	1.283664	-0.052441	-0.489568
24	8	0	2.096053	-1.237109	0.013183
25	8	0	2.002691	1.069886	-1.193254
26	1	0	-5.867263	4.143546	-0.957451
27	1	0	-6.051861	1.750799	-1.642795
28	1	0	-4.230473	0.178371	-1.180199
29	1	0	-3.799529	4.948222	0.143971
30	1	0	-1.536354	4.544798	0.973030
31	1	0	-2.006077	-4.545190	-1.132204
32	1	0	-3.856923	-0.087400	1.636028
33	1	0	-5.554127	-1.587737	2.569723
34	1	0	-5.653164	-3.982084	1.872736
35	1	0	-3.982753	-4.863162	0.269440
36	1	0	3.441490	-1.192013	-0.064243
37	1	0	-0.176917	-3.067140	-1.972671
38	1	0	0.389609	2.990615	1.310228
39	6	0	4.976749	0.522361	-0.134729
40	8	0	4.361021	0.843232	1.025187
41	8	0	4.529996	-1.187682	-0.234174
42	1	0	3.484841	1.154269	-1.205586
43	6	0	6.532307	-0.018815	1.567913
44	6	0	6.470255	0.434790	0.102478
45	1	0	7.413179	0.357434	2.094193
46	1	0	6.534818	-1.109742	1.624645
47	1	0	6.872910	1.445031	-0.036135
48	1	0	6.972865	-0.230049	-0.601359
49	8	0	4.529064	1.082301	-1.222340
50	6	0	4.759309	-1.815366	-1.504622
51	1	0	4.101491	-2.685305	-1.572720
52	1	0	4.540561	-1.121280	-2.322082
53	1	0	5.801821	-2.140881	-1.557163
54	6	0	5.222596	0.545820	2.156043
55	1	0	5.366801	1.488571	2.692327
56	1	0	4.697631	-0.158264	2.805139

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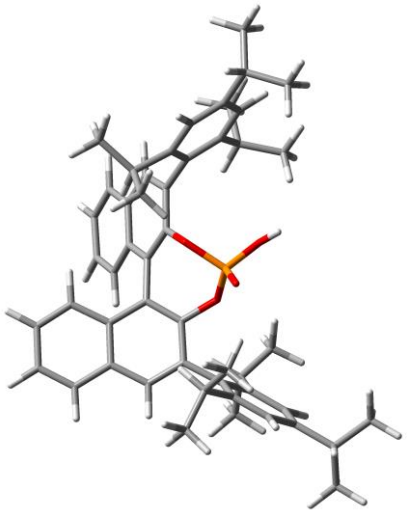
9. DFT Calculation of BINOL- and SPINOL-derived CPA-Catalyzed Reactions

Optimized structure of BINOL-derived CPA (*R*)-1aa (TRIP)



B3LYP/6-31G(d); E(B3LYP) = -2582.067793 hartree

Zero-point Energy Correction = 0.954313 hartree

Thermal Correction to Energy = 1.009099 hartree

Thermal correction to Enthalpy = 1.010043 hartree

Thermal correction to Gibbs Free Energy= 0.863516 hartree

Sum of electronic and Zero-point Energies = -2581.113480 hartree

Sum of electronic and thermal Energies = -2581.058694 hartree

Sum of electronic and thermal Enthalpies = -2581.057750 hartree

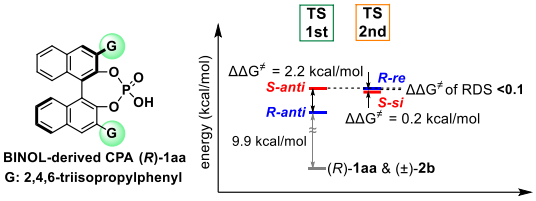
Sum of electronic and thermal Free Energies= -2581.204277 hartree

The number of Imaginary frequencies = 0

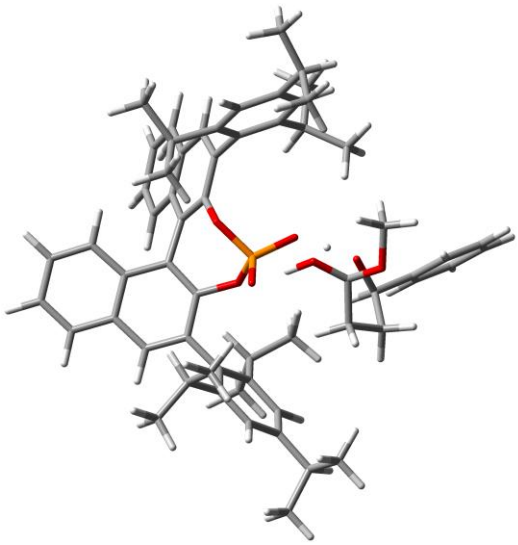
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.929521	-2.862296	-0.710095
2	6	0	-0.992836	5.227801	2.093168
3	6	0	-0.450578	4.175811	1.388406
4	6	0	-1.252494	3.074000	0.981220
5	6	0	-2.634190	3.070523	1.359274
6	6	0	-3.166811	4.181072	2.068456
7	6	0	-2.367486	5.241394	2.426403
8	1	0	-0.356209	6.052796	2.400935
9	1	0	0.606644	4.177737	1.150712
10	6	0	-0.731116	1.951483	0.245865
11	6	0	-3.444094	1.951223	1.040049
12	1	0	-4.220336	4.166811	2.336921
13	1	0	-2.783811	6.081117	2.975858
14	6	0	-2.933976	0.821497	0.434520
15	6	0	-1.558175	0.852417	0.072231
16	1	0	-4.496645	1.975781	1.308852
17	6	0	0.656656	1.947420	-0.303968
18	6	0	1.123801	2.988495	-1.182069
19	6	0	1.530534	0.915158	0.000427
20	6	0	0.273398	3.995784	-1.716092
21	6	0	2.502715	2.997961	-1.569590
22	6	0	2.900791	0.888593	-0.388077
23	6	0	0.767217	4.975750	-2.548796
24	1	0	-0.782092	3.982100	-1.471702
25	6	0	2.984777	4.035200	-2.413268
26	6	0	3.359381	1.957012	-1.130656
27	6	0	2.139108	5.008441	-2.891718
28	1	0	0.094038	5.728288	-2.950205
29	1	0	4.037207	4.033298	-2.686600
30	1	0	4.406526	1.989843	-1.418722
31	1	0	2.516877	5.791978	-3.542647
32	8	0	-1.042124	-0.284803	-0.563573
33	15	0	-0.003998	-1.204411	0.268171
34	8	0	1.084677	-0.132832	0.808203
35	8	0	-0.485189	-2.067920	1.360203
36	6	0	3.808039	-0.245688	-0.010045
37	6	0	4.204391	-0.419830	1.337099
38	6	0	4.298757	-1.127623	-1.007954
39	6	0	5.068466	-1.473031	1.657256
40	6	0	5.163089	-2.160286	-0.627965
41	6	0	5.559520	-2.357607	0.697161
42	6	0	-3.802988	-0.370170	0.155645
43	6	0	-4.234660	-1.199406	1.217437
44	6	0	-4.226858	-0.638621	-1.168778
45	6	0	-5.088850	-2.270410	0.925380
46	6	0	-5.074415	-1.725131	-1.400876
47	6	0	-5.520690	-2.555904	-0.369313
48	8	0	0.651744	-1.972769	-0.985986
49	1	0	-5.426295	-2.909095	1.738212
50	1	0	-5.400013	-1.923833	-2.419089
51	1	0	5.541087	-2.830704	-1.395581
52	1	0	5.376397	-1.604418	2.692137
53	6	0	-3.821299	0.236900	-2.354595
54	6	0	-5.041135	0.956257	-2.963796
55	6	0	-3.053653	-0.560164	-3.426348
56	1	0	-3.145842	1.016500	-1.990278
57	1	0	-5.561072	1.560811	-2.212119
58	1	0	-4.728092	1.620597	-3.778485
59	1	0	-5.764563	0.242531	-3.375192
60	1	0	-2.166456	-1.036863	-2.998595
61	1	0	-3.679075	-1.342430	-3.872733
62	1	0	-2.728628	0.104905	-4.235755
63	6	0	-3.824218	-0.968361	2.672641
64	6	0	-3.230962	-2.229210	3.329608
65	6	0	-5.007275	-0.427854	3.501540
66	1	0	-3.038599	-0.207162	2.686271
67	1	0	-2.369392	-2.592758	2.764377
68	1	0	-2.897948	-1.994116	4.347998
69	1	0	-3.969228	-3.036370	3.406867
70	1	0	-5.406786	0.502113	3.081130
71	1	0	-5.828938	-1.153496	3.536985
72	1	0	-4.693681	-0.226516	4.533042
73	6	0	3.951885	-0.984204	-2.492503
74	6	0	3.419330	-2.287603	-3.117054
75	6	0	5.164844	-0.468562	-3.294362
76	1	0	3.154974	-0.241831	-2.587192
77	1	0	2.526820	-2.639393	-2.592496
78	1	0	3.143921	-2.115416	-4.164250
79	1	0	4.166425	-3.089445	-3.103069
80	1	0	5.535199	0.484141	-2.900392
81	1	0	5.995241	-1.183911	-3.258201
82	1	0	4.896010	-0.319013	-4.347062
83	6	0	6.499178	-3.490528	1.089123
84	6	0	7.880166	-3.349068	0.421385
85	6	0	5.884203	-4.872727	0.798957
86	1	0	6.651130	-3.420845	2.174940
87	1	0	8.336482	-2.381324	0.656575
88	1	0	8.558453	-4.139429	0.764678
89	1	0	7.805231	-3.426317	-0.669872
90	1	0	4.920162	-4.991381	1.305611
91	1	0	5.717924	-5.016983	-0.275323
92	1	0	6.550976	-5.672719	1.142401
93	6	0	3.771721	0.529673	2.454074
94	6	0	4.971200	1.344842	2.978859
95	6	0	3.054157	-0.203407	3.602946
96	1	0	3.060554	1.248460	2.037930
97	1	0	5.453644	1.906893	2.171196

98	1	0	4.643482	2.059951	3.743074
99	1	0	5.729412	0.695571	3.432399
100	1	0	2.185349	-0.757116	3.235292
101	1	0	3.720434	-0.910163	4.111737
102	1	0	2.706941	0.517914	4.352456
103	6	0	-6.445038	-3.736012	-0.639248
104	6	0	-5.776235	-4.792753	-1.538737
105	6	0	-7.796732	-3.286952	-1.225749
106	1	0	-6.649708	-4.212146	0.329500
107	1	0	-4.833255	-5.141767	-1.104195
108	1	0	-6.434024	-5.660209	-1.672045
109	1	0	-5.555184	-4.386484	-2.532986
110	1	0	-8.292045	-2.562652	-0.569803
111	1	0	-7.668448	-2.814960	-2.207166
112	1	0	-8.466925	-4.145413	-1.355018

DFT calculation of real system using BINOL-derive CPA (*R*)-1aa



TS-1st-(*R*)-reaction pathway: *R-anti*/(*R*)-1aa (BINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3235.352388 hartree

Zero-point Energy Correction = 1.188487 hartree

Thermal Correction to Energy = 1.256238 hartree

Thermal correction to Enthalpy = 1.257182 hartree

Thermal correction to Gibbs Free Energy= 1.080533 hartree

Sum of electronic and Zero-point Energies = -3234.163901 hartree

Sum of electronic and thermal Energies = -3234.096150 hartree

Sum of electronic and thermal Enthalpies = -3234.095206 hartree

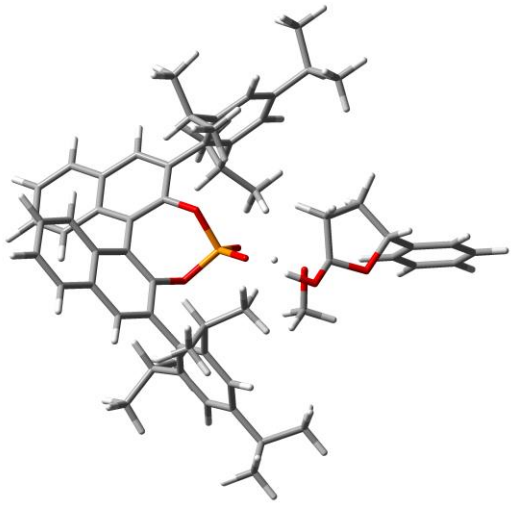
Sum of electronic and thermal Free Energies= -3234.271855 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.172926	3.757161	-1.671234
2	8	0	0.179376	3.450957	-0.033322
3	1	0	0.016874	1.901580	-2.222585
4	6	0	-0.985145	3.791751	0.781285
5	6	0	-1.978608	4.446975	-0.201154
6	6	0	-1.688173	3.786555	-1.548725
7	1	0	-1.398827	2.844129	1.143150
8	1	0	-1.800561	5.524572	-0.259471
9	1	0	-3.008470	4.292126	0.132142
10	1	0	-2.106242	4.337639	-2.395718
11	1	0	-2.058207	2.757328	-1.580107
12	8	0	0.439446	2.813780	-2.370553
13	8	0	0.326395	4.993787	-1.877497
14	6	0	1.748292	5.085845	-2.083187
15	1	0	1.960485	6.154153	-2.139757
16	1	0	2.036564	4.590877	-3.012774
17	1	0	2.282289	4.637615	-1.240704
18	1	0	0.434890	2.362372	0.160912
19	6	0	1.043707	-5.194724	3.774847
20	6	0	0.514234	-4.494273	2.713325
21	6	0	1.319053	-3.613610	1.938904
22	6	0	2.690135	-3.447159	2.318226
23	6	0	3.210543	-4.199940	3.405425
24	6	0	2.408923	-5.059828	4.119528
25	1	0	0.404282	-5.853794	4.355942
26	1	0	-0.535980	-4.602571	2.468878
27	6	0	0.810920	-2.860333	0.822668
28	6	0	3.500475	-2.518922	1.616056
29	1	0	4.256671	-4.068852	3.671871
30	1	0	2.816090	-5.624076	4.954054
31	6	0	2.997962	-1.707510	0.620344
32	6	0	1.630400	-1.890752	0.263042
33	1	0	4.547278	-2.429110	1.893077
34	6	0	-0.560473	-3.091794	0.279290
35	6	0	-0.987315	-4.395095	-0.158360
36	6	0	-1.454401	-2.037467	0.157694
37	6	0	-0.107900	-5.508966	-0.257737
38	6	0	-2.352524	-4.581395	-0.549958
39	6	0	-2.814873	-2.197096	-0.235040
40	6	0	-0.561172	-6.738900	-0.681173
41	1	0	0.938478	-5.380843	-0.007341
42	6	0	-2.792939	-5.867898	-0.963194
43	6	0	-3.236978	-3.473418	-0.543861
44	6	0	-1.920039	-6.928836	-1.025015
45	1	0	0.134425	-7.570334	-0.756728
46	1	0	-3.835595	-5.991836	-1.246140
47	1	0	-4.275147	-3.634877	-0.822097
48	1	0	-2.265980	-7.906122	-1.350280
49	8	0	1.127715	-1.099056	-0.764771
50	15	0	0.021618	0.051420	-0.425896
51	8	0	-1.041354	-0.759022	0.515527
52	8	0	0.602030	1.123404	0.494731
53	6	0	-3.764191	-1.035945	-0.299328
54	6	0	-4.247007	-0.447810	0.892792
55	6	0	-4.220506	-0.560434	-1.554318
56	6	0	-5.175469	0.596294	0.805000
57	6	0	-5.154829	0.481168	-1.581313
58	6	0	-5.650453	1.073895	-0.417066
59	6	0	3.869815	-0.698979	-0.070476
60	6	0	4.305926	0.457983	0.618695
61	6	0	4.294121	-0.927122	-1.402662
62	6	0	5.160777	1.349989	-0.041492
63	6	0	5.139794	0.002698	-2.013953
64	6	0	5.587929	1.149527	-1.353688
65	8	0	-0.568857	0.510780	-1.733138
66	1	0	5.503895	2.237309	0.485704
67	1	0	5.461841	-0.179807	-3.036250
68	1	0	-5.511259	0.833055	-2.546323
69	1	0	-5.556045	1.042248	1.721818
70	6	0	-0.584995	4.650853	1.957557
71	6	0	-0.946806	4.274805	3.254549
72	6	0	0.131960	5.840104	1.766784
73	6	0	-0.609564	5.077906	4.346483
74	1	0	-1.491071	3.346442	3.412477

75	6	0	0.476209	6.637771	2.855858
76	1	0	0.425038	6.130535	0.761579
77	6	0	0.103255	6.260078	4.149184
78	1	0	-0.897231	4.773818	5.349280
79	1	0	1.036814	7.555340	2.697553
80	1	0	0.371770	6.883680	4.997697
81	6	0	3.892706	-2.173674	-2.191281
82	6	0	5.116211	-3.060631	-2.496819
83	6	0	3.125112	-1.821792	-3.479698
84	1	0	3.219222	-2.770329	-1.569933
85	1	0	5.636874	-3.349340	-1.576740
86	1	0	4.805873	-3.976599	-3.014363
87	1	0	5.838210	-2.543448	-3.139936
88	1	0	2.237235	-1.223851	-3.254408
89	1	0	3.750645	-1.256253	-4.180906
90	1	0	2.801030	-2.736603	-3.990703
91	6	0	3.899393	0.768537	2.060262
92	6	0	3.364920	2.202311	2.235882
93	6	0	5.068435	0.514164	3.034138
94	1	0	3.084748	0.092528	2.334045
95	1	0	2.535725	2.399222	1.552784
96	1	0	2.999917	2.340854	3.260626
97	1	0	4.143499	2.955260	2.064691
98	1	0	5.433702	-0.516765	2.972116
99	1	0	5.914231	1.177412	2.815151
100	1	0	4.755453	0.700719	4.068804
101	6	0	-3.755728	-1.155310	-2.885395
102	6	0	-3.184550	-0.091666	-3.841547
103	6	0	-4.891674	-1.946723	-3.564892
104	1	0	-2.944103	-1.857406	-2.677195
105	1	0	-2.337199	0.420699	-3.379578
106	1	0	-2.833169	-0.569779	-4.764087
107	1	0	-3.938590	0.652046	-4.126076
108	1	0	-5.272646	-2.744945	-2.917879
109	1	0	-5.736780	-1.293517	-3.814458
110	1	0	-4.536873	-2.405405	-4.495739
111	6	0	-6.693842	2.183119	-0.467737
112	6	0	-8.024452	1.683822	-1.062857
113	6	0	-6.189368	3.426640	-1.222996
114	1	0	-6.892039	2.486876	0.569511
115	1	0	-8.409015	0.823940	-0.503832
116	1	0	-8.782708	2.475825	-1.037457
117	1	0	-7.899635	1.373989	-2.107130
118	1	0	-5.266970	3.814817	-0.776132
119	1	0	-5.979774	3.197906	-2.274586
120	1	0	-6.939922	4.225860	-1.199752
121	6	0	-3.830032	-0.939001	2.278823
122	6	0	-5.024638	-1.544980	3.042018
123	6	0	-3.146206	0.166618	3.105440
124	1	0	-3.097669	-1.740800	2.151538
125	1	0	-5.483632	-2.361695	2.473765
126	1	0	-4.697882	-1.945241	4.009435
127	1	0	-5.801927	-0.796555	3.236644
128	1	0	-2.259431	0.543938	2.586337
129	1	0	-3.825156	1.007159	3.294437
130	1	0	-2.827923	-0.226718	4.078474
131	6	0	6.509891	2.153358	-2.034027
132	6	0	5.841596	2.806164	-3.258877
133	6	0	7.864731	1.526721	-2.413954
134	1	0	6.710293	2.951033	-1.305238
135	1	0	4.891794	3.279038	-2.985108
136	1	0	6.494167	3.572451	-3.694944
137	1	0	5.629766	2.065428	-4.038889
138	1	0	8.361893	1.098383	-1.536752
139	1	0	7.739831	0.724374	-3.150825
140	1	0	8.531698	2.279579	-2.851475

TS-2nd-(*R*)-reaction pathway: *R-re*/(*R*)-1aa (BINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3235.348681 hartree

Zero-point Energy Correction = 1.189109 hartree

Thermal Correction to Energy = 1.257015 hartree

Thermal correction to Enthalpy = 1.257959 hartree

Thermal correction to Gibbs Free Energy= 1.080296 hartree

Sum of electronic and Zero-point Energies = -3234.159572 hartree

Sum of electronic and thermal Energies = -3234.091666 hartree

Sum of electronic and thermal Enthalpies = -3234.090722 hartree

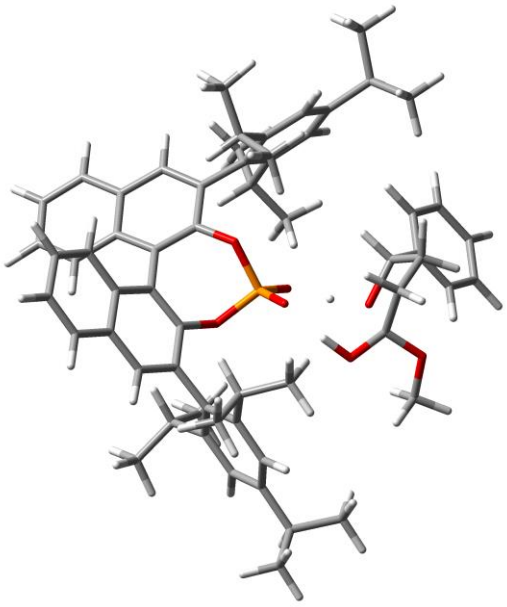
Sum of electronic and thermal Free Energies= -3234.268385 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.802911	2.351559	-0.770639
2	8	0	3.807279	3.252682	-0.697108
3	8	0	2.502296	1.958649	0.869821
4	1	0	0.970759	2.175654	-1.330048
5	6	0	5.113297	2.602602	-0.866585
6	6	0	4.808611	1.089939	-0.846563
7	6	0	3.345204	1.026686	-1.293160
8	1	0	5.456902	2.906555	-1.861907
9	1	0	4.918584	0.689494	0.164219
10	1	0	5.486748	0.539530	-1.504005
11	1	0	2.799273	0.159491	-0.920826
12	1	0	3.246795	1.053353	-2.384290
13	8	0	1.688220	2.889005	-1.230392
14	6	0	2.002756	3.076573	1.633395
15	1	0	2.785385	3.835127	1.669831
16	1	0	1.780831	2.708446	2.637276
17	1	0	1.101307	3.487876	1.171509
18	6	0	6.092211	3.102121	0.168065
19	6	0	5.864794	2.902095	1.537478
20	6	0	7.256153	3.763409	-0.235883
21	6	0	6.785693	3.356878	2.478982
22	1	0	4.962821	2.391459	1.862600
23	6	0	8.184841	4.211793	0.705837
24	1	0	7.437662	3.930843	-1.295230
25	6	0	7.949958	4.010819	2.065573
26	1	0	6.597195	3.199001	3.537543
27	1	0	9.085651	4.721992	0.375865
28	1	0	8.668192	4.362142	2.801429
29	1	0	1.746425	1.151993	0.893071
30	6	0	-4.202326	-4.322504	3.167586
31	6	0	-3.860637	-3.360961	2.242150
32	6	0	-2.596381	-3.383850	1.590453
33	6	0	-1.672565	-4.416331	1.953838

34	6	0	-2.063757	-5.405481	2.896218
35	6	0	-3.303338	-5.365676	3.490891
36	1	0	-5.171015	-4.275601	3.657820
37	1	0	-4.558417	-2.563881	2.013955
38	6	0	-2.195324	-2.401067	0.618128
39	6	0	-0.375805	-4.424582	1.380178
40	1	0	-1.353052	-6.188613	3.149630
41	1	0	-3.588690	-6.122451	4.216465
42	6	0	0.061396	-3.424732	0.536683
43	6	0	-0.873806	-2.404895	0.194334
44	1	0	0.300315	-5.236453	1.634249
45	6	0	-3.156110	-1.392125	0.081233
46	6	0	-4.395621	-1.784686	-0.536980
47	6	0	-2.857882	-0.038414	0.143684
48	6	0	-4.728142	-3.137644	-0.824871
49	6	0	-5.331168	-0.768549	-0.917078
50	6	0	-3.768091	0.990021	-0.237025
51	6	0	-5.928582	-3.466494	-1.415248
52	1	0	-4.017250	-3.919516	-0.585157
53	6	0	-6.569107	-1.142651	-1.506515
54	6	0	-4.996876	0.595662	-0.723669
55	6	0	-6.868119	-2.463085	-1.748648
56	1	0	-6.152968	-4.507493	-1.631812
57	1	0	-7.271347	-0.357798	-1.777528
58	1	0	-5.724799	1.354059	-0.999859
59	1	0	-7.814566	-2.736510	-2.206988
60	8	0	-0.442277	-1.415152	-0.681059
61	15	0	-0.248653	0.113069	-0.133130
62	8	0	-1.642418	0.357539	0.686731
63	8	0	0.833806	0.178318	0.941300
64	6	0	-3.411716	2.442162	-0.114215
65	6	0	-3.327275	3.047275	1.161247
66	6	0	-3.192428	3.219839	-1.279170
67	6	0	-3.023054	4.410822	1.244314
68	6	0	-2.898143	4.580017	-1.135180
69	6	0	-2.804273	5.198598	0.113700
70	6	0	1.454757	-3.445924	-0.022830
71	6	0	2.566451	-3.185602	0.813884
72	6	0	1.662002	-3.787246	-1.382087
73	6	0	3.854767	-3.287756	0.271765
74	6	0	2.969731	-3.870881	-1.869335
75	6	0	4.083959	-3.630205	-1.061081
76	8	0	-0.084433	0.987816	-1.345649
77	1	0	4.712112	-3.100947	0.914684
78	1	0	3.120220	-4.144244	-2.910999
79	1	0	-2.733569	5.172957	-2.031370
80	1	0	-2.963409	4.879406	2.224667
81	6	0	0.510084	-4.107443	-2.334895
82	6	0	0.551084	-5.580288	-2.788522
83	6	0	0.478600	-3.153012	-3.543761
84	1	0	-0.430233	-3.970051	-1.794605
85	1	0	0.524421	-6.261150	-1.930226
86	1	0	-0.309217	-5.807173	-3.429844
87	1	0	1.459977	-5.800916	-3.360849
88	1	0	0.403516	-2.111718	-3.216943
89	1	0	1.377816	-3.255723	-4.163166
90	1	0	-0.387095	-3.374775	-4.179434
91	6	0	5.503540	-3.759200	-1.599067
92	6	0	5.763520	-2.826015	-2.795771
93	6	0	5.842037	-5.218909	-1.958941
94	1	0	6.183367	-3.454827	-0.791159
95	1	0	5.556643	-1.781626	-2.535548
96	1	0	6.808096	-2.896219	-3.122326
97	1	0	5.130212	-3.086071	-3.651958
98	1	0	5.700662	-5.880853	-1.097738
99	1	0	5.200952	-5.585215	-2.769540
100	1	0	6.883847	-5.306044	-2.290745
101	6	0	2.422445	-2.822551	2.293027
102	6	0	3.222802	-1.565435	2.682037
103	6	0	2.823181	-4.006945	3.196441
104	1	0	1.369670	-2.597140	2.483519
105	1	0	2.931373	-0.711006	2.066680
106	1	0	3.027007	-1.310260	3.730656
107	1	0	4.304191	-1.718082	2.581592
108	1	0	2.227874	-4.900967	2.982242
109	1	0	3.878352	-4.271029	3.054453
110	1	0	2.680295	-3.751076	4.253421
111	6	0	-3.277200	2.642126	-2.693740
112	6	0	-1.994413	2.887162	-3.510325
113	6	0	-4.512716	3.183260	-3.441281
114	1	0	-3.393717	1.558327	-2.611767
115	1	0	-1.129571	2.448121	-3.007243
116	1	0	-2.087911	2.422610	-4.499832
117	1	0	-1.804112	3.955635	-3.666961
118	1	0	-5.440969	2.964558	-2.901015
119	1	0	-4.454989	4.270934	-3.569749
120	1	0	-4.586334	2.732265	-4.438334
121	6	0	-3.597038	2.281054	2.456046
122	6	0	-4.864337	2.805336	3.160558
123	6	0	-2.384954	2.300975	3.406256
124	1	0	-3.787304	1.234720	2.201679
125	1	0	-5.737174	2.746208	2.500640
126	1	0	-5.076899	2.214248	4.059831
127	1	0	-4.750044	3.851459	3.468504
128	1	0	-1.500652	1.882605	2.916367
129	1	0	-2.148500	3.319426	3.737676
130	1	0	-2.593250	1.702666	4.301635
131	6	0	-2.481865	6.681238	0.247680
132	6	0	-3.572066	7.564611	-0.388105
133	6	0	-1.092847	7.022565	-0.323808
134	1	0	-2.460653	6.909925	1.322358
135	1	0	-4.556024	7.350895	0.043586
136	1	0	-3.351718	8.627268	-0.229207
137	1	0	-3.638677	7.396667	-1.469566
138	1	0	-0.309605	6.421269	0.150662
139	1	0	-1.047768	6.831473	-1.402279
140	1	0	-0.856905	8.081515	-0.162552

TS-1st-(*S*)-reaction pathway: *S-anti*/(*R*)-1aa (BINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3235.350722 hartree

Zero-point Energy Correction = 1.188705 hartree

Thermal Correction to Energy = 1.256319 hartree

Thermal correction to Enthalpy = 1.257264 hartree

Thermal correction to Gibbs Free Energy= 1.082333 hartree

Sum of electronic and Zero-point Energies = -3234.162017 hartree

Sum of electronic and thermal Energies = -3234.094403 hartree

Sum of electronic and thermal Enthalpies = -3234.093458 hartree

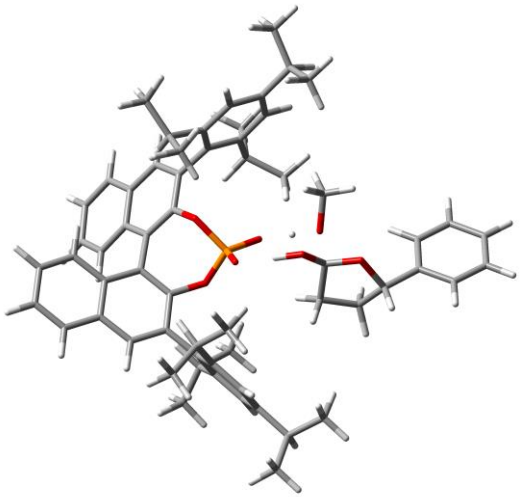
Sum of electronic and thermal Free Energies= -3234.268389 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.408319	-3.913496	1.011597
2	8	0	1.366686	-3.180981	-0.158080
3	6	0	-3.278171	5.679260	1.796112
4	6	0	-2.396064	4.834964	1.158393
5	6	0	-2.794972	3.535496	0.739311
6	6	0	-4.130850	3.115117	1.035936
7	6	0	-5.023033	4.017702	1.675609
8	6	0	-4.610870	5.276392	2.046260
9	1	0	-2.944447	6.663092	2.114799
10	1	0	-1.376386	5.157740	0.983815
11	6	0	-1.912266	2.618370	0.067056
12	6	0	-4.534325	1.797053	0.705600
13	1	0	-6.037462	3.684375	1.881362
14	1	0	-5.298880	5.955336	2.542485
15	6	0	-3.662662	0.867448	0.176396
16	6	0	-2.339771	1.311448	-0.114381
17	1	0	-5.561154	1.503303	0.905165
18	6	0	-0.570431	3.048248	-0.422171
19	6	0	-0.429484	4.178887	-1.302990
20	6	0	0.576390	2.357511	-0.054001
21	6	0	-1.536769	4.836618	-1.907716
22	6	0	0.883967	4.652553	-1.618798
23	6	0	1.893070	2.804480	-0.367727
24	6	0	-1.354880	5.919782	-2.739119
25	1	0	-2.538194	4.468028	-1.720192
26	6	0	1.037461	5.785777	-2.462747
27	6	0	2.010834	3.963643	-1.106668
28	6	0	-0.057015	6.412729	-3.010507
29	1	0	-2.218049	6.396772	-3.195455
30	1	0	2.043424	6.137094	-2.679972
31	1	0	3.002651	4.343547	-1.338155
32	1	0	0.071590	7.273283	-3.661247
33	8	0	-1.458805	0.394423	-0.684193
34	15	0	-0.226409	-0.155794	0.236939
35	8	0	0.470132	1.229223	0.749832
36	8	0	-0.672527	-0.894251	1.472303
37	6	0	3.119987	2.062952	0.072772
38	6	0	3.497521	2.049312	1.438519
39	6	0	3.940979	1.429809	-0.891001
40	6	0	4.683178	1.407928	1.808015
41	6	0	5.124012	0.810544	-0.463072
42	6	0	5.518889	0.786342	0.875283
43	6	0	-4.120852	-0.535598	-0.096420
44	6	0	-4.427925	-1.406163	0.980775
45	6	0	-4.315925	-0.969496	-1.428355
46	6	0	-4.931314	-2.679586	0.694361
47	6	0	-4.820690	-2.255177	-1.653659
48	6	0	-5.140608	-3.126343	-0.612691
49	8	0	0.679439	-0.915908	-0.733926
50	1	0	-5.169583	-3.341605	1.522800
51	1	0	-4.981278	-2.585526	-2.677781
52	1	0	5.766709	0.341095	-1.205176
53	1	0	4.971919	1.412962	2.856369
54	1	0	-0.845473	-2.445160	1.162483
55	6	0	2.736104	-3.068729	0.345032
56	6	0	2.703541	-3.691688	1.763001
57	6	0	1.253035	-3.562139	2.226080
58	1	0	2.949209	-1.997323	0.411866
59	1	0	2.994189	-4.744789	1.717203
60	1	0	3.406457	-3.178182	2.425025
61	1	0	1.004142	-4.239040	3.048038
62	1	0	1.008666	-2.538337	2.524167
63	8	0	-0.813073	-3.415198	0.867734
64	8	0	0.486530	-5.233352	0.726127
65	6	0	-0.349143	-5.707252	-0.345707
66	1	0	-0.091123	-6.760240	-0.465861
67	1	0	-1.404318	-5.600903	-0.086876
68	1	0	-0.133620	-5.157462	-1.266377
69	1	0	0.987526	-2.139249	-0.447890
70	6	0	3.720256	-3.727601	-0.595225
71	6	0	3.520932	-5.038816	-1.048459
72	6	0	4.875060	-3.042562	-0.984753
73	6	0	4.458863	-5.647553	-1.879962
74	1	0	2.628157	-5.576840	-0.744784
75	6	0	5.821387	-3.656191	-1.809393
76	1	0	5.029708	-2.021581	-0.646405
77	6	0	5.613828	-4.958730	-2.261469
78	1	0	4.290677	-6.662632	-2.230313
79	1	0	6.715032	-3.111878	-2.103252
80	1	0	6.345020	-5.436001	-2.908402
81	6	0	6.831011	0.133422	1.293036
82	6	0	6.620915	-1.009610	2.303802
83	6	0	7.830359	1.171779	1.838612
84	1	0	7.275849	-0.305512	0.389012
85	1	0	5.959985	-1.783385	1.897229
86	1	0	7.577581	-1.481921	2.557167
87	1	0	6.175159	-0.642062	3.235657
88	1	0	8.010941	1.967920	1.108266
89	1	0	7.453901	1.639877	2.755838
90	1	0	8.791344	0.698974	2.074814
91	6	0	2.686013	2.758626	2.522629
92	6	0	3.476184	3.936304	3.128035
93	6	0	2.206211	1.788722	3.618982
94	1	0	1.792448	3.184075	2.058498
95	1	0	3.781934	4.648731	2.353555
96	1	0	2.861761	4.473261	3.860818
97	1	0	4.382116	3.592584	3.641128
98	1	0	1.598101	0.985813	3.192233
99	1	0	3.048825	1.337153	4.156803
100	1	0	1.593575	2.322534	4.355419
101	6	0	3.601911	1.396104	-2.383184
102	6	0	3.423656	-0.040670	-2.909095
103	6	0	4.646775	2.163244	-3.217560
104	1	0	2.643380	1.900795	-2.524285
105	1	0	2.632346	-0.559289	-2.360100
106	1	0	3.143498	-0.019104	-3.969432
107	1	0	4.345873	-0.626859	-2.824650
108	1	0	4.743900	3.203042	-2.884479
109	1	0	5.638446	1.700289	-3.147353
110	1	0	4.358685	2.171583	-4.275582
111	6	0	-4.258263	-1.002880	2.447744
112	6	0	-3.447520	-2.026772	3.263819
113	6	0	-5.625706	-0.755652	3.117886
114	1	0	-3.698427	-0.064402	2.478333
115	1	0	-2.462000	-2.187924	2.822629
116	1	0	-3.304368	-1.655993	4.286022
117	1	0	-3.957765	-2.994630	3.335662
118	1	0	-6.207580	0.006241	2.588095
119	1	0	-6.226976	-1.672905	3.139396
120	1	0	-5.491519	-0.419250	4.153267
121	6	0	-5.703646	-4.511805	-0.902690
122	6	0	-7.105356	-4.704626	-0.294119
123	6	0	-4.746266	-5.627840	-0.443780
124	1	0	-5.805745	-4.595694	-1.993485
125	1	0	-7.798434	-3.932397	-0.645251
126	1	0	-7.515781	-5.683654	-0.569622
127	1	0	-7.075400	-4.652953	0.800650

128	1	0	-3.764306	-5.521101	-0.918158
129	1	0	-4.597580	-5.601721	0.642224
130	1	0	-5.146819	-6.615436	-0.703573
131	6	0	-4.041832	-0.074228	-2.636127
132	6	0	-5.342006	0.253334	-3.397344
133	6	0	-2.984484	-0.680422	-3.578347
134	1	0	-3.640610	0.876296	-2.274183
135	1	0	-6.078843	0.727987	-2.739485
136	1	0	-5.136688	0.938404	-4.229033
137	1	0	-5.801819	-0.649716	-3.816063
138	1	0	-2.051389	-0.878506	-3.042862
139	1	0	-3.331896	-1.620524	-4.023789
140	1	0	-2.767034	0.013103	-4.399759

TS-2nd-(*S*)-reaction pathway: *S*-*si*/(*R*)-1aa (BINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3235.349372 hartree

Zero-point Energy Correction =1.189023 hartree

Thermal Correction to Energy = 1.256845 hartree

Thermal correction to Enthalpy = 1.257789 hartree

Thermal correction to Gibbs Free Energy= 1.080712 hartree

Sum of electronic and Zero-point Energies = -3234.160349 hartree

Sum of electronic and thermal Energies = -3234.092527 hartree

Sum of electronic and thermal Enthalpies = -3234.091583 hartree

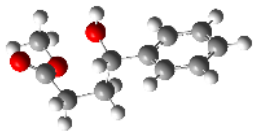
Sum of electronic and thermal Free Energies= -3234.268660 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.593780	0.163254	-0.920658
2	8	0	4.914947	-0.080134	-1.087346
3	8	0	3.060805	-1.140759	0.021213
4	1	0	1.952467	0.301169	-1.917569
5	6	0	5.715335	0.652770	-0.100558
6	6	0	4.686275	1.237039	0.889430
7	6	0	3.412159	1.329746	0.044731
8	1	0	6.198864	1.460136	-0.662545
9	1	0	4.540318	0.557531	1.733116
10	1	0	5.016605	2.201633	1.284213
11	1	0	2.487855	1.271249	0.619347
12	1	0	3.381927	2.244692	-0.556914
13	8	0	2.934851	0.090640	-2.066566
14	6	0	3.129555	-2.408014	-0.670980
15	1	0	2.590773	-3.138474	-0.065053
16	1	0	2.670922	-2.326219	-1.659292
17	1	0	4.180773	-2.682472	-0.765870
18	6	0	6.775854	-0.243233	0.491683
19	6	0	6.429841	-1.406145	1.195055
20	6	0	8.126839	0.090605	0.357102
21	6	0	7.418939	-2.214597	1.751219
22	1	0	5.382936	-1.675882	1.302384
23	6	0	9.119336	-0.713761	0.921343
24	1	0	8.405959	0.985453	-0.194694
25	6	0	8.766907	-1.869105	1.618065
26	1	0	7.138903	-3.114719	2.291965
27	1	0	10.164934	-0.439779	0.810143
28	1	0	9.536806	-2.499440	2.054792
29	6	0	-6.661553	1.549016	-1.535213
30	6	0	-5.597187	0.912944	-0.935087
31	6	0	-4.401474	1.616953	-0.621612
32	6	0	-4.321844	3.000110	-0.984843
33	6	0	-5.445150	3.631804	-1.583741
34	6	0	-6.594793	2.926032	-1.851733
35	1	0	-7.559550	0.985059	-1.772761
36	1	0	-5.662887	-0.144771	-0.708651
37	6	0	-3.264146	0.996256	0.005043
38	6	0	-3.116172	3.711911	-0.760102
39	1	0	-5.369971	4.685530	-1.841722
40	1	0	-7.444335	3.417370	-2.318044
41	6	0	-1.981947	3.101170	-0.267297
42	6	0	-2.085796	1.724749	0.087506
43	1	0	-3.082708	4.769115	-1.008891
44	6	0	-3.326360	-0.394649	0.544242
45	6	0	-4.318986	-0.784528	1.511322
46	6	0	-2.399012	-1.344850	0.140220
47	6	0	-5.199581	0.139779	2.139099
48	6	0	-4.409884	-2.162203	1.892913
49	6	0	-2.457612	-2.717000	0.522090
50	6	0	-6.138485	-0.280380	3.055474
51	1	0	-5.119100	1.193400	1.899250
52	6	0	-5.403204	-2.566260	2.825498
53	6	0	-3.487650	-3.096331	1.357212
54	6	0	-6.255315	-1.648716	3.394331
55	1	0	-6.792647	0.448461	3.526387
56	1	0	-5.464321	-3.618518	3.093100
57	1	0	-3.580094	-4.140685	1.643775
58	1	0	-7.005929	-1.967836	4.112196
59	8	0	-0.954175	1.113686	0.616971
60	15	0	-0.174813	-0.004512	-0.288359
61	8	0	-1.403114	-0.977834	-0.754716
62	8	0	0.433979	0.559045	-1.542038
63	6	0	-1.445408	-3.715230	0.041412
64	6	0	-1.441593	-4.130572	-1.313188
65	6	0	-0.516307	-4.275837	0.950947
66	6	0	-0.513406	-5.090377	-1.727249
67	6	0	0.388338	-5.237902	0.480215
68	6	0	0.411802	-5.661593	-0.849054
69	6	0	-0.708916	3.876494	-0.082399
70	6	0	0.053637	4.278738	-1.207974
71	6	0	-0.298194	4.255032	1.216795
72	6	0	1.196096	5.060514	-1.002647
73	6	0	0.857040	5.032447	1.362468
74	6	0	1.617201	5.452823	0.271088
75	8	0	0.753168	-0.704875	0.701350
76	1	0	1.771126	5.376567	-1.869174
77	1	0	1.167572	5.332179	2.361262
78	1	0	1.094724	-5.681651	1.179042
79	1	0	-0.523119	-5.408811	-2.766759
80	1	0	2.013164	-0.948826	0.321726
81	6	0	-2.450570	-3.605905	-2.334755
82	6	0	-3.407266	-4.724895	-2.793486
83	6	0	-1.765865	-2.932442	-3.539084
84	1	0	-3.065371	-2.844153	-1.848071
85	1	0	-3.929144	-5.175531	-1.941719
86	1	0	-4.161531	-4.325766	-3.482547
87	1	0	-2.868883	-5.524672	-3.315800

88	1	0	-1.123489	-2.108489	-3.214997
89	1	0	-1.153967	-3.643802	-4.106927
90	1	0	-2.519836	-2.526995	-4.224475
91	6	0	1.398356	-6.727068	-1.310201
92	6	0	2.331197	-6.216032	-2.423902
93	6	0	0.677984	-8.017199	-1.747040
94	1	0	2.027138	-6.979934	-0.445084
95	1	0	2.879140	-5.321969	-2.105549
96	1	0	3.064585	-6.984190	-2.696999
97	1	0	1.769513	-5.956502	-3.328795
98	1	0	0.042289	-8.406197	-0.944206
99	1	0	0.040176	-7.838745	-2.620878
100	1	0	1.403403	-8.794444	-2.016339
101	6	0	-0.466852	-3.899638	2.433428
102	6	0	0.927772	-3.421017	2.878820
103	6	0	-0.948839	-5.067410	3.318078
104	1	0	-1.150587	-3.062401	2.594547
105	1	0	1.236800	-2.546719	2.299978
106	1	0	0.904835	-3.135408	3.937623
107	1	0	1.686265	-4.205820	2.769148
108	1	0	-1.960826	-5.388344	3.046841
109	1	0	-0.290089	-5.939006	3.221373
110	1	0	-0.958667	-4.770970	4.373961
111	6	0	-0.336655	3.914883	-2.641882
112	6	0	0.836329	3.334427	-3.453493
113	6	0	-0.943380	5.127380	-3.377488
114	1	0	-1.102006	3.135508	-2.594591
115	1	0	1.276865	2.474675	-2.944451
116	1	0	0.478492	2.999000	-4.434152
117	1	0	1.622695	4.077774	-3.633105
118	1	0	-1.820461	5.524390	-2.855153
119	1	0	-0.213246	5.941573	-3.463322
120	1	0	-1.252378	4.845946	-4.391489
121	6	0	2.854921	6.318914	0.470415
122	6	0	2.713830	7.691154	-0.215004
123	6	0	4.139436	5.604925	0.008621
124	1	0	2.951290	6.499861	1.549878
125	1	0	1.821669	8.219154	0.138596
126	1	0	3.588267	8.319712	-0.007319
127	1	0	2.630027	7.586162	-1.303107
128	1	0	4.273154	4.654478	0.538553
129	1	0	4.110619	5.389128	-1.066162
130	1	0	5.021627	6.227842	0.200087
131	6	0	-1.087718	3.883241	2.471736
132	6	0	-1.654308	5.135619	3.169937
133	6	0	-0.253955	3.031007	3.447233
134	1	0	-1.945358	3.276501	2.168883
135	1	0	-2.283654	5.718615	2.488085
136	1	0	-2.264684	4.848862	4.034855
137	1	0	-0.855027	5.793932	3.530463
138	1	0	0.095651	2.114458	2.962660
139	1	0	0.619814	3.580536	3.817800
140	1	0	-0.858794	2.746929	4.316987

Optimization of 2b



B3LYP/6-31G(d); E(B3LYP) = -653.274726 hartree

Zero-point Energy Correction = 0.234057 hartree

Thermal Correction to Energy = 0.247971 hartree

Thermal correction to Enthalpy = 0.248915 hartree

Thermal correction to Gibbs Free Energy= 0.191349 hartree

Sum of electronic and Zero-point Energies = -653.040668 hartree

Sum of electronic and thermal Energies = -653.026754 hartree

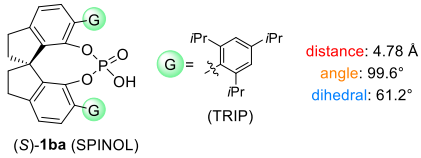
Sum of electronic and thermal Enthalpies = -653.025810 hartree

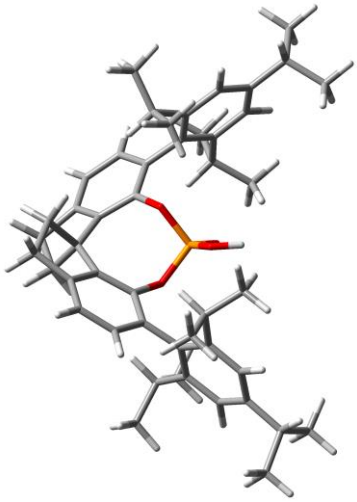
Sum of electronic and thermal Free Energies= -653.083376 hartree

The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.145559	-7.189336	-1.331531
2	8	0	-2.382908	-6.447537	0.909662
3	6	0	-3.636772	-6.205161	0.281979
4	6	0	-3.672751	-7.028859	-1.019504
5	6	0	-2.460584	-6.731717	-1.920072
6	1	0	-3.713200	-5.140261	0.018305
7	1	0	-3.689589	-8.094816	-0.768823
8	1	0	-4.594410	-6.811168	-1.571482
9	1	0	-2.583169	-7.253118	-2.878401
10	1	0	-2.377321	-5.661606	-2.133667
11	8	0	-0.137355	-6.497962	-1.201896
12	8	0	-1.145795	-8.487883	-1.037720
13	6	0	0.031886	-8.992576	-0.380058
14	1	0	-0.156670	-10.055145	-0.227728
15	1	0	0.916350	-8.839789	-1.002215
16	1	0	0.164104	-8.481318	0.576258
17	1	0	-1.964030	-5.580516	1.091839
18	6	0	-4.806848	-6.565530	1.190496
19	6	0	-4.611256	-7.328036	2.346058
20	6	0	-6.107230	-6.158020	0.862548
21	6	0	-5.694122	-7.681768	3.153856
22	1	0	-3.601400	-7.626055	2.606429
23	6	0	-7.190380	-6.510585	1.668079
24	1	0	-6.273630	-5.551914	-0.025975
25	6	0	-6.986692	-7.277175	2.817861
26	1	0	-5.525705	-8.272553	4.050997
27	1	0	-8.192266	-6.183368	1.400879
28	1	0	-7.828542	-7.551025	3.448547

Optimized structure of SPINOL-derived CPA (*S*)-1ba (TRIP)





B3LYP/6-31G(d); E(B3LYP) = -2468.936485 hartree

Zero-point Energy Correction = 0.961056 hartree

Thermal Correction to Energy = 1.013669 hartree

Thermal correction to Enthalpy = 1.014613 hartree

Thermal correction to Gibbs Free Energy= 0.874815 hartree

Sum of electronic and Zero-point Energies = -2467.975429 hartree

Sum of electronic and thermal Energies = -2467.922816 hartree

Sum of electronic and thermal Enthalpies = -2467.921872 hartree

Sum of electronic and thermal Free Energies= -2468.061670 hartree

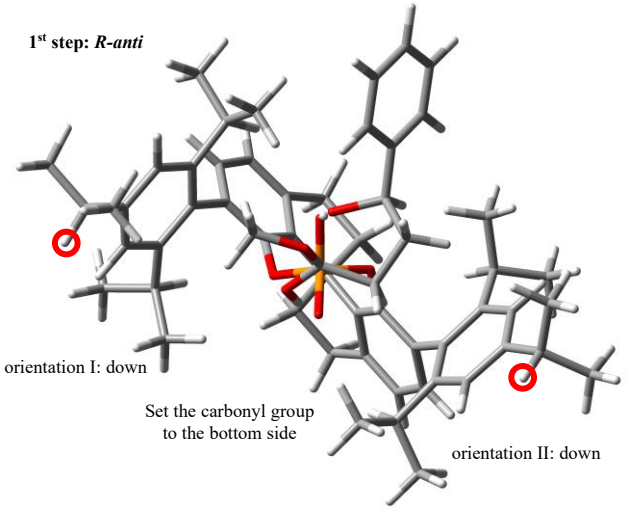
The number of Imaginary frequencies = 0

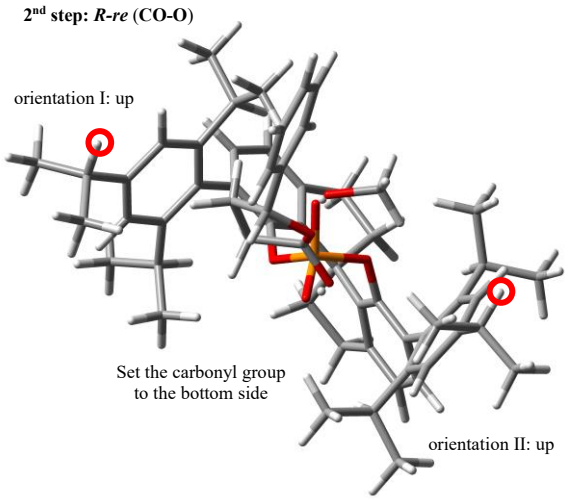
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.245628	2.659809	-0.599023
2	6	0	1.851110	1.453784	-0.257001
3	6	0	3.802239	2.066702	-1.505940
4	6	0	3.163066	3.215797	-1.972527
5	6	0	1.880384	3.504861	-1.522440
6	1	0	4.822574	1.862277	-1.811455
7	1	0	3.672265	3.878222	-2.668197
8	6	0	0.983660	4.670694	-1.880954
9	1	0	1.343270	5.607497	-1.433002
10	1	0	0.933374	4.840346	-2.962669
11	6	0	0.000430	3.351371	-0.053752
12	6	0	-0.376096	4.244674	-1.282889
13	1	0	-0.927012	3.633827	-2.007225
14	1	0	-1.013325	5.090239	-1.006094
15	6	0	0.375678	4.270834	1.159077
16	1	0	0.954174	3.681883	1.880051
17	1	0	0.988491	5.126455	0.860099
18	6	0	-0.978788	4.669847	1.779079
19	1	0	-1.381022	5.580422	1.313194
20	1	0	-0.909955	4.871288	2.854206
21	6	0	-1.841652	3.466573	1.471088
22	6	0	-1.221292	2.638520	0.521043
23	6	0	-3.083134	3.134321	1.998144
24	1	0	-3.575610	3.784848	2.716592
25	6	0	-1.806850	1.413174	0.206644
26	8	0	1.140220	0.550387	0.547915
27	8	0	-1.139266	0.548406	-0.670862
28	15	0	0.054459	-0.425387	-0.158741
29	8	0	-0.497511	-1.191067	1.103967
30	8	0	0.542999	-1.232194	-1.306187
31	6	0	3.160802	1.137939	-0.669069
32	6	0	-3.072044	1.049247	0.710536
33	6	0	3.890130	-0.096237	-0.221034
34	6	0	4.227819	-0.258740	1.145571
35	6	0	4.314839	-1.068640	-1.166192
36	6	0	4.963595	-1.384508	1.533858
37	6	0	5.052809	-2.168863	-0.717827
38	6	0	5.388372	-2.352326	0.625445
39	1	0	5.225653	-1.504556	2.582892
40	1	0	5.373251	-2.908458	-1.446446
41	6	0	-3.697716	1.953386	1.584850
42	1	0	-4.686586	1.705293	1.956078
43	6	0	-3.807330	-0.205764	0.330710
44	6	0	-4.090335	-1.195246	1.306669
45	6	0	-4.339386	-0.342587	-0.976919
46	6	0	-4.909025	-2.276386	0.953247
47	6	0	-5.143833	-1.448346	-1.273453
48	6	0	-5.456568	-2.422627	-0.322347
49	1	0	-5.146567	-3.023296	1.707638
50	1	0	-5.561046	-1.532375	-2.273790
51	6	0	3.881313	0.769948	2.223099
52	6	0	5.154689	1.428205	2.792127
53	6	0	3.019162	0.167110	3.348610
54	1	0	3.295985	1.569427	1.762622
55	1	0	5.747178	1.896815	1.998268
56	1	0	4.891964	2.202638	3.523375
57	1	0	5.795260	0.696373	3.298097
58	1	0	2.099685	-0.269395	2.948046
59	1	0	3.558817	-0.614626	3.896406
60	1	0	2.742685	0.943828	4.072488
61	6	0	4.025368	-0.962502	-2.665910
62	6	0	3.462377	-2.264224	-3.267067
63	6	0	5.288615	-0.547038	-3.450549
64	1	0	3.266478	-0.188159	-2.809747
65	1	0	2.604132	-2.641722	-2.709281
66	1	0	3.140729	-2.087116	-4.300268
67	1	0	4.218160	-3.058450	-3.298250
68	1	0	5.709539	0.399764	-3.096925
69	1	0	6.072008	-1.308874	-3.355984
70	1	0	5.057540	-0.436721	-4.517168
71	6	0	6.192707	-3.558990	1.090993
72	6	0	7.586133	-3.611883	0.436834
73	6	0	5.427962	-4.877255	0.866283
74	1	0	6.342789	-3.447739	2.173822
75	1	0	8.146540	-2.689689	0.625500
76	1	0	8.168296	-4.453024	0.832485
77	1	0	7.511993	-3.740811	-0.649412
78	1	0	4.455769	-4.856856	1.371571
79	1	0	5.247123	-5.054780	-0.200460
80	1	0	5.998589	-5.729378	1.255559
81	6	0	-3.575303	-1.120770	2.746822
82	6	0	-2.900549	-2.425662	3.212581
83	6	0	-4.706324	-0.753234	3.730802
84	1	0	-2.817031	-0.334481	2.793825
85	1	0	-2.103424	-2.737121	2.533920
86	1	0	-2.458229	-2.281147	4.205395
87	1	0	-3.619115	-3.249971	3.295806
88	1	0	-5.182158	0.198886	3.476098
89	1	0	-5.488272	-1.522296	3.734348
90	1	0	-4.313752	-0.671123	4.751657
91	6	0	-4.135110	0.709512	-2.067943
92	6	0	-5.463136	1.412613	-2.414889
93	6	0	-3.470954	0.123700	-3.327380
94	1	0	-3.463982	1.479708	-1.680929
95	1	0	-5.913316	1.870169	-1.526715

96	1	0	-5.295656	2.202738	-3.156991
97	1	0	-6.193085	0.710654	-2.835130
98	1	0	-2.508934	-0.338894	-3.088368
99	1	0	-4.101017	-0.634878	-3.806364
100	1	0	-3.293400	0.915703	-4.065216
101	6	0	-6.407780	-3.572226	-0.633053
102	6	0	-5.949901	-4.424203	-1.830248
103	6	0	-7.846302	-3.059999	-0.845690
104	1	0	-6.420904	-4.226497	0.249727
105	1	0	-4.951647	-4.842898	-1.662334
106	1	0	-6.642571	-5.257852	-1.996727
107	1	0	-5.914301	-3.834828	-2.753888
108	1	0	-8.193991	-2.486944	0.020690
109	1	0	-7.906736	-2.406345	-1.723981
110	1	0	-8.537398	-3.897052	-1.002647
111	1	0	-0.409563	-2.190578	1.037576

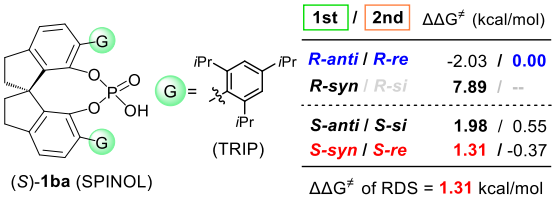
DFT calculation for full conformational search of real system using SPINOL-derive CPA (*S*)-1ba/racemic-2b

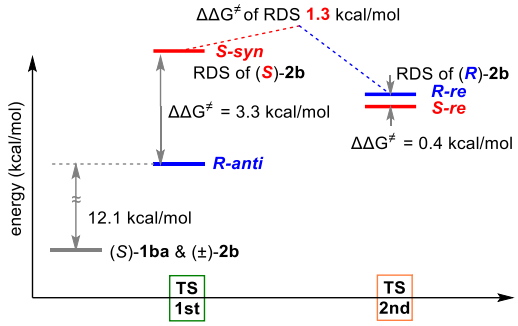
TS 1st	orientation I		Orientation II		$\Delta\Delta G^{\neq}$ (a.u.)	$\Delta\Delta G^{\neq}$ (kcal/mol)			**TS 2nd**	orientation I		Orientation II		$\Delta\Delta G^{\neq}$ (a.u.)	$\Delta\Delta G^{\neq}$ (kcal/mol)	
***R*-anti**	-3.0	up	23.0	up	-3121.122551	2.01	-0.02	***R*,*R*-Int.**	***R*-re** (CO-O)	-9.4	up	10.8	up	-3121.122518	2.03	0.00
	-5.8	up	148.2	down	-3121.125271	0.30	-1.73			-8.6	up	-175.0	down	-3121.121986	2.36	0.33
	-179.4	down	15.7	up	-3121.124951	0.50	-1.53			177.9	down	11.8	up	-3121.119926	3.65	1.63
	-179.1	down	170.2	down	-3121.125747	0.00	-2.03			178.5	down	-175.9	down	-3121.121201	2.85	0.83
									***R*-re** (CO-C)	-3.5	up	6.3	up	-3121.116296	5.93	3.90
										-2.7	up	-178.5	down	-3121.115067	6.70	4.68
										-178.3	down	4.8	up	-3121.116093	6.06	4.03
										178.4	down	-179.4	down	-3121.114932	6.79	4.76
***R*-syn**	-7.3	up	-1.1	up	-3121.109942	9.92	7.89	***R*,*S*-Int.**								
	-7.0	up	-179.3	down	-3121.109217	10.37	8.35									
	-175.4	down	-1.8	up	-3121.109650	10.10	8.08									
	-175.1	down	-179.4	down	-3121.109103	10.44	8.42									
***S*-anti**	-14.1	up	26.5	up	-3121.119369	4.00	1.98	***S*,*S*-Int.**	***S*-si** (CO-O)	-3.7	up	9.6	up	-3121.121638	2.58	0.55
	-16.8	up	154.6	down	-3121.118986	4.24	2.22			-4.2	up	-179.3	down	-3121.120753	3.13	1.11
	-177.1	down	90.4	up	-3121.110928	9.30	7.27			178.9	down	10.9	up	-3121.120044	3.58	1.55
	-176.8	down	158.7	down	-3121.119162	4.13	2.11			-179.1	down	176.9	down	-3121.119879	3.68	1.66
									***S*-si** (CO-C)	-6.5	up	4.9	up	-3121.111179	9.14	7.12
										-5.9	up	176.4	down	-3121.111472	8.96	6.93
										-176.2	down	-5.8	up	-3121.109908	9.94	7.91
										174.9	down	175.0	down	-3121.110365	9.65	7.63
***S*-syn**	0.5	up	6.1	up	-3121.119489	3.93	1.90	***S*,*R*-Int.**	***S*-re** (CO-O)	-9.4	up	11.0	up	-3121.123110	1.65	-0.37
	1.3	up	177.4	down	-3121.119101	4.17	2.14			-10.3	up	-175.3	down	-3121.122797	1.85	-0.18
	179.6	down	5.5	up	-3121.119592	3.86	1.84			-178.9	down	10.2	up	-3121.122226	2.21	0.18
	180.0	down	178.5	down	-3121.120428	3.34	1.31			177.8	down	-176.8	down	-3121.121452	2.70	0.67
									***S*-re** (CO-C)	-5.2	up	-0.8	up	-3121.113849	7.47	5.44
										-2.9	up	168.7	down	-3121.112511	8.31	6.28
										-178.0	down	-1.5	up	-3121.110893	9.32	7.30
										-178.3	down	167.6	down	-3121.111975	8.64	6.62



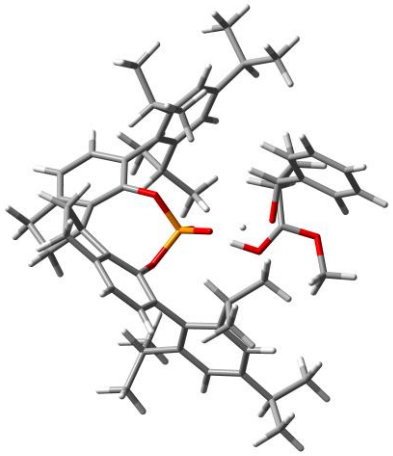


DFT calculation of real system using SPINOL-derive CPA (*S*)-1ba





TS-1st-(*R*)-reaction pathway: *R*-*anti*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.217549 hartree

Zero-point Energy Correction = 1.194953 hartree

Thermal Correction to Energy = 1.260650 hartree

Thermal correction to Enthalpy = 1.091802 hartree

Thermal correction to Gibbs Free Energy= 1.091012 hartree

Sum of electronic and Zero-point Energies = -3121.022596 hartree

Sum of electronic and thermal Energies = -3120.956899 hartree

Sum of electronic and thermal Enthalpies = -3120.955955 hartree

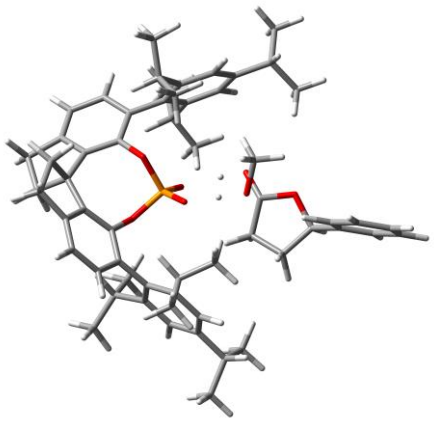
Sum of electronic and thermal Free Energies= -3121.125747 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075361	2.971503	-1.713550
2	8	0	0.275983	2.772905	-0.055046
3	6	0	-0.869642	3.219641	0.732853
4	6	0	-1.860520	3.804502	-0.295587
5	6	0	-1.588229	3.030418	-1.585037
6	1	0	-1.302774	2.321146	1.185012
7	1	0	-1.671797	4.871763	-0.443421
8	1	0	-2.888333	3.685243	0.055159
9	1	0	-2.005166	3.514883	-2.472443
10	1	0	-1.975784	2.008974	-1.529317
11	8	0	0.526656	1.977270	-2.347122
12	8	0	0.438403	4.184717	-2.004951
13	6	0	1.855906	4.239478	-2.250017
14	1	0	2.089270	5.300735	-2.344774
15	1	0	2.106531	3.711580	-3.172293
16	1	0	2.405965	3.802353	-1.412598
17	1	0	0.485085	1.684610	0.227790
18	1	0	0.116357	1.073551	-2.125390
19	6	0	-1.208649	-3.707676	0.500576
20	6	0	-1.787832	-2.458203	0.280384
21	6	0	-3.671285	-3.515623	-0.776618
22	6	0	-3.061149	-4.763743	-0.659719
23	6	0	-1.826116	-4.852058	-0.029092
24	1	0	-4.652111	-3.439032	-1.235451
25	1	0	-3.550418	-5.651014	-1.053937
26	6	0	-0.965405	-6.076127	0.191923
27	1	0	-1.372555	-6.713277	0.989747
28	1	0	-0.891299	-6.703626	-0.703722
29	6	0	0.009974	-4.119266	1.322932
30	6	0	0.387428	-5.457732	0.600537
31	1	0	0.971194	-5.219965	-0.296087
32	1	0	0.995891	-6.114549	1.229637
33	6	0	-0.372889	-4.423895	2.809855
34	1	0	-0.930606	-3.570176	3.211704
35	1	0	-1.005772	-5.311667	2.906365
36	6	0	0.982910	-4.555059	3.539279
37	1	0	1.349279	-5.591202	3.521057
38	1	0	0.924442	-4.262501	4.594104
39	6	0	1.878323	-3.636312	2.735551
40	6	0	1.251554	-3.259379	1.537834
41	6	0	3.152228	-3.171586	3.040404
42	1	0	3.654028	-3.478607	3.954798
43	6	0	1.853289	-2.299136	0.727379
44	6	0	3.789739	-2.311128	2.146195
45	1	0	4.802818	-1.981381	2.351607
46	8	0	-1.119007	-1.317193	0.725971
47	8	0	1.158567	-1.826088	-0.388131
48	15	0	0.047656	-0.643702	-0.205797
49	8	0	0.604202	0.483955	0.664171
50	8	0	-0.452698	-0.293464	-1.582371
51	6	0	-3.046699	-2.334685	-0.341594
52	6	0	3.154322	-1.825567	0.991105
53	6	0	-0.440146	4.174494	1.822145
54	6	0	-0.806718	3.931171	3.149245
55	6	0	0.305337	5.322540	1.520360
56	6	0	-0.445780	4.823782	4.161168
57	1	0	-1.374864	3.036454	3.393454
58	6	0	0.673300	6.209426	2.529897
59	1	0	0.600433	5.511021	0.491847
60	6	0	0.296028	5.963866	3.853419
61	1	0	-0.738144	4.622475	5.188274
62	1	0	1.255680	7.094083	2.285765
63	1	0	0.583073	6.657286	4.639431
64	6	0	3.886687	-0.878805	0.084164
65	6	0	4.300000	0.396407	0.554468
66	6	0	4.252286	-1.288566	-1.222008
67	6	0	5.065442	1.213213	-0.284811
68	6	0	5.010929	-0.423075	-2.019092
69	6	0	5.435856	0.827644	-1.575174
70	1	0	5.385540	2.183009	0.087866
71	1	0	5.294108	-0.743599	-3.019384

72	6	0	-3.768842	-1.029717	-0.524813
73	6	0	-4.308475	-0.354405	0.598903
74	6	0	-4.025861	-0.531133	-1.827297
75	6	0	-5.101635	0.781757	0.398002
76	6	0	-4.829225	0.607941	-1.967035
77	6	0	-5.393227	1.273434	-0.877030
78	1	0	-5.532864	1.273230	1.266738
79	1	0	-5.044282	0.977223	-2.967475
80	6	0	-3.503098	-1.205153	-3.098726
81	6	0	-2.725347	-0.238377	-4.011522
82	6	0	-4.650585	-1.867901	-3.889321
83	1	0	-2.802270	-1.989282	-2.801765
84	1	0	-1.871286	0.189441	-3.483371
85	1	0	-2.344462	-0.779748	-4.886041
86	1	0	-3.358732	0.576212	-4.383856
87	1	0	-5.198831	-2.596898	-3.283143
88	1	0	-5.373309	-1.120666	-4.239024
89	1	0	-4.256850	-2.389044	-4.770364
90	6	0	-4.119920	-0.855247	2.031950
91	6	0	-5.464766	-1.255353	2.671308
92	6	0	-3.370834	0.165879	2.909304
93	1	0	-3.506514	-1.758661	1.999949
94	1	0	-5.981795	-2.007809	2.065544
95	1	0	-5.302245	-1.676269	3.671022
96	1	0	-6.135775	-0.395141	2.778898
97	1	0	-2.378539	0.375500	2.497103
98	1	0	-3.922793	1.110504	2.990993
99	1	0	-3.238118	-0.227836	3.924567
100	6	0	-6.362789	2.429162	-1.098388
101	6	0	-6.053301	3.670843	-0.245358
102	6	0	-7.817407	1.966746	-0.874314
103	1	0	-6.273815	2.725509	-2.152838
104	1	0	-5.043896	4.048535	-0.440233
105	1	0	-6.762220	4.476349	-0.470756
106	1	0	-6.131976	3.457104	0.827025
107	1	0	-8.061518	1.109127	-1.510342
108	1	0	-7.976518	1.664924	0.167907
109	1	0	-8.522600	2.775333	-1.102543
110	6	0	3.965336	0.921767	1.953506
111	6	0	3.336985	2.327958	1.927228
112	6	0	5.210895	0.931346	2.864524
113	1	0	3.224704	0.252499	2.398702
114	1	0	2.464514	2.364601	1.272524
115	1	0	3.013773	2.613436	2.935377
116	1	0	4.051230	3.088853	1.589293
117	1	0	5.666280	-0.060418	2.954214
118	1	0	5.978283	1.609965	2.472427
119	1	0	4.946161	1.273683	3.872496
120	6	0	3.908900	-2.663887	-1.796325
121	6	0	5.181890	-3.500933	-2.035990
122	6	0	3.062024	-2.560595	-3.079040
123	1	0	3.312270	-3.206884	-1.059979
124	1	0	5.763218	-3.611750	-1.113599
125	1	0	4.918780	-4.503715	-2.394698
126	1	0	5.833720	-3.039773	-2.787359
127	1	0	2.143100	-1.996183	-2.897017
128	1	0	3.613692	-2.067518	-3.888497
129	1	0	2.785423	-3.561814	-3.432360
130	6	0	6.289633	1.721313	-2.465468
131	6	0	7.692898	1.946366	-1.870378
132	6	0	5.601233	3.063689	-2.773822
133	1	0	6.419517	1.193720	-3.420471
134	1	0	8.202577	0.993438	-1.691127
135	1	0	8.312645	2.543376	-2.550568
136	1	0	7.638445	2.479518	-0.913656
137	1	0	4.619606	2.904800	-3.233817
138	1	0	5.454905	3.653788	-1.860916
139	1	0	6.209011	3.663090	-3.462614

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.215732 hartree

Zero-point Energy Correction = 1.195785 hartree

Thermal Correction to Energy = 1.261492 hartree

Thermal correction to Enthalpy = 1.262436 hartree

Thermal correction to Gibbs Free Energy= 1.093214 hartree

Sum of electronic and Zero-point Energies = -3121.019947 hartree

Sum of electronic and thermal Energies = -3120.954240 hartree

Sum of electronic and thermal Enthalpies = -3120.953296 hartree

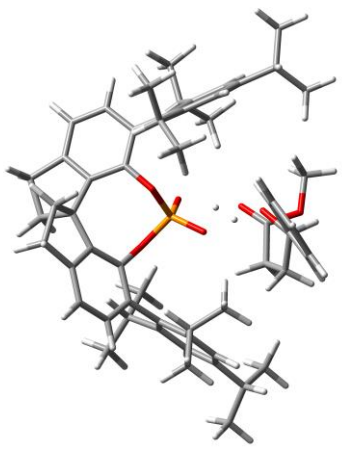
Sum of electronic and thermal Free Energies= -3121.122518 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.971144	2.134754	0.594053
2	8	0	-2.829305	3.175894	0.497221
3	8	0	-1.759848	1.648496	-1.033535
4	6	0	-4.212395	2.742459	0.732699
5	6	0	-4.145182	1.201893	0.753501
6	6	0	-2.697610	0.926124	1.170938
7	1	0	-4.466509	3.122513	1.728924
8	1	0	-4.341502	0.793444	-0.240879
9	1	0	-4.882753	0.782162	1.442487
10	1	0	-2.299470	-0.025289	0.817916
11	1	0	-2.568378	0.969355	2.258356
12	8	0	-0.782569	2.514362	1.023470
13	6	0	-1.154658	2.671264	-1.855122
14	1	0	-1.846185	3.512911	-1.905408
15	1	0	-1.007223	2.239894	-2.847412
16	1	0	-0.197920	2.989660	-1.433406
17	1	0	-1.105069	0.761979	-1.046094
18	1	0	-0.179507	1.704638	1.152399
19	6	0	4.002628	-1.539170	-0.101787
20	6	0	3.392661	-0.288063	-0.167961
21	6	0	5.247824	0.686114	1.011960
22	6	0	5.830701	-0.571617	1.168683
23	6	0	5.194868	-1.681952	0.625713
24	1	0	5.745439	1.562360	1.416468
25	1	0	6.765748	-0.676469	1.713548
26	6	0	5.597736	-3.138050	0.708863
27	1	0	6.443016	-3.360687	0.042378
28	1	0	5.909445	-3.429036	1.718636

29	6	0	3.640688	-2.868131	-0.759125
30	6	0	4.313602	-3.860960	0.249846
31	1	0	3.642240	-4.000493	1.104902
32	1	0	4.500615	-4.844673	-0.191772
33	6	0	4.317800	-3.021300	-2.161976
34	1	0	4.081808	-2.136538	-2.764292
35	1	0	5.407472	-3.099511	-2.095424
36	6	0	3.649071	-4.269569	-2.778866
37	1	0	4.191186	-5.187779	-2.512377
38	1	0	3.614355	-4.232891	-3.873896
39	6	0	2.268418	-4.240223	-2.158423
40	6	0	2.221568	-3.319210	-1.099210
41	6	0	1.140109	-4.970424	-2.512014
42	1	0	1.179189	-5.702295	-3.315171
43	6	0	0.993705	-3.034441	-0.503973
44	6	0	-0.050022	-4.757198	-1.815485
45	1	0	-0.925367	-5.351903	-2.056617
46	8	0	2.167568	-0.171478	-0.822750
47	8	0	0.916534	-2.025435	0.455358
48	15	0	0.771394	-0.467636	-0.017982
49	8	0	-0.304893	-0.321820	-1.090398
50	8	0	0.632513	0.340456	1.244594
51	6	0	4.006543	0.857960	0.378695
52	6	0	-0.166963	-3.767605	-0.826308
53	6	0	-5.141068	3.361522	-0.283236
54	6	0	-6.165025	4.214954	0.139056
55	6	0	-5.007249	3.086359	-1.651959
56	6	0	-7.048476	4.779891	-0.783202
57	1	0	-6.271754	4.441261	1.197607
58	6	0	-5.882165	3.656176	-2.574703
59	1	0	-4.214525	2.426027	-1.992160
60	6	0	-6.907125	4.502683	-2.142464
61	1	0	-7.840610	5.439195	-0.438919
62	1	0	-5.766882	3.437847	-3.633019
63	1	0	-7.590182	4.943608	-2.863449
64	6	0	-1.483926	-3.546103	-0.139206
65	6	0	-2.616233	-3.106756	-0.872624
66	6	0	-1.622676	-3.844844	1.241124
67	6	0	-3.842945	-2.974311	-0.208217
68	6	0	-2.872509	-3.692677	1.849842
69	6	0	-3.999656	-3.260136	1.148288
70	1	0	-4.713639	-2.646179	-0.772029
71	1	0	-2.968897	-3.935943	2.905012
72	6	0	3.373553	2.216373	0.311313
73	6	0	3.206412	2.864323	-0.936324
74	6	0	2.963167	2.874011	1.501474
75	6	0	2.597730	4.125314	-0.970927
76	6	0	2.375226	4.139310	1.405546
77	6	0	2.163505	4.779587	0.182748
78	1	0	2.472543	4.623238	-1.930772
79	1	0	2.059358	4.634102	2.319759
80	6	0	3.157048	2.278751	2.899347
81	6	0	1.857412	2.228962	3.725155
82	6	0	4.251175	3.044588	3.672474
83	1	0	3.493350	1.245303	2.786823
84	1	0	1.102060	1.625091	3.218779
85	1	0	2.058688	1.775247	4.703628
86	1	0	1.443985	3.228002	3.907134
87	1	0	5.199746	3.066453	3.124241
88	1	0	3.953582	4.084588	3.853901
89	1	0	4.433688	2.575014	4.646954
90	6	0	3.728233	2.276809	-2.248433
91	6	0	4.892923	3.123582	-2.801380
92	6	0	2.622150	2.103886	-3.305827
93	1	0	4.131696	1.282570	-2.041040
94	1	0	5.702550	3.209752	-2.068044
95	1	0	5.304123	2.666428	-3.709986
96	1	0	4.565883	4.138563	-3.056818
97	1	0	1.821544	1.460059	-2.930121
98	1	0	2.187227	3.067480	-3.598900
99	1	0	3.032462	1.641832	-4.212268
100	6	0	1.513937	6.154686	0.100010
101	6	0	2.470534	7.256768	0.596382
102	6	0	0.167775	6.219206	0.845134
103	1	0	1.313038	6.350071	-0.962959
104	1	0	3.411314	7.248473	0.034810
105	1	0	2.014247	8.248281	0.485850
106	1	0	2.713820	7.115714	1.656381
107	1	0	-0.507804	5.417918	0.529579
108	1	0	0.306526	6.120874	1.928278
109	1	0	-0.323760	7.182909	0.663906
110	6	0	-2.574721	-2.797922	-2.371416
111	6	0	-3.155474	-1.414246	-2.718056
112	6	0	-3.306885	-3.886485	-3.184158
113	1	0	-1.528410	-2.787187	-2.685891
114	1	0	-2.645075	-0.624012	-2.164142
115	1	0	-3.028279	-1.215471	-3.789375
116	1	0	-4.229362	-1.353055	-2.503259
117	1	0	-2.895675	-4.884292	-2.998859
118	1	0	-4.372942	-3.918582	-2.927792
119	1	0	-3.227614	-3.682453	-4.259083
120	6	0	-0.476191	-4.386869	2.095740
121	6	0	-0.755482	-5.834972	2.546234
122	6	0	-0.170140	-3.477549	3.301232
123	1	0	0.425979	-4.419106	1.481129
124	1	0	-0.927158	-6.491570	1.685761
125	1	0	0.097323	-6.230884	3.111270
126	1	0	-1.638949	-5.894678	3.192904
127	1	0	0.055463	-2.458263	2.974999
128	1	0	-1.012865	-3.437517	4.002226
129	1	0	0.696959	-3.860409	3.853408
130	6	0	-5.364759	-3.148830	1.815699
131	6	0	-5.340824	-2.270495	3.079452
132	6	0	-5.946227	-4.541635	2.130149
133	1	0	-6.038821	-2.668048	1.092942
134	1	0	-4.945825	-1.271513	2.862634
135	1	0	-6.351416	-2.156808	3.489662
136	1	0	-4.714229	-2.710399	3.864000
137	1	0	-6.010215	-5.156173	1.225621
138	1	0	-5.317137	-5.076069	2.852002
139	1	0	-6.952500	-4.457291	2.558671

TS-1st-(*R*)-reaction pathway: *R-syn*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.201932 hartree

Zero-point Energy Correction = 1.194156 hartree

Thermal Correction to Energy = 1.259923 hartree

Thermal correction to Enthalpy = 1.260867 hartree

Thermal correction to Gibbs Free Energy= 1.091990 hartree

Sum of electronic and Zero-point Energies = -3121.007775 hartree

Sum of electronic and thermal Energies = -3120.942008 hartree

Sum of electronic and thermal Enthalpies = -3120.941064 hartree

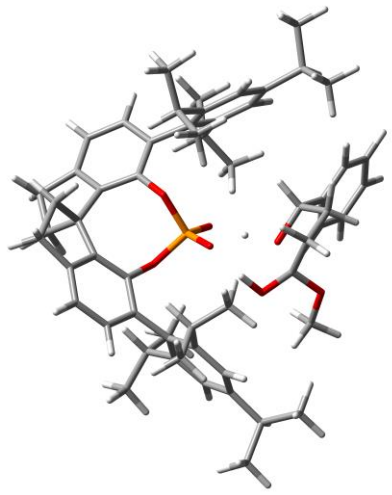
Sum of electronic and thermal Free Energies= -3121.109942 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.247075	3.501819	0.882853
2	6	0	-1.846580	2.354127	0.360630
3	6	0	-3.782553	2.734389	1.740387
4	6	0	-3.154639	3.814205	2.357359
5	6	0	-1.882743	4.181580	1.935576
6	1	0	-4.788382	2.454412	2.039187
7	1	0	-3.657088	4.360019	3.152142
8	6	0	-1.005487	5.292394	2.468104
9	1	0	-1.374798	6.280092	2.158075
10	1	0	-0.964574	5.302887	3.563491
11	6	0	-0.002710	4.282694	0.461905
12	6	0	0.357463	4.972155	1.823113
13	1	0	0.903834	4.254135	2.445561
14	1	0	0.995372	5.851081	1.690862
15	6	0	-0.343909	5.385123	-0.596004
16	1	0	-0.873586	4.917884	-1.434050
17	1	0	-0.988497	6.170940	-0.190179
18	6	0	1.033196	5.904515	-1.067128
19	1	0	1.378783	6.744410	-0.448409
20	1	0	1.015875	6.265163	-2.102124
21	6	0	1.918138	4.687596	-0.899645
22	6	0	1.251251	3.688561	-0.171777
23	6	0	3.212230	4.480047	-1.360415
24	1	0	3.741961	5.258157	-1.904553
25	6	0	1.835759	2.430335	-0.057475
26	6	0	3.833803	3.257051	-1.103653
27	1	0	4.862100	3.103746	-1.414439
28	8	0	-1.205144	1.636464	-0.642026
29	8	0	1.096933	1.383913	0.505206
30	15	0	0.034644	0.594134	-0.455141
31	8	0	0.551159	0.341849	-1.844885
32	8	0	-0.386613	-0.640137	0.354677
33	6	0	-3.140152	1.959588	0.760353
34	6	0	3.158979	2.193853	-0.483252
35	6	0	3.854386	0.882524	-0.259716
36	6	0	4.278332	0.088044	-1.357411
37	6	0	4.145324	0.458400	1.060586
38	6	0	4.950280	-1.112890	-1.103155
39	6	0	4.812088	-0.757289	1.253078
40	6	0	5.219311	-1.564310	0.191151
41	1	0	5.272425	-1.715674	-1.948448
42	1	0	5.037166	-1.079025	2.267843
43	6	0	-3.850372	0.764664	0.196279
44	6	0	-4.245032	0.732498	-1.165931
45	6	0	-4.208031	-0.308249	1.051358
46	6	0	-4.972862	-0.365217	-1.637567
47	6	0	-4.939146	-1.380441	0.522543
48	6	0	-5.339616	-1.432296	-0.812905
49	1	0	-5.285682	-0.370764	-2.678851
50	1	0	-5.220834	-2.198624	1.182310
51	6	0	-3.848161	-0.351114	2.538992
52	6	0	-2.947719	-1.549164	2.884376
53	6	0	-5.108496	-0.337616	3.427062
54	1	0	-3.274175	0.546380	2.777797
55	1	0	-2.019695	-1.515185	2.307614
56	1	0	-2.684263	-1.534520	3.948884
57	1	0	-3.446438	-2.505532	2.685282
58	1	0	-5.744771	0.529100	3.214244
59	1	0	-5.716890	-1.237260	3.276419
60	1	0	-4.828060	-0.300899	4.486714
61	6	0	-3.978272	1.886033	-2.134257
62	6	0	-5.296600	2.558670	-2.568668
63	6	0	-3.151141	1.447293	-3.357464
64	1	0	-3.396729	2.646924	-1.608839
65	1	0	-5.869635	2.906012	-1.701518
66	1	0	-5.090612	3.424924	-3.209263
67	1	0	-5.934645	1.870587	-3.135928
68	1	0	-2.186660	1.030733	-3.053343
69	1	0	-3.680566	0.695926	-3.955947
70	1	0	-2.955882	2.307153	-4.009867
71	6	0	-6.197972	-2.582465	-1.325934
72	6	0	-5.576433	-3.298174	-2.538379
73	6	0	-7.629338	-2.107810	-1.646540
74	1	0	-6.271488	-3.317621	-0.512420
75	1	0	-4.582300	-3.691742	-2.300418
76	1	0	-6.206451	-4.137842	-2.855693
77	1	0	-5.471314	-2.621756	-3.394622
78	1	0	-8.093340	-1.635663	-0.773832
79	1	0	-7.628118	-1.373727	-2.461085
80	1	0	-8.258974	-2.951039	-1.955755
81	6	0	4.063055	0.500141	-2.815559
82	6	0	3.446537	-0.619879	-3.672717
83	6	0	5.383174	0.977458	-3.456986
84	1	0	3.355683	1.333029	-2.830994
85	1	0	2.526413	-0.999696	-3.226428
86	1	0	3.207319	-0.234007	-4.671090
87	1	0	4.139769	-1.459537	-3.809011
88	1	0	5.835970	1.808032	-2.905258
89	1	0	6.119444	0.164801	-3.486871
90	1	0	5.210340	1.310521	-4.487743
91	6	0	3.830424	1.305162	2.294283
92	6	0	5.127297	1.807441	2.961072
93	6	0	2.938647	0.564189	3.307489
94	1	0	3.279904	2.191766	1.971739
95	1	0	5.741307	2.376046	2.253719
96	1	0	4.894026	2.460722	3.810985
97	1	0	5.735442	0.975783	3.336529
98	1	0	2.004793	0.236374	2.841674
99	1	0	3.446077	-0.315649	3.722273
100	1	0	2.689248	1.223168	4.148370
101	6	0	5.935868	-2.883693	0.446519
102	6	0	7.352139	-2.900505	-0.158553
103	6	0	5.109672	-4.086289	-0.048049
104	1	0	6.042802	-2.986660	1.535236
105	1	0	7.953453	-2.066683	0.219823
106	1	0	7.869160	-3.835477	0.089582
107	1	0	7.319550	-2.818846	-1.251501
108	1	0	4.113879	-4.094813	0.409014
109	1	0	4.980042	-4.054861	-1.136860
110	1	0	5.608747	-5.030904	0.200577
111	6	0	-0.118949	-3.003375	-2.006257
112	6	0	-0.230469	-3.845279	0.284935
113	6	0	-1.594035	-3.076922	-1.625224
114	1	0	-2.128752	-3.611984	-2.413998
115	1	0	-1.989168	-2.060253	-1.574974
116	8	0	0.369908	-2.030310	-2.752041
117	8	0	0.326300	-4.224558	-2.384048
118	6	0	1.689995	-4.299461	-2.841888
119	1	0	1.895664	-5.365366	-2.949952
120	1	0	1.802081	-3.790354	-3.800939
121	1	0	2.365241	-3.854519	-2.106055
122	1	0	0.298679	-1.077967	-2.384750
123	6	0	-0.025289	-3.772620	1.782098
124	6	0	-0.850331	-4.535050	2.620807
125	6	0	1.024212	-3.039431	2.348208
126	6	0	-0.637347	-4.557386	3.998640
127	1	0	-1.664379	-5.117842	2.196925
128	6	0	1.231099	-3.057614	3.728971
129	1	0	1.675615	-2.447852	1.713663

130	6	0	0.404427	-3.815284	4.558353
131	1	0	-1.287913	-5.152453	4.634171
132	1	0	2.042484	-2.473273	4.153678
133	1	0	0.569196	-3.828059	5.632404
134	1	0	0.224791	-4.771552	-0.077709
135	8	0	0.479851	-2.795683	-0.425406
136	1	0	0.109787	-1.758674	-0.044403
137	6	0	-1.686952	-3.773505	-0.245842
138	1	0	-2.317202	-3.188672	0.427050
139	1	0	-2.113417	-4.777725	-0.322779

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.212139 hartree

Zero-point Energy Correction = 1.194935 hartree

Thermal Correction to Energy = 1.260562 hartree

Thermal correction to Enthalpy = 1.261506 hartree

Thermal correction to Gibbs Free Energy= 1.091990 hartree

Sum of electronic and Zero-point Energies = -3121.017204 hartree

Sum of electronic and thermal Energies = -3120.951577 hartree

Sum of electronic and thermal Enthalpies = -3120.950633 hartree

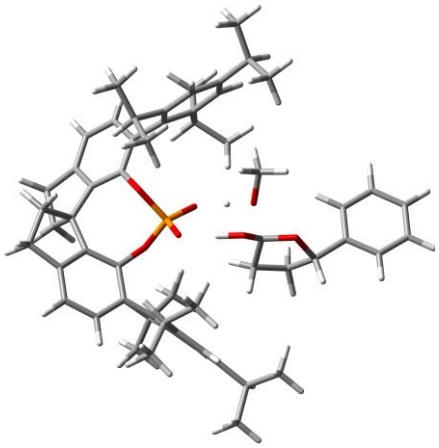
Sum of electronic and thermal Free Energies= -3121.119369 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.409583	-3.201517	0.730268
2	8	0	0.743819	-2.603347	-0.380907
3	6	0	2.069232	-2.875834	0.138532
4	6	0	1.852816	-3.556378	1.518183
5	6	0	0.462982	-3.113539	1.969077
6	1	0	2.555044	-1.903223	0.279118
7	1	0	1.885603	-4.643520	1.407436
8	1	0	2.631505	-3.263048	2.227409
9	1	0	0.044746	-3.752348	2.752178
10	1	0	0.458011	-2.076250	2.316183
11	8	0	-1.482821	-2.441299	0.595611
12	8	0	-0.593432	-4.479173	0.346544
13	6	0	-1.433104	-4.692696	-0.801791
14	1	0	-1.411101	-5.768917	-0.976567
15	1	0	-2.451621	-4.353319	-0.606915
16	1	0	-1.029036	-4.161231	-1.667841
17	1	0	0.597665	-1.479571	-0.605859
18	1	0	-1.328260	-1.512882	0.969296
19	6	0	-2.226825	3.433800	-0.154348
20	6	0	-2.493640	2.068760	-0.260338
21	6	0	-4.666291	2.425871	0.708194
22	6	0	-4.379753	3.773599	0.913543
23	6	0	-3.148486	4.266495	0.501229
24	1	0	-5.631951	2.031625	1.008709
25	1	0	-5.108295	4.421862	1.394263
26	6	0	-2.589344	5.661940	0.667581
27	1	0	-3.062888	6.372832	-0.024085
28	1	0	-2.747241	6.055522	1.678347
29	6	0	-1.087616	4.285593	-0.706614
30	6	0	-1.097262	5.458557	0.332671
31	1	0	-0.555351	5.137474	1.229692
32	1	0	-0.608012	6.360452	-0.047426
33	6	0	-1.441226	4.854871	-2.121724
34	1	0	-1.734415	4.023270	-2.772676
35	1	0	-2.273381	5.564755	-2.092208
36	6	0	-0.121510	5.476714	-2.624384
37	1	0	-0.030582	6.528328	-2.318605
38	1	0	-0.034484	5.459854	-3.716988
39	6	0	0.921396	4.609648	-1.953557
40	6	0	0.337863	3.802629	-0.962408
41	6	0	2.285442	4.546592	-2.208486
42	1	0	2.744896	5.193677	-2.951613
43	6	0	1.111321	2.818845	-0.345315
44	8	0	-1.527784	1.235111	-0.831334
45	8	0	0.514880	1.949230	0.569922
46	15	0	-0.323622	0.632365	0.098560
47	8	0	0.497162	-0.231326	-0.865064
48	8	0	-0.830673	-0.026543	1.355505
49	6	0	-3.726921	1.532113	0.165408
50	6	0	2.497335	2.723635	-0.586779
51	6	0	2.888211	-3.722667	-0.818579
52	6	0	2.372553	-4.197480	-2.027447
53	6	0	4.208293	-4.046679	-0.472919
54	6	0	3.158830	-4.984230	-2.872627
55	1	0	1.358466	-3.939164	-2.309960
56	6	0	4.993204	-4.832256	-1.316161
57	1	0	4.627435	-3.681748	0.461950
58	6	0	4.469565	-5.305681	-2.521490
59	1	0	2.743165	-5.342984	-3.810752
60	1	0	6.014317	-5.073299	-1.032123
61	1	0	5.080065	-5.916651	-3.180899
62	6	0	-4.096206	0.078794	0.092616
63	6	0	-4.271735	-0.564411	-1.157164
64	6	0	-4.384115	-0.632085	1.288508
65	6	0	-4.733588	-1.885169	-1.181275
66	6	0	-4.859172	-1.945354	1.199987
67	6	0	-5.046670	-2.594724	-0.020551
68	1	0	-4.876096	-2.373117	-2.143832
69	1	0	-5.086396	-2.473821	2.121340
70	6	0	3.061312	3.635559	-1.494531
71	1	0	4.132596	3.593288	-1.665391
72	6	0	3.384504	1.700930	0.058753
73	6	0	4.071415	0.756250	-0.747710
74	6	0	3.611396	1.719384	1.458304
75	6	0	4.951499	-0.143509	-0.131846
76	6	0	4.507268	0.800754	2.015795
77	6	0	5.192663	-0.139483	1.243377
78	1	0	5.480423	-0.864867	-0.750958
79	1	0	4.687565	0.838935	3.087053
80	6	0	-4.038352	0.139683	-2.494108
81	6	0	-5.353171	0.281963	-3.287019
82	6	0	-2.955038	-0.561012	-3.335807
83	1	0	-3.682318	1.152281	-2.291233
84	1	0	-6.111173	0.817669	-2.704471
85	1	0	-5.181683	0.839196	-4.216198
86	1	0	-5.770345	-0.695279	-3.557594
87	1	0	-2.006665	-0.608579	-2.792910
88	1	0	-3.251613	-1.582547	-3.603867
89	1	0	-2.785449	-0.011772	-4.270180
90	6	0	-4.215708	-0.033239	2.689156

91	6	0	-3.258444	-0.856553	3.573130
92	6	0	-5.575902	0.138546	3.396349
93	1	0	-3.768070	0.957782	2.586843
94	1	0	-2.264515	-0.904482	3.123569
95	1	0	-3.161319	-0.382690	4.557865
96	1	0	-3.623478	-1.877962	3.734274
97	1	0	-6.268670	0.750299	2.808074
98	1	0	-6.060256	-0.829990	3.570295
99	1	0	-5.442142	0.622607	4.371478
100	6	0	-5.632234	-3.999233	-0.118932
101	6	0	-7.172999	-3.940947	-0.177912
102	6	0	-5.172251	-4.946394	1.001753
103	1	0	-5.286839	-4.423440	-1.072978
104	1	0	-7.514121	-3.313830	-1.008642
105	1	0	-7.599072	-4.943617	-0.307607
106	1	0	-7.579450	-3.517160	0.748444
107	1	0	-4.080881	-4.966367	1.093563
108	1	0	-5.581598	-4.649822	1.974539
109	1	0	-5.518864	-5.967282	0.802999
110	6	0	3.930147	0.687944	-2.271807
111	6	0	3.435091	-0.682132	-2.766923
112	6	0	5.253395	1.067291	-2.968665
113	1	0	3.177823	1.417117	-2.578435
114	1	0	2.453518	-0.910316	-2.344839
115	1	0	3.338142	-0.670495	-3.859678
116	1	0	4.123840	-1.493087	-2.506683
117	1	0	5.608337	2.057259	-2.659993
118	1	0	6.047705	0.347536	-2.737258
119	1	0	5.122327	1.078555	-4.057557
120	6	0	2.969474	2.747863	2.390332
121	6	0	4.030472	3.692927	2.989888
122	6	0	2.126839	2.084096	3.495951
123	1	0	2.292748	3.370483	1.800911
124	1	0	4.600351	4.199549	2.202742
125	1	0	3.551831	4.460169	3.610654
126	1	0	4.744170	3.151691	3.622293
127	1	0	1.348581	1.446413	3.066962
128	1	0	2.746146	1.473350	4.164406
129	1	0	1.638034	2.849751	4.110870
130	6	0	6.223612	-1.083897	1.849930
131	6	0	5.706428	-1.833536	3.090079
132	6	0	7.531984	-0.334825	2.174845
133	1	0	6.459673	-1.835735	1.083750
134	1	0	4.784816	-2.384985	2.870366
135	1	0	6.454756	-2.551373	3.446315
136	1	0	5.491314	-1.146754	3.916730
137	1	0	7.934419	0.159963	1.284417
138	1	0	7.362860	0.435894	2.936382
139	1	0	8.293475	-1.025720	2.557139

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.214009 hartree

Zero-point Energy Correction = 1.195722 hartree

Thermal Correction to Energy = 1.261463 hartree

Thermal correction to Enthalpy = 1.262408 hartree

Thermal correction to Gibbs Free Energy= 1.092371 hartree

Sum of electronic and Zero-point Energies = -3121.018287 hartree

Sum of electronic and thermal Energies = -3120.952546 hartree

Sum of electronic and thermal Enthalpies = -3120.951602 hartree

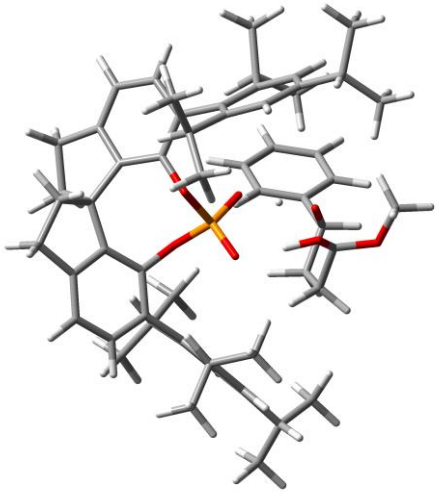
Sum of electronic and thermal Free Energies= -3121.121638 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.031208	2.702585	0.875972
2	8	0	1.166714	4.036168	1.079361
3	8	0	-0.387331	2.574926	-0.024589
4	6	0	2.070603	4.629700	0.089496
5	6	0	2.302458	3.514181	-0.949533
6	6	0	2.077384	2.240199	-0.130777
7	1	0	3.000638	4.837528	0.631724
8	1	0	1.570462	3.589285	-1.758196
9	1	0	3.301643	3.577442	-1.388620
10	1	0	1.758094	1.379135	-0.717711
11	1	0	2.969159	1.953403	0.436181
12	8	0	0.806011	2.061443	2.013940
13	6	0	-1.560109	2.960975	0.729428
14	1	0	-2.416845	2.868032	0.063031
15	1	0	-1.687456	2.314757	1.600199
16	1	0	-1.420616	3.995757	1.044229
17	1	0	-0.489794	1.530411	-0.361920
18	1	0	0.696229	1.065001	1.846297
19	6	0	0.542565	-4.135794	0.073667
20	6	0	1.309202	-2.979348	-0.067199
21	6	0	3.152307	-4.076504	1.018927
22	6	0	2.360956	-5.193676	1.281589
23	6	0	1.051478	-5.211912	0.818292
24	1	0	4.189701	-4.070247	1.336515
25	1	0	2.769742	-6.036060	1.834208
26	6	0	-0.000825	-6.284388	0.998108
27	1	0	0.212873	-7.167257	0.379422
28	1	0	-0.062903	-6.636192	2.034442
29	6	0	-0.796335	-4.538749	-0.538079
30	6	0	-1.287535	-5.568166	0.534658
31	1	0	-1.729431	-5.017433	1.372899
32	1	0	-2.049002	-6.250612	0.144564
33	6	0	-0.577927	-5.279810	-1.901235
34	1	0	0.062057	-4.659010	-2.538729
35	1	0	-0.084985	-6.248654	-1.776491
36	6	0	-1.988425	-5.380728	-2.517336
37	1	0	-2.503583	-6.295733	-2.192767
38	1	0	-1.971981	-5.402084	-3.613171
39	6	0	-2.666480	-4.142328	-1.974567
40	6	0	-1.911637	-3.575898	-0.934757
41	6	0	-3.864644	-3.565104	-2.376061
42	1	0	-4.466363	-4.016340	-3.161175
43	6	0	-2.301134	-2.348745	-0.397225
44	6	0	-4.288646	-2.393246	-1.752621
45	1	0	-5.238109	-1.949695	-2.036003
46	8	0	0.746051	-1.864932	-0.691403
47	8	0	-1.503361	-1.757161	0.580001
48	15	0	-0.195115	-0.852857	0.191244
49	8	0	-0.570168	0.250607	-0.795974
50	8	0	0.445537	-0.460853	1.494498
51	6	0	2.645890	-2.931773	0.380641
52	6	0	-3.511264	-1.735572	-0.783607
53	6	0	1.502736	5.925484	-0.436027
54	6	0	2.228611	7.112415	-0.297548

55	6	0	0.259548	5.960703	-1.083844
56	6	0	1.731414	8.315313	-0.803619
57	1	0	3.189742	7.096811	0.211551
58	6	0	-0.242298	7.161443	-1.581525
59	1	0	-0.313479	5.044358	-1.194092
60	6	0	0.493558	8.342142	-1.445081
61	1	0	2.308466	9.229013	-0.689877
62	1	0	-1.208407	7.177132	-2.079002
63	1	0	0.101335	9.277127	-1.835990
64	6	0	3.558566	-1.754864	0.184713
65	6	0	3.967242	-1.377297	-1.118446
66	6	0	4.114117	-1.086742	1.309684
67	6	0	4.917611	-0.358575	-1.265309
68	6	0	5.075414	-0.090526	1.100723
69	6	0	5.500149	0.288625	-0.175630
70	1	0	5.239091	-0.081506	-2.267267
71	1	0	5.513520	0.395765	1.968587
72	6	0	-4.021437	-0.441637	-0.218563
73	6	0	-4.234776	0.668459	-1.076630
74	6	0	-4.403926	-0.350545	1.144427
75	6	0	-4.843345	1.818801	-0.556481
76	6	0	-4.989385	0.831657	1.611143
77	6	0	-5.233055	1.927003	0.779143
78	1	0	-5.025703	2.661744	-1.220473
79	1	0	-5.288217	0.884931	2.655237
80	6	0	6.600115	1.322741	-0.383524
81	6	0	7.971870	0.763667	0.044639
82	6	0	6.313722	2.660324	0.321808
83	1	0	6.651528	1.525265	-1.462382
84	1	0	8.202583	-0.164965	-0.488417
85	1	0	8.770396	1.486169	-0.164164
86	1	0	7.989238	0.544154	1.118852
87	1	0	5.358818	3.086608	-0.006863
88	1	0	6.269359	2.541679	1.410608
89	1	0	7.102866	3.389090	0.101563
90	6	0	3.468910	-2.075881	-2.384478
91	6	0	4.620771	-2.792010	-3.118148
92	6	0	2.727683	-1.108722	-3.326952
93	1	0	2.754562	-2.848359	-2.091575
94	1	0	5.125349	-3.507933	-2.459691
95	1	0	4.237096	-3.340542	-3.987052
96	1	0	5.374288	-2.082504	-3.479968
97	1	0	1.869402	-0.653393	-2.824210
98	1	0	3.386646	-0.307866	-3.684631
99	1	0	2.357312	-1.647222	-4.208015
100	6	0	3.727111	-1.415740	2.754658
101	6	0	3.305250	-0.167507	3.552955
102	6	0	4.869312	-2.139989	3.497602
103	1	0	2.861518	-2.082049	2.728644
104	1	0	2.509054	0.380545	3.047020
105	1	0	2.935166	-0.465424	4.541197
106	1	0	4.145245	0.518971	3.714136
107	1	0	5.172677	-3.062930	2.993089
108	1	0	5.757041	-1.500273	3.574535
109	1	0	4.557309	-2.399837	4.516474
110	6	0	-4.264445	-1.514553	2.126249
111	6	0	-5.644527	-2.008571	2.605219
112	6	0	-3.356677	-1.159382	3.319431
113	1	0	-3.795214	-2.350535	1.603517
114	1	0	-6.278278	-2.298154	1.759383
115	1	0	-5.530861	-2.881345	3.259759
116	1	0	-6.177297	-1.236041	3.172262
117	1	0	-2.358771	-0.865685	2.981054
118	1	0	-3.776018	-0.339957	3.915865
119	1	0	-3.247794	-2.026198	3.982626
120	6	0	-3.843074	0.675644	-2.557718
121	6	0	-2.863381	1.814386	-2.901829
122	6	0	-5.083337	0.745628	-3.471593
123	1	0	-3.322022	-0.259064	-2.776218
124	1	0	-1.943143	1.723808	-2.319880
125	1	0	-2.595166	1.768901	-3.964511
126	1	0	-3.302529	2.802727	-2.717851
127	1	0	-5.780670	-0.076054	-3.275580
128	1	0	-5.632970	1.683758	-3.328839
129	1	0	-4.785198	0.692378	-4.525694
130	6	0	-5.923540	3.184930	1.291788
131	6	0	-5.150126	3.852772	2.443872
132	6	0	-7.381282	2.900207	1.702803
133	1	0	-5.952316	3.899487	0.457305
134	1	0	-4.126801	4.105921	2.144422
135	1	0	-5.648514	4.777434	2.758600
136	1	0	-5.087778	3.195239	3.318715
137	1	0	-7.947731	2.463432	0.873151
138	1	0	-7.425330	2.197138	2.542973
139	1	0	-7.884961	3.823883	2.012694

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.211215 hartree

Zero-point Energy Correction = 1.194562 hartree

Thermal Correction to Energy = 1.260494 hartree

Thermal correction to Enthalpy = 1.261439 hartree

Thermal correction to Gibbs Free Energy= 1.090787 hartree

Sum of electronic and Zero-point Energies = -3121.016654 hartree

Sum of electronic and thermal Energies = -3120.950721 hartree

Sum of electronic and thermal Enthalpies = -3120.949777 hartree

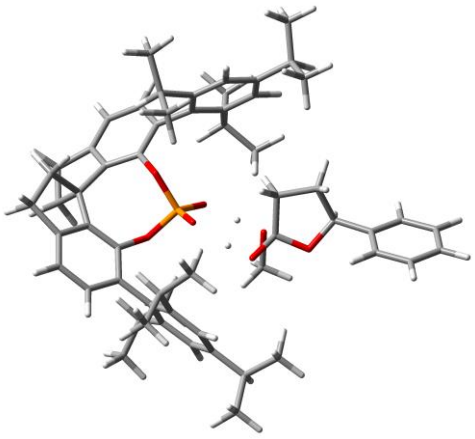
Sum of electronic and thermal Free Energies= -3121.120428 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.252509	3.125042	1.390299
2	6	0	-1.861141	2.155282	0.597085
3	6	0	-3.807999	2.228858	1.998049
4	6	0	-3.161368	3.092726	2.882844
5	6	0	-1.878549	3.532522	2.578109
6	1	0	-4.829289	1.924297	2.200385
7	1	0	-3.664941	3.424474	3.787611
8	6	0	-0.974327	4.456982	3.366047
9	1	0	-1.334930	5.494767	3.336151
10	1	0	-0.913512	4.178125	4.424529
11	6	0	-0.010693	3.978460	1.154974
12	6	0	0.379068	4.309006	2.633931
13	1	0	0.937024	3.461678	3.048880
14	1	0	1.013956	5.197198	2.711705

15	6	0	-0.399949	5.303411	0.412894
16	1	0	-0.993878	5.047666	-0.472023
17	1	0	-1.002907	5.969702	1.037205
18	6	0	0.945137	5.917558	-0.023791
19	1	0	1.362045	6.568011	0.758145
20	1	0	0.857898	6.530285	-0.928406
21	6	0	1.804611	4.691484	-0.235899
22	6	0	1.200418	3.555264	0.326989
23	6	0	3.027147	4.596186	-0.888477
24	1	0	3.504194	5.477419	-1.310210
25	6	0	1.782388	2.303504	0.125142
26	8	0	-1.163372	1.647556	-0.500558
27	8	0	1.126932	1.169142	0.612319
28	15	0	-0.051930	0.471305	-0.289245
29	8	0	0.434609	0.076643	-1.656492
30	8	0	-0.603336	-0.624303	0.625962
31	6	0	-3.173279	1.710015	0.857077
32	6	0	3.030387	2.174754	-0.518939
33	6	0	-3.909788	0.760733	-0.043873
34	6	0	-4.229580	1.145492	-1.370016
35	6	0	-4.359035	-0.496457	0.442405
36	6	0	-4.966886	0.268066	-2.173896
37	6	0	-5.101485	-1.325334	-0.405013
38	6	0	-5.414402	-0.970532	-1.718721
39	1	0	-5.209728	0.566932	-3.191271
40	1	0	-5.442092	-2.284339	-0.023561
41	6	0	3.640037	3.348378	-0.991775
42	1	0	4.611806	3.264804	-1.468016
43	6	0	3.765297	0.873497	-0.680239
44	6	0	3.955433	0.308764	-1.965893
45	6	0	4.386727	0.276759	0.446165
46	6	0	4.757983	-0.834016	-2.086622
47	6	0	5.175809	-0.864391	0.264923
48	6	0	5.382092	-1.436245	-0.993736
49	1	0	4.916358	-1.260812	-3.074405
50	1	0	5.666263	-1.301751	1.131186
51	6	0	-3.859405	2.506303	-1.962283
52	6	0	-5.119865	3.348655	-2.246086
53	6	0	-2.985782	2.373054	-3.224286
54	1	0	-3.275131	3.058377	-1.222725
55	1	0	-5.719673	3.483073	-1.338797
56	1	0	-4.840809	4.341574	-2.620023
57	1	0	-5.759203	2.876539	-3.001342
58	1	0	-2.080187	1.796519	-3.015762
59	1	0	-3.527535	1.878964	-4.039779
60	1	0	-2.685806	3.365263	-3.583973
61	6	0	-4.081201	-0.994480	1.863494
62	6	0	-3.511787	-2.425606	1.891410
63	6	0	-5.347911	-0.930654	2.742744
64	1	0	-3.324366	-0.343429	2.309108
65	1	0	-2.653879	-2.527863	1.224410
66	1	0	-3.184229	-2.679146	2.906390
67	1	0	-4.262575	-3.169237	1.596653
68	1	0	-5.764122	0.080284	2.800731
69	1	0	-6.132768	-1.585229	2.344363
70	1	0	-5.122625	-1.262411	3.763891
71	6	0	-6.217428	-1.892475	-2.626770
72	6	0	-7.636712	-2.143202	-2.083149
73	6	0	-5.484026	-3.221569	-2.888185
74	1	0	-6.321964	-1.380964	-3.593594
75	1	0	-8.175795	-1.200834	-1.936755
76	1	0	-8.215103	-2.763755	-2.778497
77	1	0	-7.607436	-2.663227	-1.118137
78	1	0	-4.485215	-3.044310	-3.302163
79	1	0	-5.366614	-3.798082	-1.962463
80	1	0	-6.045046	-3.842149	-3.597705
81	6	0	3.371115	0.922534	-3.240726
82	6	0	2.618355	-0.096823	-4.116364
83	6	0	4.472637	1.610615	-4.075053
84	1	0	2.643502	1.683182	-2.946211
85	1	0	1.806664	-0.567946	-3.559572
86	1	0	2.178615	0.413805	-4.981583
87	1	0	3.282742	-0.878232	-4.505289
88	1	0	5.001484	2.381114	-3.504429
89	1	0	5.219026	0.883003	-4.416811
90	1	0	4.039019	2.086765	-4.962882
91	6	0	4.310604	0.895329	1.843345
92	6	0	5.647589	1.573436	2.206612
93	6	0	3.892222	-0.110626	2.929718
94	1	0	3.550034	1.679410	1.829128
95	1	0	5.914286	2.338744	1.469436
96	1	0	5.582289	2.055729	3.189728
97	1	0	6.466133	0.844483	2.242830
98	1	0	2.929105	-0.573689	2.692594
99	1	0	4.629692	-0.911449	3.059711
100	1	0	3.792474	0.398423	3.896074
101	6	0	6.292584	-2.643530	-1.185189
102	6	0	5.816542	-3.874441	-0.392442
103	6	0	7.756974	-2.305451	-0.844282
104	1	0	6.257482	-2.906833	-2.251309
105	1	0	4.797154	-4.158281	-0.676602
106	1	0	6.471996	-4.733418	-0.580159
107	1	0	5.822857	-3.681989	0.687054
108	1	0	8.112001	-1.452038	-1.432024
109	1	0	7.868838	-2.049593	0.216121
110	1	0	8.411643	-3.160517	-1.052316
111	6	0	0.154959	-3.195982	-1.461203
112	8	0	-0.470295	-2.993432	0.075691
113	6	0	0.500528	-3.702219	0.916304
114	6	0	1.658726	-3.097174	-1.152227
115	1	0	2.155260	-3.904215	-1.696855
116	1	0	2.040210	-2.146258	-1.526496
117	8	0	-0.440303	-2.297817	-2.236905
118	8	0	-0.182336	-4.472343	-1.770997
119	6	0	-1.547036	-4.690473	-2.171954
120	1	0	-1.654726	-5.773586	-2.245530
121	1	0	-1.742920	-4.223286	-3.139480
122	1	0	-2.234807	-4.290703	-1.421953
123	1	0	-0.531687	-1.869587	0.317369
124	1	0	-0.087443	-1.360697	-2.080116
125	6	0	0.242043	-3.554032	2.396885
126	6	0	0.343692	-2.325003	3.065933
127	6	0	-0.077596	-4.700672	3.135742
128	6	0	0.126105	-2.254470	4.441631
129	1	0	0.555252	-1.417992	2.510594
130	6	0	-0.286122	-4.631373	4.513624
131	1	0	-0.162002	-5.658160	2.626586
132	6	0	-0.184903	-3.404811	5.170226
133	1	0	0.199506	-1.294449	4.945264
134	1	0	-0.530472	-5.532493	5.069655
135	1	0	-0.349233	-3.344135	6.242842
136	1	0	0.361476	-4.752183	0.645560
137	6	0	1.851506	-3.215942	0.377193
138	1	0	2.656284	-3.903386	0.651433
139	1	0	2.096122	-2.239229	0.804188

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1ba (SPINOL-TRIP)



B3LYP/6-31G(d); E(B3LYP) = -3122.215322 hartree

Zero-point correction= 1.195975 hartree

Thermal correction to Energy= 1.261942 hartree

Thermal correction to Enthalpy= 1.262886 hartree

Thermal correction to Gibbs Free Energy= 1.092212 hartree

Sum of electronic and Zero-point Energies= -3121.019347 hartree

Sum of electronic and thermal Energies= -3120.953380 hartree

Sum of electronic and thermal Enthalpies= -3120.952436 hartree

Sum of electronic and thermal Free Energies= -3121.123110 hartree

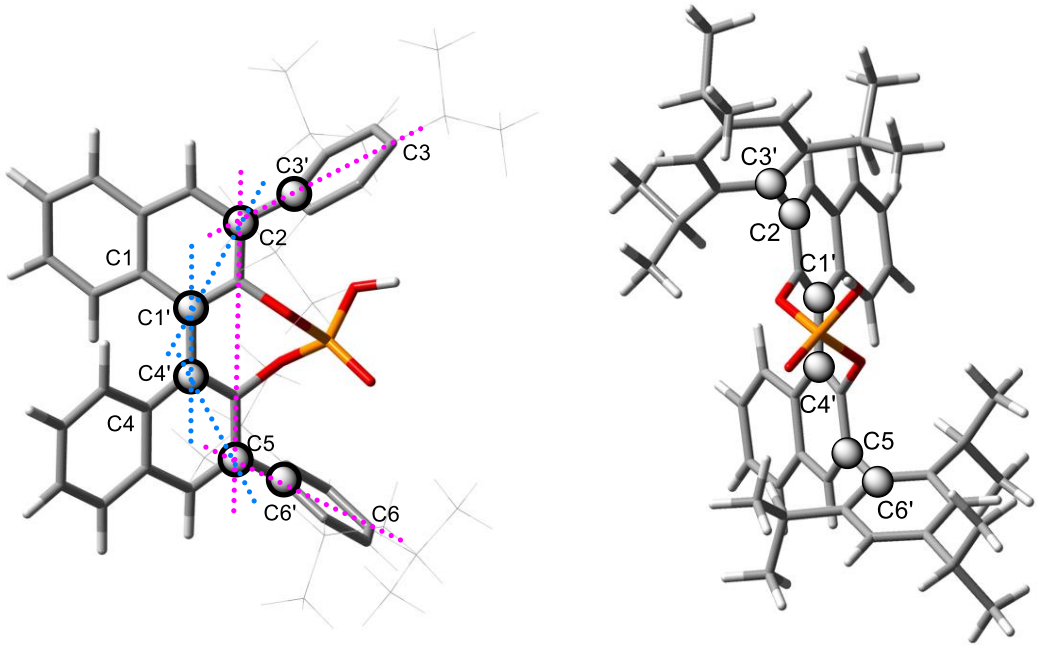
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.753138	-0.746831	-0.072823
2	8	0	4.003582	-1.164333	-0.373315
3	8	0	2.102800	-0.382048	-1.634852
4	6	0	4.870634	-0.000790	-0.507632
5	6	0	4.301869	0.979804	0.538888
6	6	0	2.796035	0.652332	0.558018
7	1	0	4.727251	0.402606	-1.517239
8	1	0	4.759906	0.775176	1.511568
9	1	0	4.513708	2.018979	0.275555
10	1	0	2.376592	0.602580	1.564914
11	1	0	2.201324	1.367506	-0.011596
12	8	0	2.016464	-1.718456	0.417071
13	6	0	2.020706	-1.533252	-2.500848
14	1	0	1.432607	-2.328253	-2.034592
15	1	0	1.549076	-1.206341	-3.430000
16	1	0	3.037042	-1.878827	-2.693609
17	1	0	1.114085	-1.349377	0.724722
18	1	0	1.101841	0.008663	-1.482358
19	6	0	-3.843910	1.713244	-0.634816
20	6	0	-2.563751	2.113854	-0.253840
21	6	0	-2.816794	4.144160	-1.516341
22	6	0	-4.046785	3.705496	-2.007320
23	6	0	-4.548813	2.484789	-1.572984
24	1	0	-2.435458	5.114611	-1.817296
25	1	0	-4.602130	4.316471	-2.714787
26	6	0	-5.829553	1.789865	-1.982495
27	1	0	-6.711171	2.279329	-1.545250
28	1	0	-5.976256	1.793482	-3.068824
29	6	0	-4.736840	0.573630	-0.146241
30	6	0	-5.633344	0.368011	-1.413002
31	1	0	-5.086231	-0.249508	-2.134465
32	1	0	-6.573872	-0.141929	-1.182286
33	6	0	-5.634506	1.040502	1.050582
34	1	0	-4.992800	1.498539	1.812035
35	1	0	-6.379346	1.784217	0.750974
36	6	0	-6.252802	-0.261628	1.603543
37	1	0	-7.194902	-0.506056	1.092674
38	1	0	-6.483114	-0.199564	2.673397
39	6	0	-5.177368	-1.282611	1.302401
40	6	0	-4.233901	-0.756964	0.405658
41	6	0	-5.039449	-2.573576	1.798979
42	1	0	-5.780478	-2.992232	2.475601
43	6	0	-3.086198	-1.492274	0.117578
44	6	0	-3.928136	-3.328254	1.422435
45	1	0	-3.819923	-4.344299	1.789840
46	8	0	-1.807413	1.286747	0.575798
47	8	0	-2.116444	-0.926497	-0.706904
48	15	0	-0.959607	0.049949	-0.077263
49	8	0	-0.213937	-0.586989	1.068430
50	8	0	-0.168453	0.509192	-1.295134
51	6	0	-2.030462	3.353770	-0.663037
52	6	0	-2.910593	-2.801961	0.610283
53	6	0	6.307625	-0.411205	-0.313459
54	6	0	7.309555	0.194888	-1.078621
55	6	0	6.665563	-1.355572	0.657275
56	6	0	8.652219	-0.124439	-0.869917
57	1	0	7.038612	0.919788	-1.843321
58	6	0	8.005802	-1.683318	0.857626
59	1	0	5.889590	-1.844794	1.238270
60	6	0	9.002866	-1.065563	0.098577
61	1	0	9.420853	0.354691	-1.470255
62	1	0	8.272391	-2.423950	1.606833
63	1	0	10.046826	-1.321715	0.257604
64	6	0	-0.693294	3.858286	-0.200785
65	6	0	-0.493126	4.188387	1.164347
66	6	0	0.354544	4.081061	-1.130895
67	6	0	0.735598	4.723328	1.564795
68	6	0	1.563025	4.621317	-0.670982
69	6	0	1.780278	4.952433	0.667041
70	1	0	0.870954	4.983560	2.611603
71	1	0	2.362319	4.803249	-1.386420
72	6	0	-1.688543	-3.616800	0.306570
73	6	0	-0.807506	-4.000252	1.352844
74	6	0	-1.418349	-4.033266	-1.019640
75	6	0	0.323761	-4.760306	1.038911
76	6	0	-0.261873	-4.781257	-1.274696
77	6	0	0.630426	-5.148668	-0.266608
78	1	0	0.995422	-5.047506	1.843470
79	1	0	-0.056938	-5.103448	-2.293999
80	6	0	3.093168	5.586925	1.108911
81	6	0	3.755821	4.836610	2.278198
82	6	0	2.903547	7.077294	1.454332
83	1	0	3.780275	5.534755	0.252472
84	1	0	3.915414	3.780036	2.035871
85	1	0	4.728413	5.281684	2.519970
86	1	0	3.139902	4.879254	3.183915
87	1	0	2.472928	7.626529	0.610086
88	1	0	2.229223	7.199559	2.310364
89	1	0	3.862553	7.542803	1.713004
90	6	0	-1.584444	4.038139	2.224952
91	6	0	-2.019502	5.411365	2.775343
92	6	0	-1.158411	3.091275	3.363292
93	1	0	-2.464779	3.596574	1.752661
94	1	0	-2.361700	6.071286	1.970099
95	1	0	-2.842509	5.293730	3.490984
96	1	0	-1.197756	5.918214	3.295133
97	1	0	-0.886435	2.107124	2.971056
98	1	0	-0.302242	3.489963	3.920930
99	1	0	-1.981925	2.960194	4.076090
100	6	0	0.219644	3.793070	-2.628444
101	6	0	1.381141	2.952321	-3.190550
102	6	0	0.095720	5.102877	-3.435917
103	1	0	-0.692947	3.211461	-2.780335
104	1	0	1.494038	2.014842	-2.642947
105	1	0	1.187467	2.709237	-4.242558

106	1	0	2.335132	3.492330	-3.154425
107	1	0	-0.746615	5.716638	-3.100480
108	1	0	1.003719	5.710497	-3.337593
109	1	0	-0.047990	4.885641	-4.501536
110	6	0	-2.375392	-3.763749	-2.182110
111	6	0	-3.010784	-5.077289	-2.682611
112	6	0	-1.706662	-2.998864	-3.339389
113	1	0	-3.191996	-3.137814	-1.814382
114	1	0	-3.528574	-5.600857	-1.871182
115	1	0	-3.739883	-4.873583	-3.476565
116	1	0	-2.255154	-5.759419	-3.090118
117	1	0	-1.305883	-2.041651	-2.993298
118	1	0	-0.890824	-3.577625	-3.789831
119	1	0	-2.437952	-2.794820	-4.131273
120	6	0	-1.043453	-3.644899	2.824132
121	6	0	0.153842	-2.922641	3.470920
122	6	0	-1.414241	-4.902043	3.638012
123	1	0	-1.888585	-2.954798	2.877945
124	1	0	0.369110	-1.989514	2.946339
125	1	0	-0.078975	-2.681638	4.515678
126	1	0	1.058798	-3.541645	3.471386
127	1	0	-2.289717	-5.413334	3.222071
128	1	0	-0.588448	-5.623561	3.649840
129	1	0	-1.639415	-4.634816	4.677800
130	6	0	1.870480	-5.973271	-0.586727
131	6	0	1.710199	-7.431722	-0.113757
132	6	0	3.160083	-5.351751	-0.019037
133	1	0	1.967901	-5.993583	-1.681472
134	1	0	0.823476	-7.897905	-0.557428
135	1	0	2.586905	-8.030001	-0.391144
136	1	0	1.601929	-7.480733	0.976532
137	1	0	3.270551	-4.305198	-0.320030
138	1	0	3.167099	-5.379823	1.077036
139	1	0	4.037976	-5.909935	-0.366726

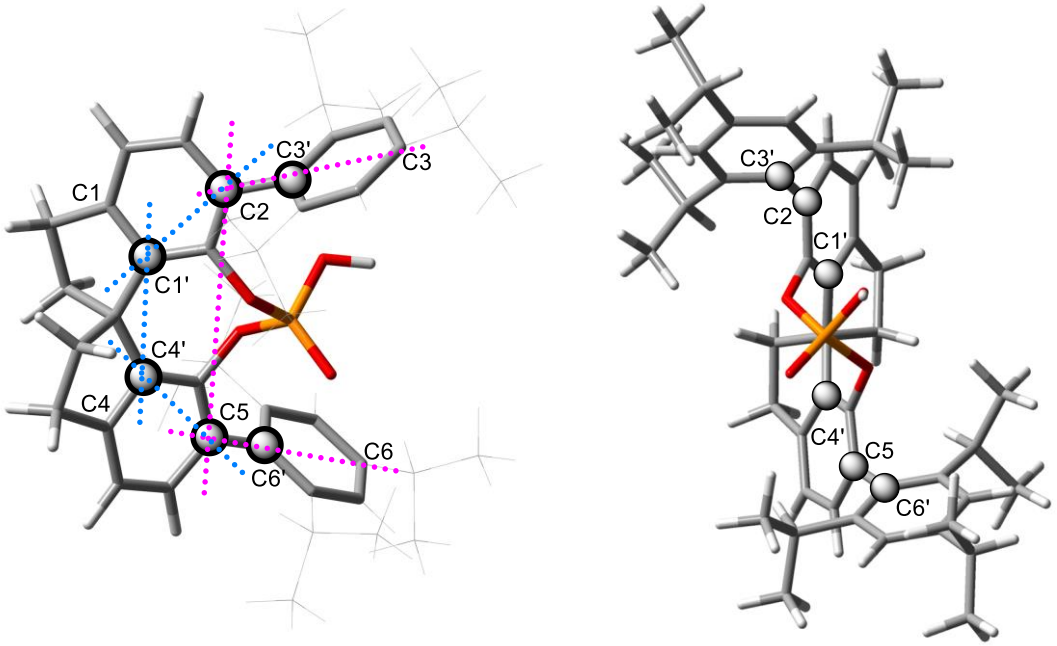
10. Structural Properties of CPAs Derived from BINOL and SPINOL Backbones

BINOL-derived CPA (*R*)-1aa



length of C2-C5: 5.89 Å
angle (average) of C3'-C2-C5 / C2-C5-C6': 123.7°
dihedral angle of C2-C1'-C4'-C5: 64.7°

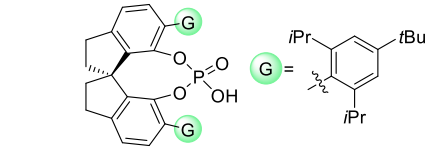
SPINOL-derived CPA (*S*)-1ba



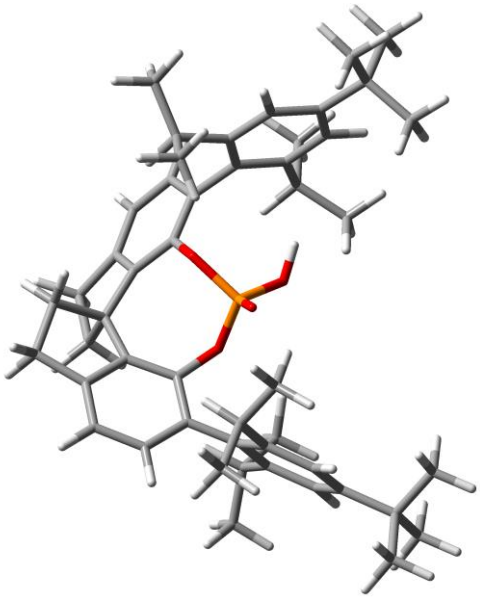
length of C2-C5: 6.38 Å
angle (average) of C3'-C2-C5 / C2-C5-C6': 114.6°
dihedral angle of C2-C1'-C4'-C5: 46.0°

11. DFT Calculation of SPINOL-derived CPAs Having Bulky Substituents

Optimized structure of SPINOL-derived CPA (*S*)-1bd



(*S*)-**1bd** (SPINOL)



E(RB3LYP) = -2547.55701922 Hartree

Zero-point correction= 1.017548 Hartree

Thermal correction to Energy= 1.072477 Hartree

Thermal correction to Enthalpy= 1.073421 Hartree

Thermal correction to Gibbs Free Energy= 0.930016 Hartree

Sum of electronic and zero-point Energies= -2546.539472 Hartree

Sum of electronic and thermal Energies= -2546.484542 Hartree

Sum of electronic and thermal Enthalpies= -2546.483598 Hartree

Sum of electronic and thermal Free Energies= -2546.627003 Hartree

The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.526613	-1.289948	-0.695755
2	6	0	-1.186971	2.993795	0.538045
3	6	0	-1.742845	1.749544	0.245189
4	6	0	-3.720794	2.317197	1.475268
5	6	0	-3.137887	3.517612	1.883415
6	6	0	-1.868984	3.846899	1.420752
7	1	0	-4.724834	2.068117	1.803936
8	1	0	-3.675306	4.184389	2.553203
9	6	0	-1.024773	5.060109	1.748256
10	1	0	-1.403830	5.962198	1.247995
11	1	0	-1.010609	5.279717	2.821891
12	6	0	0.052901	3.709565	0.000807
13	6	0	0.364808	4.656976	1.206476
14	1	0	0.911346	4.090225	1.968833
15	1	0	0.983751	5.512098	0.917287
16	6	0	-0.305474	4.574079	-1.257485
17	1	0	-0.851831	3.946985	-1.971255
18	1	0	-0.942100	5.428433	-1.009041
19	6	0	1.058623	4.977045	-1.856899
20	1	0	1.435774	5.905816	-1.406260
21	1	0	1.012613	5.148028	-2.938350
22	6	0	1.930051	3.794879	-1.494366
23	6	0	1.305652	3.006043	-0.514548
24	6	0	3.169129	3.434672	-2.012049
25	1	0	3.664336	4.058374	-2.752020
26	6	0	1.892807	1.798226	-0.152323
27	6	0	3.766455	2.247064	-1.586456
28	1	0	4.735482	1.961868	-1.983736
29	8	0	-0.985898	0.828493	-0.501188
30	8	0	1.250696	0.985406	0.784218
31	15	0	0.080649	-0.054699	0.339947
32	8	0	0.663853	-0.882843	-0.905232
33	8	0	-0.392845	-0.792724	1.522713
34	6	0	-3.032669	1.388504	0.677752
35	6	0	3.130465	1.381631	-0.683330
36	6	0	3.725883	0.047606	-0.333082
37	6	0	3.854688	-0.967448	-1.325880
38	6	0	4.164958	-0.219589	0.985204
39	6	0	4.375851	-2.211829	-0.953044
40	6	0	4.687171	-1.483526	1.292476
41	6	0	4.795424	-2.506886	0.350259
42	1	0	4.465553	-2.976361	-1.718675
43	1	0	5.016357	-1.659472	2.309836
44	6	0	-3.681908	0.088764	0.299284
45	6	0	-4.059607	-0.148377	-1.042476
46	6	0	-3.977885	-0.885721	1.287301
47	6	0	-4.711069	-1.345034	-1.369998
48	6	0	-4.637111	-2.055556	0.901353
49	6	0	-5.014495	-2.320793	-0.420028
50	1	0	-4.991812	-1.501717	-2.405369
51	1	0	-4.857772	-2.791417	1.668838
52	6	0	-3.625874	-0.710989	2.766713
53	6	0	-4.889988	-0.443120	3.609842
54	6	0	-2.846915	-1.910295	3.339980
55	1	0	-2.970478	0.159140	2.858354
56	1	0	-5.576314	-1.298036	3.573604
57	1	0	-5.442121	0.435057	3.256675
58	1	0	-1.936734	-2.087961	2.764048
59	1	0	-3.449884	-2.826461	3.347153
60	6	0	-3.833051	0.868259	-2.162535
61	6	0	-2.950902	0.301945	-3.291674
62	6	0	-5.170986	1.398340	-2.716258
63	1	0	-3.304926	1.728959	-1.743757
64	1	0	-3.435360	-0.540890	-3.798944
65	1	0	-1.989257	-0.043639	-2.900924
66	1	0	-5.780244	1.842817	-1.921222
67	1	0	-5.760562	0.598778	-3.180007
68	6	0	3.507038	-0.746155	-2.804147
69	6	0	4.795313	-0.579963	-3.638513
70	6	0	2.634238	-1.859286	-3.417498
71	1	0	2.936687	0.182951	-2.884014
72	1	0	5.390253	-1.501092	-3.627121
73	1	0	5.430879	0.224988	-3.254873
74	1	0	1.686163	-1.977048	-2.885178
75	1	0	3.145328	-2.828771	-3.428568
76	6	0	4.151275	0.837479	2.089717
77	6	0	3.372957	0.380715	3.338163
78	6	0	5.588840	1.260481	2.455794
79	1	0	3.648759	1.727726	1.703666
80	1	0	3.857221	-0.471047	3.830551
81	1	0	2.349269	0.091848	3.083483
82	1	0	6.129012	1.635219	1.579029
83	1	0	6.161803	0.421132	2.867552
84	1	0	-4.622363	-0.274449	4.660194
85	1	0	-2.560486	-1.702324	4.378409
86	1	0	-4.993695	2.166409	-3.479286
87	1	0	-2.757882	1.073493	-4.047596

88	1	0	2.397425	-1.607774	-4.457870
89	1	0	4.550226	-0.351302	-4.682633
90	1	0	3.326246	1.196102	4.070105
91	1	0	5.572573	2.055487	3.211045
92	6	0	5.350700	-3.903489	0.684688
93	6	0	6.599941	-4.183860	-0.184262
94	1	0	7.386975	-3.446431	0.010891
95	1	0	7.003473	-5.178988	0.039256
96	1	0	6.369619	-4.151537	-1.254334
97	6	0	5.757310	-4.034240	2.164782
98	1	0	6.548403	-3.325678	2.435562
99	1	0	4.907384	-3.872849	2.837347
100	1	0	6.140488	-5.043381	2.353405
101	6	0	4.269491	-4.969762	0.387034
102	1	0	3.374362	-4.801656	0.996582
103	1	0	3.964616	-4.960088	-0.664701
104	1	0	4.651226	-5.972706	0.613820
105	6	0	-5.729888	-3.639330	-0.767991
106	6	0	-4.818299	-4.832628	-0.394902
107	1	0	-4.571676	-4.838706	0.671756
108	1	0	-5.315876	-5.782116	-0.629298
109	1	0	-3.876312	-4.794316	-0.953694
110	6	0	-6.068834	-3.747261	-2.266880
111	1	0	-6.740035	-2.944243	-2.592403
112	1	0	-5.169008	-3.715127	-2.891637
113	1	0	-6.573934	-4.699928	-2.463700
114	6	0	-7.051565	-3.736317	0.030526
115	1	0	-7.569742	-4.675600	-0.199967
116	1	0	-6.877811	-3.708190	1.111181
117	1	0	-7.722771	-2.907104	-0.221298

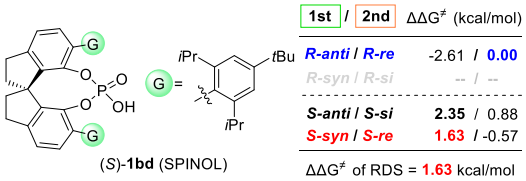
DFT calculation for all conformations of real system using Cy-SPINOL-derived CPA (*S*)-1bd

TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-anti	up	up	-3199.692163	-2.59
	up	down	-3199.692191	-2.61
	down	up	-3199.691950	-2.46
	down	down	-3199.692144	-2.58
S-anti	up	up	-3199.684283	2.35
	up	down	-3199.684180	2.42
	down	up	-3199.683759	2.68
	down	down	-3199.683107	3.09
S-syn	up	up	-3199.68538	1.66
	up	down	-3199.685436	1.63
	down	down	-3199.685107	1.84
	down	up	-3199.685173	1.79

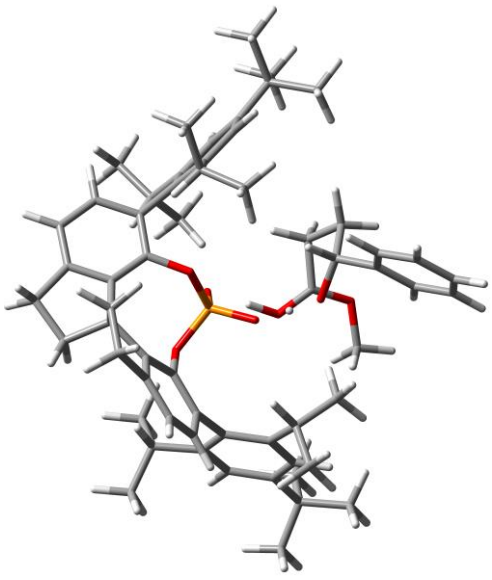
TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-re	up	up	-3199.688032	0.00
	up	down	-3199.687747	0.18
	down	up	-3199.687644	0.24
	down	down	-3199.687453	0.36
S-si	up	up	-3199.686632	0.88
	up	down	-3199.686294	1.09
	down	up	-3199.686600	0.90
	down	down	-3199.686177	1.16
S-re	up	up	-3199.688944	-0.57
	up	down	-3199.688381	-0.22
	down	up	-3199.688449	-0.26
	down	down	-3199.687898	0.08

* Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using SPINOL-derived CPA (*S*)-1bd



TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1bd (SPINOL)

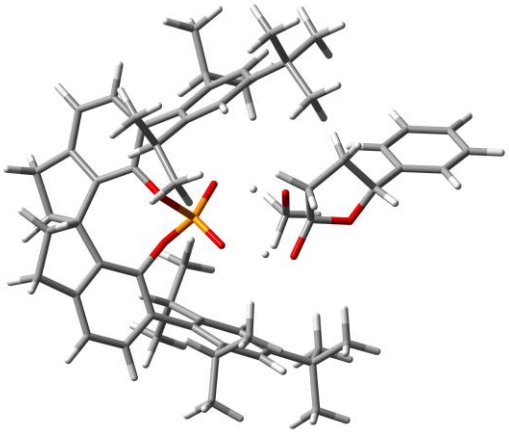


E(RB3LYP) = -3200.83786196 Hartree
Zero-point correction= 1.250976 Hartree
Thermal correction to Energy= 1.319163 Hartree
Thermal correction to Enthalpy= 1.320107 Hartree
Thermal correction to Gibbs Free Energy= 1.145671 Hartree
Sum of electronic and zero-point Energies= -3199.586886 Hartree
Sum of electronic and thermal Energies= -3199.518699 Hartree
Sum of electronic and thermal Enthalpies= -3199.517755 Hartree
Sum of electronic and thermal Free Energies= -3199.692191 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.112774	-2.961103	-1.507571
2	8	0	-0.200766	-2.705750	0.152069
3	6	0	0.976165	-3.090501	0.926028
4	6	0	1.956342	-3.690546	-0.104587
5	6	0	1.629159	-2.979274	-1.417304
6	1	0	1.396104	-2.163495	1.330609
7	1	0	1.792652	-4.767581	-0.202986
8	1	0	2.989268	-3.530471	0.212728
9	1	0	2.033764	-3.491487	-2.294875
10	1	0	1.993280	-1.947924	-1.416050
11	8	0	-0.528984	-2.006613	-2.162449
12	8	0	-0.378307	-4.196508	-1.737970
13	6	0	-1.800425	-4.294691	-1.939425
14	1	0	-2.009157	-5.364166	-1.988112
15	1	0	-2.090299	-3.807734	-2.872892
16	1	0	-2.336674	-3.839832	-1.102113
17	1	0	-0.437668	-1.616758	0.396848
18	1	0	-0.135973	-1.085065	-1.986498
19	6	0	1.089409	3.834887	0.415643
20	6	0	1.703759	2.594437	0.241819

21	6	0	3.537583	3.661204	-0.891049
22	6	0	2.890973	4.893974	-0.820336
23	6	0	1.663017	4.972422	-0.174950
24	1	0	4.513771	3.593298	-1.360843
25	1	0	3.346530	5.777165	-1.261331
26	6	0	0.767850	6.178549	0.003517
27	1	0	1.166409	6.864101	0.764717
28	1	0	0.661655	6.761156	-0.918822
29	6	0	-0.128617	4.247683	1.238487
30	6	0	-0.558884	5.538688	0.461238
31	1	0	-1.147788	5.240838	-0.413836
32	1	0	-1.178583	6.205083	1.068907
33	6	0	0.268560	4.633732	2.702733
34	1	0	0.856912	3.816018	3.134668
35	1	0	0.877075	5.542471	2.746209
36	6	0	-1.078971	4.760736	3.447901
37	1	0	-1.476851	5.783322	3.385348
38	1	0	-0.995052	4.522510	4.514618
39	6	0	-1.958081	3.777201	2.705199
40	6	0	-1.339384	3.362346	1.515801
41	6	0	-3.211359	3.288423	3.054437
42	1	0	-3.708005	3.623624	3.961738
43	6	0	-1.923440	2.346769	0.762317
44	6	0	-3.834979	2.364989	2.214807
45	1	0	-4.832827	2.012981	2.455185
46	8	0	1.077073	1.453741	0.747222
47	8	0	-1.233803	1.846892	-0.343982
48	15	0	-0.083559	0.707334	-0.135389
49	8	0	-0.594123	-0.400259	0.786620
50	8	0	0.399706	0.319989	-1.508204
51	6	0	2.956259	2.482188	-0.395147
52	6	0	-3.202997	1.843804	1.073437
53	6	0	0.601257	-4.013457	2.061951
54	6	0	1.006510	-3.717257	3.366846
55	6	0	-0.130123	-5.185518	1.824758
56	6	0	0.698181	-4.581667	4.419844
57	1	0	1.563278	-2.803505	3.561673
58	6	0	-0.445763	-6.044270	2.875472
59	1	0	-0.455524	-5.414736	0.813834
60	6	0	-0.029425	-5.746139	4.176278
61	1	0	1.020076	-4.339269	5.429090
62	1	0	-1.017649	-6.947898	2.681189
63	1	0	-0.275441	-6.417550	4.994628
64	6	0	-3.912287	0.823185	0.231059
65	6	0	-4.263372	-0.439353	0.768295
66	6	0	-4.312086	1.144915	-1.091646
67	6	0	-4.997900	-1.337042	-0.020181
68	6	0	-5.035455	0.206535	-1.831285
69	6	0	-5.398828	-1.046043	-1.324773
70	1	0	-5.261215	-2.293347	0.416838
71	1	0	-5.336950	0.475641	-2.839784
72	6	0	3.720698	1.196509	-0.536667
73	6	0	4.308252	0.589283	0.601626
74	6	0	3.979470	0.654113	-1.818610
75	6	0	5.147798	-0.515470	0.428379
76	6	0	4.836314	-0.451095	-1.931546
77	6	0	5.453290	-1.048706	-0.830135
78	1	0	5.609863	-0.948195	1.311749
79	1	0	5.036797	-0.833093	-2.925983
80	6	0	3.400293	1.246022	-3.106952
81	6	0	4.496003	1.928939	-3.951978
82	6	0	2.652079	0.203970	-3.959765
83	1	0	2.667326	2.007208	-2.828251
84	1	0	5.247055	1.203813	-4.288676
85	1	0	5.020737	2.709198	-3.390530
86	1	0	1.828585	-0.237744	-3.395731
87	1	0	3.315520	-0.597070	-4.308091
88	6	0	4.117203	1.133475	2.018426
89	6	0	3.413392	0.116524	2.936926
90	6	0	5.451784	1.604249	2.630033
91	1	0	3.470709	2.012372	1.961532
92	1	0	4.001758	-0.803081	3.046106
93	1	0	2.427498	-0.144175	2.538963
94	1	0	5.935743	2.353022	1.993166
95	1	0	6.155228	0.773618	2.761645
96	6	0	-3.896430	-0.876338	2.189192
97	6	0	-5.134289	-0.888890	3.110687
98	6	0	-3.207476	-2.253225	2.233212
99	1	0	-3.182282	-0.153042	2.591096
100	1	0	-5.874088	-1.620713	2.763690
101	1	0	-5.631676	0.085928	3.148915
102	1	0	-2.340274	-2.286787	1.571623
103	1	0	-3.889610	-3.062753	1.945870
104	6	0	-4.038206	2.503335	-1.739466
105	6	0	-3.204337	2.374688	-3.028434
106	6	0	-5.349874	3.271487	-1.999455
107	1	0	-3.456299	3.107267	-1.039540
108	1	0	-3.744695	1.821155	-3.805956
109	1	0	-2.259911	1.858562	-2.834010
110	1	0	-5.923093	3.401804	-1.074558
111	1	0	-5.990770	2.745861	-2.717256
112	1	0	4.057474	2.392304	-4.844107
113	1	0	2.229716	0.686607	-4.849479
114	1	0	5.282644	2.054392	3.615823
115	1	0	3.271984	0.539591	3.939110
116	1	0	-2.863341	-2.467590	3.252051
117	1	0	-4.848575	-1.162832	4.133812
118	1	0	-2.975035	3.368530	-3.432725
119	1	0	-5.136551	4.265919	-2.410658
120	6	0	-6.216111	-2.021504	-2.192127
121	6	0	-5.440395	-2.334171	-3.493468
122	1	0	-4.472845	-2.798466	-3.269825
123	1	0	-6.013151	-3.025108	-4.124760
124	1	0	-5.244798	-1.430589	-4.079575
125	6	0	-6.499780	-3.353704	-1.472541
126	1	0	-5.574937	-3.877892	-1.204845
127	1	0	-7.084140	-3.206968	-0.557235
128	1	0	-7.076521	-4.014248	-2.130231
129	6	0	-7.574383	-1.373671	-2.553060
130	1	0	-8.152661	-1.149328	-1.649434
131	1	0	-7.443478	-0.437614	-3.105745
132	1	0	-8.168923	-2.051482	-3.178503
133	6	0	6.483634	-2.187752	-0.962436
134	6	0	7.861775	-1.666823	-0.485629
135	1	0	7.832850	-1.347491	0.561467
136	1	0	8.621912	-2.452830	-0.576962
137	1	0	8.184257	-0.809294	-1.086895
138	6	0	6.634113	-2.679802	-2.414722
139	1	0	5.686513	-3.055823	-2.817570
140	1	0	6.996778	-1.888114	-3.079529
141	1	0	7.360118	-3.499955	-2.453879
142	6	0	6.075244	-3.397440	-0.091230
143	1	0	6.842341	-4.179889	-0.142190
144	1	0	5.951027	-3.124865	0.961859
145	1	0	5.132213	-3.832321	-0.441295

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1bd (SPINOL)



E(RB3LYP) = -3200.83603328 Hartree

Zero-point correction= 1.252076 (Hartree)

Thermal correction to Energy= 1.320179 (Hartree)

Thermal correction to Enthalpy= 1.321123 (Hartree)

Thermal correction to Gibbs Free Energy= 1.148001 (Hartree)

Sum of electronic and zero-point Energies= -3199.583957 (Hartree)

Sum of electronic and thermal Energies= -3199.515855 (Hartree)

Sum of electronic and thermal Enthalpies= -3199.514910 (Hartree)

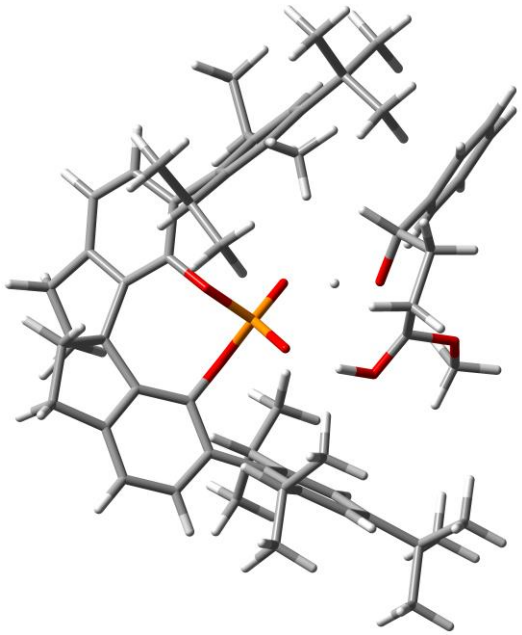
Sum of electronic and thermal Free Energies= -3199.688032 (Hartree)

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.481027	2.762399	0.607949
2	8	0	-0.609505	4.104341	0.503797
3	8	0	-0.574192	2.232746	-1.024019
4	6	0	-2.002116	4.519125	0.720862
5	6	0	-2.806295	3.203632	0.747817
6	6	0	-1.762162	2.169374	1.179549
7	1	0	-2.009731	4.986867	1.712023
8	1	0	-3.190805	2.966654	-0.247245
9	1	0	-3.656403	3.272991	1.431690
10	1	0	-1.958644	1.155069	0.831625
11	1	0	-1.638435	2.139945	2.268063
12	8	0	0.714140	2.413020	1.041280
13	6	0	0.493846	2.753111	-1.845516
14	1	0	0.360365	3.832388	-1.925542
15	1	0	0.401862	2.284249	-2.827395
16	1	0	1.466667	2.522104	-1.404008
17	1	0	-0.511061	1.134407	-1.032368
18	1	0	0.758830	1.405400	1.182580
19	6	0	2.604655	-3.504803	-0.104008
20	6	0	2.738507	-2.117668	-0.136983
21	6	0	4.810077	-2.282653	1.074193
22	6	0	4.647281	-3.662218	1.199466
23	6	0	3.534924	-4.264456	0.623681
24	1	0	5.685464	-1.804244	1.502830
25	1	0	5.380123	-4.251990	1.744701
26	6	0	3.119412	-5.718591	0.667117
27	1	0	3.737052	-6.333763	-0.002509
28	1	0	3.216067	-6.151801	1.669335
29	6	0	1.616456	-4.436947	-0.800388
30	6	0	1.655442	-5.656494	0.183189
31	1	0	0.993952	-5.444464	1.031026
32	1	0	1.310667	-6.583440	-0.285286
33	6	0	2.141332	-4.890511	-2.203720
34	1	0	2.412310	-3.999996	-2.782348
35	1	0	3.029287	-5.526437	-2.133304
36	6	0	0.932356	-5.594080	-2.858931
37	1	0	0.912252	-6.665837	-2.616292
38	1	0	0.942663	-5.520920	-3.952636
39	6	0	-0.242666	-4.863849	-2.244409
40	6	0	0.176618	-4.077114	-1.159553
41	6	0	-1.579628	-4.891196	-2.622958
42	1	0	-1.913077	-5.518168	-3.446333
43	6	0	-0.733795	-3.209093	-0.559435
44	6	0	-2.496730	-4.104441	-1.925290
45	1	0	-3.549027	-4.149812	-2.187151
46	8	0	1.765232	-1.361416	-0.789569
47	8	0	-0.288606	-2.332222	0.428792
48	15	0	0.400057	-0.913438	-0.000608
49	8	0	-0.433261	-0.213583	-1.070814
50	8	0	0.666740	-0.177515	1.286093
51	6	0	3.852605	-1.474334	0.440595
52	6	0	-2.099999	-3.221144	-0.908186
53	6	0	-2.417206	5.540341	-0.310012
54	6	0	-2.780542	6.828878	0.093678
55	6	0	-2.460013	5.218624	-1.674465
56	6	0	-3.188411	7.781192	-0.842769
57	1	0	-2.742967	7.090636	1.148758
58	6	0	-2.858149	6.170063	-2.611356
59	1	0	-2.179007	4.221146	-2.000245
60	6	0	-3.226060	7.453595	-2.197656
61	1	0	-3.470065	8.777435	-0.512889
62	1	0	-2.884916	5.909871	-3.666127
63	1	0	-3.539272	8.193144	-2.929596
64	6	0	-3.123565	-2.359095	-0.227040
65	6	0	-3.848722	-1.385253	-0.956747
66	6	0	-3.429919	-2.561859	1.143256
67	6	0	-4.851188	-0.649608	-0.307139
68	6	0	-4.435147	-1.794898	1.737433
69	6	0	-5.170741	-0.830355	1.039706
70	1	0	-5.398699	0.082046	-0.890187
71	1	0	-4.659782	-1.974110	2.785204
72	6	0	4.034723	0.014155	0.401653
73	6	0	4.273399	0.673112	-0.825870
74	6	0	4.014729	0.771311	1.602679
75	6	0	4.444909	2.065172	-0.836370
76	6	0	4.206732	2.153182	1.531488
77	6	0	4.408419	2.836840	0.327111
78	1	0	4.630187	2.545741	-1.790904
79	1	0	4.188833	2.718021	2.458652
80	6	0	4.429108	-0.080497	-2.148184
81	6	0	3.416057	0.372444	-3.215817
82	6	0	5.874165	0.028062	-2.676245
83	1	0	4.241462	-1.140567	-1.959797
84	1	0	3.555209	1.426584	-3.486137
85	1	0	2.390456	0.236033	-2.860506
86	1	0	6.594277	-0.336970	-1.935421
87	1	0	6.139143	1.064891	-2.915332
88	6	0	3.825709	0.142626	2.986772
89	6	0	5.140366	0.189768	3.793356
90	6	0	2.681902	0.783249	3.795803
91	1	0	3.558834	-0.908004	2.849278
92	1	0	5.443969	1.224274	3.995062
93	1	0	5.965268	-0.294983	3.259263
94	1	0	1.731755	0.682148	3.267811
95	1	0	2.861649	1.846207	3.995724
96	6	0	-3.612677	-1.107078	-2.443989
97	6	0	-4.778729	-1.637330	-3.304459
98	6	0	-3.381602	0.385410	-2.747166
99	1	0	-2.703386	-1.632379	-2.745976
100	1	0	-5.714441	-1.118457	-3.062694
101	1	0	-4.949252	-2.708008	-3.150635
102	1	0	-2.551828	0.781049	-2.158294
103	1	0	-4.273704	0.990324	-2.543390
104	6	0	-2.745990	-3.627165	2.001675
105	6	0	-2.029501	-3.016633	3.221276
106	6	0	-3.743477	-4.721714	2.431762

107	1	0	-1.983429	-4.119784	1.394373
108	1	0	-2.739127	-2.546027	3.912870
109	1	0	-1.300543	-2.262916	2.910359
110	1	0	-4.221535	-5.186806	1.562202
111	1	0	-4.536840	-4.317433	3.071709
112	1	0	-1.498043	-3.797726	3.778908
113	1	0	-3.228535	-5.507653	2.997810
114	1	0	-3.138203	0.515884	-3.808923
115	1	0	-4.574120	-1.477520	-4.370315
116	1	0	2.588073	0.279484	4.765981
117	1	0	5.017664	-0.316259	4.758850
118	1	0	5.995065	-0.566356	-3.590336
119	1	0	3.539602	-0.218589	-4.131780
120	6	0	4.604830	4.364211	0.331759
121	6	0	3.412163	5.045074	1.045083
122	1	0	3.335843	4.738151	2.093009
123	1	0	3.533689	6.135530	1.026872
124	1	0	2.461300	4.794487	0.563660
125	6	0	4.707542	4.947313	-1.090574
126	1	0	5.570681	4.549641	-1.636451
127	1	0	3.806462	4.741969	-1.680106
128	1	0	4.826724	6.035476	-1.036029
129	6	0	5.911708	4.705451	1.087273
130	1	0	6.066168	5.791502	1.116861
131	1	0	5.886549	4.342407	2.120193
132	1	0	6.779665	4.251531	0.595004
133	6	0	-6.288870	-0.046835	1.752711
134	6	0	-7.378794	-1.035341	2.232585
135	1	0	-6.974362	-1.779292	2.926709
136	1	0	-8.184360	-0.498044	2.748697
137	1	0	-7.817506	-1.574020	1.384985
138	6	0	-6.958210	0.992935	0.833995
139	1	0	-6.240424	1.735891	0.467186
140	1	0	-7.435291	0.524053	-0.033878
141	1	0	-7.736917	1.529773	1.387930
142	6	0	-5.706980	0.698685	2.976729
143	1	0	-6.497128	1.251098	3.500337
144	1	0	-5.248732	0.011395	3.694983
145	1	0	-4.938110	1.417003	2.668108

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1bd (SPINOL)



E(RB3LYP) = -3200.83186885 Hartree

Zero-point correction= 1.251294 Hartree

Thermal correction to Energy= 1.319319 Hartree

Thermal correction to Enthalpy= 1.320264 Hartree

Thermal correction to Gibbs Free Energy= 1.147586 Hartree

Sum of electronic and zero-point Energies= -3199.580575 Hartree

Sum of electronic and thermal Energies= -3199.512550 Hartree

Sum of electronic and thermal Enthalpies= -3199.511605 Hartree

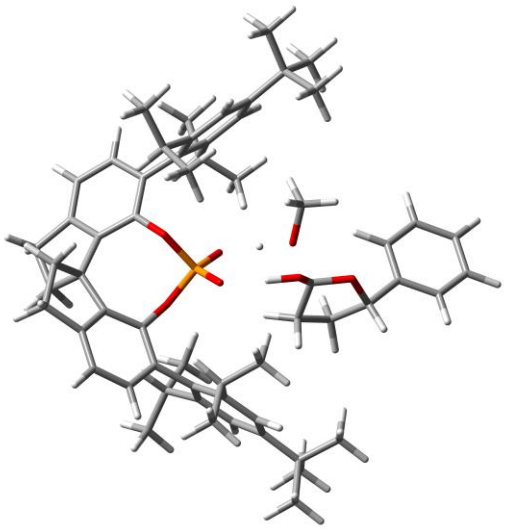
Sum of electronic and thermal Free Energies= -3199.684283 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.578435	-3.060481	0.725209
2	8	0	0.577406	-2.549221	-0.426729
3	6	0	1.892893	-2.936393	0.046493
4	6	0	1.681809	-3.528134	1.468605
5	6	0	0.330768	-2.991049	1.937902
6	1	0	2.478458	-2.011738	0.113851
7	1	0	1.656095	-4.619779	1.418436
8	1	0	2.492110	-3.236625	2.142002
9	1	0	-0.101857	-3.583996	2.748824
10	1	0	0.393018	-1.946860	2.256777
11	8	0	-1.611102	-2.244827	0.599053
12	8	0	-0.835459	-4.334630	0.375233
13	6	0	-1.663132	-4.534238	-0.784209
14	1	0	-1.796950	-5.613867	-0.859249
15	1	0	-2.624664	-4.032299	-0.666424
16	1	0	-1.152626	-4.156215	-1.674244
17	1	0	0.510269	-1.426184	-0.641234
18	1	0	-1.397057	-1.324003	0.962170
19	6	0	-2.026846	3.647149	-0.223630
20	6	0	-2.370220	2.295942	-0.280720
21	6	0	-4.491949	2.802639	0.733039
22	6	0	-4.129476	4.138791	0.884356
23	6	0	-2.885415	4.550202	0.424346
24	1	0	-5.468452	2.470862	1.071339
25	1	0	-4.809478	4.841041	1.360302
26	6	0	-2.250498	5.918902	0.526699
27	1	0	-2.700631	6.627111	-0.183188
28	1	0	-2.365826	6.358571	1.524136
29	6	0	-0.853381	4.414931	-0.824841
30	6	0	-0.779669	5.623051	0.170978
31	1	0	-0.237105	5.304861	1.068632
32	1	0	-0.250301	6.482462	-0.251216
33	6	0	-1.194841	4.951849	-2.254741
34	1	0	-1.536861	4.113800	-2.872719
35	1	0	-1.990065	5.703394	-2.241367
36	6	0	0.149046	5.488276	-2.791922
37	1	0	0.294644	6.545094	-2.528113
38	1	0	0.223835	5.425293	-3.883772
39	6	0	1.155710	4.596872	-2.097394
40	6	0	0.541661	3.849500	-1.078522
41	6	0	2.515074	4.465833	-2.351863
42	1	0	3.000785	5.068324	-3.115535
43	6	0	1.270868	2.848949	-0.435062
44	8	0	-1.466613	1.397327	-0.854907
45	8	0	0.636188	2.029786	0.500907
46	15	0	-0.272543	0.749461	0.058248
47	8	0	0.488250	-0.163001	-0.907907
48	8	0	-0.791134	0.129989	1.330857
49	6	0	-3.618334	1.841484	0.194608
50	6	0	2.651346	2.686802	-0.673082
51	6	0	2.563544	-3.897305	-0.920275
52	6	0	2.065882	-4.115175	-2.208882
53	6	0	3.730681	-4.567882	-0.526706
54	6	0	2.715677	-4.990004	-3.082383
55	1	0	1.170124	-3.593260	-2.526329
56	6	0	4.383393	-5.437300	-1.400731
57	1	0	4.133884	-4.415377	0.471496

58	6	0	3.875695	-5.653727	-2.683321
59	1	0	2.312838	-5.148951	-4.079316
60	1	0	5.286182	-5.948436	-1.076802
61	1	0	4.381085	-6.332925	-3.364515
62	6	0	-4.082517	0.413378	0.179874
63	6	0	-4.349676	-0.255303	-1.036201
64	6	0	-4.393494	-0.234174	1.406733
65	6	0	-4.937069	-1.528796	-1.005659
66	6	0	-4.992249	-1.495501	1.373153
67	6	0	-5.290192	-2.169285	0.183429
68	1	0	-5.144738	-2.010982	-1.954558
69	1	0	-5.242655	-1.963554	2.320656
70	6	0	3.252395	3.546535	-1.608342
71	1	0	4.320937	3.454465	-1.776847
72	6	0	3.496847	1.648207	0.001730
73	6	0	4.163121	0.668025	-0.775295
74	6	0	3.714817	1.684304	1.402665
75	6	0	5.019769	-0.242864	-0.138206
76	6	0	4.579640	0.751346	1.980447
77	6	0	5.258201	-0.222030	1.237631
78	1	0	5.524256	-0.977223	-0.756013
79	1	0	4.746274	0.808149	3.052600
80	6	0	-4.116194	0.383451	2.782127
81	6	0	-5.422586	0.687369	3.543612
82	6	0	-3.191074	-0.498274	3.643777
83	1	0	-3.591964	1.330048	2.632514
84	1	0	-5.979646	-0.231178	3.764373
85	1	0	-6.086734	1.343996	2.970985
86	1	0	-2.225349	-0.635952	3.153032
87	1	0	-3.630416	-1.483353	3.841603
88	6	0	-4.083562	0.375166	-2.403489
89	6	0	-3.069305	-0.441890	-3.226300
90	6	0	-5.391917	0.592617	-3.189828
91	1	0	-3.645035	1.362884	-2.244808
92	1	0	-3.450234	-1.445302	-3.453509
93	1	0	-2.122594	-0.546117	-2.688355
94	1	0	-6.098968	1.206332	-2.620290
95	1	0	-5.887990	-0.356816	-3.423814
96	6	0	3.102458	2.750084	2.312966
97	6	0	2.233365	2.136274	3.426897
98	6	0	4.191465	3.670596	2.900736
99	1	0	2.449826	3.383607	1.708489
100	1	0	2.828223	1.513841	4.106798
101	1	0	1.432337	1.521243	3.007039
102	1	0	4.784692	4.139922	2.107785
103	1	0	4.881043	3.118519	3.550394
104	6	0	4.024430	0.561758	-2.297880
105	6	0	5.362712	0.856600	-3.005722
106	6	0	3.463357	-0.798342	-2.747662
107	1	0	3.307286	1.314743	-2.629679
108	1	0	6.122383	0.105478	-2.758491
109	1	0	5.765745	1.835893	-2.723176
110	1	0	2.466011	-0.955944	-2.329805
111	1	0	4.105174	-1.633355	-2.445868
112	1	0	1.772980	2.929817	4.028266
113	1	0	3.735465	4.467221	3.501299
114	1	0	3.379073	-0.827164	-3.841173
115	1	0	5.228907	0.846339	-4.094257
116	1	0	-5.202852	1.179358	4.498981
117	1	0	-3.012314	-0.016160	4.612945
118	1	0	-5.187220	1.102383	-4.139336
119	1	0	-2.864665	0.057034	-4.181648
120	6	0	6.246302	-1.176394	1.935061
121	6	0	6.895855	-2.171542	0.954663
122	1	0	6.151100	-2.799960	0.453221
123	1	0	7.480325	-1.658551	0.182690
124	1	0	7.578670	-2.834265	1.498872
125	6	0	7.376431	-0.347607	2.592540
126	1	0	6.987043	0.349944	3.341202
127	1	0	8.094972	-1.009014	3.092646
128	1	0	7.918501	0.237693	1.841213
129	6	0	5.513251	-1.985957	3.029902
130	1	0	5.045490	-1.335544	3.776031
131	1	0	4.725752	-2.611543	2.592591
132	1	0	6.215047	-2.646144	3.554470
133	6	0	-6.030455	-3.520114	0.224526
134	6	0	-5.323632	-4.499845	1.190238
135	1	0	-5.304540	-4.123292	2.217660
136	1	0	-5.848435	-5.463065	1.203017
137	1	0	-4.287098	-4.681115	0.886247
138	6	0	-6.109860	-4.189635	-1.161120
139	1	0	-6.675664	-3.583975	-1.877469
140	1	0	-5.114731	-4.372589	-1.583430
141	1	0	-6.618505	-5.156885	-1.076832
142	6	0	-7.474802	-3.276858	0.726588
143	1	0	-8.031082	-4.221665	0.775234
144	1	0	-7.480549	-2.830037	1.726554
145	1	0	-8.013226	-2.598462	0.054985

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1bd (SPINOL)



E(RB3LYP) = -3200.83440625 Hartree

Zero-point correction= 1.252124 Hartree

Thermal correction to Energy= 1.320235 Hartree

Thermal correction to Enthalpy= 1.321179 Hartree

Thermal correction to Gibbs Free Energy= 1.147774 Hartree

Sum of electronic and zero-point Energies= -3199.582283 Hartree

Sum of electronic and thermal Energies= -3199.514171 Hartree

Sum of electronic and thermal Enthalpies= -3199.513227 Hartree

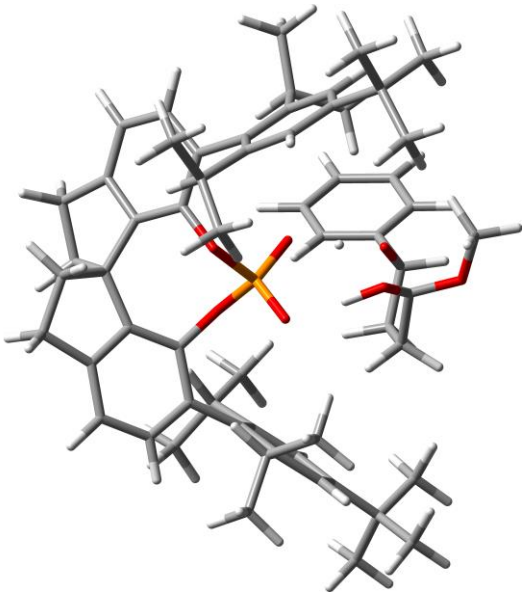
Sum of electronic and thermal Free Energies= -3199.686632 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.934066	-4.152948	0.085119
2	6	0	1.587106	-2.926048	-0.031421
3	6	0	3.504784	-3.848467	1.087799
4	6	0	2.820169	-5.039018	1.326857
5	6	0	1.529293	-5.181021	0.833487
6	1	0	4.529422	-3.743422	1.428768
7	1	0	3.296804	-5.841902	1.883891
8	6	0	0.583988	-6.353694	0.980303
9	1	0	0.898704	-7.205090	0.360633
10	1	0	0.532448	-6.719779	2.012249
11	6	0	-0.343926	-4.679866	-0.561324
12	6	0	-0.756039	-5.763879	0.490232

13	1	0	-1.271368	-5.268948	1.321282
14	1	0	-1.436105	-6.513709	0.074361
15	6	0	-0.022240	-5.381111	-1.925341
16	1	0	0.569009	-4.694111	-2.541694
17	1	0	0.559653	-6.298905	-1.797322
18	6	0	-1.401202	-5.612258	-2.576946
19	1	0	-1.831777	-6.576989	-2.273614
20	1	0	-1.356884	-5.619250	-3.672202
21	6	0	-2.209909	-4.452280	-2.039731
22	6	0	-1.539112	-3.827161	-0.976486
23	6	0	-3.448155	-3.988649	-2.466544
24	1	0	-3.983802	-4.486585	-3.271046
25	6	0	-2.058848	-2.650277	-0.437232
26	6	0	-3.998505	-2.870333	-1.843542
27	1	0	-4.978502	-2.515866	-2.147496
28	8	0	0.930354	-1.865868	-0.658664
29	8	0	-1.344907	-1.994709	0.563573
30	15	0	-0.126108	-0.960360	0.209763
31	8	0	-0.589090	0.107257	-0.779203
32	8	0	0.443179	-0.516607	1.529655
33	6	0	2.903849	-2.753728	0.443669
34	6	0	-3.312654	-2.152262	-0.848705
35	6	0	3.705318	-1.495299	0.269801
36	6	0	4.109003	-1.075315	-1.019474
37	6	0	4.172849	-0.781083	1.405872
38	6	0	4.968381	0.026162	-1.146963
39	6	0	5.042717	0.297513	1.217162
40	6	0	5.469808	0.723962	-0.046838
41	1	0	5.270609	0.317050	-2.146786
42	1	0	5.409780	0.814138	2.099468
43	6	0	-3.958559	-0.920074	-0.285345
44	6	0	-4.262510	0.172579	-1.135176
45	6	0	-4.378991	-0.877477	1.068512
46	6	0	-4.994194	1.254942	-0.623258
47	6	0	-5.087274	0.237187	1.526649
48	6	0	-5.426338	1.317386	0.703431
49	1	0	-5.232543	2.068270	-1.299939
50	1	0	-5.409107	0.243758	2.564306
51	6	0	0.742726	2.688500	0.933129
52	8	0	0.751568	4.027714	1.138646
53	8	0	-0.642853	2.434651	0.001003
54	1	0	0.539426	1.024322	1.892504
55	6	0	1.609082	4.704200	0.159948
56	6	0	1.968635	3.613316	-0.869153
57	6	0	1.846026	2.324145	-0.052111
58	1	0	2.503825	5.005323	0.717229
59	1	0	1.252875	3.617211	-1.695569
60	1	0	2.967434	3.769966	-1.285104
61	1	0	1.618911	1.437550	-0.643669
62	1	0	2.749024	2.120144	0.532718
63	8	0	0.551517	2.026176	2.064568
64	6	0	-1.860719	2.708312	0.731596
65	1	0	-2.691803	2.547769	0.045636
66	1	0	-1.950684	2.044559	1.593941
67	1	0	-1.819667	3.748029	1.058311
68	6	0	0.925221	5.935467	-0.382531
69	6	0	-0.300518	5.844615	-1.057743
70	6	0	1.524969	7.189570	-0.232495
71	6	0	-0.908899	6.988058	-1.571316
72	1	0	-0.776377	4.875314	-1.176465
73	6	0	0.921073	8.335630	-0.754277
74	1	0	2.471129	7.271377	0.297897
75	6	0	-0.298310	8.236827	-1.423430
76	1	0	-1.860247	6.905947	-2.090243
77	1	0	1.400731	9.302888	-0.631390
78	1	0	-0.773332	9.126988	-1.826942
79	1	0	-0.640933	1.387418	-0.339615
80	6	0	-4.150653	-2.030200	2.047460
81	6	0	-3.308223	-1.600457	3.263585
82	6	0	-5.487214	-2.659279	2.490451
83	1	0	-3.591923	-2.813163	1.530537
84	1	0	-3.817377	-0.830904	3.856718
85	1	0	-2.336210	-1.208530	2.950527
86	1	0	-6.070937	-2.999821	1.627740
87	1	0	-6.104849	-1.947533	3.051003
88	6	0	-3.843038	0.233997	-2.607844
89	6	0	-5.065247	0.190506	-3.547703
90	6	0	-2.973062	1.466090	-2.924109
91	1	0	-3.228059	-0.642714	-2.822715
92	1	0	-5.706399	1.069758	-3.411019
93	1	0	-5.683630	-0.696508	-3.372071
94	1	0	-2.060897	1.462043	-2.322816
95	1	0	-3.510658	2.405577	-2.745323
96	6	0	3.787624	-1.147940	2.842338
97	6	0	4.977617	-1.760062	3.610664
98	6	0	3.228567	0.051336	3.631028
99	1	0	2.991228	-1.894860	2.797214
100	1	0	5.796325	-1.036681	3.709537
101	1	0	5.381947	-2.646811	3.111878
102	1	0	2.391855	0.517910	3.109028
103	1	0	3.992564	0.818212	3.808471
104	6	0	3.706723	-1.811593	-2.298656
105	6	0	2.902866	-0.913425	-3.257887
106	6	0	4.935225	-2.420341	-3.004686
107	1	0	3.058669	-2.646587	-2.023676
108	1	0	3.492632	-0.052626	-3.596307
109	1	0	1.993137	-0.542977	-2.776201
110	1	0	5.486675	-3.088581	-2.333752
111	1	0	5.630698	-1.646336	-3.350241
112	1	0	2.870578	-0.282949	4.612066
113	1	0	4.669179	-2.053289	4.621527
114	1	0	4.622923	-3.000685	-3.881502
115	1	0	2.606810	-1.479575	-4.149663
116	1	0	-4.742076	0.175121	-4.595691
117	1	0	-2.678999	1.454677	-3.980853
118	1	0	-3.130595	-2.458748	3.923115
119	1	0	-5.304996	-3.523736	3.140498
120	6	0	6.484818	1.876589	-0.173273
121	6	0	5.952324	3.142033	0.538615
122	1	0	5.746755	2.962732	1.598715
123	1	0	6.687639	3.953582	0.475234
124	1	0	5.024328	3.492989	0.071323
125	6	0	6.778140	2.244476	-1.640246
126	1	0	7.222557	1.407706	-2.190301
127	1	0	5.871563	2.557285	-2.171495
128	1	0	7.489342	3.077586	-1.678090
129	6	0	7.815570	1.447730	0.491421
130	1	0	8.559563	2.250661	0.415467
131	1	0	7.680402	1.214477	1.552741
132	1	0	8.225586	0.556233	0.003569
133	6	0	-6.258538	2.486014	1.264821
134	6	0	-5.521905	3.127589	2.464259
135	1	0	-6.119368	3.944854	2.886778
136	1	0	-5.334621	2.404237	3.264238
137	1	0	-4.554836	3.542937	2.156909
138	6	0	-6.512695	3.585704	0.216205
139	1	0	-5.577840	4.025132	-0.150693
140	1	0	-7.072624	3.206315	-0.645988
141	1	0	-7.103205	4.393346	0.663573
142	6	0	-7.631112	1.951114	1.739867
143	1	0	-8.240690	2.767846	2.146195
144	1	0	-8.182115	1.496025	0.908935
145	1	0	-7.522907	1.193380	2.522716

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1bd (SPINOL)



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Zero-point correction= 1.251140 Hartree

Thermal correction to Energy= 1.319388 Hartree

Thermal correction to Enthalpy= 1.320332 Hartree

Thermal correction to Gibbs Free Energy= 1.146183 Hartree

Sum of electronic and zero-point Energies= -3199.580479 Hartree

Sum of electronic and thermal Energies= -3199.512231 Hartree

Sum of electronic and thermal Enthalpies= -3199.511287 Hartree

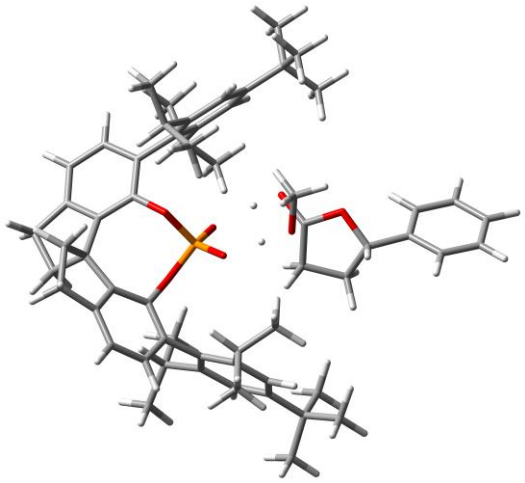
Sum of electronic and thermal Free Energies= -3199.685436 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.353903	3.271555	1.243717
2	6	0	-1.946840	2.216709	0.554163
3	6	0	-3.864148	2.352166	1.991677
4	6	0	-3.229370	3.314243	2.778199
5	6	0	-1.968920	3.765195	2.404463
6	1	0	-4.868737	2.032022	2.247369
7	1	0	-3.724588	3.710122	3.661554
8	6	0	-1.079848	4.784108	3.085646
9	1	0	-1.472089	5.803907	2.967584
10	1	0	-0.991844	4.606404	4.163854
11	6	0	-0.142585	4.134912	0.907057
12	6	0	0.263903	4.607446	2.342747
13	1	0	0.852714	3.815843	2.820410
14	1	0	0.875035	5.515362	2.328091
15	6	0	-0.582789	5.377659	0.058903
16	1	0	-1.180716	5.027611	-0.790333
17	1	0	-1.197129	6.078299	0.632441
18	6	0	0.737229	5.989850	-0.450785
19	1	0	1.144922	6.717662	0.265039
20	1	0	0.619856	6.518525	-1.403725
21	6	0	1.630111	4.775111	-0.569881
22	6	0	1.067434	3.674499	0.097054
23	6	0	2.846921	4.659802	-1.229883
24	1	0	3.292457	5.515103	-1.731809
25	6	0	1.682656	2.426251	-0.008562
26	8	0	-1.257119	1.637002	-0.511996
27	8	0	1.068539	1.319215	0.582230
28	15	0	-0.109246	0.512362	-0.226608
29	8	0	0.356777	0.014979	-1.568129
30	8	0	-0.609003	-0.512411	0.791255
31	6	0	-3.236017	1.752994	0.886913
32	6	0	2.925025	2.278365	-0.659070
33	6	0	-3.953470	0.694806	0.099855
34	6	0	-4.315858	0.933702	-1.251352
35	6	0	-4.340880	-0.523225	0.710161
36	6	0	-5.028384	-0.044741	-1.948116
37	6	0	-5.064534	-1.462916	-0.037927
38	6	0	-5.418508	-1.258427	-1.371707
39	1	0	-5.296129	0.158883	-2.981166
40	1	0	-5.351281	-2.385463	0.453172
41	6	0	3.494438	3.425532	-1.236827
42	1	0	4.461232	3.329136	-1.720883
43	6	0	3.694367	0.989334	-0.737172
44	6	0	3.884651	0.340981	-1.979626
45	6	0	4.355864	0.491993	0.415355
46	6	0	4.735556	-0.773835	-2.042597
47	6	0	5.189461	-0.622741	0.292298
48	6	0	5.410576	-1.274719	-0.928548
49	1	0	4.878488	-1.245042	-3.008098
50	1	0	5.707835	-0.976451	1.178243
51	6	0	0.194476	-3.240741	-1.101530
52	8	0	-0.352229	-2.913159	0.454650
53	6	0	0.688201	-3.503088	1.301317
54	6	0	1.708869	-3.084070	-0.887987
55	1	0	2.193639	-3.929206	-1.383272
56	1	0	2.045099	-2.165433	-1.370620
57	8	0	-0.465166	-2.425727	-1.913822
58	8	0	-0.129132	-4.544372	-1.274023
59	6	0	-1.508142	-4.823456	-1.577239
60	1	0	-1.593025	-5.910705	-1.551148
61	1	0	-1.767476	-4.445956	-2.568780
62	1	0	-2.162613	-4.372977	-0.825982
63	1	0	-0.461269	-1.787469	0.597589
64	1	0	-0.132809	-1.469502	-1.851555
65	6	0	0.517105	-3.193464	2.769828
66	6	0	0.654626	-1.898191	3.291303
67	6	0	0.243091	-4.249722	3.648359
68	6	0	0.517967	-1.674671	4.661087
69	1	0	0.832299	-1.058585	2.628532
70	6	0	0.114548	-4.027025	5.019767
71	1	0	0.131305	-5.257352	3.254339
72	6	0	0.251939	-2.735819	5.529390
73	1	0	0.618419	-0.665037	5.049745
74	1	0	-0.095288	-4.859841	5.685550
75	1	0	0.150152	-2.555981	6.596367
76	1	0	0.560882	-4.579519	1.158045
77	6	0	1.992399	-3.053360	0.630784
78	1	0	2.824995	-3.700617	0.919284
79	1	0	2.246832	-2.036899	0.944258
80	6	0	3.244882	0.832633	-3.281266
81	6	0	4.295188	1.490991	-4.200893
82	6	0	2.503308	-0.277406	-4.049537
83	1	0	2.498818	1.588926	-3.024207
84	1	0	5.058935	0.766548	-4.509567
85	1	0	4.809890	2.322437	-3.708291
86	1	0	1.719342	-0.720999	-3.433469
87	1	0	3.181444	-1.069976	-4.388529
88	6	0	4.275031	1.212490	1.763175
89	6	0	4.180523	0.266839	2.972809
90	6	0	5.467970	2.178085	1.923659
91	1	0	3.365946	1.818791	1.768828
92	1	0	5.100061	-0.310603	3.124060
93	1	0	3.351059	-0.440579	2.869919
94	1	0	5.499138	2.908374	1.108138
95	1	0	6.417919	1.629700	1.921035
96	6	0	-4.015248	2.245780	-1.978363
97	6	0	-3.164726	2.029646	-3.244525
98	6	0	-5.314866	3.009083	-2.305271
99	1	0	-3.437261	2.886461	-1.308533

100	1	0	-3.702217	1.439822	-3.996929
101	1	0	-2.231379	1.511997	-3.006140
102	1	0	-5.899602	3.203181	-1.398937
103	1	0	-5.951047	2.444864	-2.997495
104	6	0	-4.018499	-0.872119	2.165598
105	6	0	-5.275994	-0.791862	3.056491
106	6	0	-3.369812	-2.261087	2.316674
107	1	0	-3.293268	-0.142688	2.535481
108	1	0	-6.027604	-1.524821	2.738534
109	1	0	-5.747597	0.195771	3.021099
110	1	0	-2.509979	-2.373053	1.654016
111	1	0	-4.078373	-3.069207	2.096633
112	1	0	2.027878	0.145898	-4.942586
113	1	0	3.818345	1.880066	-5.108754
114	1	0	5.397301	2.728349	2.870159
115	1	0	4.014552	0.848884	3.887105
116	1	0	-2.914604	2.994750	-3.702596
117	1	0	-5.085334	3.973378	-2.775393
118	1	0	-3.024738	-2.403469	3.347598
119	1	0	-5.020802	-1.007268	4.101511
120	6	0	6.396737	-2.456440	-1.006071
121	6	0	5.954725	-3.582072	-0.042171
122	1	0	6.673851	-4.410191	-0.066180
123	1	0	5.885052	-3.231829	0.992879
124	1	0	4.974322	-3.979754	-0.329358
125	6	0	6.490199	-3.053635	-2.423156
126	1	0	5.522091	-3.431595	-2.771381
127	1	0	6.851972	-2.320200	-3.152347
128	1	0	7.193775	-3.894037	-2.424386
129	6	0	7.807294	-1.966154	-0.598270
130	1	0	7.820746	-1.571361	0.422986
131	1	0	8.529085	-2.790985	-0.648207
132	1	0	8.152791	-1.170583	-1.268130
133	6	0	-6.201390	-2.291646	-2.202669
134	6	0	-7.530501	-1.666063	-2.688620
135	1	0	-7.360670	-0.777175	-3.304904
136	1	0	-8.096033	-2.387575	-3.291617
137	1	0	-8.156054	-1.368446	-1.839204
138	6	0	-5.356081	-2.710831	-3.428898
139	1	0	-4.406401	-3.158637	-3.113733
140	1	0	-5.898098	-3.447854	-4.034847
141	1	0	-5.120768	-1.857005	-4.072372
142	6	0	-6.538465	-3.560998	-1.397582
143	1	0	-5.635006	-4.072284	-1.045704
144	1	0	-7.164374	-3.337439	-0.526220
145	1	0	-7.091854	-4.264465	-2.030372

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1bd (SPINOL)



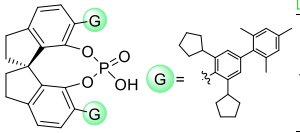
E(RB3LYP) = -3200.83559846 Hartree

Zero-point correction= 1.252032 Hartree
Thermal correction to Energy= 1.320402 Hartree
Thermal correction to Enthalpy= 1.321346 Hartree
Thermal correction to Gibbs Free Energy= 1.146654 Hartree
Sum of electronic and zero-point Energies= -3199.583567 Hartree
Sum of electronic and thermal Energies= -3199.515197 Hartree
Sum of electronic and thermal Enthalpies= -3199.514252 Hartree
Sum of electronic and thermal Free Energies= -3199.688944 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.775490	2.115232	-0.037094
2	8	0	-2.565403	3.173675	-0.325564
3	8	0	-1.443924	1.465413	-1.609214
4	6	0	-3.940234	2.711917	-0.468348
5	6	0	-4.031878	1.569189	0.563721
6	6	0	-2.608173	0.979541	0.574713
7	1	0	-4.049807	2.311400	-1.483365
8	1	0	-4.291552	1.986098	1.541807
9	1	0	-4.799058	0.840039	0.291526
10	1	0	-2.236112	0.764047	1.578306
11	1	0	-2.526660	0.062978	-0.011010
12	8	0	-0.617750	2.487897	0.459502
13	6	0	-0.727728	2.381051	-2.463200
14	1	0	0.193093	2.719543	-1.980584
15	1	0	-0.498194	1.849111	-3.388915
16	1	0	-1.381534	3.230023	-2.666718
17	1	0	-0.085870	1.666827	0.757044
18	1	0	-0.834542	0.577814	-1.466906
19	6	0	2.276057	-3.633628	-0.685034
20	6	0	0.992312	-3.248740	-0.300070
21	6	0	0.058687	-5.041675	-1.601029
22	6	0	1.322421	-5.362586	-2.097190
23	6	0	2.425085	-4.647881	-1.645032
24	1	0	-0.802880	-5.622260	-1.914713
25	1	0	1.437323	-6.165072	-2.821779
26	6	0	3.876050	-4.788641	-2.052593
27	1	0	4.325515	-5.699960	-1.633748
28	1	0	3.999036	-4.850330	-3.140121
29	6	0	3.654630	-3.209948	-0.181210
30	6	0	4.515175	-3.517518	-1.452109
31	1	0	4.414686	-2.682684	-2.155081
32	1	0	5.578474	-3.632890	-1.219952
33	6	0	4.125862	-4.131755	0.995563
34	1	0	3.334809	-4.165030	1.753536
35	1	0	4.320526	-5.158677	0.671307
36	6	0	5.369759	-3.421752	1.570988
37	1	0	6.286815	-3.739163	1.054685
38	1	0	5.521250	-3.630615	2.636310
39	6	0	5.060516	-1.964517	1.306002
40	6	0	3.990332	-1.841999	0.405650
41	6	0	5.673688	-0.834851	1.835010
42	1	0	6.517788	-0.925694	2.514295
43	6	0	3.462088	-0.579261	0.144789
44	6	0	5.185436	0.424973	1.487957
45	1	0	5.668300	1.314409	1.881264
46	8	0	0.832461	-2.154138	0.548909
47	8	0	2.349350	-0.475985	-0.687035
48	15	0	0.837759	-0.642456	-0.074823
49	8	0	0.571702	0.281639	1.087085
50	8	0	-0.063396	-0.549646	-1.299467
51	6	0	-0.146530	-3.963298	-0.725424
52	6	0	4.054041	0.587055	0.671999
53	6	0	-4.888606	3.864675	-0.261887
54	6	0	-6.054252	3.948074	-1.030655
55	6	0	-4.648411	4.831585	0.722885
56	6	0	-6.976099	4.973155	-0.812166

57	1	0	-6.241928	3.208176	-1.805886
58	6	0	-5.563529	5.862117	0.933313
59	1	0	-3.734254	4.783807	1.306889
60	6	0	-6.731669	5.933263	0.170245
61	1	0	-7.878229	5.025740	-1.415611
62	1	0	-5.363399	6.612522	1.693412
63	1	0	-7.443950	6.736755	0.336992
64	6	0	-1.536770	-3.639836	-0.258298
65	6	0	-1.891865	-3.826583	1.102287
66	6	0	-2.531566	-3.226727	-1.178284
67	6	0	-3.212191	-3.600729	1.499273
68	6	0	-3.841736	-3.018248	-0.721120
69	6	0	-4.217016	-3.200615	0.611401
70	1	0	-3.464417	-3.763593	2.543383
71	1	0	-4.587418	-2.714653	-1.447019
72	6	0	3.512531	1.959630	0.401669
73	6	0	2.992477	2.746180	1.463707
74	6	0	3.549843	2.501659	-0.903323
75	6	0	2.512326	4.027377	1.181755
76	6	0	3.039690	3.788760	-1.127933
77	6	0	2.505876	4.576116	-0.105644
78	1	0	2.118589	4.615860	2.005065
79	1	0	3.084149	4.182122	-2.137670
80	6	0	-2.256428	-3.026531	-2.671469
81	6	0	-2.886962	-4.156928	-3.512056
82	6	0	-2.740756	-1.662365	-3.197671
83	1	0	-1.174379	-3.055374	-2.821581
84	1	0	-3.980106	-4.151947	-3.420685
85	1	0	-2.537030	-5.146393	-3.200232
86	1	0	-2.302896	-0.839704	-2.629161
87	1	0	-3.832905	-1.569142	-3.157109
88	6	0	-0.904629	-4.320858	2.160869
89	6	0	-0.733483	-3.308527	3.309544
90	6	0	-1.307841	-5.709319	2.696921
91	1	0	0.073342	-4.439606	1.689165
92	1	0	-1.667765	-3.168487	3.867115
93	1	0	-0.410634	-2.335548	2.928270
94	1	0	-1.389027	-6.440015	1.884249
95	1	0	-2.273485	-5.678848	3.215568
96	6	0	4.193059	1.769389	-2.082405
97	6	0	3.215673	1.552427	-3.252574
98	6	0	5.467357	2.499135	-2.554197
99	1	0	4.505575	0.779984	-1.739533
100	1	0	2.878240	2.504361	-3.681070
101	1	0	2.338335	0.986107	-2.926612
102	1	0	6.184440	2.613318	-1.733560
103	1	0	5.239458	3.500384	-2.938915
104	6	0	2.954350	2.271029	2.919636
105	6	0	3.973058	3.049212	3.778379
106	6	0	1.550905	2.357002	3.549285
107	1	0	3.240111	1.216734	2.941109
108	1	0	3.719484	4.115326	3.825029
109	1	0	4.989572	2.972060	3.376512
110	1	0	0.840107	1.743798	2.991762
111	1	0	1.175437	3.386596	3.583564
112	1	0	1.584796	1.986705	4.581538
113	1	0	3.984387	2.663810	4.805341
114	1	0	3.704818	0.988077	-4.056189
115	1	0	5.957122	1.936324	-3.358490
116	1	0	-2.445492	-1.543751	-4.247496
117	1	0	-2.640004	-4.030434	-4.573377
118	1	0	-0.559603	-6.075791	3.410407
119	1	0	0.022103	-3.665380	4.020348
120	6	0	-5.662649	-3.019851	1.111918
121	6	0	-6.609212	-2.511614	0.007842
122	1	0	-6.679052	-3.216779	-0.827862
123	1	0	-7.618483	-2.382783	0.415296
124	1	0	-6.286781	-1.542729	-0.391903
125	6	0	-5.696468	-2.003445	2.277215
126	1	0	-5.076526	-2.325050	3.120018
127	1	0	-5.332752	-1.021310	1.953501
128	1	0	-6.721963	-1.879726	2.646736
129	6	0	-6.198471	-4.382457	1.614090
130	1	0	-7.227504	-4.279453	1.980898
131	1	0	-6.197021	-5.124084	0.807213
132	1	0	-5.588853	-4.779430	2.432464
133	6	0	1.951585	5.994140	-0.336141
134	6	0	1.933848	6.382453	-1.826940
135	1	0	1.514940	7.388729	-1.941907
136	1	0	2.940351	6.394415	-2.260337
137	1	0	1.315922	5.696674	-2.418195
138	6	0	0.503043	6.084834	0.200841
139	1	0	-0.147601	5.346781	-0.279631
140	1	0	0.457291	5.904828	1.279637
141	1	0	0.091786	7.084765	0.013358
142	6	0	2.838297	7.014976	0.416629
143	1	0	2.453938	8.033541	0.278593
144	1	0	2.865009	6.809795	1.492050
145	1	0	3.869551	6.987229	0.045963

DFT calculation of real system using SPINOL-derived CPA (*S*)-1be

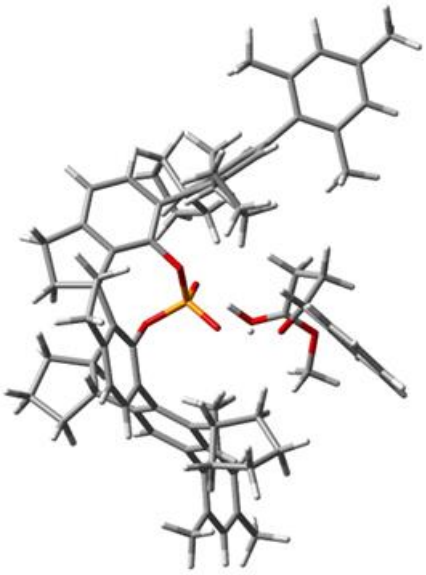


(*S*)-**1be** (SPINOL)

1st / 2nd	ΔΔG≠ (kcal/mol) (c)
R-anti* / *R-re	-0.30 / **0.00**
R-syn / *R-si*	-- / --
S-anti* / *S-si	**5.05** / 3.21
S-syn* / *S-re	**3.54** / 0.47

ΔΔG≠ of RDS = **3.54** kcal/mol

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1be (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3893.99550452 hartree

Zero-point Energy Correction = 1.501031 hartree

Thermal Correction to Energy = 1.582038 hartree

Thermal correction to Enthalpy = 1.582982 hartree

Thermal correction to Gibbs Free Energy= 1.372274 hartree

Sum of electronic and Zero-point Energies = -3892.494473 hartree

Sum of electronic and thermal Energies = -3892.413467 hartree

Sum of electronic and thermal Enthalpies = -3892.412523 hartree

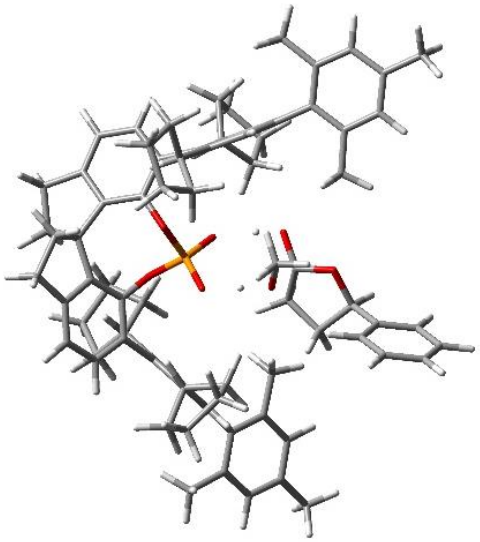
Sum of electronic and thermal Free Energies= -3892.623231 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.058630	-2.910367	-0.811692
2	8	0	-0.399811	-2.474902	0.794053
3	6	0	0.759688	-2.787824	1.629642
4	6	0	1.762587	-3.478855	0.682621
5	6	0	1.457334	-2.902985	-0.700228
6	1	0	1.166124	-1.824973	1.956343
7	1	0	1.605551	-4.561101	0.685043
8	1	0	2.788154	-3.285438	1.003406
9	1	0	1.879397	-3.497984	-1.514852
10	1	0	1.811727	-1.872708	-0.798849
11	8	0	-0.700046	-2.042379	-1.581566
12	8	0	-0.526006	-4.172735	-0.910793
13	6	0	-1.938875	-4.331138	-1.134715
14	1	0	-2.123194	-5.402899	-1.050686
15	1	0	-2.212489	-3.976195	-2.129622
16	1	0	-2.510929	-3.789089	-0.376954
17	1	0	-0.601778	-1.364914	0.908600
18	1	0	-0.306897	-1.106057	-1.518529
19	6	0	1.115332	4.018686	0.368403
20	6	0	1.691652	2.751761	0.248149
21	6	0	3.465078	3.693968	-1.078531
22	6	0	2.850515	4.943854	-1.056211
23	6	0	1.673910	5.098465	-0.334149
24	1	0	4.406529	3.566659	-1.604110
25	1	0	3.292600	5.782023	-1.589165
26	6	0	0.827184	6.341173	-0.175062
27	1	0	1.293983	7.055659	0.517803
28	1	0	0.679313	6.872795	-1.122090
29	6	0	-0.042312	4.517348	1.230288
30	6	0	-0.483945	5.772543	0.401793
31	1	0	-1.134774	5.441114	-0.415669
32	1	0	-1.046300	6.492701	1.003858
33	6	0	0.435531	4.974295	2.648962
34	1	0	1.025635	4.167306	3.098434
35	1	0	1.066312	5.868121	2.610961
36	6	0	-0.871027	5.178714	3.450126
37	1	0	-1.242790	6.208564	3.355022
38	1	0	-0.740842	4.991756	4.522429
39	6	0	-1.814572	4.186771	2.802365
40	6	0	-1.261044	3.687999	1.613287
41	6	0	-3.067420	3.760323	3.228431
42	1	0	-3.512711	4.157337	4.137468
43	6	0	-1.907486	2.656194	0.939859
44	6	0	-3.758968	2.820249	2.462015
45	1	0	-4.757452	2.514030	2.758895
46	8	0	1.071910	1.666397	0.871569
47	8	0	-1.273885	2.060167	-0.153684
48	15	0	-0.163036	0.891549	0.117374
49	8	0	-0.675072	-0.094566	1.166466
50	8	0	0.248590	0.348210	-1.225778
51	6	0	2.900175	2.568306	-0.452978
52	6	0	-3.191651	2.224062	1.324222
53	6	0	0.353473	-3.600848	2.836412
54	6	0	0.693482	-3.165257	4.120919
55	6	0	-0.346584	-4.806362	2.688779
56	6	0	0.348266	-3.922777	5.242782
57	1	0	1.229055	-2.226842	4.245584
58	6	0	-0.699026	-5.558801	3.807143
59	1	0	-0.618922	-5.145309	1.693153
60	6	0	-0.350316	-5.119857	5.088171
61	1	0	0.619829	-3.572521	6.234965
62	1	0	-1.246055	-6.489458	3.681281
63	1	0	-0.624130	-5.708753	5.959466
64	6	0	-3.956378	1.193626	0.547982
65	6	0	-4.992558	-0.992324	0.382137
66	6	0	-5.156629	0.532784	-1.454962
67	6	0	-5.444725	-0.722107	-0.912176
68	1	0	-5.215329	-1.962619	0.819705
69	1	0	-5.524575	0.764598	-2.450876
70	6	0	3.687677	1.289087	-0.537449
71	6	0	5.389963	-0.163980	0.404275
72	6	0	4.841156	-0.339717	-1.919444
73	6	0	5.642476	-0.737573	-0.844921
74	1	0	5.993806	-0.478974	1.251928
75	1	0	5.012851	-0.796100	-2.891115
76	6	0	-6.213136	-1.743213	-1.692564
77	6	0	-7.656013	-3.689874	-3.157272
78	6	0	6.789022	-1.685525	-1.045391
79	6	0	8.983792	-3.430665	-1.435411
80	6	0	-4.423824	1.497240	-0.756112
81	6	0	-4.196792	2.847427	-1.416151
82	6	0	-3.460747	2.821324	-2.774453
83	6	0	-5.487076	3.636898	-1.754167
84	1	0	-3.604830	3.474769	-0.743382
85	6	0	-3.655955	4.250099	-3.315719
86	1	0	-3.939586	2.093510	-3.443040
87	1	0	-2.410698	2.532161	-2.672489
88	6	0	-5.042652	4.715419	-2.776943
89	1	0	-5.956358	4.062299	-0.860107

90	1	0	-6.223343	2.962673	-2.207963
91	1	0	-2.863940	4.902796	-2.927648
92	1	0	-3.592411	4.295501	-4.408387
93	1	0	-4.963130	5.700397	-2.303644
94	1	0	-5.776817	4.817269	-3.583667
95	6	0	-4.258029	-0.062680	1.129119
96	6	0	-3.846846	-0.436272	2.547118
97	6	0	-5.045067	-0.439110	3.546367
98	6	0	-3.197836	-1.854951	2.714093
99	1	0	-3.118687	0.297989	2.894495
100	6	0	-4.665627	-1.476355	4.612697
101	1	0	-5.959123	-0.761036	3.030083
102	1	0	-5.243574	0.556136	3.959742
103	6	0	-4.029383	-2.600887	3.781095
104	1	0	-2.165832	-1.734887	3.054642
105	1	0	-3.146428	-2.403588	1.770207
106	1	0	-3.923662	-1.053146	5.304005
107	1	0	-5.520884	-1.808249	5.213062
108	1	0	-3.425399	-3.295370	4.375114
109	1	0	-4.824350	-3.190919	3.303610
110	6	0	4.434320	0.845970	0.582007
111	6	0	4.276926	1.461452	1.962842
112	6	0	3.757859	0.488910	3.054325
113	6	0	5.561675	2.033913	2.603619
114	1	0	3.565660	2.289543	1.899642
115	6	0	4.165221	1.129414	4.411002
116	1	0	4.241768	-0.488331	2.934359
117	1	0	2.678358	0.330939	2.961457
118	6	0	5.143454	2.287708	4.062087
119	1	0	5.919654	2.935046	2.093030
120	1	0	6.370610	1.292885	2.563193
121	1	0	3.293312	1.504170	4.957811
122	1	0	4.644969	0.388458	5.060154
123	1	0	4.623097	3.251240	4.130430
124	1	0	5.998450	2.339694	4.744934
125	6	0	3.861653	0.654564	-1.793935
126	6	0	3.047002	1.043964	-3.019014
127	6	0	3.844774	1.778047	-4.133446
128	6	0	2.386898	-0.122092	-3.789384
129	1	0	2.231873	1.696412	-2.694197
130	6	0	3.042853	1.554649	-5.447810
131	1	0	4.846904	1.340054	-4.217380
132	1	0	3.982104	2.839046	-3.899949
133	6	0	1.918428	0.545741	-5.091394
134	1	0	1.570031	-0.575114	-3.222496
135	1	0	3.123285	-0.905660	-4.013209
136	1	0	2.629068	2.490988	-5.837402
137	1	0	3.696102	1.152948	-6.230819
138	1	0	0.978341	1.078986	-4.904628
139	1	0	1.725042	-0.173839	-5.894728
140	6	0	7.754007	-3.909884	-0.980769
141	1	0	7.640797	-4.972575	-0.773828
142	6	0	6.658234	-3.062619	-0.780994
143	6	0	9.098775	-2.060012	-1.684769
144	1	0	10.050764	-1.661133	-2.030996
145	6	0	8.027562	-1.180614	-1.501005
146	6	0	-5.632525	-2.355227	-2.825228
147	6	0	-6.362506	-3.318928	-3.530359
148	1	0	-5.904895	-3.790471	-4.398568
149	6	0	-8.220793	-3.058510	-2.046102
150	1	0	-9.235659	-3.316041	-1.747452
151	6	0	-7.525038	-2.097038	-1.306461
152	6	0	5.354986	-3.637234	-0.277274
153	1	0	5.120228	-3.271597	0.730244
154	1	0	4.516095	-3.351771	-0.921383
155	1	0	5.396572	-4.730192	-0.233854
156	6	0	8.217660	0.293819	-1.782628
157	1	0	7.566354	0.639157	-2.594074
158	1	0	7.974486	0.906413	-0.906798
159	1	0	9.252802	0.505046	-2.068651
160	6	0	10.148440	-4.364081	-1.672563
161	1	0	10.235394	-4.633055	-2.733945
162	1	0	11.098437	-3.903284	-1.379078
163	1	0	10.036494	-5.296054	-1.108550
164	6	0	-8.207637	-1.439828	-0.125531
165	1	0	-7.806953	-1.795141	0.831728
166	1	0	-8.074645	-0.352895	-0.136236
167	1	0	-9.281248	-1.654057	-0.132047
168	6	0	-4.242484	-1.991309	-3.303251
169	1	0	-4.233323	-1.027529	-3.827505
170	1	0	-3.526902	-1.900016	-2.480430
171	1	0	-3.867458	-2.743475	-4.005823
172	6	0	-8.414417	-4.753356	-3.917460
173	1	0	-8.080526	-4.817757	-4.958663
174	1	0	-8.271232	-5.745716	-3.468323
175	1	0	-9.491687	-4.553506	-3.919534

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1be (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3893.99523492 hartree

Zero-point Energy Correction = 1.501708 hartree

Thermal Correction to Energy = 1.582967 hartree

Thermal correction to Enthalpy = 1.583911 hartree

Thermal correction to Gibbs Free Energy= 1.372482 hartree

Sum of electronic and Zero-point Energies = -3892.493527 hartree

Sum of electronic and thermal Energies = -3892.412268 hartree

Sum of electronic and thermal Enthalpies = -3892.411324 hartree

Sum of electronic and thermal Free Energies= -3892.622753 hartree

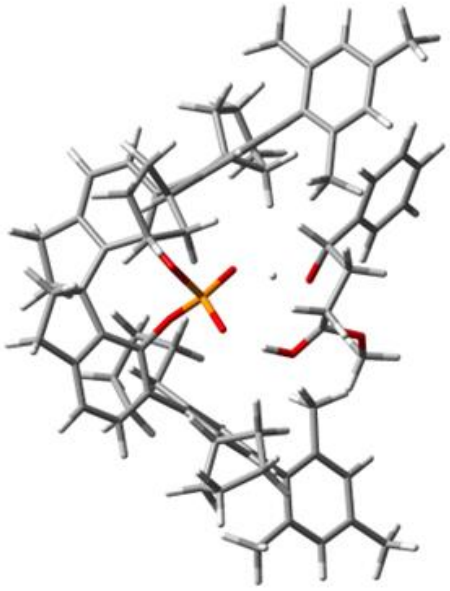
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.480325	2.598583	-0.318993
2	8	0	-0.853608	3.890066	-0.185204
3	8	0	-0.282118	2.074223	1.305455
4	6	0	0.300190	4.789104	-0.325732
5	6	0	1.528939	3.857355	-0.316710
6	6	0	0.955852	2.529421	-0.821245
7	1	0	0.184200	5.251265	-1.312790
8	1	0	1.919372	3.746261	0.697940
9	1	0	2.330755	4.250631	-0.946691
10	1	0	1.487075	1.643645	-0.472520
11	1	0	0.907898	2.491201	-1.915424
12	8	0	-1.441533	1.853735	-0.831665

13	6	0	-1.504080	2.122606	2.073095	82	6	0	-5.695457	-2.507756	2.478278
14	1	0	-1.817156	3.164577	2.142062	83	1	0	-3.693744	-2.823588	1.787873
15	1	0	-1.275940	1.726443	3.064949	84	6	0	-4.146751	-2.091465	4.369774
16	1	0	-2.283740	1.524461	1.595123	85	1	0	-4.321479	-0.224385	3.251105
17	1	0	0.062346	1.026760	1.287224	86	1	0	-2.732113	-0.981891	3.072879
18	1	0	-1.102846	0.908385	-1.009422	87	6	0	-5.392667	-2.925000	3.936569
19	6	0	-1.175817	-4.347914	0.085774	88	1	0	-6.082976	-3.331325	1.868271
20	6	0	-1.787481	-3.094846	0.107305	89	1	0	-6.450736	-1.712330	2.458679
21	6	0	-3.552699	-3.934647	-1.294036	90	1	0	-3.305279	-2.757682	4.593043
22	6	0	-2.907807	-5.165836	-1.404510	91	1	0	-4.332082	-1.507175	5.277656
23	6	0	-1.713815	-5.362794	-0.720843	92	1	0	-5.170209	-3.996733	3.990908
24	1	0	-4.500053	-3.775884	-1.800436	93	1	0	-6.253750	-2.751926	4.591094
25	1	0	-3.336889	-5.955689	-2.016165	94	6	0	-3.193477	-1.157344	-3.017628
26	6	0	-0.822274	-6.584844	-0.707931	95	6	0	-4.145177	-1.676470	-4.129439
27	1	0	-1.250749	-7.386964	-0.090345	96	6	0	-2.407256	0.015425	-3.701954
28	1	0	-0.671791	-7.005656	-1.708766	97	1	0	-2.470757	-1.948678	-2.808873
29	6	0	0.009522	-4.893251	0.875939	98	6	0	-3.356960	-1.449428	-5.425691
30	6	0	0.480010	-6.034980	-0.090249	99	1	0	-5.067159	-1.079121	-4.144649
31	1	0	1.104051	-5.593982	-0.876325	100	1	0	-4.437637	-2.721123	-3.974127
32	1	0	1.076993	-6.796722	0.420625	101	6	0	-2.739516	-0.054837	-5.215845
33	6	0	-0.439354	-5.520252	2.238047	102	1	0	-1.338823	-0.117760	-3.514091
34	1	0	-1.052957	-4.789192	2.776907	103	1	0	-2.678457	0.987040	-3.279380
35	1	0	-1.039296	-6.425913	2.104400	104	1	0	-2.564453	-2.205015	-5.514840
36	6	0	0.879550	-5.765120	3.004451	105	1	0	-3.976554	-1.516584	-6.327574
37	1	0	1.289348	-6.761804	2.788924	106	1	0	-1.863280	0.121469	-5.849727
38	1	0	0.752973	-5.707545	4.091818	107	1	0	-3.480212	0.712525	-5.477019
39	6	0	1.778259	-4.670003	2.470497	108	6	0	3.612675	0.038948	2.714103
40	6	0	1.202208	-4.063688	1.343102	109	6	0	4.680922	-0.083145	3.834894
41	6	0	3.013149	-4.246470	2.947685	110	6	0	3.013523	1.435004	2.995132
42	1	0	3.473526	-4.727436	3.807315	111	1	0	2.818265	-0.685702	2.915563
43	6	0	1.809451	-2.936519	0.791978	112	6	0	4.085620	0.658622	5.063104
44	6	0	3.667426	-3.201479	2.294636	113	1	0	5.606897	0.404257	3.504880
45	1	0	4.655656	-2.896232	2.624349	114	1	0	4.933780	-1.125272	4.055373
46	8	0	-1.190094	-2.071112	0.842819	115	6	0	2.861040	1.451920	4.525881
47	8	0	1.160565	-2.242552	-0.230865	116	1	0	2.069755	1.594356	2.467930
48	15	0	-0.005801	-1.163584	0.158092	117	1	0	3.710070	2.224500	2.683174
49	8	0	0.461460	-0.257132	1.293719	118	1	0	3.784043	-0.043188	5.848173
50	8	0	-0.440992	-0.524688	-1.134462	119	1	0	4.829301	1.326785	5.511519
51	6	0	-3.003320	-2.865266	-0.566402	120	1	0	1.931316	0.941560	4.805802
52	6	0	3.077343	-2.503827	1.227849	121	1	0	2.803545	2.467125	4.934258
53	6	0	0.265332	5.864899	0.731558	122	6	0	4.091899	-2.790837	-1.572719
54	6	0	0.190455	7.209225	0.354279	123	6	0	3.357598	-2.527358	-2.906866
55	6	0	0.323530	5.544188	2.095540	124	6	0	5.347419	-3.580590	-2.026789
56	6	0	0.182850	8.220586	1.317215	125	1	0	3.469663	-3.483594	-0.999715
57	1	0	0.136354	7.467777	-0.700876	126	6	0	3.487992	-3.867012	-3.650806
58	6	0	0.305836	6.551392	3.058157	127	1	0	3.871897	-1.731953	-3.463544
59	1	0	0.381771	4.503305	2.400973	128	1	0	2.322075	-2.209464	-2.754212
60	6	0	0.238279	7.892950	2.671473	129	6	0	4.882914	-4.425993	-3.246366
61	1	0	0.127335	9.260722	1.007891	130	1	0	5.758115	-4.192281	-1.215888
62	1	0	0.348012	6.290561	4.112268	131	1	0	6.138982	-2.884397	-2.326985
63	1	0	0.227967	8.677037	3.423692	132	1	0	2.697244	-4.549579	-3.314339
64	6	0	3.839506	-1.385362	0.577580	133	1	0	3.373644	-3.761878	-4.735220
65	6	0	-3.757049	-1.566405	-0.531131	134	1	0	4.821411	-5.491007	-2.997238
66	6	0	-5.449522	0.704067	-0.560332	135	1	0	5.599953	-4.341344	-4.070468
67	6	0	5.508958	0.602308	-0.559262	136	6	0	6.428079	1.630278	-1.145892
68	6	0	4.967908	0.759618	0.720128	137	6	0	7.753252	1.745593	-0.671937
69	1	0	5.209701	1.661288	1.276342	138	6	0	5.982634	2.483719	-2.177264
70	6	0	4.138643	-0.205257	1.306110	139	6	0	8.598240	2.709516	-1.231114
71	6	0	5.182125	-0.556172	-1.267191	140	6	0	6.859359	3.437709	-2.705088
72	1	0	5.599863	-0.691975	-2.261430	141	6	0	8.173402	3.566403	-2.249856
73	6	0	4.362178	-1.555208	-0.729215	142	1	0	9.618991	2.789323	-0.861069
74	6	0	-5.260859	-0.038071	0.609072	143	1	0	6.503129	4.098435	-3.493671
75	1	0	-5.801651	0.257700	1.504903	144	6	0	-6.416962	1.849488	-0.608545
76	6	0	-4.437045	-1.170965	0.647629	145	6	0	-7.744237	1.617100	-1.030644
77	6	0	-4.747925	0.312499	-1.702676	146	6	0	-6.020269	3.151027	-0.241002
78	1	0	-4.876301	0.891250	-2.614296	147	6	0	-8.644034	2.686223	-1.079034
79	6	0	-3.899183	-0.801314	-1.715941	148	6	0	-6.951988	4.193489	-0.307925
80	6	0	-4.349965	-1.962074	1.942788	149	6	0	-8.267672	3.985237	-0.726702
81	6	0	-3.803120	-1.188636	3.164252	150	1	0	-9.666723	2.497598	-1.401379

151	1	0	-6.637038	5.196079	-0.023385
152	6	0	-4.615909	3.436365	0.239919
153	1	0	-4.450327	3.019381	1.242061
154	1	0	-3.855171	2.996409	-0.411591
155	1	0	-4.433645	4.514247	0.298029
156	6	0	-8.208894	0.231956	-1.425239
157	1	0	-7.660412	-0.146377	-2.296031
158	1	0	-8.048367	-0.493256	-0.619083
159	1	0	-9.274987	0.234498	-1.673418
160	6	0	-9.247597	5.132001	-0.822335
161	1	0	-8.991350	5.937920	-0.126143
162	1	0	-9.258440	5.565802	-1.831577
163	1	0	-10.270009	4.806049	-0.600924
164	6	0	4.572171	2.393479	-2.717495
165	1	0	4.418182	1.483700	-3.310213
166	1	0	3.833542	2.363774	-1.909307
167	1	0	4.347065	3.249744	-3.361926
168	6	0	8.283364	0.837904	0.417280
169	1	0	7.830356	1.057744	1.391472
170	1	0	8.068465	-0.214873	0.203778
171	1	0	9.367032	0.951099	0.522470
172	6	0	9.115242	4.579188	-2.859183
173	1	0	9.709467	4.134740	-3.669104
174	1	0	8.569975	5.428076	-3.285529
175	1	0	9.821452	4.968652	-2.117617

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1be (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3893.98967222 hartree

Zero-point Energy Correction = 1.501491 hartree

Thermal Correction to Energy = 1.582099 hartree

Thermal correction to Enthalpy = 1.583043 hartree

Thermal correction to Gibbs Free Energy= 1.374961 hartree

Sum of electronic and Zero-point Energies = -3892.488181 hartree

Sum of electronic and thermal Energies = -3892.407573 hartree

Sum of electronic and thermal Enthalpies = -3892.406629 hartree

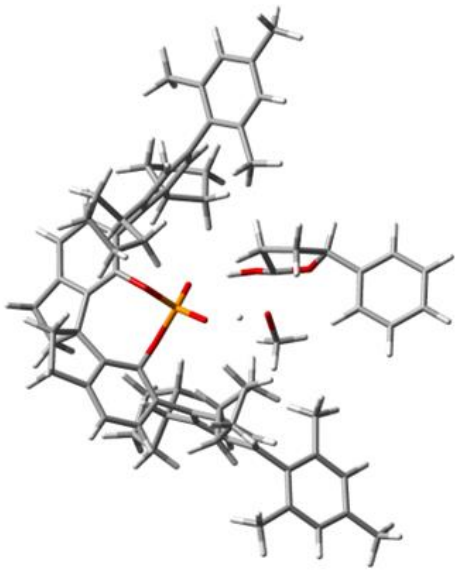
Sum of electronic and thermal Free Energies= -3892.614712 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.629059	-2.685777	-1.286055
2	8	0	-0.376567	-2.373713	0.042235
3	6	0	-1.737221	-2.731494	-0.322211
4	6	0	-1.672511	-3.173859	-1.810683
5	6	0	-0.419151	-2.504779	-2.369290
6	1	0	-2.333564	-1.816879	-0.231482
7	1	0	-1.577537	-4.261216	-1.871313
8	1	0	-2.578731	-2.883573	-2.345999
9	1	0	-0.065456	-2.965931	-3.295715
10	1	0	-0.562098	-1.433494	-2.536295
11	8	0	1.653273	-1.852440	-1.169570
12	8	0	0.963168	-3.985356	-1.158791
13	6	0	2.053010	-4.299113	-0.277985
14	1	0	2.084798	-5.388627	-0.237405
15	1	0	2.992618	-3.905399	-0.670094
16	1	0	1.870347	-3.890221	0.719382
17	1	0	-0.304366	-1.264084	0.385430
18	1	0	1.373764	-0.905623	-1.395182
19	6	0	1.644260	4.058231	-0.162555
20	6	0	2.161840	2.768857	-0.051727
21	6	0	4.093378	3.452677	-1.313808
22	6	0	3.524704	4.703055	-1.552255
23	6	0	2.295347	4.998250	-0.977056
24	1	0	5.077522	3.225057	-1.711003
25	1	0	4.045241	5.434187	-2.165909
26	6	0	1.478605	6.267753	-1.086975
27	1	0	1.933771	7.089720	-0.516901
28	1	0	1.388984	6.617077	-2.122127
29	6	0	0.489579	4.737704	0.561281
30	6	0	0.121939	5.845318	-0.481935
31	1	0	-0.510002	5.400267	-1.259283
32	1	0	-0.433549	6.675635	-0.034826
33	6	0	0.995651	5.415365	1.880422
34	1	0	1.561580	4.676597	2.459732
35	1	0	1.657841	6.264627	1.686904
36	6	0	-0.291268	5.797905	2.638248
37	1	0	-0.640257	6.801251	2.356169
38	1	0	-0.156388	5.807052	3.726015
39	6	0	-1.262446	4.730409	2.185603
40	6	0	-0.753450	4.027058	1.081440
41	6	0	-2.508447	4.418888	2.714609
42	1	0	-2.913743	4.976127	3.555542
43	6	0	-1.450198	2.920892	0.592654
44	8	0	1.422239	1.793798	0.630841
45	8	0	-0.901057	2.170575	-0.450126
46	15	0	0.234025	1.018860	-0.194316
47	8	0	-0.288308	-0.047176	0.775771
48	8	0	0.686640	0.551159	-1.553289
49	6	0	3.423700	2.449910	-0.592585
50	6	0	-2.727521	2.597956	1.091683
51	6	0	-2.305434	-3.806826	0.583813
52	6	0	-1.504804	-4.547334	1.457636
53	6	0	-3.675887	-4.094435	0.509421
54	6	0	-2.062967	-5.558070	2.243696
55	1	0	-0.447238	-4.321233	1.528689
56	6	0	-4.231913	-5.106285	1.291796
57	1	0	-4.316908	-3.522278	-0.156943
58	6	0	-3.426158	-5.842816	2.163207
59	1	0	-1.428072	-6.121807	2.922536
60	1	0	-5.296430	-5.314082	1.222532
61	1	0	-3.859046	-6.628788	2.776289
62	6	0	4.114504	1.133414	-0.392671
63	6	0	-3.240415	3.383875	2.137467
64	1	0	-4.233056	3.151742	2.510606
65	6	0	-3.599000	1.502178	0.553864
66	6	0	-5.526745	-0.387627	-0.307590
67	6	0	5.668314	-1.211842	-0.044895
68	6	0	5.148627	-0.865775	-1.296291
69	1	0	5.348738	-1.517593	-2.142530
70	6	0	4.388894	0.292411	-1.500772
71	6	0	5.381251	-0.367206	1.031388

72	1	0	5.789706	-0.612001	2.007896
73	6	0	4.611628	0.791623	0.890199
74	6	0	-4.864607	-0.533956	0.918035
75	1	0	-5.106432	-1.388685	1.542721
76	6	0	-3.916061	0.390276	1.374092
77	6	0	-5.180309	0.708175	-1.104438
78	1	0	-5.691566	0.843599	-2.053373
79	6	0	-4.227877	1.652925	-0.706087
80	6	0	4.380563	1.654645	2.120422
81	6	0	3.634751	0.965179	3.285061
82	6	0	5.665552	2.192632	2.805791
83	1	0	3.782898	2.524612	1.835227
84	6	0	3.817834	1.952693	4.449238
85	1	0	4.114052	0.005318	3.521357
86	1	0	2.586979	0.761794	3.044024
87	6	0	5.245995	2.538615	4.263046
88	1	0	6.080764	3.051541	2.267103
89	1	0	6.441458	1.418677	2.806539
90	1	0	3.069981	2.752067	4.368384
91	1	0	3.676972	1.485488	5.430132
92	1	0	5.255633	3.619331	4.441930
93	1	0	5.948834	2.099339	4.979829
94	6	0	3.933594	0.625036	-2.917725
95	6	0	5.093704	1.058205	-3.856694
96	6	0	3.218049	-0.527142	-3.706114
97	1	0	3.228521	1.456913	-2.861856
98	6	0	4.535138	0.830517	-5.266776
99	1	0	5.968032	0.413236	-3.694006
100	1	0	5.414871	2.090073	-3.677599
101	6	0	3.816901	-0.524215	-5.137033
102	1	0	2.142608	-0.327460	-3.724380
103	1	0	3.346503	-1.497461	-3.220346
104	1	0	3.813779	1.621595	-5.513043
105	1	0	5.306948	0.837026	-6.045187
106	1	0	3.059205	-0.681717	-5.912720
107	1	0	4.550956	-1.334243	-5.240899
108	6	0	-3.938600	2.824898	-1.629406
109	6	0	-3.351355	2.449592	-3.009109
110	6	0	-5.162521	3.696549	-2.010232
111	1	0	-3.213970	3.485165	-1.144593
112	6	0	-3.445400	3.763908	-3.804964
113	1	0	-3.971955	1.673332	-3.477818
114	1	0	-2.331785	2.059193	-2.933890
115	6	0	-4.727430	4.475897	-3.281136
116	1	0	-5.466864	4.354781	-1.189018
117	1	0	-6.022483	3.054920	-2.234924
118	1	0	-2.561717	4.379994	-3.597760
119	1	0	-3.467337	3.598995	-4.887692
120	1	0	-4.522432	5.527532	-3.052717
121	1	0	-5.524995	4.471596	-4.032182
122	6	0	-3.300702	0.199770	2.754903
123	6	0	-4.296623	0.442224	3.934296
124	6	0	-2.705175	-1.190601	3.069250
125	1	0	-2.477478	0.910927	2.861280
126	6	0	-3.817328	-0.466770	5.103298
127	1	0	-5.315843	0.177750	3.630286
128	1	0	-4.319746	1.500583	4.215540
129	6	0	-2.529751	-1.152972	4.593891
130	1	0	-1.768129	-1.360804	2.533495
131	1	0	-3.400001	-1.993811	2.795149
132	1	0	-3.647626	0.096321	6.027472
133	1	0	-4.580439	-1.220696	5.330691
134	1	0	-1.651479	-0.544319	4.845983
135	1	0	-2.373381	-2.144872	5.032154
136	6	0	6.517625	-2.431807	0.133948
137	6	0	7.745529	-2.551710	-0.560130
138	6	0	6.117690	-3.468993	1.007258
139	6	0	8.522474	-3.701123	-0.387975
140	6	0	6.923004	-4.606250	1.138962
141	6	0	8.126417	-4.748610	0.447183
142	1	0	9.470352	-3.775603	-0.918355
143	1	0	6.597781	-5.402303	1.807101
144	6	0	-6.589706	-1.353433	-0.733331
145	6	0	-7.747488	-1.529563	0.066168
146	6	0	-6.472132	-2.085553	-1.936864
147	6	0	-8.728802	-2.438677	-0.336467
148	6	0	-7.475959	-2.996006	-2.292024
149	6	0	-8.610142	-3.194633	-1.506405
150	1	0	-9.618502	-2.554122	0.280302
151	1	0	-7.364089	-3.562217	-3.215191
152	6	0	-5.303463	-1.918565	-2.885848
153	1	0	-5.516231	-1.165011	-3.655847
154	1	0	-4.395623	-1.593445	-2.372987
155	1	0	-5.094289	-2.858090	-3.409262
156	6	0	-7.984187	-0.731439	1.332339
157	1	0	-7.430762	-1.136611	2.188344
158	1	0	-7.673243	0.311613	1.219816
159	1	0	-9.046371	-0.745881	1.597393
160	6	0	-9.670083	-4.198683	-1.895298
161	1	0	-10.677333	-3.818538	-1.690122
162	1	0	-9.613757	-4.449187	-2.959729
163	1	0	-9.559200	-5.135238	-1.332302
164	6	0	4.845467	-3.392988	1.826098
165	1	0	5.017272	-2.899057	2.791570
166	1	0	4.059930	-2.827545	1.319756
167	1	0	4.469641	-4.398505	2.046761
168	6	0	8.271278	-1.453189	-1.461278
169	1	0	7.792777	-1.461717	-2.448410
170	1	0	8.097754	-0.460237	-1.035259
171	1	0	9.347574	-1.574186	-1.621830
172	6	0	8.964532	-5.998585	0.582070
173	1	0	10.031465	-5.780831	0.461768
174	1	0	8.824201	-6.473203	1.559304
175	1	0	8.698453	-6.742471	-0.181294

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1be (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = - 3893.99025248 hartree

Zero-point Energy Correction = 1.501912 hartree

Thermal Correction to Energy = 1.583073 hartree

Thermal correction to Enthalpy = 1.584018 hartree

Thermal correction to Gibbs Free Energy= 1.371627 hartree

Sum of electronic and Zero-point Energies = -3892.488341 hartree

Sum of electronic and thermal Energies = -3892.407179 hartree

Sum of electronic and thermal Enthalpies = -3892.406235 hartree

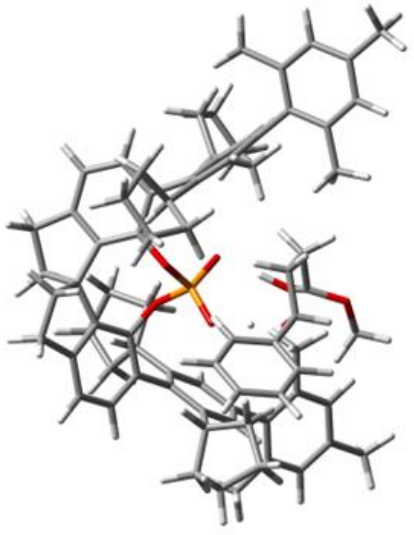
Sum of electronic and thermal Free Energies= -3892.618625 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.315972	-4.226992	-0.271556
2	6	0	-1.902296	-2.970238	-0.129521
3	6	0	-3.784796	-3.712394	-1.428971
4	6	0	-3.150101	-4.925147	-1.696328
5	6	0	-1.912519	-5.175713	-1.116269
6	1	0	-4.775832	-3.524587	-1.830125
7	1	0	-3.627547	-5.663744	-2.335545
8	6	0	-1.033147	-6.400656	-1.248813
9	1	0	-1.452292	-7.256845	-0.701906
10	1	0	-0.918151	-6.720901	-2.290830
11	6	0	-0.129887	-4.863381	0.443941
12	6	0	0.296907	-5.927531	-0.621678
13	1	0	0.912849	-5.435501	-1.383265
14	1	0	0.887675	-6.741071	-0.188993
15	6	0	-0.607335	-5.593508	1.745913
16	1	0	-1.216498	-4.897600	2.334435
17	1	0	-1.221235	-6.473596	1.531345
18	6	0	0.692431	-5.920426	2.508618
19	1	0	1.100113	-6.895345	2.206158
20	1	0	0.548227	-5.963584	3.594355
21	6	0	1.605220	-4.789572	2.089647
22	6	0	1.072565	-4.100124	0.989173
23	6	0	2.820244	-4.407358	2.644715
24	1	0	3.247078	-4.951203	3.483792
25	6	0	1.710025	-2.948495	0.524589
26	6	0	3.494269	-3.318027	2.097372
27	1	0	4.464509	-3.032965	2.492160
28	8	0	-1.218440	-1.979786	0.581344
29	8	0	1.122928	-2.226782	-0.513301
30	15	0	-0.060924	-1.129079	-0.212212
31	8	0	0.415001	-0.099445	0.810608
32	8	0	-0.526408	-0.639525	-1.556287
33	6	0	-3.174543	-2.699044	-0.670212
34	6	0	2.954422	-2.548050	1.051700
35	6	0	-3.945637	-1.432471	-0.430352
36	6	0	-5.378847	-0.100475	1.007472
37	6	0	-5.134808	0.497773	-1.296371
38	6	0	-5.729681	0.739227	-0.053629
39	1	0	-5.833321	0.072910	1.979389
40	1	0	-5.383088	1.151581	-2.129079
41	6	0	3.785774	-1.400291	0.551625
42	6	0	5.076821	0.597799	1.046813
43	6	0	5.392228	-0.523588	-1.043785
44	6	0	5.761480	0.502547	-0.169394
45	1	0	5.338863	1.402998	1.728804
46	1	0	5.910992	-0.605161	-1.995467
47	6	0	-0.410028	2.620617	-1.027153
48	8	0	-0.159772	3.925386	-1.286114
49	8	0	0.911638	2.137480	-0.077718
50	1	0	-0.497181	0.906264	-1.923539
51	6	0	-0.857013	4.794364	-0.331582
52	6	0	-1.400666	3.835730	0.746176
53	6	0	-1.548813	2.517125	-0.019638
54	1	0	-1.687279	5.235722	-0.895090
55	1	0	-0.679036	3.728036	1.560208
56	1	0	-2.339057	4.202025	1.168954
57	1	0	-1.489535	1.622148	0.600898
58	1	0	-2.481528	2.475755	-0.593482
59	8	0	-0.360049	1.891854	-2.129215
60	6	0	2.150812	2.138082	-0.821709
61	1	0	2.947943	1.875361	-0.126572
62	1	0	2.108491	1.418041	-1.641821
63	1	0	2.293634	3.145030	-1.214203
64	6	0	0.057284	5.895240	0.147531
65	6	0	1.250531	5.602956	0.823808
66	6	0	-0.289889	7.232529	-0.067689
67	6	0	2.075835	6.631412	1.273776
68	1	0	1.531937	4.567520	0.993150
69	6	0	0.531454	8.264793	0.390624
70	1	0	-1.208789	7.469015	-0.599556
71	6	0	1.717168	7.965562	1.060733
72	1	0	3.000143	6.392919	1.793171
73	1	0	0.246971	9.299126	0.217569
74	1	0	2.361186	8.766048	1.414725
75	1	0	0.714775	1.129830	0.315075
76	6	0	-6.741322	1.830318	0.125661
77	6	0	-8.671559	3.881883	0.448204
78	6	0	6.904933	1.418378	-0.493612
79	6	0	9.109211	3.093269	-1.092959
80	6	0	4.425474	-1.481458	-0.710541
81	6	0	4.141502	-2.596056	-1.703671
82	6	0	3.562384	-2.135333	-3.061147
83	6	0	5.365710	-3.443674	-2.132706
84	1	0	3.414102	-3.283803	-1.264726
85	6	0	3.660502	-3.397281	-3.938958
86	1	0	4.185869	-1.331544	-3.476475
87	1	0	2.541618	-1.751850	-2.968927
88	6	0	4.922535	-4.159947	-3.435973
89	1	0	5.677828	-4.140479	-1.346912
90	1	0	6.221890	-2.788959	-2.333008
91	1	0	2.765152	-4.013782	-3.793898
92	1	0	3.709843	-3.160086	-5.007151
93	1	0	4.688774	-5.213717	-3.248175
94	1	0	5.725866	-4.148479	-4.180682
95	6	0	4.089706	-0.323145	1.424358
96	6	0	3.395697	-0.143715	2.768250
97	6	0	4.302875	-0.364164	4.011979
98	6	0	2.788009	1.252674	3.037629
99	1	0	2.565730	-0.853883	2.822664
100	6	0	3.628832	0.415598	5.177086
101	1	0	5.304981	0.034619	3.813150
102	1	0	4.427173	-1.428657	4.236225
103	6	0	2.454153	1.201254	4.536632
104	1	0	1.914299	1.449300	2.410702
105	1	0	3.528075	2.041226	2.843793
106	1	0	3.276019	-0.255049	5.967875
107	1	0	4.346307	1.099000	5.645510
108	1	0	1.513659	0.654406	4.677596
109	1	0	2.317429	2.194385	4.978876
110	6	0	-4.500314	-1.178861	0.849805
111	6	0	-4.208938	-2.053572	2.058722
112	6	0	-3.512851	-1.337387	3.238136
113	6	0	-5.448824	-2.702549	2.731480
114	1	0	-3.548155	-2.868519	1.751799
115	6	0	-3.622388	-2.359931	4.380628
116	1	0	-4.059400	-0.419266	3.494453
117	1	0	-2.482052	-1.055976	3.001623
118	6	0	-5.007401	-3.037879	4.185095
119	1	0	-5.791498	-3.583225	2.177323
120	1	0	-6.284994	-1.994578	2.742241
121	1	0	-2.821756	-3.104009	4.279746
122	1	0	-3.509882	-1.905767	5.371279
123	1	0	-4.945517	-4.118714	4.352062
124	1	0	-5.738180	-2.654156	4.905836
125	6	0	-4.252642	-0.569527	-1.512155
126	6	0	-3.697620	-0.783694	-2.915083
127	6	0	-4.756206	-1.325558	-3.923285
128	6	0	-3.116826	0.497071	-3.613836
129	1	0	-2.887086	-1.511323	-2.849166

130	6	0	-4.283104	-0.820312	-5.293433
131	1	0	-5.742367	-0.898713	-3.695608
132	1	0	-4.856016	-2.414990	-3.873936
133	6	0	-3.821465	0.612352	-4.984822
134	1	0	-2.039340	0.369175	-3.746375
135	1	0	-3.248499	1.400173	-3.011100
136	1	0	-3.434306	-1.423322	-5.643921
137	1	0	-5.061958	-0.870333	-6.063331
138	1	0	-3.172689	1.036386	-5.759176
139	1	0	-4.700965	1.266749	-4.908467
140	6	0	7.875843	3.270702	-1.722356
141	1	0	7.763985	4.067007	-2.456082
142	6	0	6.773621	2.455295	-1.440933
143	6	0	8.149833	1.215216	0.144481
144	6	0	9.224343	2.054129	-0.165981
145	1	0	10.181253	1.882978	0.324123
146	6	0	-7.996899	1.738890	-0.520179
147	6	0	-8.932870	2.762328	-0.346801
148	1	0	-9.897141	2.679189	-0.845448
149	6	0	-7.430632	3.953088	1.081871
150	1	0	-7.200746	4.816728	1.703750
151	6	0	-6.466998	2.947079	0.943109
152	6	0	-5.152827	3.092757	1.678645
153	1	0	-5.142082	2.517817	2.613559
154	1	0	-4.311750	2.730591	1.081198
155	1	0	-4.971043	4.140627	1.941581
156	6	0	-8.367230	0.547078	-1.377921
157	1	0	-7.850253	0.557194	-2.344980
158	1	0	-8.103725	-0.397789	-0.891188
159	1	0	-9.442962	0.539517	-1.580775
160	6	0	-9.711049	4.962803	0.634764
161	1	0	-10.463407	4.669352	1.379233
162	1	0	-9.258543	5.898294	0.980198
163	1	0	-10.246680	5.170641	-0.298460
164	6	0	5.461896	2.729800	-2.142466
165	1	0	5.009531	1.819804	-2.548300
166	1	0	4.730919	3.170225	-1.453023
167	1	0	5.600935	3.436388	-2.966640
168	6	0	8.354294	0.090600	1.137019
169	1	0	7.781202	0.246143	2.058790
170	1	0	8.029718	-0.872276	0.726816
171	1	0	9.410242	0.005210	1.412181
172	6	0	10.277590	4.004122	-1.390772
173	1	0	10.194748	4.449835	-2.387730
174	1	0	10.334577	4.830154	-0.668842
175	1	0	11.230104	3.465145	-1.338974

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1be (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3893.99032101 hartree

Zero-point Energy Correction = 1.501064 hartree

Thermal Correction to Energy = 1.582241 hartree

Thermal correction to Enthalpy = 1.583185 hartree

Thermal correction to Gibbs Free Energy= 1.373218 hartree

Sum of electronic and Zero-point Energies = -3892.489257 hartree

Sum of electronic and thermal Energies = -3892.408080hartree

Sum of electronic and thermal Enthalpies = -3892.407136 hartree

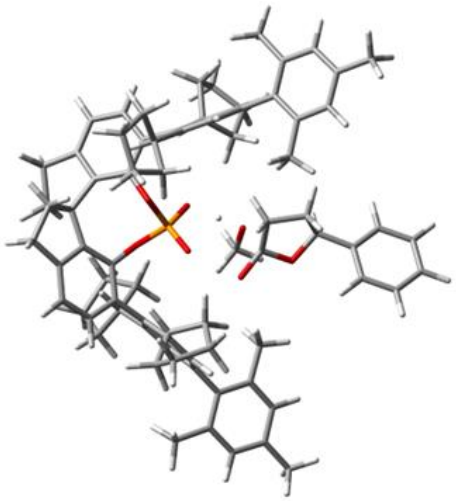
Sum of electronic and thermal Free Energies= -3892.617103 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.314238	3.780856	0.716880
2	6	0	-1.966205	2.624234	0.300436
3	6	0	-3.814569	3.144197	1.742221
4	6	0	-3.118072	4.232308	2.271389
5	6	0	-1.863822	4.543640	1.758529
6	1	0	-4.814166	2.920201	2.101657
7	1	0	-3.561302	4.830685	3.063697
8	6	0	-0.916248	5.656354	2.156253
9	1	0	-1.285327	6.636527	1.823365
10	1	0	-0.784509	5.724873	3.242414
11	6	0	-0.095291	4.496652	0.149276
12	6	0	0.387946	5.266668	1.422821
13	1	0	0.975570	4.582763	2.046161
14	1	0	1.022555	6.124433	1.178749
15	6	0	-0.540767	5.528497	-0.943541
16	1	0	-1.192980	5.017641	-1.661379
17	1	0	-1.103199	6.366947	-0.521713
18	6	0	0.767483	5.950664	-1.639510
19	1	0	1.235513	6.805443	-1.130798
20	1	0	0.616116	6.250507	-2.682815
21	6	0	1.615109	4.705191	-1.512524
22	6	0	1.060262	3.812990	-0.580547
23	6	0	2.790207	4.393908	-2.184349
24	1	0	3.227650	5.089922	-2.895816
25	6	0	1.640017	2.552463	-0.411504
26	8	0	-1.332768	1.789448	-0.623840
27	8	0	1.026747	1.634977	0.445341
28	15	0	-0.224448	0.713535	-0.094605
29	8	0	0.168047	-0.138387	-1.271380
30	8	0	-0.725654	0.016935	1.169433
31	6	0	-3.252353	2.297450	0.772693
32	6	0	2.847318	2.218097	-1.057357
33	6	0	-4.026521	1.119325	0.259592
34	6	0	3.408262	3.173133	-1.923806
35	1	0	4.346695	2.929322	-2.412244
36	6	0	3.638765	0.952767	-0.859439
37	6	0	0.066853	-3.107259	0.119094
38	8	0	-0.435176	-2.378345	1.531135
39	6	0	0.674240	-2.642328	2.456694
40	6	0	1.581273	-2.847552	0.195763
41	1	0	2.079769	-3.792853	-0.031159
42	1	0	1.862310	-2.118122	-0.565146
43	8	0	-0.661161	-2.577961	-0.860215
44	8	0	-0.192964	-4.420423	0.332889
45	6	0	-1.563147	-4.837076	0.198261
46	1	0	-1.576371	-5.882642	0.509202
47	1	0	-1.894295	-4.745492	-0.837973
48	1	0	-2.210003	-4.241957	0.849067
49	1	0	-0.583623	-1.266631	1.347288
50	1	0	-0.346512	-1.645619	-1.100333
51	6	0	0.532034	-1.930507	3.781378
52	6	0	0.674524	-0.540545	3.912955
53	6	0	0.280863	-2.695020	4.928607
54	6	0	0.564592	0.061327	5.166506

55	1	0	0.835638	0.077124	3.036606
56	6	0	0.176815	-2.093077	6.183207
57	1	0	0.168237	-3.773034	4.838144
58	6	0	0.319172	-0.710648	6.304202
59	1	0	0.669563	1.139358	5.252223
60	1	0	-0.015349	-2.703356	7.061499
61	1	0	0.237951	-0.236528	7.278696
62	1	0	0.611805	-3.719367	2.633593
63	6	0	1.917410	-2.337325	1.614170
64	1	0	2.804719	-2.815869	2.035875
65	1	0	2.105226	-1.260063	1.592259
66	6	0	-5.551754	-1.065771	-0.699547
67	6	0	5.588698	-1.096587	-0.740221
68	6	0	-4.359086	0.049311	1.127403
69	6	0	-5.116662	-1.016587	0.626324
70	1	0	-5.367248	-1.842976	1.287215
71	6	0	-5.225408	0.005639	-1.534162
72	1	0	-5.574048	-0.013263	-2.563585
73	6	0	-4.477741	1.099710	-1.085239
74	6	0	4.729666	-0.981284	-1.837528
75	1	0	4.850398	-1.674125	-2.666119
76	6	0	3.754387	0.021836	-1.922382
77	6	0	5.407155	-0.212953	0.327864
78	1	0	6.068033	-0.294405	1.186935
79	6	0	4.450146	0.810481	0.293406
80	6	0	4.388690	1.799358	1.447138
81	6	0	4.369091	1.208498	2.873284
82	6	0	5.589045	2.778927	1.514793
83	1	0	3.481604	2.402311	1.344670
84	6	0	4.616598	2.435208	3.771985
85	1	0	5.181946	0.481830	2.998040
86	1	0	3.432109	0.690609	3.105156
87	6	0	5.549168	3.372267	2.947586
88	1	0	5.539760	3.542593	0.731241
89	1	0	6.519046	2.218437	1.357633
90	1	0	3.664088	2.939296	3.976742
91	1	0	5.043891	2.161989	4.742727
92	1	0	5.161856	4.396969	2.942036
93	1	0	6.554801	3.422108	3.379030
94	6	0	2.892294	0.112974	-3.173189
95	6	0	3.639861	0.609606	-4.443012
96	6	0	2.245901	-1.203736	-3.658946
97	1	0	2.068071	0.802079	-2.968349
98	6	0	2.799687	0.108309	-5.651982
99	1	0	4.646638	0.174400	-4.469220
100	1	0	3.765692	1.697250	-4.439885
101	6	0	1.721167	-0.835716	-5.055800
102	1	0	1.456996	-1.547006	-2.985303
103	1	0	2.997067	-2.001206	-3.738460
104	1	0	2.341916	0.938287	-6.201020
105	1	0	3.436819	-0.424333	-6.367229
106	1	0	0.768310	-0.302732	-4.952321
107	1	0	1.531940	-1.712849	-5.684414
108	6	0	-3.950568	0.011158	2.594253
109	6	0	-5.138752	0.261987	3.570600
110	6	0	-3.326324	-1.342904	3.084241
111	1	0	-3.205881	0.790902	2.762242
112	6	0	-4.746628	-0.475418	4.858649
113	1	0	-6.057270	-0.178047	3.159757
114	1	0	-5.334108	1.329304	3.723446
115	6	0	-4.132266	-1.780829	4.328768
116	1	0	-2.280366	-1.174307	3.350266
117	1	0	-3.326483	-2.106775	2.301935
118	1	0	-3.988361	0.101017	5.406319
119	1	0	-5.592375	-0.635439	5.537643
120	1	0	-3.512931	-2.299184	5.069286
121	1	0	-4.938113	-2.470508	4.041721
122	6	0	-4.213063	2.236419	-2.059429
123	6	0	-3.434981	1.857583	-3.339857
124	6	0	-5.480816	2.924188	-2.630367
125	1	0	-3.632381	3.011535	-1.550826
126	6	0	-3.586406	3.105647	-4.226939
127	1	0	-3.908529	0.990968	-3.820419
128	1	0	-2.395051	1.591278	-3.130843
129	6	0	-5.000727	3.671866	-3.904399
130	1	0	-5.952006	3.588156	-1.897149
131	1	0	-6.226750	2.165230	-2.893765
132	1	0	-2.817452	3.841197	-3.958272
133	1	0	-3.453110	2.885190	-5.291695
134	1	0	-4.959800	4.754473	-3.741301
135	1	0	-5.696074	3.509414	-4.735318
136	6	0	-6.339272	-2.232924	-1.210549
137	6	0	-7.704431	-2.370067	-0.880408
138	6	0	-5.715153	-3.204725	-2.021269
139	6	0	-8.416035	-3.474247	-1.360430
140	6	0	-6.463524	-4.296236	-2.475822
141	6	0	-7.815709	-4.449907	-2.160678
142	1	0	-9.469282	-3.572221	-1.102658
143	1	0	-5.973531	-5.047387	-3.093208
144	6	0	6.721378	-2.081434	-0.747784
145	6	0	7.910303	-1.759671	-1.440171
146	6	0	6.626869	-3.313201	-0.070168
147	6	0	8.968195	-2.673863	-1.444961
148	6	0	7.707844	-4.201240	-0.102070
149	6	0	8.887583	-3.904284	-0.786965
150	1	0	9.882473	-2.414297	-1.975939
151	1	0	7.622701	-5.150589	0.423721
152	6	0	8.066983	-0.439290	-2.162778
153	1	0	7.367058	-0.347741	-3.001736
154	1	0	7.869260	0.409649	-1.498380
155	1	0	9.081410	-0.331768	-2.559465
156	6	0	5.376933	-3.691917	0.690518
157	1	0	5.203247	-3.020468	1.540061
158	1	0	4.488551	-3.630886	0.052316
159	1	0	5.448649	-4.712893	1.078711
160	6	0	10.033503	-4.888203	-0.835506
161	1	0	9.992744	-5.593136	0.001601
162	1	0	10.013514	-5.479383	-1.761051
163	1	0	11.002530	-4.377701	-0.801008
164	6	0	-4.255938	-3.089720	-2.406327
165	1	0	-4.088973	-2.276085	-3.122736
166	1	0	-3.614610	-2.873557	-1.545349
167	1	0	-3.904766	-4.015417	-2.874555
168	6	0	-8.413417	-1.339267	-0.028752
169	1	0	-8.044675	-1.337106	1.003969
170	1	0	-8.261110	-0.325384	-0.415649
171	1	0	-9.490051	-1.534699	0.002313
172	6	0	-8.612365	-5.619329	-2.692000
173	1	0	-9.094781	-5.373285	-3.647795
174	1	0	-7.974689	-6.492679	-2.867182
175	1	0	-9.406029	-5.914085	-1.996607

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1be (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3893.99441179 hartree

Zero-point Energy Correction = 1.502060 hartree

Thermal Correction to Energy = 1.583252 hartree

Thermal correction to Enthalpy = 1.584196 hartree

Thermal correction to Gibbs Free Energy= 1.372407 hartree

Sum of electronic and Zero-point Energies = -3892.492352 hartree

Sum of electronic and thermal Energies = -3892.411160 hartree

Sum of electronic and thermal Enthalpies = -3892.410215 hartree

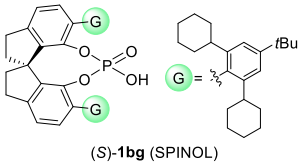
Sum of electronic and thermal Free Energies= -3892.622004 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.465609	2.499323	-0.230116
2	8	0	0.824748	3.761384	-0.548665
3	8	0	0.229678	1.779631	-1.790531
4	6	0	-0.379523	4.547104	-0.791860
5	6	0	-1.391779	3.952425	0.209024
6	6	0	-0.969220	2.473618	0.314070
7	1	0	-0.702662	4.343023	-1.819595
8	1	0	-1.286092	4.458228	1.173661
9	1	0	-2.421746	4.085972	-0.130603
10	1	0	-0.953348	2.099513	1.339849
11	1	0	-1.604120	1.806816	-0.270945
12	8	0	1.445922	1.835882	0.341900
13	6	0	1.429527	1.731491	-2.589007
14	1	0	2.212495	1.163239	-2.080631
15	1	0	1.169541	1.255654	-3.537219
16	1	0	1.759313	2.756860	-2.758736
17	1	0	1.109909	0.927266	0.675012
18	1	0	-0.104378	0.763339	-1.623305
19	6	0	-1.284097	-4.295967	-0.862966
20	6	0	-1.869219	-3.086367	-0.492379
21	6	0	-3.735582	-3.545858	-1.936986
22	6	0	-3.102626	-4.691793	-2.419989
23	6	0	-1.874236	-5.059083	-1.883029
24	1	0	-4.718351	-3.276095	-2.311122
25	1	0	-3.573740	-5.290649	-3.195641
26	6	0	-0.994883	-6.238131	-2.242119
27	1	0	-1.418715	-7.182320	-1.872233
28	1	0	-0.873043	-6.353026	-3.325441
29	6	0	-0.101262	-5.061159	-0.276889
30	6	0	0.331403	-5.897275	-1.526819
31	1	0	0.951891	-5.266427	-2.173719
32	1	0	0.919689	-6.779990	-1.257012
33	6	0	-0.581459	-6.031373	0.856846
34	1	0	-1.198547	-5.465241	1.564264
35	1	0	-1.188349	-6.856646	0.471778
36	6	0	0.716000	-6.493160	1.552271
37	1	0	1.132422	-7.388811	1.069665
38	1	0	0.563454	-6.747622	2.607456
39	6	0	1.623374	-5.296580	1.369811
40	6	0	1.095517	-4.414793	0.414008
41	6	0	2.821971	-5.010541	2.012571
42	1	0	3.242682	-5.699907	2.740536
43	6	0	1.724067	-3.189503	0.192963
44	6	0	3.481957	-3.820405	1.709271
45	1	0	4.432404	-3.595438	2.183534
46	8	0	-1.202553	-2.253502	0.407925
47	8	0	1.139745	-2.286785	-0.694674
48	15	0	-0.028958	-1.263735	-0.160525
49	8	0	0.430774	-0.439653	1.016164
50	8	0	-0.494426	-0.544902	-1.419680
51	6	0	-3.129977	-2.702683	-0.991136
52	6	0	2.943855	-2.872372	0.822544
53	6	0	-0.071808	6.012908	-0.627075
54	6	0	-0.673214	6.946280	-1.477756
55	6	0	0.770937	6.464293	0.396885
56	6	0	-0.449709	8.312880	-1.302219
57	1	0	-1.319416	6.603023	-2.282861
58	6	0	1.003670	7.828578	0.564820
59	1	0	1.257654	5.742507	1.045944
60	6	0	0.390574	8.756636	-0.280675
61	1	0	-0.924355	9.027579	-1.969034
62	1	0	1.666467	8.167848	1.356322
63	1	0	0.572334	9.819555	-0.146838
64	6	0	-3.864871	-1.479995	-0.521576
65	6	0	-5.173970	-0.341765	1.177820
66	6	0	-4.914380	0.660561	-0.978683
67	6	0	-5.456584	0.714745	0.308577
68	1	0	-5.594990	-0.316560	2.179417
69	1	0	-5.122954	1.477463	-1.665593
70	6	0	3.710447	-1.602514	0.586676
71	6	0	4.726818	0.421059	1.456673
72	6	0	5.223994	-0.281023	-0.777096
73	6	0	5.426034	0.627800	0.265468
74	1	0	4.862661	1.131470	2.268699
75	1	0	5.763719	-0.130957	-1.708964
76	6	0	6.398370	1.762034	0.133902
77	6	0	8.248658	3.891473	-0.074389
78	6	0	-6.326746	1.856846	0.736507
79	6	0	-7.977626	4.014754	1.535646
80	6	0	-4.123288	-0.410167	-1.415336
81	6	0	-3.609031	-0.393387	-2.849365
82	6	0	-4.713594	-0.649879	-3.912667
83	6	0	-2.934182	0.943100	-3.316404
84	1	0	-2.860491	-1.181516	-2.950851
85	6	0	-4.136172	-0.052427	-5.202183
86	1	0	-5.632868	-0.116013	-3.635183
87	1	0	-4.968854	-1.711193	-4.001493
88	6	0	-3.511617	1.267739	-4.718358
89	1	0	-1.851430	0.802297	-3.354982
90	1	0	-3.115316	1.761944	-2.613343
91	1	0	-3.357712	-0.715689	-5.603154
92	1	0	-4.885750	0.087389	-5.989642
93	1	0	-2.755603	1.661756	-5.406816
94	1	0	-4.296915	2.031079	-4.637208
95	6	0	-4.393884	-1.438388	0.793608
96	6	0	-4.174011	-2.552887	1.803429
97	6	0	-3.422819	-2.138902	3.089915
98	6	0	-5.456967	-3.209116	2.368998
99	1	0	-3.592039	-3.349523	1.331136
100	6	0	-3.629954	-3.333700	4.044304
101	1	0	-3.883760	-1.234422	3.508902

102	1	0	-2.370295	-1.911364	2.898433
103	6	0	-4.975395	-3.995044	3.612861
104	1	0	-5.960691	-3.843313	1.630912
105	1	0	-6.173587	-2.432772	2.663964
106	1	0	-2.805672	-4.048701	3.935410
107	1	0	-3.635969	-3.022870	5.094647
108	1	0	-4.819161	-5.050982	3.364619
109	1	0	-5.722254	-3.971390	4.413817
110	6	0	4.388143	-1.397271	-0.640828
111	6	0	4.280776	-2.371624	-1.802918
112	6	0	3.709230	-1.787383	-3.114238
113	6	0	5.617800	-2.997604	-2.273065
114	1	0	3.625868	-3.197596	-1.510870
115	6	0	4.001542	-2.883702	-4.156169
116	1	0	4.243984	-0.862943	-3.372096
117	1	0	2.644886	-1.546201	-3.028776
118	6	0	5.325720	-3.560099	-3.689551
119	1	0	5.980236	-3.761518	-1.576318
120	1	0	6.392398	-2.223312	-2.324211
121	1	0	3.185093	-3.616109	-4.155725
122	1	0	4.068176	-2.486647	-5.174998
123	1	0	5.216143	-4.649958	-3.668106
124	1	0	6.152889	-3.344753	-4.374768
125	6	0	3.865944	-0.667814	1.640959
126	6	0	3.156986	-0.810354	2.981752
127	6	0	4.105252	-1.179791	4.157510
128	6	0	2.399813	0.471836	3.481173
129	1	0	2.414960	-1.605712	2.891439
130	6	0	3.370385	-0.679224	5.408224
131	1	0	5.059971	-0.646986	4.051618
132	1	0	4.333752	-2.251010	4.185750
133	6	0	2.816155	0.683236	4.957855
134	1	0	1.323607	0.301147	3.389631
135	1	0	2.627463	1.348556	2.868235
136	1	0	2.545553	-1.361608	5.655589
137	1	0	4.016460	-0.613026	6.291462
138	1	0	1.990293	1.038801	5.584332
139	1	0	3.613245	1.436183	5.022986
140	6	0	-7.628061	1.993827	0.203047
141	6	0	-8.426971	3.065276	0.613842
142	1	0	-9.432017	3.156147	0.205230
143	6	0	-6.693161	3.857343	2.059467
144	1	0	-6.323225	4.580033	2.784841
145	6	0	-5.862908	2.795707	1.682241
146	6	0	6.949909	4.013496	-0.573155
147	1	0	6.646631	4.947236	-1.043865
148	6	0	6.020163	2.971323	-0.484247
149	6	0	8.605187	2.684588	0.533089
150	1	0	9.611336	2.566943	0.932069
151	6	0	7.706127	1.619406	0.646449
152	6	0	8.151354	0.335930	1.313223
153	1	0	7.592231	0.141084	2.236247
154	1	0	7.990318	-0.532430	0.664118
155	1	0	9.215138	0.378307	1.567766
156	6	0	4.632736	3.158910	-1.055101
157	1	0	4.494016	2.554476	-1.961090
158	1	0	3.850521	2.854909	-0.352855
159	1	0	4.460785	4.205512	-1.326693
160	6	0	9.245968	5.019055	-0.210280
161	1	0	9.830284	4.927250	-1.136067
162	1	0	8.747418	5.994091	-0.237923
163	1	0	9.958815	5.026812	0.621613
164	6	0	-4.488127	2.680387	2.304713
165	1	0	-4.454118	1.901648	3.076859
166	1	0	-3.728640	2.413850	1.563236
167	1	0	-4.195961	3.623601	2.778064
168	6	0	-8.188153	0.991167	-0.783306
169	1	0	-7.710988	1.071226	-1.767428
170	1	0	-8.032595	-0.038557	-0.443689
171	1	0	-9.262583	1.146498	-0.923776
172	6	0	-8.847643	5.184006	1.935337
173	1	0	-8.758346	6.012295	1.219269
174	1	0	-9.905965	4.902534	1.971323
175	1	0	-8.567816	5.574223	2.919637

DFT calculation of real system using SPINOL-derived CPA (*S*)-1bg

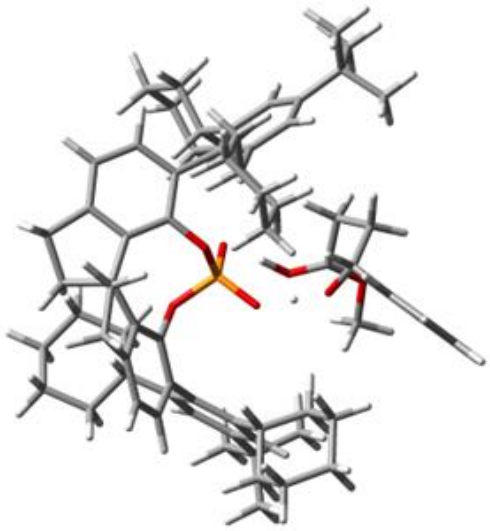


(*S*)-**1bg** (SPINOL)

1st / 2nd	ΔΔG‡ (kcal/mol)
R-anti / *R-re*	-1.93 / **0.00**
R-syn / *R-si*	-- / --
S-anti / *S-si*	**2.24** / 0.19
S-syn / *S-re*	**1.90** / -0.27

ΔΔG‡ of RDS = **1.90** kcal/mol

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1bg (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3667.78658495 hartree

Zero-point Energy Correction = 1.517614 hartree

Thermal Correction to Energy = 1.592386 hartree

Thermal correction to Enthalpy = 1.593330 hartree

Thermal correction to Gibbs Free Energy= 1.404519 hartree

Sum of electronic and Zero-point Energies = -3666.268971 hartree

Sum of electronic and thermal Energies = -3666.194199 hartree

Sum of electronic and thermal Enthalpies = -3666.193255 hartree

Sum of electronic and thermal Free Energies= -3666.382065 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.154667	2.297739	-2.657605
2	8	0	0.158574	2.734257	-1.035309
3	6	0	-1.018022	3.401115	-0.485892
4	6	0	-1.996679	3.533982	-1.672096
5	6	0	-1.671363	2.350376	-2.581752
6	1	0	-1.439778	2.719582	0.260520
7	1	0	-1.829428	4.477784	-2.198990
8	1	0	-3.030288	3.519789	-1.318548
9	1	0	-2.077178	2.459993	-3.591405
10	1	0	-2.034450	1.409418	-2.158849
11	8	0	0.487966	1.160978	-2.872600
12	8	0	0.335764	3.335602	-3.366618
13	6	0	1.757669	3.343743	-3.592355
14	1	0	1.966394	4.302290	-4.069087
15	1	0	2.046425	2.521300	-4.249747
16	1	0	2.295348	3.265361	-2.643875
17	1	0	0.392901	1.832992	-0.370874
18	1	0	0.095713	0.386893	-2.341836
19	6	0	-1.130814	-3.157094	1.824456
20	6	0	-1.743070	-2.087983	1.170242
21	6	0	-3.581156	-3.513979	0.560301
22	6	0	-2.935361	-4.617884	1.114584
23	6	0	-1.707013	-4.434512	1.737571
24	1	0	-4.559194	-3.636219	0.105484
25	1	0	-3.392815	-5.602828	1.063188
26	6	0	-0.814702	-5.470378	2.384157
27	1	0	-1.214395	-5.793178	3.355828
28	1	0	-0.709875	-6.373715	1.772294
29	6	0	0.086434	-3.208189	2.744609
30	6	0	0.513355	-4.703827	2.548572
31	1	0	1.101837	-4.782365	1.626963
32	1	0	1.132599	-5.074613	3.371024
33	6	0	-0.311232	-2.974778	4.240975
34	1	0	-0.896216	-2.050064	4.309079
35	1	0	-0.923271	-3.787107	4.645332
36	6	0	1.035824	-2.797298	4.975871
37	1	0	1.429186	-3.760393	5.330056
38	1	0	0.953195	-2.150406	5.857020
39	6	0	1.918745	-2.198094	3.902239
40	6	0	1.300004	-2.288551	2.645818
41	6	0	3.176787	-1.620807	4.028546
42	1	0	3.672335	-1.569721	4.994998
43	6	0	1.889968	-1.661181	1.550493
44	6	0	3.807778	-1.119266	2.889879
45	1	0	4.810595	-0.712281	2.969122
46	8	0	-1.112025	-0.843131	1.177850
47	8	0	1.203089	-1.635160	0.335240
48	15	0	0.048779	-0.511803	0.070918
49	8	0	0.545588	0.877606	0.472477
50	8	0	-0.435077	-0.710617	-1.341372
51	6	0	-2.998324	-2.235380	0.545962
52	6	0	3.177656	-1.094525	1.634276
53	6	0	-0.645709	4.708539	0.173920
54	6	0	-1.068063	4.979714	1.478834
55	6	0	0.093153	5.678019	-0.518329
56	6	0	-0.768351	6.202832	2.083399
57	1	0	-1.632818	4.228913	2.026892
58	6	0	0.400441	6.895241	0.086405
59	1	0	0.429775	5.468793	-1.529882
60	6	0	-0.032424	7.162534	1.388898
61	1	0	-1.103541	6.399998	3.098108
62	1	0	0.977451	7.638197	-0.458098
63	1	0	0.206541	8.113024	1.858377
64	6	0	3.901447	-0.520656	0.450566
65	6	0	4.284604	0.847036	0.429727
66	6	0	4.289919	-1.360986	-0.619829
67	6	0	-3.770897	-1.111544	-0.084567
68	6	0	-4.350985	-0.104214	0.727937
69	6	0	-4.049035	-1.125067	-1.473105
70	6	0	5.437572	0.511521	-1.717143
71	6	0	-5.541337	0.813412	-1.218268
72	6	0	-5.208369	0.832903	0.141964
73	1	0	-5.661123	1.582714	0.785296
74	6	0	-4.930010	-0.168290	-2.001072
75	1	0	-5.149219	-0.216240	-3.061395
76	6	0	5.040820	-0.824933	-1.675489
77	1	0	5.331630	-1.492766	-2.477832
78	6	0	5.039759	1.321424	-0.647098
79	1	0	5.334080	2.366967	-0.640287
80	6	0	6.292090	1.097502	-2.856909
81	6	0	7.623539	1.632774	-2.277832
82	1	0	8.242903	2.062592	-3.075209
83	1	0	7.456952	2.412013	-1.526841
84	1	0	8.193793	0.827070	-1.801507
85	6	0	5.529526	2.259367	-3.535931
86	1	0	5.294304	3.059712	-2.826333
87	1	0	6.132759	2.694138	-4.342765
88	1	0	4.587409	1.903941	-3.969317
89	6	0	6.627544	0.052490	-3.937967
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91	1	0	5.724095	-0.352331	-4.408079
92	1	0	7.232145	0.516089	-4.726161

93	6	0	-6.578330	1.807523	-1.776758
94	6	0	-7.934421	1.567047	-1.069390
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96	1	0	-8.695860	2.256380	-1.455343
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98	6	0	-6.124947	3.262238	-1.514833
99	1	0	-5.951029	3.453135	-0.450710
100	1	0	-5.197184	3.486498	-2.053742
101	1	0	-6.890098	3.969218	-1.858576
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105	1	0	-7.530659	2.377122	-3.642608
106	6	0	3.989887	-2.856914	-0.654052
107	6	0	3.170367	-3.279982	-1.895038
108	6	0	5.283273	-3.701879	-0.547618
109	1	0	3.386073	-3.110801	0.222194
110	6	0	2.869491	-4.787096	-1.883701
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112	1	0	2.238873	-2.705010	-1.929708
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114	1	0	5.944664	-3.470471	-1.394710
115	1	0	5.832898	-3.420875	0.359983
116	6	0	4.152884	-5.623471	-1.766875
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118	1	0	2.208967	-5.015952	-1.033598
119	1	0	5.914581	-5.780288	-0.498584
120	1	0	4.419427	-5.459084	0.373225
121	1	0	3.909896	-6.693143	-1.718292
122	1	0	4.759069	-5.481921	-2.674391
123	6	0	3.937411	1.825126	1.550251
124	6	0	5.183830	2.199862	2.390907
125	6	0	3.251711	3.118780	1.052578
126	1	0	3.222478	1.335874	2.219725
127	6	0	4.826681	3.127863	3.561946
128	1	0	5.917848	2.698022	1.740512
129	1	0	5.677635	1.294990	2.766279
130	6	0	2.878513	4.041402	2.223613
131	1	0	3.925734	3.664276	0.375808
132	1	0	2.359770	2.864119	0.474118
133	6	0	4.103660	4.393605	3.079501
134	1	0	5.734038	3.394189	4.120351
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136	1	0	2.402399	4.953426	1.843281
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141	6	0	-3.417984	1.277910	2.662311
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143	1	0	-3.462438	-0.851914	2.525012
144	6	0	-3.178003	1.326480	4.179246
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146	1	0	-2.463925	1.360582	2.128877
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148	1	0	-6.153873	0.562498	2.764220
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150	6	0	-4.479704	1.123986	4.968404
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152	1	0	-2.460536	0.538969	4.453658
153	1	0	-6.135406	-0.283225	5.091327
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161	6	0	-3.877833	-4.210727	-3.883722
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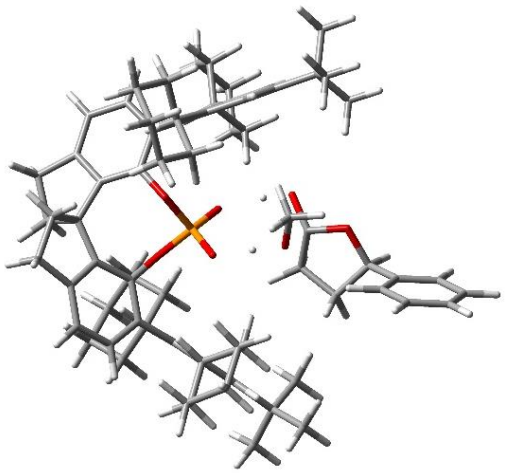
164	6	0	-2.074546	-2.558665	-4.539316
165	1	0	-3.411771	-0.895094	-4.213262
166	1	0	-1.934967	-0.829977	-3.243167
167	6	0	-3.114660	-3.565651	-5.049487
168	1	0	-4.656940	-4.885381	-4.262656
169	1	0	-3.183905	-4.832017	-3.298307
170	1	0	-1.573189	-2.068276	-5.384086
171	1	0	-1.292101	-3.091979	-3.980518
172	1	0	-2.632682	-4.338417	-5.662556
173	1	0	-3.829673	-3.046730	-5.706040

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1bg (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3667.78446830 hartree

Zero-point Energy Correction = 1.518547 hartree

Thermal Correction to Energy = 1.593332 hartree

Thermal correction to Enthalpy = 1.594276 hartree

Thermal correction to Gibbs Free Energy= 1.405483 hartree

Sum of electronic and Zero-point Energies = -3666.265922 hartree

Sum of electronic and thermal Energies = -3666.191136 hartree

Sum of electronic and thermal Enthalpies = -3666.190192 hartree

Sum of electronic and thermal Free Energies= -3666.378985 hartree

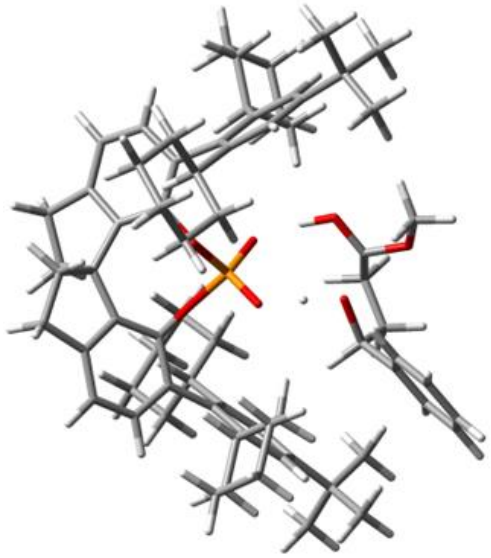
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.209459	2.930741	-1.003756
2	8	0	0.222737	4.280236	-1.097039
3	8	0	0.414620	2.650329	0.673469
4	6	0	1.559741	4.770654	-1.455730
5	6	0	2.477158	3.536698	-1.337789
6	6	0	1.512469	2.367881	-1.557939
7	1	0	1.479369	5.082459	-2.503440
8	1	0	2.923243	3.481765	-0.341597
9	1	0	3.287813	3.574484	-2.070180
10	1	0	1.816033	1.436161	-1.081155
11	1	0	1.343453	2.168395	-2.622129
12	8	0	-0.967988	2.425792	-1.319856
13	6	0	-0.662610	3.187781	1.471662
14	1	0	-0.643557	4.273625	1.373188
15	1	0	-0.471898	2.895738	2.506425
16	1	0	-1.624564	2.792046	1.136567
17	1	0	0.454883	1.560492	0.838336
18	1	0	-0.925125	1.408992	-1.316986
19	6	0	-2.112253	-3.502235	0.632626
20	6	0	-2.415755	-2.147648	0.511675
21	6	0	-4.488467	-2.703272	-0.572990

22	6	0	-4.160769	-4.058936	-0.544063	91	1	0	-2.622274	0.522932	5.365630
23	6	0	-2.963061	-4.450308	0.042756	92	1	0	-2.949057	-1.044890	4.637209
24	1	0	-5.430099	-2.387856	-1.011977	93	1	0	-6.744945	-0.633285	4.748761
25	1	0	-4.833186	-4.793355	-0.980700	94	1	0	-5.479817	-1.756652	4.262465
26	6	0	-2.368304	-5.837726	0.146290	95	1	0	-4.740832	-0.494783	6.266886
27	1	0	-2.880870	-6.439861	0.909853	96	1	0	-5.049513	1.036560	5.453235
28	1	0	-2.441367	-6.395755	-0.794287	97	6	0	-3.859935	-0.445544	-2.806322
29	6	0	-0.992332	-4.215656	1.384559	98	6	0	-5.194697	-0.679246	-3.556618
30	6	0	-0.908848	-5.540330	0.551081	99	6	0	-2.836160	0.216116	-3.758913
31	1	0	-0.306244	-5.353575	-0.345593	100	1	0	-3.450491	-1.428527	-2.552959
32	1	0	-0.435247	-6.355817	1.106332	101	6	0	-4.998838	-1.505949	-4.836993
33	6	0	-1.412043	-4.558570	2.853418	102	1	0	-5.635244	0.294713	-3.815576
34	1	0	-1.778174	-3.645765	3.337542	103	1	0	-5.918442	-1.173717	-2.896202
35	1	0	-2.212707	-5.303491	2.897069	104	6	0	-2.635866	-0.618479	-5.034285
36	6	0	-0.104173	-5.023472	3.530459	105	1	0	-3.179330	1.220970	-4.042930
37	1	0	0.043922	-6.106449	3.416001	106	1	0	-1.884139	0.334074	-3.235637
38	1	0	-0.089801	-4.818116	4.607172	107	6	0	-3.960532	-0.866094	-5.769600
39	6	0	0.949755	-4.236921	2.781062	108	1	0	-5.958612	-1.624884	-5.357274
40	6	0	0.401593	-3.641924	1.633148	109	1	0	-4.664210	-2.517908	-4.564336
41	6	0	2.291606	-4.061441	3.097428	110	1	0	-1.919998	-0.117122	-5.699083
42	1	0	2.725340	-4.541694	3.971208	111	1	0	-2.184513	-1.584600	-4.764190
43	6	0	1.179603	-2.750367	0.895399	112	1	0	-3.798171	-1.500362	-6.651048
44	6	0	3.083356	-3.264698	2.270005	113	1	0	-4.352446	0.092453	-6.142276
45	1	0	4.141992	-3.156901	2.483917	114	6	0	3.161212	-3.284844	-1.671976
46	8	0	-1.522254	-1.211967	1.030458	115	6	0	2.331024	-2.956126	-2.934754
47	8	0	0.601101	-2.053606	-0.165425	116	6	0	4.267490	-4.315056	-2.004927
48	15	0	-0.255662	-0.692795	0.129696	117	1	0	2.483689	-3.779830	-0.969655
49	8	0	0.503820	0.235565	1.074090	118	6	0	1.752806	-4.228693	-3.573149
50	8	0	-0.666030	-0.157922	-1.216695	119	1	0	2.967665	-2.445275	-3.671967
51	6	0	-3.617545	-1.715137	-0.085805	120	1	0	1.526724	-2.261260	-2.671270
52	6	0	2.548684	-2.563888	1.176663	121	6	0	3.685531	-5.584303	-2.646330
53	6	0	1.929646	5.965639	-0.611501	122	1	0	4.996719	-3.863988	-2.693138
54	6	0	2.172486	7.200570	-1.220694	123	1	0	4.820426	-4.569190	-1.091426
55	6	0	2.051419	5.859846	0.781637	124	6	0	2.850093	-5.254893	-3.892245
56	6	0	2.539206	8.311857	-0.458606	125	1	0	1.195220	-3.971190	-4.483041
57	1	0	2.072794	7.294886	-2.299731	126	1	0	1.024756	-4.678909	-2.881472
58	6	0	2.408372	6.969596	1.544820	127	1	0	4.494754	-6.281006	-2.901972
59	1	0	1.864051	4.905680	1.265886	128	1	0	3.050243	-6.101344	-1.911631
60	6	0	2.656021	8.198427	0.926283	129	1	0	2.409055	-6.170324	-4.308060
61	1	0	2.726992	9.264057	-0.947193	130	1	0	3.511401	-4.845499	-4.671034
62	1	0	2.496765	6.876214	2.623924	131	6	0	3.839541	-0.107331	2.353820
63	1	0	2.937335	9.061908	1.522982	132	6	0	5.078998	-0.384384	3.241160
64	6	0	3.440694	-1.687594	0.344884	133	6	0	3.438649	1.379744	2.490382
65	6	0	4.065992	-0.548142	0.908906	134	1	0	3.005985	-0.689498	2.759376
66	6	0	3.731708	-2.040249	-0.998310	135	6	0	4.825406	-0.009606	4.709498
67	6	0	-3.976092	-0.264770	-0.221455	136	1	0	5.931769	0.194785	2.857336
68	6	0	-4.251146	0.515359	0.924897	137	1	0	5.370951	-1.439058	3.167924
69	6	0	-4.082790	0.329070	-1.507556	138	6	0	3.166866	1.752777	3.956415
70	6	0	-4.679187	2.483546	-0.480856	139	1	0	4.243999	2.023342	2.107422
71	6	0	5.257413	-0.123594	-1.199307	140	1	0	2.553022	1.574522	1.880379
72	6	0	4.622615	-1.251468	-1.731324	141	6	0	4.378040	1.452472	4.851604
73	1	0	4.839588	-1.546115	-2.754080	142	1	0	5.729595	-0.190992	5.305455
74	6	0	4.957116	0.200805	0.124885	143	1	0	4.044678	-0.668173	5.117937
75	1	0	5.432459	1.060749	0.582153	144	1	0	2.896677	2.815030	4.029706
76	6	0	-4.585853	1.869415	0.769699	145	1	0	2.297281	1.183611	4.315974
77	1	0	-4.794895	2.445360	1.664435	146	1	0	4.145357	1.679547	5.900229
78	6	0	-4.436921	1.677726	-1.599251	147	1	0	5.210285	2.113462	4.565957
79	1	0	-4.517358	2.116767	-2.588837	148	6	0	-5.054907	3.965457	-0.665727
80	6	0	-4.268696	-0.072027	2.333709	149	6	0	-5.176230	4.712580	0.676059
81	6	0	-3.275034	0.619471	3.295156	150	1	0	-5.966447	4.294179	1.309728
82	6	0	-5.695377	-0.061916	2.934193	151	1	0	-4.236919	4.688283	1.240630
83	1	0	-3.966717	-1.122626	2.272420	152	1	0	-5.425378	5.763868	0.491777
84	6	0	-3.313154	-0.008283	4.697702	153	6	0	-6.418163	4.057161	-1.392685
85	1	0	-3.522273	1.688245	3.375918	154	1	0	-6.699206	5.105983	-1.552005
86	1	0	-2.264613	0.552374	2.877693	155	1	0	-6.386779	3.566446	-2.371213
87	6	0	-5.728368	-0.687490	4.337451	156	1	0	-7.209825	3.578327	-0.804667
88	1	0	-6.063123	0.972673	2.989943	157	6	0	-3.975998	4.678183	-1.516025
89	1	0	-6.379463	-0.596897	2.263183	158	1	0	-2.985034	4.592650	-1.058592
90	6	0	-4.731872	-0.003654	5.285002	159	1	0	-3.906165	4.254492	-2.522779

160	1	0	-4.219696	5.742970	-1.620845
161	6	0	6.258838	0.674370	-2.055343
162	6	0	5.578246	1.142895	-3.362889
163	1	0	5.213937	0.301144	-3.960285
164	1	0	4.721060	1.792310	-3.148794
165	1	0	6.286277	1.708493	-3.981284
166	6	0	6.796020	1.919898	-1.324798
167	1	0	5.989909	2.609572	-1.048377
168	1	0	7.343780	1.655742	-0.413393
169	1	0	7.488093	2.462818	-1.978716
170	6	0	7.461759	-0.233243	-2.408542
171	1	0	8.187372	0.312360	-3.024912
172	1	0	7.973350	-0.573621	-1.501100
173	1	0	7.147659	-1.121405	-2.966624

TS-1st-(*S*)-reaction pathway: *S*-*anti*/(*S*)-1bg (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3667.78073088 hartree

Zero-point Energy Correction = 1.517554 hartree

Thermal Correction to Energy = 1.592400 hartree

Thermal correction to Enthalpy = 1.593344 hartree

Thermal correction to Gibbs Free Energy= 1.405322 hartree

Sum of electronic and Zero-point Energies = -3666.263177 hartree

Sum of electronic and thermal Energies = -3666.188331 hartree

Sum of electronic and thermal Enthalpies = -3666.187387 hartree

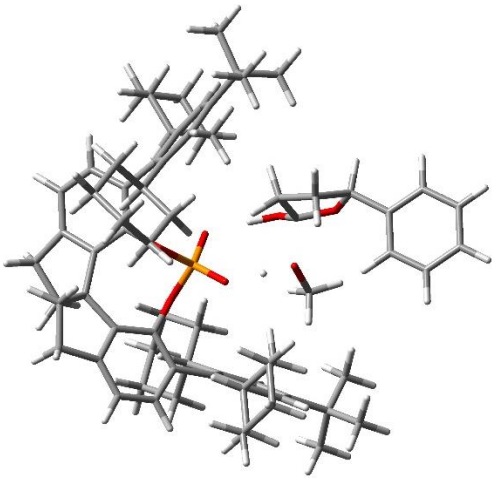
Sum of electronic and thermal Free Energies= -3666.375409 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.338228	2.863363	-1.890215
2	8	0	0.636527	2.727603	-0.512871
3	6	0	2.015853	2.930340	-0.924242
4	6	0	2.007833	2.944871	-2.479382
5	6	0	0.671606	2.322363	-2.885909
6	1	0	2.567467	2.052814	-0.568903
7	1	0	2.068129	3.972935	-2.845353
8	1	0	2.855947	2.385689	-2.881843
9	1	0	0.367190	2.600138	-3.898980
10	1	0	0.680808	1.232044	-2.807098
11	8	0	-1.455236	2.209100	-1.613090
12	8	0	-0.505002	4.191001	-2.051013
13	6	0	-1.489577	4.826066	-1.220013
14	1	0	-1.433405	5.886751	-1.467012
15	1	0	-2.484721	4.432682	-1.436209
16	1	0	-1.251557	4.672439	-0.163772
17	1	0	0.509130	1.709781	0.014388
18	1	0	-1.296165	1.207792	-1.597555
19	6	0	-1.950304	-3.372786	0.750801
20	6	0	-2.325665	-2.036667	0.619392
21	6	0	-4.470463	-2.730193	-0.214010
22	6	0	-4.066363	-4.064091	-0.210650
23	6	0	-2.797451	-4.378435	0.258416
24	1	0	-5.474228	-2.477209	-0.539544
25	1	0	-4.739686	-4.840771	-0.565052
26	6	0	-2.123437	-5.731259	0.331885
27	1	0	-2.555193	-6.355579	1.126611
28	1	0	-2.225439	-6.297606	-0.601092
29	6	0	-0.764441	-4.021212	1.456375
30	6	0	-0.658809	-5.355114	0.643364
31	1	0	-0.117708	-5.155850	-0.289018
32	1	0	-0.114424	-6.134914	1.184836
33	6	0	-1.126107	-4.354563	2.944106
34	1	0	-1.515861	-3.448711	3.422946
35	1	0	-1.894444	-5.129398	3.024077
36	6	0	0.217376	-4.751464	3.588232
37	1	0	0.410883	-5.828271	3.483770
38	1	0	0.255442	-4.529374	4.661020
39	6	0	1.210688	-3.931352	2.795648
40	6	0	0.608497	-3.383918	1.650707
41	6	0	2.551889	-3.699084	3.072492
42	1	0	3.028560	-4.146391	3.941260
43	6	0	1.328210	-2.480843	0.866271
44	8	0	-1.416770	-1.039847	0.990093
45	8	0	0.704127	-1.876795	-0.226364
46	15	0	-0.271129	-0.574787	-0.080808
47	8	0	0.454931	0.579168	0.619235
48	8	0	-0.824398	-0.312608	-1.457546
49	6	0	-3.608808	-1.682160	0.154077
50	6	0	2.692198	-2.226773	1.118537
51	6	0	2.589139	4.183114	-0.284995
52	6	0	1.998340	4.762603	0.843955
53	6	0	3.760271	4.756909	-0.799374
54	6	0	2.561464	5.893159	1.439317
55	1	0	1.092905	4.326801	1.251888
56	6	0	4.326944	5.882975	-0.201009
57	1	0	4.236363	4.327117	-1.676948
58	6	0	3.727498	6.457335	0.920925
59	1	0	2.084951	6.332769	2.311792
60	1	0	5.233991	6.313786	-0.616856
61	1	0	4.165058	7.336704	1.385735
62	6	0	-4.111721	-0.271540	0.050749
63	6	0	-4.302912	0.509268	1.220186
64	6	0	-4.519259	0.251194	-1.202835
65	6	0	3.282974	-2.884431	2.211460
66	1	0	4.339918	-2.720191	2.396625
67	6	0	3.553317	-1.316617	0.293014
68	6	0	4.161026	-0.184579	0.891889
69	6	0	3.874161	-1.645951	-1.048470
70	6	0	5.432197	0.253145	-1.167732
71	6	0	-5.330139	2.300270	-0.113653
72	6	0	-5.111989	1.521777	-1.251273
73	1	0	-5.421619	1.896272	-2.220029
74	6	0	-4.902430	1.766606	1.107070
75	1	0	-5.061146	2.338337	2.017045
76	6	0	5.078648	0.571888	0.145572
77	1	0	5.542375	1.423655	0.629765
78	6	0	4.794011	-0.853065	-1.741538
79	1	0	5.046021	-1.138852	-2.758902
80	6	0	6.519774	1.011949	-1.952693
81	6	0	7.695444	0.045411	-2.237750
82	1	0	8.489877	0.560878	-2.792035
83	1	0	8.123330	-0.334101	-1.303026
84	1	0	7.375878	-0.816641	-2.832371
85	6	0	7.074265	2.219616	-1.172803

86	1	0	7.559409	1.913503	-0.239308
87	1	0	7.826229	2.737658	-1.779289
88	1	0	6.289819	2.943356	-0.924639
89	6	0	5.956425	1.525115	-3.297932
90	1	0	5.556063	0.712729	-3.913060
91	1	0	5.150261	2.250482	-3.136914
92	1	0	6.744078	2.022870	-3.876871
93	6	0	-6.059228	3.657111	-0.151531
94	6	0	-5.209562	4.745180	0.544564
95	1	0	-5.738891	5.706018	0.533729
96	1	0	-4.996677	4.496377	1.588927
97	1	0	-4.250248	4.881295	0.033110
98	6	0	-6.351505	4.128442	-1.588819
99	1	0	-7.017789	3.438295	-2.118110
100	1	0	-6.845069	5.106932	-1.564918
101	1	0	-5.433283	4.232994	-2.178505
102	6	0	-7.408600	3.519012	0.594763
103	1	0	-7.954366	4.470948	0.583613
104	1	0	-8.040128	2.758579	0.121545
105	1	0	-7.262314	3.226942	1.640089
106	6	0	3.321254	-2.882577	-1.750973
107	6	0	2.503822	-2.537626	-3.017532
108	6	0	4.438765	-3.899781	-2.086717
109	1	0	2.638290	-3.392935	-1.065561
110	6	0	1.947907	-3.802432	-3.690666
111	1	0	3.143466	-2.001545	-3.734270
112	1	0	1.684143	-1.862405	-2.749265
113	6	0	3.875179	-5.161035	-2.759198
114	1	0	5.174859	-3.433214	-2.756886
115	1	0	4.980232	-4.166064	-1.169870
116	6	0	3.058448	-4.813150	-4.012262
117	1	0	1.402610	-3.531176	-4.603923
118	1	0	1.212885	-4.271074	-3.019428
119	1	0	4.693008	-5.847865	-3.014010
120	1	0	3.231285	-5.695200	-2.044543
121	1	0	2.631315	-5.723091	-4.453717
122	1	0	3.729623	-4.383283	-4.771348
123	6	0	3.897227	0.239000	2.337577
124	6	0	5.165327	0.105056	3.216792
125	6	0	3.321401	1.668560	2.454538
126	1	0	3.140407	-0.429599	2.758193
127	6	0	4.892657	0.490796	4.678564
128	1	0	5.957595	0.753503	2.815675
129	1	0	5.554737	-0.919716	3.162979
130	6	0	3.057664	2.059430	3.917569
131	1	0	4.016483	2.393582	2.009261
132	1	0	2.388400	1.721462	1.885508
133	6	0	4.314126	1.908602	4.786686
134	1	0	5.816595	0.408478	5.266108
135	1	0	4.180373	-0.225333	5.114630
136	1	0	2.684823	3.090954	3.961473
137	1	0	2.258757	1.420614	4.322023
138	1	0	4.086736	2.149049	5.833494
139	1	0	5.072820	2.634047	4.456374
140	6	0	-4.387007	-0.521285	-2.517045
141	6	0	-5.772946	-0.929943	-3.077185
142	6	0	-3.594676	0.238133	-3.607273
143	1	0	-3.828718	-1.441373	-2.319289
144	6	0	-5.652115	-1.759225	-4.364668
145	1	0	-6.359256	-0.022833	-3.283470
146	1	0	-6.337418	-1.489281	-2.320828
147	6	0	-3.471115	-0.590450	-4.896392
148	1	0	-4.091757	1.190653	-3.839431
149	1	0	-2.599671	0.482729	-3.229044
150	6	0	-4.842846	-1.017120	-5.437436
151	1	0	-6.651398	-2.010173	-4.744586
152	1	0	-5.156826	-2.713888	-4.133327
153	1	0	-2.924948	-0.016240	-5.656573
154	1	0	-2.867036	-1.486064	-4.690502
155	1	0	-4.724795	-1.645593	-6.329893
156	1	0	-5.400940	-0.123524	-5.755425
157	6	0	-3.938696	0.016116	2.617574
158	6	0	-2.884825	0.915156	3.305728
159	6	0	-5.183244	-0.145908	3.523136
160	1	0	-3.494601	-0.979752	2.530148
161	6	0	-2.510441	0.382295	4.697157
162	1	0	-3.283432	1.935283	3.406752
163	1	0	-1.993526	0.982355	2.673008
164	6	0	-4.803967	-0.678603	4.913897
165	1	0	-5.689723	0.823562	3.633560
166	1	0	-5.904232	-0.818977	3.041541
167	6	0	-3.746735	0.206280	5.591171
168	1	0	-1.787297	1.056337	5.174720
169	1	0	-2.002150	-0.587060	4.584578
170	1	0	-5.699760	-0.753517	5.544487
171	1	0	-4.408649	-1.700570	4.813278
172	1	0	-3.460359	-0.218803	6.562180
173	1	0	-4.184466	1.194213	5.800352

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1bg (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3667.78289566 hartree

Zero-point Energy Correction = 1.518508 hartree

Thermal Correction to Energy = 1.593401hartree

Thermal correction to Enthalpy = 1.594345 hartree

Thermal correction to Gibbs Free Energy= 1.404206 hartree

Sum of electronic and Zero-point Energies = -3666.264388 hartree

Sum of electronic and thermal Energies = -3666.189495 hartree

Sum of electronic and thermal Enthalpies = -3666.188551 hartree

Sum of electronic and thermal Free Energies= -3666.378690 hartree

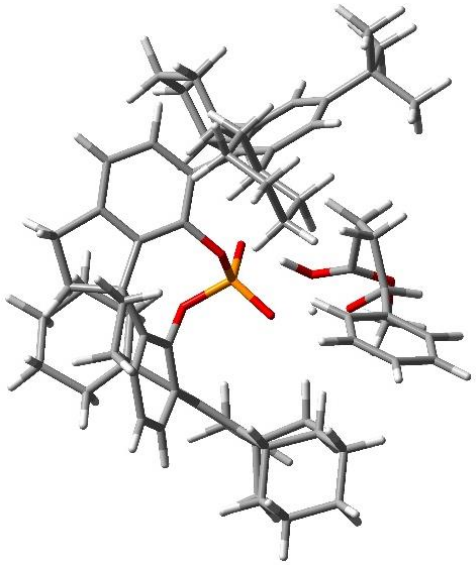
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.209347	-3.846914	0.271279
2	6	0	-1.786859	-2.577905	0.300058
3	6	0	-3.780759	-3.469749	-0.703758
4	6	0	-3.170888	-4.713324	-0.862161
5	6	0	-1.879603	-4.893143	-0.382035
6	1	0	-4.805795	-3.331210	-1.031728
7	1	0	-3.705728	-5.527435	-1.345165
8	6	0	-1.006987	-6.127677	-0.451306
9	1	0	-1.358858	-6.909320	0.236611
10	1	0	-0.996617	-6.573913	-1.452498
11	6	0	0.047584	-4.396764	0.939273
12	6	0	0.374762	-5.583457	-0.027778
13	1	0	0.904245	-5.188329	-0.902502
14	1	0	1.015811	-6.339227	0.436607

15	6	0	-0.290155	-4.967459	2.359329	84	1	0	-4.878964	3.990083	-0.225797
16	1	0	-0.829315	-4.199786	2.926635	85	6	0	-7.787948	2.080137	-0.428813
17	1	0	-0.927202	-5.855909	2.312537	86	1	0	-8.233255	1.252514	0.134795
18	6	0	1.084185	-5.227283	3.009294	87	1	0	-8.485689	2.926510	-0.399704
19	1	0	1.453645	-6.235729	2.775568	88	1	0	-7.692579	1.759967	-1.471627
20	1	0	1.058564	-5.148006	4.102285	89	6	0	-6.658316	2.976454	1.613897
21	6	0	1.948070	-4.161444	2.372368	90	1	0	-7.125321	2.205601	2.236836
22	6	0	1.297355	-3.585905	1.269473	91	1	0	-5.725387	3.286471	2.099141
23	6	0	3.217648	-3.738283	2.746073	92	1	0	-7.330169	3.842394	1.603023
24	1	0	3.736054	-4.199894	3.582910	93	6	0	6.416285	2.149007	-1.577637
25	6	0	1.877413	-2.491494	0.627553	94	6	0	5.714417	2.727814	-2.828908
26	6	0	3.823840	-2.711953	2.024562	95	1	0	6.363838	3.457527	-3.328023
27	1	0	4.829141	-2.395080	2.284693	96	1	0	5.467949	1.948826	-3.557517
28	8	0	-1.051730	-1.512012	0.822589	97	1	0	4.782263	3.237438	-2.557745
29	8	0	1.187820	-1.880932	-0.417544	98	6	0	6.763494	3.320581	-0.639411
30	15	0	0.032687	-0.752049	-0.144051	99	1	0	7.301278	2.983019	0.253621
31	8	0	0.573147	0.379073	0.728350	100	1	0	7.409345	4.034390	-1.163311
32	8	0	-0.537794	-0.404591	-1.491981	101	1	0	5.868279	3.863022	-0.313842
33	6	0	-3.103049	-2.365319	-0.159333	102	6	0	7.739368	1.470245	-2.007056
34	6	0	3.166717	-2.040379	0.978673	103	1	0	7.565254	0.650615	-2.711801
35	6	0	-3.828962	-1.053655	-0.066792	104	1	0	8.401860	2.196530	-2.494279
36	6	0	-4.167601	-0.508787	1.194981	105	1	0	8.266485	1.057302	-1.139393
37	6	0	-4.295749	-0.409753	-1.245105	106	6	0	3.948344	-2.235308	-1.926570
38	6	0	3.885576	-0.912695	0.296943	107	6	0	3.103022	-1.853192	-3.164525
39	6	0	4.280371	0.228283	1.039689	108	6	0	5.210768	-3.021276	-2.356438
40	6	0	4.289457	-1.027861	-1.058455	109	1	0	3.343881	-2.927850	-1.334055
41	6	0	-0.561513	2.858027	-1.266253	110	6	0	2.746519	-3.087648	-4.006566
42	8	0	-0.458870	4.161511	-1.621374	111	1	0	3.665296	-1.143849	-3.789292
43	8	0	0.802777	2.593594	-0.309368	112	1	0	2.189720	-1.342891	-2.841269
44	1	0	-0.505942	1.086675	-2.032719	113	6	0	4.847880	-4.254003	-3.199646
45	6	0	-1.243793	5.015404	-0.723727	114	1	0	5.873755	-2.367181	-2.940533
46	6	0	-1.692949	4.080250	0.417691	115	1	0	5.778181	-3.322558	-1.466415
47	6	0	-1.685627	2.701772	-0.249452	116	6	0	3.998470	-3.874108	-4.421666
48	1	0	-2.111245	5.335220	-1.312682	117	1	0	2.175081	-2.783256	-4.892864
49	1	0	-0.977683	4.114455	1.243910	118	1	0	2.083969	-3.741428	-3.420119
50	1	0	-2.673141	4.368216	0.806854	119	1	0	5.761779	-4.774012	-3.515740
51	1	0	-1.530987	1.870179	0.437991	120	1	0	4.285336	-4.964653	-2.575842
52	1	0	-2.606309	2.512391	-0.811308	121	1	0	3.716991	-4.774162	-4.983858
53	8	0	-0.435714	2.059921	-2.316545	122	1	0	4.603643	-3.256933	-5.102924
54	6	0	2.034487	2.686618	-1.062573	123	6	0	3.873403	0.460557	2.495318
55	1	0	2.854802	2.564902	-0.356133	124	6	0	5.087854	0.440245	3.455400
56	1	0	2.079142	1.909838	-1.828684	125	6	0	3.073670	1.771282	2.692222
57	1	0	2.060747	3.674416	-1.523953	126	1	0	3.205648	-0.351946	2.797200
58	6	0	-0.445932	6.230807	-0.317865	127	6	0	4.664640	0.633658	4.920032
59	6	0	0.765783	6.102640	0.376304	128	1	0	5.788959	1.238816	3.172778
60	6	0	-0.921962	7.510463	-0.619308	129	1	0	5.639273	-0.502018	3.344459
61	6	0	1.482092	7.234577	0.759633	130	6	0	2.646545	1.958598	4.156493
62	1	0	1.146129	5.112598	0.611207	131	1	0	3.686817	2.632204	2.386855
63	6	0	-0.209770	8.646449	-0.228486	132	1	0	2.190017	1.753642	2.048302
64	1	0	-1.856257	7.620092	-1.165489	133	6	0	3.849362	1.921406	5.109062
65	6	0	0.994873	8.510231	0.460488	134	1	0	5.551230	0.644057	5.567718
66	1	0	2.421410	7.122766	1.294673	135	1	0	4.057584	-0.227567	5.235943
67	1	0	-0.593919	9.634183	-0.468457	136	1	0	2.101627	2.905338	4.268238
68	1	0	1.553866	9.391850	0.762366	137	1	0	1.941007	1.160321	4.428782
69	1	0	0.719346	1.594858	0.146684	138	1	0	3.516519	2.011881	6.151267
70	6	0	-5.469933	1.272785	0.114464	139	1	0	4.495145	2.790187	4.910434
71	6	0	5.506065	1.104370	-0.904172	140	6	0	-3.965106	-0.905025	-2.652571
72	6	0	-5.105775	0.724083	-1.121454	141	6	0	-5.199479	-1.500092	-3.374282
73	1	0	-5.475318	1.186096	-2.032360	142	6	0	-3.336779	0.191708	-3.543747
74	6	0	-4.967318	0.642668	1.253930	143	1	0	-3.216935	-1.699207	-2.566273
75	1	0	-5.221766	1.030644	2.233569	144	6	0	-4.835123	-2.050466	-4.762385
76	6	0	5.075833	-0.017952	-1.621531	145	1	0	-5.966180	-0.718358	-3.480433
77	1	0	5.382662	-0.130748	-2.657307	146	1	0	-5.654462	-2.291037	-2.765762
78	6	0	5.085161	1.199953	0.424091	147	6	0	-2.955804	-0.357885	-4.926565
79	1	0	5.390544	2.053461	1.019002	148	1	0	-4.049575	1.018673	-3.677228
80	6	0	-6.420344	2.483889	0.173606	149	1	0	-2.456454	0.608377	-3.049664
81	6	0	-5.838356	3.661176	-0.643104	150	6	0	-4.164051	-0.982281	-5.638658
82	1	0	-5.673649	3.392858	-1.691596	151	1	0	-5.733060	-2.442743	-5.258046
83	1	0	-6.524739	4.516659	-0.622696	152	1	0	-4.148480	-2.901119	-4.639875

153	1	0	-2.525141	0.444141	-5.539830
154	1	0	-2.167987	-1.115484	-4.807208
155	1	0	-3.861598	-1.415130	-6.601202
156	1	0	-4.896382	-0.193076	-5.867439
157	6	0	-3.754745	-1.153703	2.514817
158	6	0	-2.870341	-0.226121	3.380309
159	6	0	-4.975925	-1.648520	3.327524
160	1	0	-3.156420	-2.042227	2.293188
161	6	0	-2.446554	-0.908754	4.690147
162	1	0	-3.424210	0.693892	3.618820
163	1	0	-1.985468	0.070568	2.806902
164	6	0	-4.543934	-2.332285	4.634109
165	1	0	-5.633048	-0.799469	3.564771
166	1	0	-5.570038	-2.338568	2.714742
167	6	0	-3.658145	-1.413004	5.487765
168	1	0	-1.851051	-0.215160	5.298072
169	1	0	-1.787502	-1.757781	4.454731
170	1	0	-5.428497	-2.646570	5.203575
171	1	0	-3.986504	-3.250098	4.393883
172	1	0	-3.328289	-1.936720	6.394542
173	1	0	-4.253372	-0.550653	5.824682

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1bg (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3667.77999606 hartree

Zero-point Energy Correction = 1.517549 hartree

Thermal Correction to Energy = 1.592480 hartree

Thermal correction to Enthalpy = 1.593424 hartree

Thermal correction to Gibbs Free Energy= 1.404042 hartree

Sum of electronic and Zero-point Energies = -3666.262447 hartree

Sum of electronic and thermal Energies = -3666.187516 hartree

Sum of electronic and thermal Enthalpies = -3666.186572 hartree

Sum of electronic and thermal Free Energies= -3666.375954 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.243769	1.433506	3.034312
2	6	0	-1.877251	1.127101	1.832499
3	6	0	-3.793429	0.336069	3.040135
4	6	0	-3.118321	0.496855	4.250956
5	6	0	-1.838631	1.039847	4.242546
6	1	0	-4.812796	-0.036103	3.043074
7	1	0	-3.598428	0.213772	5.184578
8	6	0	-0.907230	1.308131	5.406048
9	1	0	-1.260461	2.147642	6.020958
10	1	0	-0.820384	0.445364	6.076866
11	6	0	-0.005853	2.274272	3.332745
12	6	0	0.425842	1.647774	4.699910
13	1	0	0.989886	0.728234	4.504708
14	1	0	1.067727	2.315404	5.283280
15	6	0	-0.418696	3.770465	3.557903
16	1	0	-1.039825	4.092879	2.714107
17	1	0	-1.002680	3.909637	4.472594
18	6	0	0.911401	4.548851	3.551176
19	1	0	1.354777	4.594007	4.555996
20	1	0	0.795897	5.584621	3.211844
21	6	0	1.760861	3.723209	2.611775
22	6	0	1.178849	2.464773	2.386530
23	6	0	2.957237	4.073601	1.999112
24	1	0	3.416892	5.040910	2.186238
25	6	0	1.756301	1.605573	1.450105
26	8	0	-1.204781	1.374331	0.634673
27	8	0	1.129452	0.387229	1.177715
28	15	0	-0.092199	0.314455	0.086956
29	8	0	0.328861	0.790945	-1.276770
30	8	0	-0.606260	-1.120097	0.222714
31	6	0	-3.188020	0.609298	1.801490
32	6	0	2.976570	1.926124	0.820260
33	6	0	-3.948830	0.381614	0.526980
34	6	0	-4.275242	1.472429	-0.315323
35	6	0	-4.416905	-0.916120	0.185821
36	6	0	3.565524	3.161235	1.138769
37	1	0	4.517030	3.408765	0.678609
38	6	0	3.709127	1.017031	-0.127069
39	6	0	3.825264	1.348780	-1.497679
40	6	0	4.415144	-0.103519	0.380957
41	6	0	0.020041	-1.971665	-3.020766
42	8	0	-0.404006	-2.739138	-1.584495
43	6	0	0.678178	-3.707179	-1.399906
44	6	0	1.552433	-1.971936	-2.884331
45	1	0	1.959524	-2.325131	-3.835263
46	1	0	1.899117	-0.950819	-2.720125
47	8	0	-0.656954	-0.831143	-3.054555
48	8	0	-0.372405	-2.854940	-3.969165
49	6	0	-1.779662	-2.884857	-4.269352
50	1	0	-1.911476	-3.734510	-4.940722
51	1	0	-2.087051	-1.960251	-4.762587
52	1	0	-2.362692	-3.028155	-3.355776
53	1	0	-0.484271	-1.965918	-0.740054
54	1	0	-0.269227	-0.141098	-2.421926
55	6	0	0.635333	-4.434635	-0.076561
56	6	0	0.777407	-3.777667	1.155096
57	6	0	0.501967	-5.829428	-0.086307
58	6	0	0.783888	-4.507948	2.343738
59	1	0	0.852259	-2.696419	1.191363
60	6	0	0.518645	-6.560355	1.102388
61	1	0	0.389307	-6.349001	-1.035278
62	6	0	0.659517	-5.899109	2.322328
63	1	0	0.887438	-3.984936	3.290542
64	1	0	0.417894	-7.641969	1.073375
65	1	0	0.669822	-6.462838	3.251406
66	1	0	0.517054	-4.436081	-2.199207
67	6	0	1.940522	-2.892584	-1.706764
68	1	0	2.784624	-3.546997	-1.940624
69	1	0	2.223457	-2.294343	-0.835559
70	6	0	-5.507852	-0.018823	-1.827476
71	6	0	5.360561	-0.540101	-1.845320

72	6	0	5.215718	-0.852042	-0.487172
73	1	0	5.772216	-1.689638	-0.077410
74	6	0	4.645389	0.560578	-2.320722
75	1	0	4.734554	0.842409	-3.363274
76	6	0	-5.038720	1.244473	-1.468750
77	1	0	-5.274429	2.097582	-2.093989
78	6	0	-5.180913	-1.077861	-0.973604
79	1	0	-5.533133	-2.076285	-1.215591
80	6	0	-6.353930	-0.273162	-3.088831
81	6	0	-6.607028	1.013962	-3.896446
82	1	0	-7.209367	0.782619	-4.782609
83	1	0	-7.154904	1.760737	-3.310610
84	1	0	-5.671745	1.469450	-4.240737
85	6	0	-5.619486	-1.278569	-4.007552
86	1	0	-5.451146	-2.237531	-3.506056
87	1	0	-6.208687	-1.473197	-4.912577
88	1	0	-4.643607	-0.883831	-4.313299
89	6	0	-7.725456	-0.861818	-2.681391
90	1	0	-8.338432	-1.056431	-3.570443
91	1	0	-7.617756	-1.805195	-2.136205
92	1	0	-8.273347	-0.164919	-2.036846
93	6	0	6.316710	-1.364296	-2.729527
94	6	0	5.908835	-2.855821	-2.710044
95	1	0	6.610801	-3.451689	-3.306473
96	1	0	5.903345	-3.266032	-1.694915
97	1	0	4.907160	-2.993554	-3.133648
98	6	0	7.757223	-1.227248	-2.179721
99	1	0	8.459500	-1.801924	-2.796436
100	1	0	8.078678	-0.179563	-2.184358
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103	1	0	5.324399	-0.966716	-4.650775
104	1	0	6.657912	0.146462	-4.289495
105	1	0	7.001213	-1.514916	-4.784310
106	6	0	4.421019	-0.444367	1.869107
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108	6	0	5.708347	0.084314	2.549527
109	1	0	3.580814	0.073653	2.342397
110	6	0	4.218795	-2.204947	3.693975
111	1	0	5.058383	-2.528045	1.737321
112	1	0	3.312368	-2.311786	1.720209
113	6	0	5.711154	-0.188642	4.061603
114	1	0	6.581349	-0.397348	2.084977
115	1	0	5.808848	1.160124	2.359329
116	6	0	5.492303	-1.676932	4.371310
117	1	0	4.100209	-3.278916	3.887791
118	1	0	3.341092	-1.708752	4.135288
119	1	0	6.654218	0.158393	4.503792
120	1	0	4.910759	0.399845	4.534192
121	1	0	5.443372	-1.837484	5.456175
122	1	0	6.357337	-2.252412	4.008784
123	6	0	3.143693	2.570156	-2.111635
124	6	0	4.163795	3.699017	-2.407646
125	6	0	2.339518	2.257665	-3.395186
126	1	0	2.424103	2.957028	-1.382709
127	6	0	3.479853	4.959338	-2.958923
128	1	0	4.900586	3.332736	-3.137918
129	1	0	4.729370	3.946635	-1.501274
130	6	0	1.642312	3.515305	-3.936999
131	1	0	3.008443	1.861734	-4.173079
132	1	0	1.596835	1.487269	-3.175846
133	6	0	2.641954	4.649133	-4.207448
134	1	0	4.232908	5.726045	-3.184762
135	1	0	2.827329	5.382138	-2.180744
136	1	0	1.089266	3.269863	-4.853104
137	1	0	0.895599	3.852810	-3.203869
138	1	0	2.116385	5.551168	-4.547315
139	1	0	3.313351	4.351306	-5.027155
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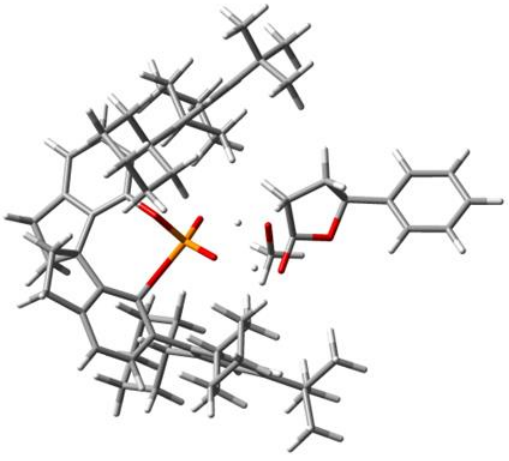
141	6	0	-5.428692	-2.645679	1.757487
142	6	0	-3.525834	-3.325360	0.244007
143	1	0	-3.418025	-1.885750	1.811079
144	6	0	-5.149092	-3.851906	2.667316
145	1	0	-6.177309	-2.924044	1.001312
146	1	0	-5.876661	-1.830648	2.339586
147	6	0	-3.229340	-4.526171	1.156011
148	1	0	-4.216694	-3.647720	-0.548825
149	1	0	-2.610638	-2.989236	-0.251080
150	6	0	-4.489266	-5.002288	1.893260
151	1	0	-6.081498	-4.192213	3.137204
152	1	0	-4.483681	-3.537579	3.485163
153	1	0	-2.799283	-5.346192	0.567050
154	1	0	-2.462390	-4.240752	1.889498
155	1	0	-4.245760	-5.828691	2.573984
156	1	0	-5.207805	-5.402216	1.161557
157	6	0	-3.880101	2.914344	-0.008210
158	6	0	-3.005588	3.542323	-1.119172
159	6	0	-5.113813	3.806035	0.273508
160	1	0	-3.282208	2.923868	0.908026
161	6	0	-2.598078	4.981194	-0.768048
162	1	0	-3.564519	3.551761	-2.066011
163	1	0	-2.117719	2.922421	-1.279989
164	6	0	-4.704606	5.246619	0.619070
165	1	0	-5.769773	3.818376	-0.608503
166	1	0	-5.703333	3.371749	1.091243
167	6	0	-3.820901	5.863279	-0.475689
168	1	0	-2.003972	5.412309	-1.584474
169	1	0	-1.942427	4.964235	0.115781
170	1	0	-5.599231	5.862644	0.779808
171	1	0	-4.152147	5.246580	1.570766
172	1	0	-3.504509	6.873748	-0.184951
173	1	0	-4.412989	5.974835	-1.396667

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1bg (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3667.78401199 hartree

Zero-point Energy Correction = 1.518896 hartree

Thermal Correction to Energy = 1.593894 hartree

Thermal correction to Enthalpy = 1.594838 hartree

Thermal correction to Gibbs Free Energy= 1.404594 hartree
Sum of electronic and Zero-point Energies = -3666.265116 hartree
Sum of electronic and thermal Energies = -3666.190118 hartree
Sum of electronic and thermal Enthalpies = -3666.189174 hartree
Sum of electronic and thermal Free Energies= -3666.379418 hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.084906	3.005443	0.007163
2	8	0	-0.048589	4.334137	-0.241530
3	8	0	-0.286996	2.338497	-1.575937
4	6	0	-1.412692	4.842892	-0.300118
5	6	0	-2.151270	3.976075	0.739877
6	6	0	-1.421929	2.621789	0.658462
7	1	0	-1.799379	4.635489	-1.305309
8	1	0	-2.036666	4.425822	1.731156
9	1	0	-3.219708	3.904529	0.521470
10	1	0	-1.230166	2.171248	1.634086
11	1	0	-1.963724	1.890036	0.057647
12	8	0	1.069166	2.558375	0.450381
13	6	0	0.817150	2.625391	-2.459168
14	1	0	1.759219	2.280597	-2.024597
15	1	0	0.621168	2.108852	-3.401129
16	1	0	0.846542	3.704042	-2.617879
17	1	0	0.977073	1.578455	0.724529
18	1	0	-0.368526	1.260949	-1.464683
19	6	0	-0.610231	-3.982684	-0.804048
20	6	0	-1.348999	-2.882020	-0.371279
21	6	0	-3.243997	-3.652301	-1.632901
22	6	0	-2.482566	-4.685696	-2.179051
23	6	0	-1.163368	-4.839255	-1.769632
24	1	0	-4.288202	-3.551452	-1.910817
25	1	0	-2.922685	-5.362894	-2.907036
26	6	0	-0.140657	-5.856192	-2.229589
27	1	0	-0.358957	-6.856171	-1.829350
28	1	0	-0.112943	-5.954900	-3.320984
29	6	0	0.735818	-4.542252	-0.347214
30	6	0	1.174656	-5.292325	-1.648778
31	1	0	1.608054	-4.565214	-2.345286
32	1	0	1.929703	-6.060394	-1.454368
33	6	0	0.539861	-5.585476	0.806733
34	1	0	-0.077553	-5.130697	1.590310
35	1	0	0.032841	-6.494589	0.469103
36	6	0	1.962910	-5.839853	1.346860
37	1	0	2.460531	-6.651430	0.797198
38	1	0	1.969210	-6.127279	2.404592
39	6	0	2.641785	-4.509489	1.104592
40	6	0	1.875213	-3.713879	0.238437
41	6	0	3.841988	-4.037361	1.622934
42	1	0	4.450748	-4.659913	2.274142
43	6	0	2.262496	-2.396359	0.002539
44	6	0	4.255562	-2.744547	1.301460
45	1	0	5.200254	-2.372385	1.686115
46	8	0	-0.755346	-1.952502	0.481873
47	8	0	1.452451	-1.594358	-0.798755
48	15	0	0.193586	-0.775513	-0.141738
49	8	0	0.604582	0.082898	1.028219
50	8	0	-0.473528	-0.106633	-1.337115
51	6	0	-2.695733	-2.707548	-0.749880
52	6	0	3.467855	-1.881149	0.522547
53	6	0	-1.415508	6.327294	-0.040100
54	6	0	-2.325734	7.145252	-0.717898
55	6	0	-0.556747	6.898340	0.907846
56	6	0	-2.389922	8.512531	-0.445009
57	1	0	-2.987329	6.710783	-1.464350
58	6	0	-0.612802	8.266285	1.171783
59	1	0	0.165859	6.270780	1.420582
60	6	0	-1.532072	9.075991	0.500220
61	1	0	-3.102428	9.136682	-0.977466
62	1	0	0.063848	8.701469	1.902325
63	1	0	-1.574613	10.141570	0.708811
64	6	0	-3.561242	-1.595613	-0.229268
65	6	0	-3.914188	-1.549380	1.144599
66	6	0	-4.110867	-0.635223	-1.114522
67	6	0	3.913980	-0.468408	0.286421
68	6	0	4.028883	0.436090	1.375955
69	6	0	4.266933	-0.033825	-1.012030
70	6	0	-5.381281	0.378963	0.730140
71	6	0	4.796544	2.204588	-0.151655
72	6	0	-5.006945	0.322150	-0.613656
73	1	0	-5.427257	1.035755	-1.313022
74	6	0	-4.806975	-0.568464	1.584961
75	1	0	-5.072258	-0.558551	2.638304
76	6	0	4.470713	1.738108	1.126798
77	1	0	4.555021	2.416595	1.970203
78	6	0	4.691530	1.290174	-1.201517
79	1	0	4.962362	1.596824	-2.205753
80	6	0	3.714819	0.049826	2.821217
81	6	0	5.004920	-0.036663	3.674575
82	6	0	2.696379	0.990797	3.507476
83	1	0	3.258113	-0.944643	2.819050
84	6	0	4.710997	-0.477511	5.116779
85	1	0	5.494575	0.948138	3.687149
86	1	0	5.720869	-0.725644	3.208330
87	6	0	2.399766	0.542688	4.947749
88	1	0	3.087001	2.018173	3.528727
89	1	0	1.773662	1.006705	2.922161
90	6	0	3.679982	0.440580	5.788753
91	1	0	5.641257	-0.499711	5.699895
92	1	0	4.324425	-1.507572	5.106152
93	1	0	1.691435	1.238645	5.416546
94	1	0	1.901830	-0.437837	4.924413
95	1	0	3.448309	0.078331	6.799033
96	1	0	4.115150	1.444420	5.908390
97	6	0	4.270418	-0.969608	-2.217138
98	6	0	3.356363	-0.488986	-3.367599
99	6	0	5.705247	-1.219303	-2.742684
100	1	0	3.885294	-1.942915	-1.897170
101	6	0	3.368171	-1.474205	-4.547096
102	1	0	3.696103	0.495246	-3.722646
103	1	0	2.335368	-0.363333	-2.991253
104	6	0	5.714949	-2.202266	-3.923784
105	1	0	6.151281	-0.265567	-3.059779
106	1	0	6.334334	-1.599050	-1.927538
107	6	0	4.792837	-1.733193	-5.058822
108	1	0	2.734771	-1.094502	-5.359649
109	1	0	2.919703	-2.425659	-4.224149
110	1	0	6.740052	-2.333805	-4.294463
111	1	0	5.381572	-3.190416	-3.573220
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113	1	0	5.195710	-0.804338	-5.490352
114	6	0	-3.788989	-0.602416	-2.608079
115	6	0	-4.985717	-1.073515	-3.471451
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117	1	0	-2.956130	-1.289233	-2.789527
118	6	0	-4.633460	-1.105042	-4.967072
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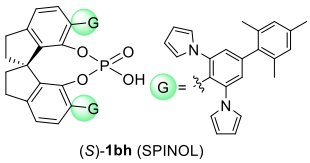
120	1	0	-5.324985	-2.064161	-3.145828
121	6	0	-2.952388	0.754068	-4.595595
122	1	0	-4.122947	1.526112	-2.956823
123	1	0	-2.466433	1.118291	-2.512551
124	6	0	-4.120355	0.255974	-5.459057
125	1	0	-5.508713	-1.416187	-5.552583
126	1	0	-3.857826	-1.866455	-5.136251
127	1	0	-2.637032	1.753446	-4.924693
128	1	0	-2.086171	0.090998	-4.735464

129	1	0	-3.818254	0.191071	-6.512551
130	1	0	-4.940260	0.988800	-5.414007
131	6	0	-3.388366	-2.546943	2.171892
132	6	0	-2.563698	-1.859775	3.286354
133	6	0	-4.514160	-3.409883	2.790934
134	1	0	-2.714769	-3.243160	1.663822
135	6	0	-2.006826	-2.883212	4.287270
136	1	0	-3.201090	-1.142606	3.824303
137	1	0	-1.746474	-1.287120	2.835864
138	6	0	-3.953118	-4.431930	3.792633
139	1	0	-5.239413	-2.762156	3.304081
140	1	0	-5.066969	-3.922950	1.993438
141	6	0	-3.119616	-3.753180	4.890036
142	1	0	-1.453095	-2.366961	5.082288
143	1	0	-1.279026	-3.528313	3.772537
144	1	0	-4.773643	-5.009498	4.238418
145	1	0	-3.321143	-5.153884	3.254295
146	1	0	-2.694067	-4.507113	5.565248
147	1	0	-3.778899	-3.120924	5.503960
148	6	0	5.267781	3.658079	-0.343061
149	6	0	4.209524	4.630635	0.231010
150	1	0	4.067652	4.488119	1.307086
151	1	0	4.524450	5.669755	0.072166
152	1	0	3.235217	4.486424	-0.247435
153	6	0	6.606390	3.862307	0.406223
154	1	0	6.955279	4.896734	0.294659
155	1	0	6.504850	3.656952	1.477132
156	1	0	7.382819	3.196948	0.011156
157	6	0	5.488895	4.013755	-1.825687
158	1	0	6.269201	3.395871	-2.284302
159	1	0	4.570866	3.895919	-2.413128
160	1	0	5.805020	5.059663	-1.912018
161	6	0	-6.396207	1.398813	1.279646
162	6	0	-7.633570	0.641817	1.819842
163	1	0	-8.372274	1.347593	2.220099
164	1	0	-8.113623	0.060434	1.024476
165	1	0	-7.363647	-0.052177	2.622584
166	6	0	-6.874969	2.392597	0.204145
167	1	0	-6.042771	2.967426	-0.219136
168	1	0	-7.391628	1.886823	-0.619231
169	1	0	-7.579250	3.106457	0.646600
170	6	0	-5.757413	2.210776	2.430686
171	1	0	-5.423073	1.567275	3.250602
172	1	0	-4.886940	2.775451	2.076640
173	1	0	-6.480461	2.926086	2.841969

DFT calculation of real system using SPINOL-derived CPA (*S*)-1bh

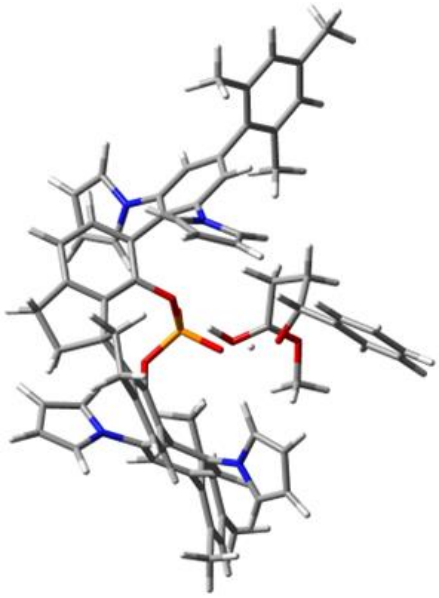


(*S*)-**1bh** (SPINOL)

1st / 2nd	ΔΔG≠ (kcal/mol)
R-anti / R-re	-0.84 / **0.00**
R-syn / R-si	-- / --
S-anti / S-si	**2.06** / 1.27
S-syn / S-re	**2.80** / -0.72

ΔΔG≠ of RDS = **2.06** kcal/mol

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1bh (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3948.43775673 hartree

Zero-point Energy Correction = 1.264313 hartree

Thermal Correction to Energy = 1.340477 hartree

Thermal correction to Enthalpy = 1.341422 hartree

Thermal correction to Gibbs Free Energy= 1.143265 hartree

Sum of electronic and Zero-point Energies = -3947.173443 hartree

Sum of electronic and thermal Energies = -3947.097279 hartree

Sum of electronic and thermal Enthalpies = -3947.096335 hartree

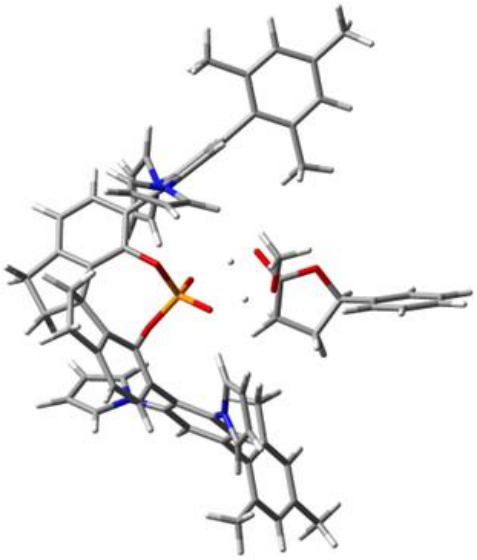
Sum of electronic and thermal Free Energies= -3947.294492 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.242198	-3.059258	-0.460450
2	8	0	-0.388468	-2.467033	1.121718
3	6	0	0.862892	-2.705520	1.845916
4	6	0	1.715574	-3.557186	0.884137
5	6	0	1.275046	-3.126470	-0.516249
6	1	0	1.325367	-1.721779	1.979319
7	1	0	1.513071	-4.621259	1.034310
8	1	0	2.781075	-3.390386	1.064336
9	1	0	1.573942	-3.831428	-1.296531
10	1	0	1.656684	-2.133786	-0.774131
11	8	0	-0.917975	-2.221788	-1.237229
12	8	0	-0.779013	-4.293362	-0.386468
13	6	0	-2.216913	-4.376813	-0.355734
14	1	0	-2.437886	-5.420995	-0.131455
15	1	0	-2.639850	-4.101082	-1.323238
16	1	0	-2.617595	-3.728964	0.428259
17	1	0	-0.564484	-1.368438	1.129179
18	1	0	-0.453130	-1.321861	-1.325763
19	6	0	1.006884	4.010669	0.072107
20	6	0	1.633506	2.767348	-0.016272
21	6	0	3.286203	3.708946	-1.500251
22	6	0	2.618788	4.930131	-1.497320
23	6	0	1.481885	5.074694	-0.710199
24	1	0	4.185700	3.590393	-2.095749
25	1	0	2.987081	5.754702	-2.102018
26	6	0	0.597380	6.290848	-0.556768
27	1	0	1.076986	7.050034	0.077604
28	1	0	0.379066	6.773583	-1.516158
29	6	0	-0.129827	4.497693	0.966796
30	6	0	-0.659304	5.703724	0.115705
31	1	0	-1.348276	5.324083	-0.646605
32	1	0	-1.205516	6.429949	0.725729
33	6	0	0.387682	5.014956	2.350152
34	1	0	1.042547	4.255438	2.791677
35	1	0	0.965370	5.940392	2.256910
36	6	0	-0.891551	5.179105	3.205008
37	1	0	-1.314211	6.188852	3.105710
38	1	0	-0.706463	5.020762	4.273768
39	6	0	-1.821087	4.134952	2.622130
40	6	0	-1.297684	3.633685	1.420993
41	6	0	-3.030848	3.660034	3.118847
42	1	0	-3.442894	4.046547	4.047460
43	6	0	-1.929215	2.564445	0.798467
44	6	0	-3.721881	2.680506	2.404614
45	1	0	-4.681699	2.325857	2.767320
46	8	0	1.102796	1.686712	0.685683
47	8	0	-1.295974	1.927126	-0.272561
48	15	0	-0.142829	0.823618	0.075130
49	8	0	-0.594304	-0.053079	1.241037
50	8	0	0.222232	0.125569	-1.213012
51	6	0	2.810510	2.603984	-0.772790
52	6	0	-3.185096	2.105759	1.241992
53	6	0	0.589606	-3.321120	3.196755
54	6	0	1.046227	-2.687387	4.356461
55	6	0	-0.107858	-4.531563	3.309143
56	6	0	0.826246	-3.260210	5.611192
57	1	0	1.568313	-1.736281	4.278528
58	6	0	-0.335512	-5.099430	4.560504
59	1	0	-0.481098	-5.018875	2.412453
60	6	0	0.135487	-4.467119	5.714915
61	1	0	1.187676	-2.758536	6.504713
62	1	0	-0.882612	-6.035229	4.637692
63	1	0	-0.041679	-4.912292	6.690257
64	6	0	-3.938941	1.071779	0.476096
65	6	0	-5.074943	-1.089430	0.293278
66	6	0	-4.940970	0.318532	-1.634390
67	6	0	-5.346056	-0.890958	-1.063955
68	1	0	-5.370220	-2.015377	0.775833
69	1	0	-5.185946	0.544692	-2.666828
70	6	0	3.632059	1.354752	-0.792108
71	6	0	5.151217	-0.219213	0.317949
72	6	0	4.928489	-0.301211	-2.060986
73	6	0	5.536906	-0.785798	-0.900052
74	1	0	5.614262	-0.553045	1.240856
75	1	0	5.181485	-0.725014	-3.027494
76	6	0	-6.062070	-1.927918	-1.870541
77	6	0	-7.409076	-3.907332	-3.380268
78	6	0	6.606644	-1.833459	-0.964151
79	6	0	8.647010	-3.790446	-1.084018
80	6	0	-4.256479	1.279032	-0.886683
81	6	0	-4.406784	-0.128208	1.060319
82	6	0	4.226783	0.830710	0.379615
83	6	0	3.998858	0.742695	-2.015395
84	6	0	7.317412	-4.118261	-1.354339
85	1	0	7.064581	-5.146110	-1.607879
86	6	0	6.294265	-3.164940	-1.307695
87	6	0	8.938228	-2.463688	-0.754746
88	1	0	9.968726	-2.182855	-0.544873
89	6	0	7.947706	-1.479549	-0.689979

90	6	0	-5.403767	-2.575402	-2.940520
91	6	0	-6.088498	-3.555590	-3.667113
92	1	0	-5.571947	-4.055414	-4.484675
93	6	0	-8.049229	-3.238848	-2.334011
94	1	0	-9.085872	-3.479506	-2.105301
95	6	0	-7.402781	-2.260668	-1.572108
96	6	0	4.876791	-3.589919	-1.619673
97	1	0	4.164493	-3.168456	-0.904097
98	1	0	4.558255	-3.254754	-2.614720
99	1	0	4.783900	-4.680387	-1.595282
100	6	0	8.342892	-0.058230	-0.349549
101	1	0	7.914126	0.660431	-1.056570
102	1	0	7.999747	0.239560	0.648225
103	1	0	9.431298	0.053746	-0.370226
104	6	0	9.741932	-4.828002	-1.170776
105	1	0	10.266152	-4.773814	-2.134326
106	1	0	10.494078	-4.685142	-0.386854
107	1	0	9.341123	-5.842394	-1.074405
108	6	0	-8.174129	-1.566918	-0.468483
109	1	0	-7.884421	-1.926283	0.526828
110	1	0	-8.009398	-0.484476	-0.475497
111	1	0	-9.247867	-1.748216	-0.579153
112	6	0	-3.979878	-2.239503	-3.332483
113	1	0	-3.930778	-1.318160	-3.926918
114	1	0	-3.327738	-2.089236	-2.467288
115	1	0	-3.552948	-3.038574	-3.947585
116	6	0	-8.116519	-4.988590	-4.163467
117	1	0	-7.740698	-5.051501	-5.190350
118	1	0	-7.970017	-5.975223	-3.703225
119	1	0	-9.196279	-4.809981	-4.208018
120	7	0	3.470848	1.190507	-3.257628
121	6	0	4.246347	1.546279	-4.352379
122	6	0	2.134026	1.295982	-3.603026
123	6	0	3.402473	1.886665	-5.382613
124	1	0	5.324235	1.551296	-4.278681
125	6	0	2.067027	1.721106	-4.909141
126	1	0	1.364211	1.022285	-2.895488
127	1	0	3.709103	2.222434	-6.364488
128	1	0	1.155632	1.888526	-5.467521
129	7	0	3.969944	1.379068	1.669822
130	6	0	3.689550	0.621976	2.795238
131	6	0	4.110924	2.700696	2.055990
132	6	0	3.635081	1.459849	3.883164
133	1	0	3.534831	-0.443350	2.707844
134	6	0	3.907111	2.778989	3.414209
135	1	0	4.364486	3.459592	1.332559
136	1	0	3.413700	1.163924	4.899880
137	1	0	3.959475	3.682307	4.007221
138	7	0	-3.940856	2.504508	-1.541808
139	6	0	-3.273217	2.607894	-2.749679
140	6	0	-4.384883	3.762881	-1.172738
141	6	0	-3.279067	3.926863	-3.136251
142	1	0	-2.810429	1.736626	-3.188651
143	6	0	-3.989592	4.659445	-2.137830
144	1	0	-4.954193	3.897360	-0.265679
145	1	0	-2.813705	4.325162	-4.027871
146	1	0	-4.196878	5.721412	-2.133759
147	7	0	-4.259550	-0.408329	2.449407
148	6	0	-5.317952	-0.790426	3.263226
149	6	0	-3.096099	-0.421875	3.200280
150	6	0	-4.826753	-1.034799	4.523349
151	1	0	-6.323479	-0.819406	2.869488
152	6	0	-3.419418	-0.807271	4.480041
153	1	0	-2.150726	-0.166334	2.747839
154	1	0	-5.412991	-1.336178	5.381473
155	1	0	-2.716918	-0.921753	5.294773

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1bh (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3948.43608343 hartree

Zero-point Energy Correction = 1.264041 hartree

Thermal Correction to Energy = 1.340517hartree

Thermal correction to Enthalpy = 1.341461 hartree

Thermal correction to Gibbs Free Energy= 1.142604 hartree

Sum of electronic and Zero-point Energies = -3947.172042 hartree

Sum of electronic and thermal Energies = -3947.095566 hartree

Sum of electronic and thermal Enthalpies = -3947.094622 hartree

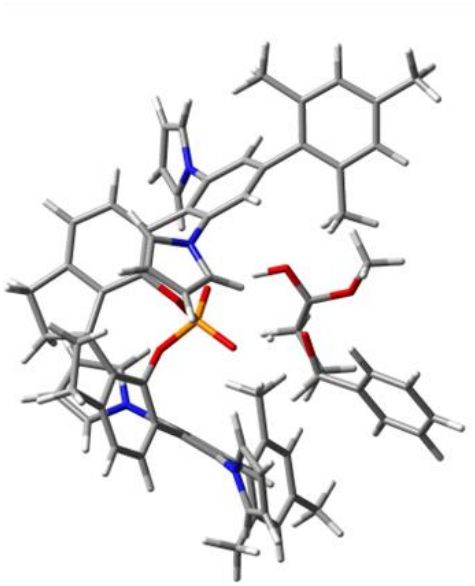
Sum of electronic and thermal Free Energies= -3947.293479 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.393574	2.700638	-0.286561
2	8	0	-0.753177	3.995443	-0.144801
3	8	0	-0.208547	2.165890	1.325057
4	6	0	0.418001	4.880196	-0.246381
5	6	0	1.632749	3.929596	-0.247460
6	6	0	1.043655	2.621107	-0.782578
7	1	0	0.320121	5.368933	-1.222303
8	1	0	2.014266	3.790995	0.767025
9	1	0	2.444737	4.323793	-0.863812
10	1	0	1.558074	1.720386	-0.446785
11	1	0	1.001166	2.605100	-1.877433
12	8	0	-1.357660	1.969461	-0.817265
13	6	0	-1.425571	2.243866	2.095618
14	1	0	-1.680502	3.296288	2.220888
15	1	0	-1.221578	1.782427	3.064190
16	1	0	-2.235365	1.716917	1.583898
17	1	0	0.099737	1.111484	1.294096
18	1	0	-1.019419	1.031138	-1.024315
19	6	0	-1.165097	-4.262015	-0.000194
20	6	0	-1.787666	-3.016112	0.002768
21	6	0	-3.458333	-3.846541	-1.524564
22	6	0	-2.792084	-5.066570	-1.613536
23	6	0	-1.648098	-5.269231	-0.848891
24	1	0	-4.361209	-3.683264	-2.104503
25	1	0	-3.167036	-5.845074	-2.272816
26	6	0	-0.759423	-6.491289	-0.784696
27	1	0	-1.234768	-7.295742	-0.205418
28	1	0	-0.541963	-6.903814	-1.776579
29	6	0	-0.026643	-4.804851	0.855428
30	6	0	0.500298	-5.951592	-0.075356
31	1	0	1.188741	-5.522748	-0.811578
32	1	0	1.045737	-6.718676	0.483466

33	6	0	-0.549794	-5.412164	2.199654
34	1	0	-1.212993	-4.686721	2.683683
35	1	0	-1.121217	-6.332726	2.042945
36	6	0	0.722671	-5.622644	3.052125
37	1	0	1.155558	-6.619855	2.889659
38	1	0	0.528600	-5.536534	4.127513
39	6	0	1.647721	-4.535944	2.546415
40	6	0	1.136650	-3.965918	1.370525
41	6	0	2.845654	-4.085017	3.091480
42	1	0	3.245437	-4.526515	4.000714
43	6	0	1.773476	-2.857470	0.821746
44	6	0	3.540783	-3.060769	2.449369
45	1	0	4.493250	-2.724404	2.847254
46	8	0	-1.229185	-1.984522	0.757710
47	8	0	1.165922	-2.165784	-0.228834
48	15	0	-0.011647	-1.092503	0.126781
49	8	0	0.430870	-0.192725	1.278911
50	8	0	-0.397100	-0.422278	-1.168538
51	6	0	-2.972833	-2.797411	-0.725899
52	6	0	3.019894	-2.421800	1.312891
53	6	0	0.385853	5.929547	0.837517
54	6	0	0.285471	7.281162	0.493093
55	6	0	0.468945	5.578337	2.192883
56	6	0	0.275629	8.269597	1.479466
57	1	0	0.213708	7.563413	-0.554906
58	6	0	0.449691	6.562535	3.179055
59	1	0	0.548929	4.532122	2.474390
60	6	0	0.355545	7.911393	2.824753
61	1	0	0.200398	9.315677	1.195487
62	1	0	0.513037	6.277848	4.225826
63	1	0	0.344747	8.677511	3.595223
64	6	0	3.808360	-1.360413	0.620726
65	6	0	-3.758980	-1.530067	-0.640977
66	6	0	-5.456617	0.771750	-0.503219
67	6	0	5.414111	0.587843	-0.735882
68	6	0	5.056137	0.748892	0.606192
69	1	0	5.370080	1.635290	1.147811
70	6	0	4.289553	-0.206861	1.284206
71	6	0	4.967484	-0.562512	-1.391664
72	1	0	5.264068	-0.757343	-2.417193
73	6	0	4.186654	-1.516226	-0.733551
74	6	0	-5.113115	0.059577	0.648502
75	1	0	-5.532402	0.344385	1.608532
76	6	0	-4.289722	-1.071403	0.587117
77	6	0	-4.937978	0.328725	-1.722673
78	1	0	-5.170841	0.863535	-2.637877
79	6	0	-4.113277	-0.798113	-1.799322
80	6	0	6.280592	1.588971	-1.435517
81	6	0	7.633237	1.740939	-1.054803
82	6	0	5.759760	2.378048	-2.483370
83	6	0	8.427380	2.679089	-1.721031
84	6	0	6.589369	3.310060	-3.116013
85	6	0	7.927608	3.475911	-2.754327
86	1	0	9.469409	2.786167	-1.425122
87	1	0	6.174882	3.922743	-3.914538
88	6	0	-6.406933	1.930978	-0.451019
89	6	0	-7.793400	1.691695	-0.571230
90	6	0	-5.932996	3.248879	-0.293959
91	6	0	-8.677115	2.774132	-0.532797
92	6	0	-6.854043	4.302542	-0.265141
93	6	0	-8.228623	4.089714	-0.385180
94	1	0	-9.744928	2.583043	-0.623095
95	1	0	-6.481756	5.318322	-0.144212
96	6	0	-4.460290	3.545431	-0.127485
97	1	0	-4.114640	3.271952	0.877940
98	1	0	-3.833397	2.991583	-0.831417
99	1	0	-4.258974	4.612998	-0.259485
100	6	0	-8.337585	0.289846	-0.740392
101	1	0	-7.948472	-0.189044	-1.646961
102	1	0	-8.060528	-0.358917	0.098823
103	1	0	-9.429571	0.302833	-0.809759
104	6	0	-9.200762	5.246733	-0.383860
105	1	0	-8.805677	6.101937	0.174785
106	1	0	-9.409153	5.593623	-1.405051
107	1	0	-10.160281	4.964143	0.063015
108	6	0	4.322062	2.248656	-2.938020
109	1	0	4.164881	1.350671	-3.548284
110	1	0	3.633177	2.174968	-2.090873
111	1	0	4.030313	3.110387	-3.547125
112	6	0	8.254374	0.900069	0.040646
113	1	0	7.920664	1.210264	1.038535
114	1	0	7.996348	-0.158989	-0.064996
115	1	0	9.345066	0.987678	0.019821
116	6	0	8.815877	4.463079	-3.474910
117	1	0	9.382486	3.974928	-4.279242
118	1	0	8.231716	5.268875	-3.931710
119	1	0	9.546019	4.916689	-2.795646
120	7	0	-3.686116	-1.196691	-3.097548
121	6	0	-4.549633	-1.402057	-4.164510
122	6	0	-2.386096	-1.391464	-3.531826
123	6	0	-3.799005	-1.736662	-5.266365
124	1	0	-5.617517	-1.316268	-4.025297
125	6	0	-2.430060	-1.722768	-4.866072
126	1	0	-1.557517	-1.242126	-2.855112
127	1	0	-4.189121	-1.970006	-6.248323
128	1	0	-1.569806	-1.927294	-5.489587
129	7	0	-4.069663	-1.776850	1.806165
130	6	0	-3.673046	-1.189197	2.995062
131	6	0	-4.355295	-3.109493	2.050218
132	6	0	-3.690782	-2.145034	3.982051
133	1	0	-3.377538	-0.151108	3.014912
134	6	0	-4.128905	-3.363437	3.382818
135	1	0	-4.710525	-3.747784	1.256243
136	1	0	-3.407331	-1.992786	5.014847
137	1	0	-4.273097	-4.315951	3.875214
138	7	0	3.846384	-2.688805	-1.468671
139	6	0	3.215617	-2.695173	-2.700594
140	6	0	4.236220	-3.982141	-1.164477
141	6	0	3.189982	-3.987696	-3.167138
142	1	0	2.795238	-1.783848	-3.099128
143	6	0	3.842898	-4.803875	-2.194790
144	1	0	4.770496	-4.191218	-0.250225
145	1	0	2.739689	-4.314861	-4.094670
146	1	0	4.013446	-5.870939	-2.249485
147	7	0	4.061189	0.021718	2.671054
148	6	0	5.070994	0.342643	3.569093
149	6	0	2.852549	0.014561	3.346926
150	6	0	4.504286	0.528913	4.806868
151	1	0	6.100395	0.372210	3.243227
152	6	0	3.099473	0.326923	4.663246
153	1	0	1.934835	-0.200307	2.820979
154	1	0	5.038818	0.773867	5.715178
155	1	0	2.350667	0.401936	5.440735

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1bh (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3948.43378881 hartree

Zero-point Energy Correction = 1.263696 hartree

Thermal Correction to Energy = 1.339884 hartree

Thermal correction to Enthalpy = 1.340828 hartree

Thermal correction to Gibbs Free Energy= 1.143600hartree

Sum of electronic and Zero-point Energies = -3947.170093 hartree

Sum of electronic and thermal Energies = -3947.093905 hartree

Sum of electronic and thermal Enthalpies = -3947.092961 hartree

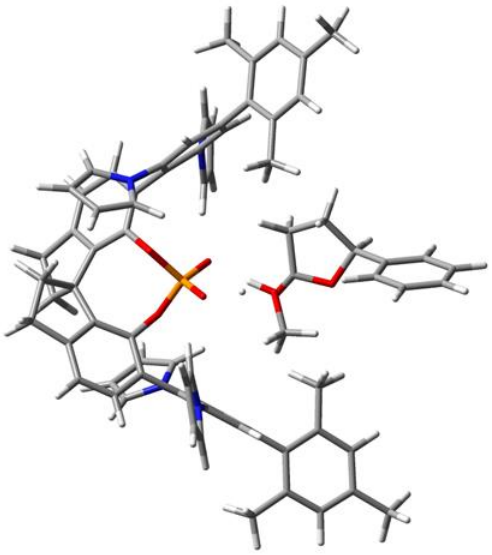
Sum of electronic and thermal Free Energies= -3947.290189 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.173023	-2.846299	-1.138402
2	8	0	-0.131294	-2.541290	0.467786
3	6	0	-1.478651	-3.024385	0.752833
4	6	0	-2.149906	-3.266573	-0.629657
5	6	0	-1.233303	-2.584512	-1.651879
6	1	0	-1.977644	-2.197244	1.267917
7	1	0	-2.205355	-4.337301	-0.839452
8	1	0	-3.164056	-2.860102	-0.650204
9	1	0	-1.339524	-2.998227	-2.658158
10	1	0	-1.390865	-1.503455	-1.699998
11	8	0	1.199585	-2.074220	-1.479027
12	8	0	0.440722	-4.169409	-1.202619
13	6	0	1.752516	-4.599400	-0.812485
14	1	0	1.742847	-5.684425	-0.923270
15	1	0	2.514565	-4.157849	-1.457934
16	1	0	1.943594	-4.333957	0.230340
17	1	0	-0.109802	-1.396006	0.686367
18	1	0	0.934226	-1.101339	-1.545199
19	6	0	1.394439	4.025576	0.121995
20	6	0	1.987935	2.770318	0.037828
21	6	0	3.688273	3.668129	-1.416558
22	6	0	3.035314	4.899112	-1.440857
23	6	0	1.896634	5.075463	-0.661892
24	1	0	4.597702	3.527861	-1.992652
25	1	0	3.423092	5.709366	-2.052786
26	6	0	1.036506	6.310376	-0.508260
27	1	0	1.540500	7.067515	0.109147
28	1	0	0.811592	6.786790	-1.469400
29	6	0	0.290307	4.541365	1.034514
30	6	0	-0.224323	5.758055	0.190889
31	1	0	-0.938891	5.397047	-0.556476
32	1	0	-0.737364	6.501447	0.809260
33	6	0	0.869328	5.048741	2.398028
34	1	0	1.526602	4.278300	2.815356
35	1	0	1.460768	5.962417	2.281068
36	6	0	-0.370863	5.236582	3.300356
37	1	0	-0.783372	6.251710	3.213070
38	1	0	-0.147957	5.078538	4.361881
39	6	0	-1.338758	4.207811	2.756508
40	6	0	-0.878949	3.700454	1.531249
41	6	0	-2.536132	3.762203	3.307090
42	1	0	-2.893740	4.154692	4.255483
43	6	0	-1.569678	2.652679	0.929448
44	8	0	1.391369	1.689133	0.694035
45	8	0	-1.029558	2.016676	-0.189331
46	15	0	0.157631	0.906485	-0.033787
47	8	0	-0.240928	-0.172766	0.984185
48	8	0	0.478942	0.438740	-1.427907
49	6	0	3.184030	2.583341	-0.680928
50	6	0	-2.825057	2.242972	1.419206
51	6	0	-1.435773	-4.225293	1.679214
52	6	0	-0.333731	-4.457958	2.510530
53	6	0	-2.539063	-5.084130	1.767256
54	6	0	-0.327591	-5.537223	3.395211
55	1	0	0.519493	-3.789931	2.460182
56	6	0	-2.536380	-6.158644	2.657117
57	1	0	-3.412005	-4.914406	1.142289
58	6	0	-1.427599	-6.392380	3.471546
59	1	0	0.538967	-5.706475	4.029250
60	1	0	-3.401441	-6.814358	2.710652
61	1	0	-1.422782	-7.231366	4.162147
62	6	0	3.969511	1.317260	-0.606977
63	6	0	-3.289265	2.815956	2.613982
64	1	0	-4.246980	2.492313	3.010176
65	6	0	-3.694287	1.295396	0.662774
66	6	0	-5.481008	-0.412254	-0.790613
67	6	0	5.643871	-0.997668	-0.419065
68	6	0	5.167434	-0.545044	-1.653021
69	1	0	5.407834	-1.088124	-2.560863
70	6	0	4.365599	0.596792	-1.757288
71	6	0	5.275396	-0.278120	0.721363
72	1	0	5.660320	-0.562741	1.695145
73	6	0	4.456769	0.849720	0.635033
74	6	0	-5.063660	-0.729990	0.506690
75	1	0	-5.401347	-1.649027	0.974462
76	6	0	-4.208368	0.108360	1.232852
77	6	0	-4.997295	0.773396	-1.351401
78	1	0	-5.331894	1.089901	-2.333647
79	6	0	-4.127022	1.608858	-0.646714
80	6	0	6.539062	-2.192426	-0.320970
81	6	0	7.827408	-2.165027	-0.902757
82	6	0	6.112116	-3.347853	0.368957
83	6	0	8.649023	-3.290755	-0.793191
84	6	0	6.964930	-4.454373	0.443901
85	6	0	8.236356	-4.450701	-0.132443
86	1	0	9.644206	-3.256370	-1.232924
87	1	0	6.623221	-5.343833	0.970412
88	6	0	-6.439655	-1.288453	-1.534930
89	6	0	-7.748025	-1.490748	-1.032287
90	6	0	-6.058038	-1.908987	-2.744353
91	6	0	-8.629580	-2.314725	-1.735789
92	6	0	-6.972962	-2.736192	-3.407168
93	6	0	-8.262959	-2.953799	-2.924022
94	1	0	-9.635578	-2.457534	-1.345155
95	1	0	-6.663357	-3.222176	-4.330463
96	6	0	-4.689351	-1.712330	-3.361889
97	1	0	-4.641535	-0.790240	-3.955385
98	1	0	-3.899299	-1.643836	-2.609439
99	1	0	-4.449763	-2.540828	-4.036346

100	6	0	-8.238237	-0.817837	0.233508
101	1	0	-7.856977	-1.308149	1.137916
102	1	0	-7.927884	0.230779	0.284448
103	1	0	-9.330999	-0.851135	0.284221
104	6	0	-9.242949	-3.831944	-3.666367
105	1	0	-10.039641	-3.235868	-4.130245
106	1	0	-8.749239	-4.398560	-4.462243
107	1	0	-9.729090	-4.548605	-2.993966
108	6	0	4.754766	-3.425733	1.034827
109	1	0	4.756911	-2.941306	2.019813
110	1	0	3.977684	-2.934296	0.442415
111	1	0	4.464591	-4.470111	1.191543
112	6	0	8.359782	-0.940282	-1.617164
113	1	0	7.932414	-0.831060	-2.621653
114	1	0	8.130603	-0.018838	-1.072051
115	1	0	9.446226	-1.006323	-1.732254
116	6	0	9.130262	-5.666763	-0.062602
117	1	0	10.186723	-5.384560	0.004150
118	1	0	8.891054	-6.291215	0.804666
119	1	0	9.019343	-6.294634	-0.956997
120	7	0	-3.911490	-0.273571	2.571323
121	6	0	-4.874315	-0.673727	3.487883
122	6	0	-2.663812	-0.370964	3.169366
123	6	0	-4.241187	-1.015537	4.658457
124	1	0	-5.921735	-0.643798	3.225713
125	6	0	-2.842344	-0.830755	4.453122
126	1	0	-1.769267	-0.113482	2.622117
127	1	0	-4.727788	-1.354026	5.563484
128	1	0	-2.051238	-1.015952	5.167239
129	7	0	-3.749484	2.828363	-1.279935
130	6	0	-3.169519	2.923120	-2.533240
131	6	0	-4.059236	4.103703	-0.837861
132	6	0	-3.095655	4.251990	-2.876320
133	1	0	-2.815460	2.035466	-3.035998
134	6	0	-3.665547	5.000906	-1.802822
135	1	0	-4.544048	4.249242	0.115454
136	1	0	-2.666427	4.645021	-3.788118
137	1	0	-3.781287	6.075291	-1.748548
138	7	0	4.011394	1.019481	-3.069288
139	6	0	4.934578	1.197168	-4.091222
140	6	0	2.744549	1.280163	-3.563890
141	6	0	4.255094	1.577565	-5.223595
142	1	0	5.989798	1.066123	-3.900394
143	6	0	2.869097	1.623031	-4.889883
144	1	0	1.875637	1.169755	-2.932193
145	1	0	4.703061	1.803408	-6.182340
146	1	0	2.050354	1.873794	-5.551228
147	7	0	4.191635	1.549633	1.849716
148	6	0	3.631476	0.981906	2.980109
149	6	0	4.597809	2.836901	2.156141
150	6	0	3.665798	1.909958	3.993915
151	1	0	3.216795	-0.014202	2.936902
152	6	0	4.283934	3.085882	3.472124
153	1	0	5.084070	3.448927	1.411766
154	1	0	3.279562	1.766956	4.994231
155	1	0	4.484396	4.006539	4.004059

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1bh (SPINOL)

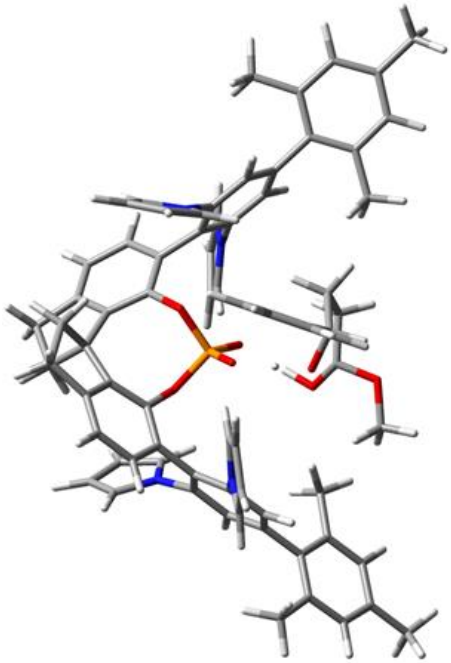


B3LYP/6-31G(d); E(B3LYP) = -3948.43571002 hartree
Zero-point Energy Correction = 1.264691 hartree
Thermal Correction to Energy = 1.340901 hartree
Thermal correction to Enthalpy = 1.341845 hartree
Thermal correction to Gibbs Free Energy= 1.144248 hartree
Sum of electronic and Zero-point Energies = -3947.171019 hartree
Sum of electronic and thermal Energies = -3947.094809 hartree
Sum of electronic and thermal Enthalpies = -3947.093865 hartree
Sum of electronic and thermal Free Energies= -3947.291462 hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.063672	-4.280405	-0.530642
2	6	0	-1.721047	-3.067261	-0.354809
3	6	0	-3.395136	-3.731224	-1.958426
4	6	0	-2.675194	-4.891075	-2.243204
5	6	0	-1.517589	-5.164544	-1.521501
6	1	0	-4.319338	-3.525013	-2.489448
7	1	0	-3.025712	-5.573802	-3.012892
8	6	0	-0.582507	-6.348550	-1.641703
9	1	0	-1.033783	-7.254245	-1.212114
10	1	0	-0.338184	-6.583142	-2.684156
11	6	0	0.071581	-4.923963	0.257275
12	6	0	0.650462	-5.890881	-0.830722
13	1	0	1.337419	-5.331171	-1.474697
14	1	0	1.210146	-6.722384	-0.390362
15	6	0	-0.484431	-5.754796	1.464219
16	1	0	-1.193069	-5.136894	2.026213
17	1	0	-1.014895	-6.654438	1.136408
18	6	0	0.756069	-6.060159	2.332829
19	1	0	1.239719	-6.998965	2.027573
20	1	0	0.511504	-6.163796	3.396270
21	6	0	1.653243	-4.873029	2.058976
22	6	0	1.184462	-4.148839	0.952559
23	6	0	2.796421	-4.468585	2.741587
24	1	0	3.159971	-5.028358	3.599453
25	6	0	1.813860	-2.956846	0.607244
26	6	0	3.484606	-3.337758	2.303580
27	1	0	4.396162	-3.031363	2.807549
28	8	0	-1.171866	-2.104321	0.493032
29	8	0	1.265978	-2.161411	-0.395307
30	15	0	0.024686	-1.147643	-0.075661

31	8	0	0.351819	-0.220521	1.093385
32	8	0	-0.319262	-0.493433	-1.390634
33	6	0	-2.935479	-2.798416	-1.015881
34	6	0	3.011008	-2.560431	1.234516
35	6	0	-3.762260	-1.603783	-0.674792
36	6	0	-5.050882	-0.331750	0.982759
37	6	0	-4.993004	0.425007	-1.284328
38	6	0	-5.441207	0.611184	0.027423
39	1	0	-5.416467	-0.260924	2.001859
40	1	0	-5.259478	1.139635	-2.056184
41	6	0	3.805444	-1.395712	0.743618
42	6	0	4.968912	0.731789	1.107299
43	6	0	5.065215	-0.293513	-1.051494
44	6	0	5.417680	0.769567	-0.215610
45	1	0	5.215081	1.541914	1.786662
46	1	0	5.433908	-0.327388	-2.071713
47	6	0	0.117556	2.598747	-0.865114
48	8	0	0.502931	3.898227	-0.945800
49	8	0	0.349571	2.212655	0.747388
50	1	0	0.491904	0.880652	-1.614120
51	6	0	-0.662664	4.792599	-0.960358
52	6	0	-1.842180	3.898865	-0.537940
53	6	0	-1.398458	2.511914	-1.008987
54	1	0	-0.780216	5.100440	-2.005951
55	1	0	-1.964467	3.915764	0.547991
56	1	0	-2.780245	4.232379	-0.989186
57	1	0	-1.831851	1.678357	-0.456395
58	1	0	-1.611416	2.352676	-2.071817
59	8	0	0.914238	1.800921	-1.567474
60	6	0	1.666963	2.564679	1.241678
61	1	0	1.745581	2.150476	2.248477
62	1	0	2.437069	2.134150	0.598765
63	1	0	1.744997	3.650396	1.260352
64	6	0	-0.403018	6.014474	-0.113500
65	6	0	-0.209577	5.913722	1.271883
66	6	0	-0.365272	7.278556	-0.710480
67	6	0	0.019236	7.054224	2.039099
68	1	0	-0.236788	4.938830	1.750778
69	6	0	-0.145671	8.424180	0.057191
70	1	0	-0.507204	7.367577	-1.785129
71	6	0	0.049262	8.313612	1.433525
72	1	0	0.171312	6.961709	3.111072
73	1	0	-0.121748	9.399096	-0.421897
74	1	0	0.224661	9.202451	2.033391
75	1	0	0.275052	1.118982	0.872033
76	6	0	-6.328658	1.760013	0.391239
77	6	0	-8.006442	3.941395	1.062650
78	6	0	6.291144	1.882078	-0.711736
79	6	0	7.978827	3.943550	-1.657190
80	6	0	4.284437	-1.355914	-0.587373
81	6	0	4.187630	-0.327375	1.586276
82	6	0	-4.233062	-1.412868	0.645226
83	6	0	-4.189254	-0.664219	-1.641261
84	6	0	6.624245	3.910736	-1.990254
85	1	0	6.215473	4.692537	-2.627799
86	6	0	5.766960	2.901826	-1.533249
87	6	0	7.662353	1.890843	-0.369138
88	6	0	8.478352	2.919051	-0.847470
89	1	0	9.535563	2.913184	-0.588190
90	6	0	-7.622117	1.864604	-0.172133
91	6	0	-8.432150	2.949358	0.175324
92	1	0	-9.428211	3.017694	-0.258476
93	6	0	-6.729229	3.818457	1.611437
94	1	0	-6.372915	4.580118	2.302707
95	6	0	-5.886987	2.744413	1.302508
96	6	0	-4.525364	2.680367	1.961778
97	1	0	-4.527906	2.017052	2.836201
98	1	0	-3.755648	2.302166	1.283041
99	1	0	-4.220485	3.672172	2.311617
100	6	0	-8.171256	0.822204	-1.124055
101	1	0	-7.762052	0.929572	-2.136269
102	1	0	-7.938062	-0.194778	-0.792655
103	1	0	-9.259105	0.912793	-1.203402
104	6	0	-8.912117	5.091413	1.436586
105	1	0	-9.619423	4.800974	2.224988
106	1	0	-8.339784	5.946345	1.811444
107	1	0	-9.505834	5.430110	0.580266
108	6	0	4.302764	2.962461	-1.909661
109	1	0	3.874610	1.979242	-2.118445
110	1	0	3.698121	3.400317	-1.105292
111	1	0	4.156576	3.589910	-2.794533
112	6	0	8.269977	0.798281	0.484426
113	1	0	7.885433	0.818303	1.511402
114	1	0	8.047929	-0.198161	0.085803
115	1	0	9.357572	0.907590	0.536263
116	6	0	8.877185	5.057580	-2.142153
117	1	0	8.464372	5.546934	-3.030455
118	1	0	9.004714	5.830839	-1.372558
119	1	0	9.877020	4.686424	-2.393798
120	7	0	-3.857815	-0.794596	-3.019363
121	6	0	-4.801068	-0.778297	-4.038200
122	6	0	-2.595929	-0.898410	-3.580818
123	6	0	-4.139001	-0.881307	-5.238267
124	1	0	-5.854509	-0.728475	-3.803891
125	6	0	-2.744334	-0.950403	-4.947432
126	1	0	-1.716819	-0.902219	-2.952793
127	1	0	-4.603919	-0.911698	-6.214899
128	1	0	-1.935611	-1.027077	-5.662073
129	7	0	-3.945046	-2.350912	1.679232
130	6	0	-3.390665	-2.028898	2.905673
131	6	0	-4.318479	-3.683854	1.698668
132	6	0	-3.396842	-3.155679	3.692967
133	1	0	-2.994552	-1.039173	3.077665
134	6	0	-3.990888	-4.204830	2.928616
135	1	0	-4.794587	-4.131092	0.839410
136	1	0	-3.006022	-3.224695	4.699286
137	1	0	-4.166016	-5.223666	3.247953
138	7	0	3.814044	-0.283319	2.960565
139	6	0	4.709029	-0.062805	3.997134
140	6	0	2.534458	-0.361130	3.486691
141	6	0	4.001668	-0.011050	5.174844
142	1	0	5.768058	0.008557	3.796203
143	6	0	2.625134	-0.193197	4.849638
144	1	0	1.684596	-0.514983	2.837876
145	1	0	4.425575	0.132707	6.159877
146	1	0	1.791281	-0.204186	5.538998
147	7	0	4.042244	-2.424395	-1.497274
148	6	0	3.541796	-2.270892	-2.778848
149	6	0	4.412541	-3.747442	-1.322982
150	6	0	3.578490	-3.492316	-3.407454
151	1	0	3.159548	-1.313590	-3.100653
152	6	0	4.136877	-4.428387	-2.485467
153	1	0	4.852487	-4.075003	-0.393538
154	1	0	3.230385	-3.695975	-4.411170
155	1	0	4.324451	-5.479832	-2.658665

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1bh (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3948.43382924 hartree

Zero-point Energy Correction = 1.264092 hartree

Thermal Correction to Energy = 1.340269 hartree

Thermal correction to Enthalpy = 1.341213 hartree

Thermal correction to Gibbs Free Energy= 1.144816hartree

Sum of electronic and Zero-point Energies = -3947.169737 hartree

Sum of electronic and thermal Energies = -3947.093560 hartree

Sum of electronic and thermal Enthalpies = -3947.092616 hartree

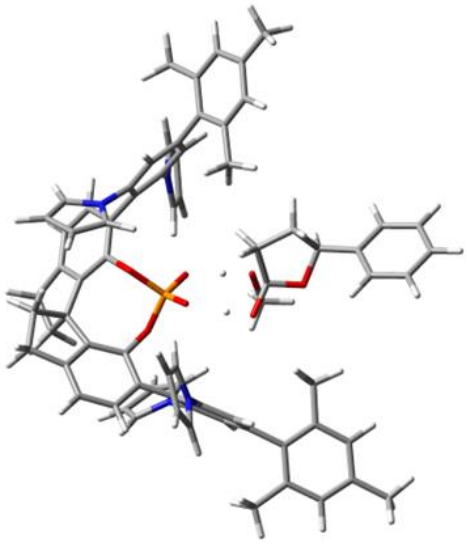
Sum of electronic and thermal Free Energies= -3947.289013 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.237349	3.707370	0.788966
2	6	0	-1.887260	2.553392	0.369916
3	6	0	-3.656879	2.967856	1.951442
4	6	0	-2.946002	4.047338	2.477662
5	6	0	-1.739423	4.415923	1.890522
6	1	0	-4.614899	2.692293	2.381371
7	1	0	-3.341523	4.593935	3.329859
8	6	0	-0.795486	5.539509	2.265896
9	1	0	-1.214929	6.518534	1.995109
10	1	0	-0.593925	5.572247	3.342904
11	6	0	-0.073136	4.468868	0.172201
12	6	0	0.469326	5.217842	1.434268
13	1	0	1.128391	4.543777	1.992655
14	1	0	1.049138	6.108456	1.170927
15	6	0	-0.612464	5.508475	-0.870825
16	1	0	-1.316872	5.003585	-1.540631
17	1	0	-1.144201	6.336775	-0.392131
18	6	0	0.633769	5.956668	-1.659388
19	1	0	1.128155	6.814339	-1.180834
20	1	0	0.399157	6.260514	-2.685958
21	6	0	1.511193	4.726929	-1.607810
22	6	0	1.045520	3.822189	-0.640698
23	6	0	2.632820	4.437152	-2.376580
24	1	0	2.990575	5.137753	-3.126508
25	6	0	1.667291	2.579538	-0.517204
26	8	0	-1.277077	1.736215	-0.585952
27	8	0	1.138014	1.634680	0.363199
28	15	0	-0.121630	0.695067	-0.089153
29	8	0	0.211782	-0.199943	-1.256452
30	8	0	-0.549229	0.017989	1.212729
31	6	0	-3.142588	2.194821	0.898593
32	6	0	2.835221	2.281341	-1.246012
33	6	0	-3.919762	1.058641	0.324383
34	6	0	3.299774	3.233335	-2.169463
35	1	0	4.190000	3.005683	-2.747029
36	6	0	3.656779	1.049867	-1.038118
37	6	0	-0.382550	-3.154648	0.079331
38	8	0	-0.689585	-2.397096	1.516490
39	6	0	0.381761	-2.887543	2.396934
40	6	0	1.155510	-3.169058	0.087818
41	1	0	1.473254	-4.170274	-0.211955
42	1	0	1.519291	-2.454267	-0.652530
43	8	0	-1.036481	-2.471226	-0.859409
44	8	0	-0.865107	-4.405792	0.273501
45	6	0	-2.296356	-4.557968	0.225080
46	1	0	-2.491946	-5.560463	0.608163
47	1	0	-2.657242	-4.470427	-0.801529
48	1	0	-2.783221	-3.810113	0.856458
49	1	0	-0.638253	-1.283401	1.360296
50	1	0	-0.550654	-1.619396	-1.108440
51	6	0	0.422015	-2.191175	3.735578
52	6	0	0.825740	-0.855345	3.881204
53	6	0	0.076916	-2.922134	4.879770
54	6	0	0.877693	-0.271488	5.146652
55	1	0	1.071376	-0.254638	3.012673
56	6	0	0.135827	-2.340207	6.146106
57	1	0	-0.240595	-3.957333	4.777739
58	6	0	0.537415	-1.010756	6.281867
59	1	0	1.186692	0.765914	5.239089
60	1	0	-0.133547	-2.923723	7.022217
61	1	0	0.584906	-0.552696	7.266295
62	1	0	0.121428	-3.936903	2.555638
63	6	0	1.631931	-2.801438	1.511399
64	1	0	2.416529	-3.467059	1.882200
65	1	0	2.028500	-1.782100	1.525304
66	6	0	-5.372991	-1.109572	-0.855087
67	6	0	5.525261	-1.101436	-0.741949
68	6	0	-4.394302	-0.021829	1.103782
69	6	0	-5.083615	-1.086877	0.512658
70	1	0	-5.380875	-1.917915	1.143691
71	6	0	-4.961187	-0.015739	-1.621320
72	1	0	-5.219196	0.042835	-2.673422
73	6	0	-4.253037	1.043213	-1.050193
74	6	0	4.901067	-0.851428	-1.966749
75	1	0	5.127927	-1.468855	-2.830029
76	6	0	3.991882	0.200625	-2.120152
77	6	0	5.186225	-0.284641	0.339749
78	1	0	5.673102	-0.428016	1.299014
79	6	0	4.279413	0.773632	0.202007
80	6	0	-6.113418	-2.252569	-1.474386
81	6	0	-7.443996	-2.532600	-1.087339
82	6	0	-5.487329	-3.058067	-2.452759
83	6	0	-8.112711	-3.611812	-1.673263
84	6	0	-6.194013	-4.133287	-3.002569
85	6	0	-7.507335	-4.428222	-2.631343
86	1	0	-9.139187	-3.816198	-1.373844
87	1	0	-5.699970	-4.757290	-3.745238
88	6	0	6.574420	-2.164343	-0.612099
89	6	0	7.936008	-1.794875	-0.550729
90	6	0	6.218178	-3.527744	-0.562589
91	6	0	8.907693	-2.794028	-0.435046
92	6	0	7.222643	-4.493354	-0.442062
93	6	0	8.575047	-4.149813	-0.379710
94	1	0	9.955235	-2.501900	-0.389706
95	1	0	6.937623	-5.542798	-0.394507
96	6	0	8.368124	-0.345937	-0.622464

97	1	0	7.922856	0.165855	-1.483166
98	1	0	8.067166	0.218749	0.267812
99	1	0	9.456366	-0.271217	-0.709854
100	6	0	4.771722	-3.963952	-0.626064
101	1	0	4.157810	-3.417895	0.097963
102	1	0	4.331699	-3.780144	-1.613728
103	1	0	4.678211	-5.034061	-0.415559
104	6	0	9.645993	-5.211432	-0.284013
105	1	0	9.277913	-6.107518	0.226994
106	1	0	9.987913	-5.523028	-1.280207
107	1	0	10.524107	-4.847468	0.260157
108	6	0	-4.071896	-2.800544	-2.926864
109	1	0	-4.031832	-1.977048	-3.651274
110	1	0	-3.393683	-2.535383	-2.110819
111	1	0	-3.670360	-3.686398	-3.430057
112	6	0	-8.181359	-1.684823	-0.071308
113	1	0	-7.886158	-1.923161	0.958411
114	1	0	-7.991724	-0.616695	-0.217619
115	1	0	-9.260579	-1.852107	-0.145183
116	6	0	-8.260864	-5.572454	-3.268491
117	1	0	-8.829463	-5.235211	-4.145651
118	1	0	-7.580676	-6.361219	-3.607268
119	1	0	-8.977864	-6.019247	-2.571071
120	7	0	4.073505	1.593438	1.350106
121	6	0	3.836911	1.106098	2.624980
122	6	0	4.239408	2.966105	1.430790
123	6	0	3.832116	2.163903	3.502793
124	1	0	3.669988	0.051554	2.784739
125	6	0	4.092612	3.343963	2.744968
126	1	0	4.466140	3.544333	0.549004
127	1	0	3.659333	2.098608	4.568731
128	1	0	4.175308	4.354810	3.121504
129	7	0	3.462824	0.409768	-3.423671
130	6	0	4.242642	0.525927	-4.566515
131	6	0	2.127892	0.486033	-3.783758
132	6	0	3.403694	0.686876	-5.643187
133	1	0	5.320501	0.513896	-4.494332
134	6	0	2.066554	0.654355	-5.147265
135	1	0	1.353999	0.375205	-3.037771
136	1	0	3.714800	0.818413	-6.671173
137	1	0	1.157352	0.737383	-5.727724
138	7	0	-3.930049	2.139969	-1.901229
139	6	0	-3.266196	2.036365	-3.110880
140	6	0	-4.361565	3.446079	-1.743659
141	6	0	-3.262281	3.273530	-3.710032
142	1	0	-2.811453	1.100835	-3.400630
143	6	0	-3.962493	4.167511	-2.844533
144	1	0	-4.926896	3.733124	-0.870113
145	1	0	-2.797500	3.514782	-4.656586
146	1	0	-4.160468	5.217482	-3.015273
147	7	0	-4.231036	-0.070063	2.517575
148	6	0	-5.278539	-0.312215	3.396725
149	6	0	-3.059323	0.044168	3.246384
150	6	0	-4.771563	-0.341265	4.673882
151	1	0	-6.288776	-0.406316	3.026057
152	6	0	-3.365534	-0.121641	4.576552
153	1	0	-2.120076	0.221762	2.747280
154	1	0	-5.347016	-0.495190	5.577276
155	1	0	-2.651195	-0.097859	5.388475

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1bh (SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3948.43553729 hartree

Zero-point Energy Correction = 1.264091 hartree

Thermal Correction to Energy = 1.340892 hartree

Thermal correction to Enthalpy = 1.341836 hartree

Thermal correction to Gibbs Free Energy= 1.140903 hartree

Sum of electronic and Zero-point Energies = -3947.171446 hartree

Sum of electronic and thermal Energies = -3947.094645 hartree

Sum of electronic and thermal Enthalpies = -3947.093701 hartree

Sum of electronic and thermal Free Energies= -3947.294634 hartree

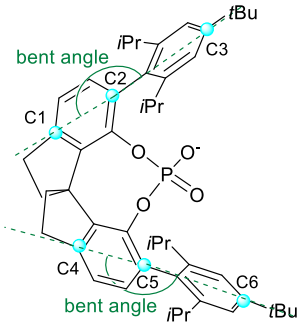
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.488353	2.598641	-0.204460
2	8	0	0.910208	3.840186	-0.528238
3	8	0	0.136250	1.912719	-1.754893
4	6	0	-0.249547	4.713803	-0.672480
5	6	0	-1.227717	4.164164	0.384942
6	6	0	-0.920297	2.654264	0.403701
7	1	0	-0.656756	4.558874	-1.678894
8	1	0	-1.003113	4.619268	1.354554
9	1	0	-2.266361	4.393388	0.134964
10	1	0	-0.897950	2.225378	1.407547
11	1	0	-1.625994	2.074310	-0.193443
12	8	0	1.449036	1.870450	0.320737
13	6	0	1.270825	1.871198	-2.642510
14	1	0	2.090378	1.304067	-2.192545
15	1	0	0.939906	1.394342	-3.567675
16	1	0	1.585218	2.896956	-2.835557
17	1	0	1.067764	0.993867	0.689554
18	1	0	-0.170777	0.893838	-1.579319
19	6	0	-1.354374	-4.172537	-0.846413
20	6	0	-1.940126	-2.956758	-0.507464
21	6	0	-3.710937	-3.364339	-2.093802
22	6	0	-3.065242	-4.518539	-2.535187
23	6	0	-1.891486	-4.920005	-1.905682
24	1	0	-4.644526	-3.058231	-2.555862
25	1	0	-3.483665	-5.096224	-3.355322
26	6	0	-1.020975	-6.123124	-2.198797
27	1	0	-1.499269	-7.051303	-1.855565
28	1	0	-0.827879	-6.246942	-3.270634
29	6	0	-0.227843	-4.955260	-0.183594

30	6	0	0.262855	-5.818597	-1.393713
31	1	0	0.955671	-5.222681	-1.998257
32	1	0	0.793483	-6.719703	-1.069928
33	6	0	-0.796302	-5.888873	0.940152
34	1	0	-1.458849	-5.303075	1.586577
35	1	0	-1.379904	-6.720087	0.531627
36	6	0	0.445342	-6.347442	1.734162
37	1	0	0.876450	-7.267051	1.313191
38	1	0	0.220045	-6.558468	2.785868
39	6	0	1.390726	-5.178322	1.569769
40	6	0	0.940770	-4.317323	0.557841
41	6	0	2.556429	-4.899082	2.274965
42	1	0	2.907126	-5.565244	3.058917
43	6	0	1.617028	-3.121589	0.328174
44	6	0	3.276820	-3.748807	1.961956
45	1	0	4.198056	-3.530343	2.492767
46	8	0	-1.304139	-2.122247	0.415124
47	8	0	1.090347	-2.211290	-0.588209
48	15	0	-0.082010	-1.174018	-0.109688
49	8	0	0.348700	-0.336530	1.072965
50	8	0	-0.486082	-0.441586	-1.382570
51	6	0	-3.163108	-2.558765	-1.082729
52	6	0	2.823684	-2.834986	0.995850
53	6	0	0.172032	6.150014	-0.499373
54	6	0	-0.417940	7.143876	-1.287238
55	6	0	1.111604	6.515287	0.473470
56	6	0	-0.087237	8.486796	-1.098743
57	1	0	-1.139209	6.866831	-2.053115
58	6	0	1.450695	7.855556	0.653445
59	1	0	1.588116	5.745330	1.072869
60	6	0	0.849020	8.844960	-0.128303
61	1	0	-0.553844	9.249464	-1.716192
62	1	0	2.187100	8.128029	1.404627
63	1	0	1.113788	9.889006	0.015020
64	6	0	-3.906311	-1.357896	-0.600332
65	6	0	-5.055866	-0.172715	1.217120
66	6	0	-5.046795	0.777560	-0.977245
67	6	0	-5.434583	0.866878	0.363458
68	1	0	-5.378667	-0.174753	2.253090
69	1	0	-5.306402	1.571108	-1.670232
70	6	0	3.660523	-1.638133	0.683546
71	6	0	4.924406	0.334039	1.408569
72	6	0	5.056699	-0.358823	-0.878007
73	6	0	5.442620	0.532344	0.126208
74	1	0	5.189623	1.013908	2.211912
75	1	0	5.472723	-0.266834	-1.876459
76	6	0	6.434599	1.625573	-0.138494
77	6	0	8.328944	3.671410	-0.596773
78	6	0	-6.263098	2.012811	0.855229
79	6	0	-7.839304	4.177341	1.775921
80	6	0	-4.320004	-0.315871	-1.463564
81	6	0	-4.310916	-1.259369	0.751311
82	6	0	4.191466	-1.426415	-0.609956
83	6	0	4.060718	-0.728924	1.691541
84	6	0	-7.587075	2.178865	0.387758
85	6	0	-8.347352	3.253072	0.859455
86	1	0	-9.369903	3.365705	0.503734
87	6	0	-6.533897	3.989999	2.233917
88	1	0	-6.118206	4.691793	2.954779
89	6	0	-5.739570	2.924060	1.797991
90	6	0	6.969026	3.882948	-0.830910
91	1	0	6.636494	4.854813	-1.191222
92	6	0	6.013552	2.882825	-0.615342
93	6	0	8.724834	2.416390	-0.125059
94	1	0	9.779405	2.229786	0.069975
95	6	0	7.804919	1.390616	0.109368
96	6	0	8.292820	0.054099	0.625071
97	1	0	7.881632	-0.173735	1.615868
98	1	0	7.993886	-0.769256	-0.034009
99	1	0	9.384103	0.043470	0.705330
100	6	0	4.558883	3.166200	-0.912065
101	1	0	4.244969	2.673580	-1.841934
102	1	0	3.890268	2.803636	-0.126497
103	1	0	4.386419	4.239741	-1.037808
104	6	0	9.346779	4.755649	-0.865568
105	1	0	9.807176	4.633991	-1.855368
106	1	0	8.889266	5.750235	-0.839549
107	1	0	10.157674	4.736455	-0.128926
108	6	0	-4.340082	2.781106	2.356668
109	1	0	-4.292286	2.022941	3.148574
110	1	0	-3.623200	2.476973	1.588332
111	1	0	-4.000004	3.726088	2.792726
112	6	0	-8.219940	1.209444	-0.588694
113	1	0	-7.858281	1.361566	-1.613298
114	1	0	-8.003967	0.168545	-0.326778
115	1	0	-9.306757	1.337530	-0.605703
116	6	0	-8.670279	5.350718	2.239824
117	1	0	-8.589331	6.196410	1.543553
118	1	0	-9.731835	5.088486	2.306377
119	1	0	-8.347125	5.707567	3.223412
120	7	0	-4.063384	-0.342777	-2.863780
121	6	0	-5.043607	-0.128449	-3.824322
122	6	0	-2.848850	-0.526882	-3.503031
123	6	0	-4.452736	-0.184653	-5.063478
124	1	0	-6.074022	0.007474	-3.530219
125	6	0	-3.062558	-0.430578	-4.858093
126	1	0	-1.950620	-0.692283	-2.927825
127	1	0	-4.962365	-0.071425	-6.011247
128	1	0	-2.301470	-0.527208	-5.621138
129	7	0	-4.035929	-2.300760	1.684638
130	6	0	-3.423109	-2.120730	2.912367
131	6	0	-4.479068	-3.609692	1.598899
132	6	0	-3.461509	-3.313400	3.594455
133	1	0	-2.968527	-1.172319	3.156996
134	6	0	-4.136560	-4.257216	2.762894
135	1	0	-5.009285	-3.951129	0.722993
136	1	0	-3.039008	-3.494245	4.573696
137	1	0	-4.354974	-5.290920	2.996218
138	7	0	3.924563	-2.327023	-1.682118
139	6	0	3.510948	-1.945957	-2.946758
140	6	0	4.166828	-3.689975	-1.691748
141	6	0	3.474519	-3.061443	-3.748372
142	1	0	3.241525	-0.918911	-3.142442
143	6	0	3.896273	-4.168144	-2.952709
144	1	0	4.526507	-4.188544	-0.805067
145	1	0	3.166589	-3.084970	-4.785102
146	1	0	4.000722	-5.196685	-3.271736
147	7	0	3.645232	-0.877929	3.045348
148	6	0	4.524422	-0.933897	4.117957
149	6	0	2.349385	-0.951926	3.526887
150	6	0	3.787463	-1.053118	5.272160
151	1	0	5.591281	-0.911783	3.949383
152	6	0	2.411479	-1.057748	4.896823
153	1	0	1.511096	-0.893275	2.848190
154	1	0	4.190974	-1.132773	6.273023
155	1	0	1.558590	-1.125474	5.559126

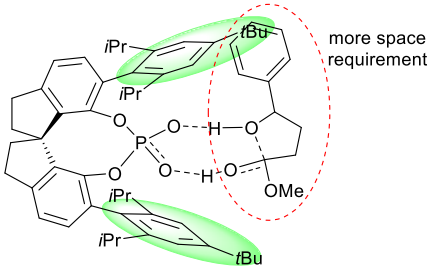
12. DFT Calculation for Distortion Analysis of SPINOL-derived CPA (*S*)-1bd in Transition States

Distortion analysis of the anion form of CPA (*S*)-1bd in the transition states.



anion form of (*S*)-**1bd**
bent angles : 176.1° and 176.1°
set to distortion energy: 0.0 kcal/mol

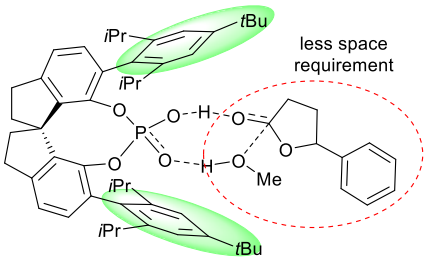
TS 1st



catalyst structure taken from TS of 1st step	distortion energy (kcal/mol)	bent angles
From ***R-anti*** (**-2.61**)*	7.9	172.1° and 175.9°
From ***S-syn*** (**1.63**)*	8.8	172.2° and 176.6°
cf. From ***S-anti*** (**2.35**)*	9.4	171.3° and 174.5°

* $\Delta\Delta G^{\neq}$ (kcal/mol) of the correspondingTSs.

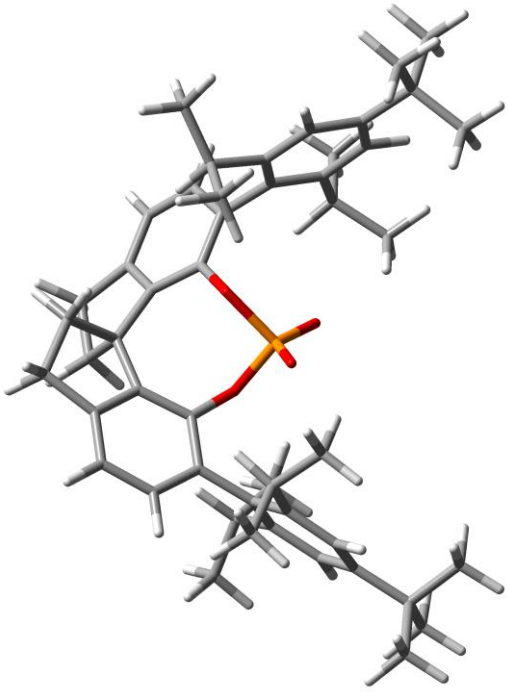
TS 2nd



catalyst structure taken from TS of 2nd step	distortion energy (kcal/mol)	bent angles
From ***R-re*** (**0.00**)*	7.1	176.4° and 177.6°
From ***S-re*** (**-0.57**)*	6.9	175.8° and 177.3°
cf. From ***S-si*** (**0.88**)*	7.8	173.0° and 173.3°

* $\Delta\Delta G^{\neq}$ (kcal/mol) of the correspondingTSs.

Optimized structure of the anion form (phosphate) of CPA (*S*)-1bd



B3LYP/6-31+G(d); E(RB3LYP) = -2547.11082979 Hartree
Zero-point correction= 1.001453 Hartree
Thermal correction to Energy= 1.056070 Hartree
Thermal correction to Enthalpy= 1.057014 Hartree
Thermal correction to Gibbs Free Energy= 0.913807 Hartree
Sum of electronic and zero-point Energies= -2546.109376 Hartree
Sum of electronic and thermal Energies= -2546.054760 Hartree
Sum of electronic and thermal Enthalpies= -2546.053816 Hartree
Sum of electronic and thermal Free Energies= -2546.197023 Hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.412586	4.497699	1.208331
2	6	0	0.000408	3.590305	-0.000850
3	6	0	-1.213440	2.883618	0.597825
4	6	0	-1.806214	3.701448	1.571037
5	6	0	-0.922900	4.893661	1.877023
6	6	0	-0.411983	4.496635	-1.210782
7	6	0	0.923353	4.892032	-1.880079
8	6	0	1.806657	3.700007	-1.573357
9	6	0	1.214236	2.883216	-0.599053
10	6	0	3.039620	3.365026	-2.126871
11	6	0	3.668210	2.190214	-1.704457
12	6	0	3.063891	1.305331	-0.796509
13	6	0	1.798803	1.654902	-0.267271
14	6	0	-1.797936	1.654986	0.267051
15	6	0	-3.063465	1.306169	0.795798
16	6	0	-3.668187	2.192217	1.702359
17	6	0	-3.039592	3.367266	2.124097
18	8	0	-1.149977	0.817326	-0.598821
19	8	0	1.151158	0.818230	0.599868
20	15	0	0.000658	-0.285050	0.001202
21	8	0	0.528836	-0.953532	-1.225897
22	8	0	-0.527467	-0.952206	1.229006
23	6	0	3.785347	0.049998	-0.395347
24	6	0	-3.785102	0.050681	0.395357
25	6	0	4.019646	-0.985335	-1.337982
26	6	0	4.759229	-2.105270	-0.945045

27	6	0	5.271257	-2.268128	0.348367
28	6	0	5.019281	-1.240377	1.259018
29	6	0	4.293971	-0.088923	0.916770
30	6	0	-4.291654	-0.089774	-0.917443
31	6	0	-5.016910	-1.241348	-1.259426
32	6	0	-5.271056	-2.267791	-0.347856
33	6	0	-4.761320	-2.103311	0.946280
34	6	0	-4.021831	-0.983221	1.339028
35	6	0	-4.104602	0.979994	-1.994454
36	6	0	-5.453880	1.583892	-2.437098
37	6	0	-3.309743	0.449819	-3.204091
38	6	0	-3.500155	-0.929533	2.776980
39	6	0	-2.713042	-2.194605	3.171312
40	6	0	-4.645093	-0.677267	3.781945
41	6	0	-6.054072	-3.544000	-0.713379
42	6	0	-5.142600	-4.781275	-0.524234
43	6	0	-6.547637	-3.537734	-2.173898
44	6	0	-7.292767	-3.679995	0.205298
45	6	0	4.108587	0.982212	1.992699
46	6	0	5.458545	1.585839	2.433611
47	6	0	3.314368	0.453809	3.203530
48	6	0	3.494998	-0.933226	-2.774888
49	6	0	2.704207	-2.197393	-3.164796
50	6	0	4.638186	-0.684913	-3.782771
51	6	0	6.054350	-3.544139	0.714261
52	6	0	6.550964	-3.535582	2.173695
53	6	0	7.290886	-3.682330	-0.206958
54	6	0	5.141744	-4.781173	0.529082
55	1	0	1.017454	5.357618	0.898431
56	1	0	1.011856	3.898567	1.904139
57	1	0	-0.818852	5.071936	2.955062
58	1	0	-1.329410	5.819304	1.441481
59	1	0	-1.011348	3.896870	-1.905963
60	1	0	-1.016837	5.356805	-0.901555
61	1	0	1.330001	5.817984	-1.445324
62	1	0	0.819064	5.069495	-2.958229
63	1	0	3.510301	4.001440	-2.874326
64	1	0	4.645594	1.932423	-2.103966
65	1	0	-4.645984	1.935248	2.101308
66	1	0	-3.510660	4.004521	2.870592
67	1	0	4.922463	-2.889218	-1.679639
68	1	0	5.391037	-1.320742	2.274981
69	1	0	-5.386933	-1.322824	-2.275925
70	1	0	-4.926377	-2.886117	1.681680
71	1	0	-3.521624	1.796833	-1.562648
72	1	0	-6.003617	1.996354	-1.582080
73	1	0	-5.291147	2.394128	-3.160891
74	1	0	-6.095799	0.833663	-2.916813
75	1	0	-3.133582	1.258827	-3.926448
76	1	0	-3.854670	-0.347523	-3.726851
77	1	0	-2.339663	0.056554	-2.886846
78	1	0	-2.796579	-0.096327	2.844205
79	1	0	-3.353621	-3.086957	3.198698
80	1	0	-1.888206	-2.356089	2.473381
81	1	0	-2.289181	-2.065654	4.176643
82	1	0	-4.245979	-0.586240	4.801351
83	1	0	-5.364361	-1.507535	3.777492
84	1	0	-5.199464	0.240512	3.552818
85	1	0	-4.256445	-4.713648	-1.165827
86	1	0	-4.793787	-4.873261	0.509780
87	1	0	-5.685403	-5.701732	-0.781203
88	1	0	-7.222975	-2.696686	-2.372998
89	1	0	-7.099752	-4.463599	-2.380747
90	1	0	-5.714987	-3.482817	-2.884817
91	1	0	-7.855785	-4.591122	-0.040631
92	1	0	-7.010128	-3.736065	1.262027
93	1	0	-7.963741	-2.820403	0.085207
94	1	0	3.525708	1.798891	1.560406
95	1	0	6.007892	1.996944	1.577690
96	1	0	5.296837	2.397040	3.156552
97	1	0	6.100376	0.835818	2.913767
98	1	0	3.139443	1.263618	3.925296
99	1	0	3.859141	-0.343483	3.726526
100	1	0	2.343742	0.060968	2.887437
101	1	0	2.792954	-0.098756	-2.842113
102	1	0	2.278942	-2.069921	-4.169742
103	1	0	3.342587	-3.091365	-3.191001
104	1	0	1.880170	-2.354843	-2.464979
105	1	0	4.237018	-0.595081	-4.801472
106	1	0	5.356082	-1.516366	-3.778352
107	1	0	5.194518	0.232406	-3.556473
108	1	0	5.719805	-3.479054	2.886235
109	1	0	7.103137	-4.461304	2.381029
110	1	0	7.227028	-2.694435	2.369926
111	1	0	7.962617	-2.822931	-0.089754
112	1	0	7.005806	-3.739925	-1.262946
113	1	0	7.853924	-4.593392	0.039165
114	1	0	4.257063	-4.712028	1.172545
115	1	0	4.790558	-4.874555	-0.504006
116	1	0	5.684596	-5.701543	0.786269

Phosphate in *R-anti*

B3LYP/6-31+G(d); E(RB3LYP) = -2547.09819535 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.183691	2.787273	-0.680063
2	6	0	1.779978	1.588462	-0.288080
3	6	0	3.645795	2.042858	-1.736025
4	6	0	3.018495	3.190380	-2.218225
5	6	0	1.783544	3.551609	-1.693858
6	1	0	4.626881	1.769436	-2.111486
7	1	0	3.494194	3.791324	-2.989336
8	6	0	0.905880	4.724013	-2.072133
9	1	0	1.305451	5.668004	-1.675294
10	1	0	0.821423	4.850607	-3.157609
11	6	0	-0.038230	3.526619	-0.140308
12	6	0	-0.437057	4.357437	-1.407832
13	1	0	-1.019101	3.715271	-2.078745
14	1	0	-1.053798	5.226796	-1.160415
15	6	0	0.345765	4.505167	1.019775
16	1	0	0.914933	3.949955	1.774208
17	1	0	0.968390	5.337589	0.677140
18	6	0	-1.009264	4.954447	1.610779
19	1	0	-1.389552	5.852582	1.104184
20	1	0	-0.943374	5.200974	2.676876
21	6	0	-1.894385	3.754204	1.350474
22	6	0	-1.266840	2.859621	0.469868
23	6	0	-3.159982	3.476157	1.853000
24	1	0	-3.663066	4.175677	2.516166
25	6	0	-1.857351	1.623183	0.219321
26	6	0	-3.787405	2.285813	1.484176
27	1	0	-4.793956	2.081600	1.834238
28	8	0	1.128136	0.784857	0.649297
29	8	0	-1.161369	0.687325	-0.548240
30	15	0	-0.032725	-0.259733	0.154902
31	8	0	-0.573447	-0.854111	1.455621
32	8	0	0.462295	-1.207743	-0.905491
33	6	0	3.038806	1.200194	-0.789761
34	6	0	-3.148948	1.316077	0.693135
35	6	0	-3.863571	0.037717	0.362276
36	6	0	-4.242281	-0.864388	1.386322
37	6	0	-4.240520	-0.241583	-0.976678
38	6	0	-4.980846	-2.008379	1.050349
39	6	0	-4.969238	-1.401198	-1.250810
40	6	0	-5.359665	-2.307523	-0.259000

41	1	0	-5.265485	-2.678667	1.853178
42	1	0	-5.252924	-1.592728	-2.281939
43	6	0	3.783984	-0.026736	-0.346234
44	6	0	4.346433	-0.086306	0.953673
45	6	0	4.050829	-1.073126	-1.261874
46	6	0	5.170072	-1.164582	1.291713
47	6	0	4.890956	-2.125847	-0.868953
48	6	0	5.483465	-2.192987	0.394110
49	1	0	5.613281	-1.176155	2.283947
50	1	0	5.098333	-2.902628	-1.596020
51	6	0	3.498492	-1.092423	-2.690222
52	6	0	4.616287	-0.852710	-3.726609
53	6	0	2.744742	-2.394270	-3.021947
54	1	0	2.774409	-0.279088	-2.782473
55	1	0	5.359806	-1.658824	-3.701895
56	1	0	5.146195	0.088997	-3.548397
57	1	0	1.906758	-2.540723	-2.338045
58	1	0	3.399586	-3.273056	-2.976515
59	6	0	4.145539	1.019501	1.991362
60	6	0	3.413137	0.507031	3.246011
61	6	0	5.479404	1.696732	2.364136
62	1	0	3.514274	1.792808	1.547345
63	1	0	3.984931	-0.279800	3.753668
64	1	0	2.428479	0.108544	2.981469
65	1	0	5.983901	2.091438	1.475223
66	1	0	6.167405	0.998777	2.855682
67	6	0	-3.901362	-0.646146	2.863040
68	6	0	-5.151355	-0.247264	3.675454
69	6	0	-3.235597	-1.874249	3.511833
70	1	0	-3.180898	0.173424	2.925720
71	1	0	-5.898330	-1.050509	3.665463
72	1	0	-5.633241	0.652357	3.278475
73	1	0	-2.360373	-2.198806	2.946579
74	1	0	-3.926977	-2.722210	3.590338
75	6	0	-3.935970	0.699739	-2.143360
76	6	0	-3.087314	0.018064	-3.233511
77	6	0	-5.231379	1.291235	-2.735114
78	1	0	-3.353610	1.541984	-1.762929
79	1	0	-3.626284	-0.812735	-3.704903
80	1	0	-2.154088	-0.371384	-2.816923
81	1	0	-5.814593	1.814400	-1.968853
82	1	0	-5.871200	0.512355	-3.166673
83	1	0	4.197224	-0.817526	-4.739554
84	1	0	2.342125	-2.340815	-4.040751
85	1	0	5.304589	2.530907	3.054506
86	1	0	3.265389	1.323654	3.963403
87	1	0	-2.908525	-1.629285	4.529394
88	1	0	-4.883719	-0.053617	4.721558
89	1	0	-2.836502	0.736663	-4.023740
90	1	0	-4.996441	2.007515	-3.532131
91	6	0	-6.181190	-3.555030	-0.633967
92	6	0	-5.393512	-4.407400	-1.656715
93	1	0	-4.436708	-4.737685	-1.235790
94	1	0	-5.969049	-5.298419	-1.937453
95	1	0	-5.175461	-3.848595	-2.572374
96	6	0	-6.496050	-4.441551	0.585858
97	1	0	-5.583504	-4.806355	1.071601
98	1	0	-7.090008	-3.907641	1.336156
99	1	0	-7.074726	-5.316574	0.268097
100	6	0	-7.523818	-3.115279	-1.265498
101	1	0	-8.110275	-2.516535	-0.559206
102	1	0	-7.370358	-2.512149	-2.166322
103	1	0	-8.120998	-3.991739	-1.547060
104	6	0	6.496759	-3.286149	0.787522
105	6	0	7.876777	-2.622485	1.017924
106	1	0	7.839200	-1.880916	1.822836
107	1	0	8.625138	-3.377286	1.290301
108	1	0	8.221134	-2.112891	0.110950
109	6	0	6.658411	-4.359965	-0.305491
110	1	0	5.710222	-4.864851	-0.523786
111	1	0	7.042710	-3.937593	-1.240467
112	1	0	7.371399	-5.122639	0.028042
113	6	0	6.057195	-3.995465	2.088592
114	1	0	6.812038	-4.729635	2.395947
115	1	0	5.923506	-3.292588	2.917335
116	1	0	5.111916	-4.530582	1.943434

Phosphate in *R-re*

B3LYP/6-31+G(d); E(RB3LYP) = -2547.09952708 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.269065	2.914407	0.580515
2	6	0	-1.857408	1.703854	0.217799
3	6	0	-3.754936	2.202082	1.609463
4	6	0	-3.141767	3.372244	2.056833
5	6	0	-1.892673	3.713774	1.552178
6	1	0	-4.739434	1.935664	1.981876
7	1	0	-3.635933	4.001430	2.793105
8	6	0	-1.016432	4.892042	1.916780
9	1	0	-1.394257	5.825861	1.476843
10	1	0	-0.962631	5.054511	2.999445
11	6	0	-0.027202	3.627649	0.051895
12	6	0	0.342926	4.491995	1.305749
13	1	0	0.896510	3.864193	2.013395
14	1	0	0.976527	5.347506	1.052338
15	6	0	-0.371850	4.576985	-1.144154
16	1	0	-0.924373	4.005463	-1.898698
17	1	0	-0.997182	5.422511	-0.841052
18	6	0	1.002053	5.000499	-1.708918
19	1	0	1.378208	5.905653	-1.211782
20	1	0	0.967294	5.224012	-2.781524
21	6	0	1.867055	3.797323	-1.399578
22	6	0	1.210289	2.931721	-0.510166
23	6	0	3.136523	3.491847	-1.875657
24	1	0	3.659293	4.171095	-2.544657
25	6	0	1.779885	1.691971	-0.225502
26	6	0	3.739559	2.298316	-1.477369
27	1	0	4.746699	2.070119	-1.811366
28	8	0	-1.192071	0.874070	-0.684328
29	8	0	1.068606	0.778011	0.550673
30	15	0	-0.053641	-0.179114	-0.153644
31	8	0	0.498266	-0.803107	-1.432545
32	8	0	-0.549472	-1.100442	0.929689
33	6	0	-3.121834	1.325019	0.714186
34	6	0	3.071846	1.355366	-0.679175
35	6	0	3.750170	0.063444	-0.324790
36	6	0	4.109026	-0.864384	-1.333280
37	6	0	4.107412	-0.209792	1.020720
38	6	0	4.809547	-2.026237	-0.976250
39	6	0	4.800070	-1.386494	1.316280
40	6	0	5.171884	-2.317599	0.340031
41	1	0	5.081678	-2.715058	-1.767768
42	1	0	5.072217	-1.570334	2.351916
43	6	0	-3.789455	0.039315	0.324917
44	6	0	-4.234776	-0.161741	-1.001457
45	6	0	-4.022112	-0.970989	1.295126
46	6	0	-4.860253	-1.370567	-1.340391
47	6	0	-4.663554	-2.148045	0.901943
48	6	0	-5.082214	-2.389532	-0.411449
49	1	0	-5.195630	-1.498037	-2.363955
50	1	0	-4.834284	-2.910871	1.655564
51	6	0	-4.131337	0.920748	-2.077656
52	6	0	-3.327704	0.463003	-3.308880
53	6	0	-5.530334	1.424777	-2.487027
54	1	0	-3.601138	1.775655	-1.650489

55	1	0	-3.810254	-0.380608	-3.817912
56	1	0	-2.315028	0.164400	-3.022461
57	1	0	-6.087249	1.794088	-1.618646
58	1	0	-6.125736	0.629161	-2.950581
59	6	0	-3.633600	-0.822576	2.769480
60	6	0	-4.888370	-0.654511	3.651767
61	6	0	-2.768059	-1.985184	3.291403
62	1	0	-3.032042	0.083729	2.872871
63	1	0	-5.519147	-1.551179	3.617553
64	1	0	-5.504984	0.191696	3.328623
65	1	0	-1.838830	-2.060066	2.723334
66	1	0	-3.291535	-2.947072	3.237550
67	6	0	3.792883	-0.651697	-2.816454
68	6	0	5.068450	-0.318279	-3.618336
69	6	0	3.077608	-1.856025	-3.457397
70	1	0	3.110352	0.197667	-2.898177
71	1	0	5.777997	-1.154494	-3.595463
72	1	0	5.586017	0.560845	-3.220397
73	1	0	2.163789	-2.103799	-2.913918
74	1	0	3.717349	-2.746558	-3.488604
75	6	0	3.817978	0.754266	2.172389
76	6	0	2.939768	0.109170	3.261486
77	6	0	5.123391	1.316939	2.770126
78	1	0	3.262721	1.606796	1.775061
79	1	0	3.452500	-0.728421	3.750248
80	1	0	2.001164	-0.260902	2.839339
81	1	0	5.728552	1.814528	2.003855
82	1	0	5.737140	0.526334	3.218071
83	1	0	2.699228	0.844483	4.039279
84	1	0	4.900043	2.049148	3.555786
85	1	0	2.803997	-1.618139	-4.492840
86	1	0	4.821638	-0.118477	-4.668392
87	1	0	-2.511170	-1.811322	4.343833
88	1	0	-4.603506	-0.486641	4.697697
89	1	0	-5.446859	2.244189	-3.211670
90	1	0	-3.247852	1.280676	-4.035933
91	6	0	-5.776238	-3.717453	-0.767001
92	6	0	-4.878092	-4.907283	-0.351671
93	1	0	-4.703241	-4.927295	0.728700
94	1	0	-5.355967	-5.855707	-0.627935
95	1	0	-3.898359	-4.858582	-0.837937
96	6	0	-6.068210	-3.842096	-2.274583
97	1	0	-6.749894	-3.059748	-2.627249
98	1	0	-5.150555	-3.790220	-2.871975
99	1	0	-6.543067	-4.808263	-2.480277
100	6	0	-7.121682	-3.806109	-0.007331
101	1	0	-7.629113	-4.752475	-0.233485
102	1	0	-6.976382	-3.754680	1.076920
103	1	0	-7.789137	-2.985087	-0.293946
104	6	0	5.965550	-3.576805	0.736246
105	6	0	7.322822	-3.153382	1.347706
106	1	0	7.189761	-2.528473	2.236874
107	1	0	7.903688	-4.036476	1.642218
108	1	0	7.915413	-2.581948	0.624264
109	6	0	6.249699	-4.497128	-0.466019
110	1	0	5.325179	-4.846343	-0.940427
111	1	0	6.855202	-3.996219	-1.229640
112	1	0	6.805416	-5.381091	-0.132534
113	6	0	5.169283	-4.389141	1.784427
114	1	0	5.730580	-5.283000	2.083794
115	1	0	4.966618	-3.804824	2.687615
116	1	0	4.204841	-4.714779	1.376749

Phosphate in *S-syn*

B3LYP/6-31+G(d); E(RB3LYP) = -2547.09677777 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.263719	2.865587	0.454684
2	6	0	-1.863024	1.628988	0.227934
3	6	0	-3.802313	2.342785	1.448802
4	6	0	-3.164490	3.532468	1.802339
5	6	0	-1.890025	3.785897	1.309101
6	1	0	-4.816651	2.160046	1.787615
7	1	0	-3.667936	4.251634	2.443914
8	6	0	-0.995160	4.983475	1.549239
9	1	0	-1.367335	5.875693	1.026539
10	1	0	-0.929009	5.248580	2.610935
11	6	0	-0.031777	3.512563	-0.169621
12	6	0	0.357971	4.513492	0.968784
13	1	0	0.924422	3.971875	1.735126
14	1	0	0.985105	5.334972	0.608394
15	6	0	-0.435320	4.319305	-1.451761
16	1	0	-1.024474	3.665817	-2.105293
17	1	0	-1.047128	5.195905	-1.218264
18	6	0	0.903884	4.666023	-2.132444
19	1	0	1.311806	5.614752	-1.755826
20	1	0	0.812359	4.773009	-3.219433
21	6	0	1.777241	3.496010	-1.738325
22	6	0	1.183847	2.756797	-0.701887
23	6	0	3.003108	3.116459	-2.270036
24	1	0	3.472228	3.697343	-3.060272
25	6	0	1.778807	1.563960	-0.288440
26	8	0	-1.165189	0.666661	-0.503793
27	8	0	1.135198	0.789036	0.679528
28	15	0	-0.042355	-0.262124	0.231377
29	8	0	0.438072	-1.256415	-0.790788
30	8	0	-0.577606	-0.792730	1.561011
31	6	0	-3.165721	1.347810	0.687991
32	6	0	3.029489	1.158065	-0.797907
33	6	0	-3.887871	0.070501	0.370278
34	6	0	-4.222512	-0.244549	-0.972449
35	6	0	-4.307129	-0.800575	1.405464
36	6	0	-4.939903	-1.412822	-1.238925
37	6	0	-5.034075	-1.953613	1.076248
38	6	0	-5.361210	-2.293372	-0.236622
39	1	0	-5.186069	-1.634529	-2.273618
40	1	0	-5.345446	-2.601957	1.886922
41	6	0	3.628886	1.975403	-1.770896
42	1	0	4.602093	1.685501	-2.154457
43	6	0	3.777329	-0.062659	-0.339479
44	6	0	3.977733	-1.153502	-1.217067
45	6	0	4.409899	-0.066504	0.930594
46	6	0	4.809906	-2.209130	-0.812151
47	6	0	5.225813	-1.145801	1.279965
48	6	0	5.456600	-2.231658	0.424345
49	1	0	4.961277	-3.026842	-1.507199
50	1	0	5.722450	-1.122614	2.245125
51	6	0	3.369372	-1.214399	-2.621161
52	6	0	4.446868	-0.985931	-3.702408
53	6	0	2.621872	-2.531581	-2.901580
54	1	0	2.632348	-0.411435	-2.703110
55	1	0	5.203024	-1.780372	-3.680062
56	1	0	4.967459	-0.031916	-3.569301
57	1	0	1.819670	-2.686235	-2.178066
58	1	0	3.291773	-3.399795	-2.881921
59	6	0	4.318350	1.131436	1.878659
60	6	0	4.186287	0.745981	3.362029
61	6	0	5.525088	2.070155	1.669317
62	1	0	3.420085	1.698278	1.621993
63	1	0	5.092786	0.267940	3.751389
64	1	0	3.346445	0.063686	3.529887
65	1	0	5.583213	2.415406	0.631632
66	1	0	6.465169	1.557274	1.906674
67	6	0	-3.886352	0.667177	-2.154063
68	6	0	-3.017913	-0.042650	-3.210107

69	6	0	-5.166506	1.249345	-2.787146
70	1	0	-3.308918	1.516106	-1.781098
71	1	0	-3.552538	-0.878145	-3.678109
72	1	0	-2.098072	-0.431300	-2.764274
73	1	0	-5.763382	1.793360	-2.046323
74	1	0	-5.800385	0.462190	-3.212383
75	6	0	-4.016222	-0.544605	2.886615
76	6	0	-5.287383	-0.104982	3.643124
77	6	0	-3.394731	-1.764729	3.592233
78	1	0	-3.284828	0.265062	2.952530
79	1	0	-6.046111	-0.896986	3.625639
80	1	0	-5.740895	0.791345	3.207228
81	1	0	-2.525627	-2.138985	3.048582
82	1	0	-4.113441	-2.587128	3.695432
83	1	0	2.169511	-2.494143	-3.899940
84	1	0	3.992751	-0.985775	-4.700781
85	1	0	5.447675	2.952170	2.317162
86	1	0	4.014718	1.645218	3.965516
87	1	0	-2.742982	0.658213	-4.008242
88	1	0	-4.911963	1.944862	-3.596484
89	1	0	-3.070148	-1.488395	4.602401
90	1	0	-5.054181	0.110793	4.693194
91	6	0	6.423066	-3.355699	0.845608
92	6	0	5.944710	-4.000834	2.167160
93	1	0	6.649499	-4.776729	2.490822
94	1	0	5.863246	-3.267101	2.975773
95	1	0	4.962609	-4.470903	2.039372
96	6	0	6.530606	-4.468192	-0.214723
97	1	0	5.562202	-4.944564	-0.406060
98	1	0	6.917793	-4.088751	-1.166898
99	1	0	7.219240	-5.246151	0.134361
100	6	0	7.834723	-2.756648	1.057070
101	1	0	7.837380	-1.988297	1.837222
102	1	0	8.542684	-3.539866	1.355703
103	1	0	8.205700	-2.296449	0.134245
104	6	0	-6.147570	-3.564638	-0.606032
105	6	0	-7.456865	-3.171816	-1.330929
106	1	0	-7.260793	-2.603078	-2.245730
107	1	0	-8.024425	-4.068428	-1.610169
108	1	0	-8.091742	-2.555100	-0.684406
109	6	0	-5.288599	-4.444812	-1.544843
110	1	0	-4.352536	-4.738992	-1.055971
111	1	0	-5.832873	-5.357044	-1.820086
112	1	0	-5.027208	-3.919659	-2.469147
113	6	0	-6.520788	-4.405770	0.629381
114	1	0	-5.632683	-4.743156	1.176107
115	1	0	-7.157702	-3.848261	1.325468
116	1	0	-7.075376	-5.297790	0.315915

Phosphate in *S-re*

B3LYP/6-31+G(d); E(RB3LYP) = -2547.09985916 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.201975	2.920506	-0.522736
2	6	0	1.767520	1.678367	-0.237103
3	6	0	3.730225	2.277984	-1.488909
4	6	0	3.130459	3.471917	-1.890141
5	6	0	1.862375	3.782094	-1.413832
6	1	0	4.737496	2.047068	-1.820355
7	1	0	3.654898	4.148514	-2.560511
8	6	0	1.003358	4.988763	-1.725696
9	1	0	1.384029	5.893061	-1.230432
10	1	0	0.970027	5.210093	-2.798800
11	6	0	-0.032404	3.624714	0.037805
12	6	0	-0.372264	4.573009	-1.160340
13	1	0	-0.927295	4.002396	-1.913704
14	1	0	-0.993817	5.421990	-0.859148
15	6	0	0.339949	4.490210	1.290343
16	1	0	0.889250	3.861461	2.000511
17	1	0	0.978054	5.342198	1.036289
18	6	0	-1.018829	4.898558	1.898185
19	1	0	-1.390591	5.833759	1.456026
20	1	0	-0.965967	5.062663	2.980663
21	6	0	-1.900767	3.724263	1.534042
22	6	0	-1.278497	2.920042	0.566082
23	6	0	-3.153336	3.388782	2.034539
24	1	0	-3.648405	4.021790	2.766928
25	6	0	-1.869545	1.711290	0.203897
26	6	0	-3.768617	2.218776	1.588996
27	1	0	-4.754827	1.956598	1.959937
28	8	0	1.054563	0.764547	0.538200
29	8	0	-1.204755	0.882543	-0.697222
30	15	0	-0.076441	-0.182370	-0.167796
31	8	0	-0.592126	-1.087826	0.922611
32	8	0	0.456309	-0.814572	-1.447227
33	6	0	3.059497	1.338971	-0.688862
34	6	0	-3.135367	1.335872	0.699284
35	6	0	3.741561	0.051552	-0.324247
36	6	0	4.114184	-0.200227	1.021084
37	6	0	4.096734	-0.887532	-1.323560
38	6	0	4.822793	-1.365182	1.325426
39	6	0	4.811429	-2.038331	-0.957663
40	6	0	5.194269	-2.305744	0.358251
41	1	0	5.109862	-1.530346	2.360134
42	1	0	5.082269	-2.735266	-1.742563
43	6	0	-3.799593	0.045226	0.320719
44	6	0	-4.043412	-0.949980	1.304161
45	6	0	-4.226292	-0.179548	-1.008038
46	6	0	-4.680184	-2.133442	0.922787
47	6	0	-4.847645	-1.393943	-1.334381
48	6	0	-5.082827	-2.396676	-0.391419
49	1	0	-4.859582	-2.883840	1.686920
50	1	0	-5.168732	-1.539004	-2.360119
51	6	0	3.767539	-0.693345	-2.806565
52	6	0	5.032889	-0.344834	-3.618590
53	6	0	3.072126	-1.914937	-3.436267
54	1	0	3.069743	0.143495	-2.890090
55	1	0	5.756012	-1.169317	-3.592933
56	1	0	5.538351	0.545913	-3.231542
57	1	0	2.165326	-2.180682	-2.889650
58	1	0	3.728804	-2.793007	-3.466132
59	6	0	3.824345	0.775692	2.162624
60	6	0	2.952018	0.138285	3.260949
61	6	0	5.128177	1.351914	2.750625
62	1	0	3.263618	1.620929	1.757418
63	1	0	3.467598	-0.695562	3.753145
64	1	0	2.011556	-0.235055	2.845690
65	1	0	5.729618	1.842170	1.976764
66	1	0	5.746523	0.570520	3.208296
67	6	0	-4.104662	0.880932	-2.103835
68	6	0	-3.290008	0.392829	-3.316165
69	6	0	-5.496092	1.384428	-2.538998
70	1	0	-3.574428	1.741249	-1.688075
71	1	0	-3.775499	-0.454204	-3.816648
72	1	0	-2.284312	0.088433	-3.011846
73	1	0	-6.060098	1.775455	-1.684781
74	1	0	-6.091357	0.582669	-2.992085
75	6	0	-3.666445	-0.782473	2.779556
76	6	0	-4.926990	-0.610095	3.652531
77	6	0	-2.798611	-1.935614	3.318665
78	1	0	-3.069250	0.127205	2.877033
79	1	0	-5.554569	-1.509216	3.624205
80	1	0	-5.544568	0.230557	3.316895
81	1	0	-1.866719	-2.012751	2.755005
82	1	0	-3.317820	-2.900256	3.272791

83	1	0	-2.546909	-1.749357	4.370220
84	1	0	-4.648991	-0.430190	4.698315
85	1	0	-3.192131	1.196643	-4.056337
86	1	0	-5.399775	2.187739	-3.279894
87	1	0	2.789488	-1.687943	-4.471628
88	1	0	4.776521	-0.158080	-4.668728
89	1	0	4.902618	2.093438	3.526827
90	1	0	2.714394	0.879122	4.034377
91	6	0	6.019661	-3.542555	0.760837
92	6	0	6.272123	-4.493732	-0.424403
93	1	0	6.847004	-4.010068	-1.221973
94	1	0	6.846280	-5.363699	-0.085661
95	1	0	5.335038	-4.863160	-0.857866
96	6	0	5.280575	-4.336593	1.863288
97	1	0	5.106555	-3.730875	2.758217
98	1	0	4.305969	-4.690285	1.507319
99	1	0	5.869423	-5.212148	2.163543
100	6	0	7.392459	-3.079410	1.305722
101	1	0	7.999135	-3.943648	1.604224
102	1	0	7.947089	-2.520871	0.543172
103	1	0	7.281640	-2.429432	2.179911
104	6	0	-5.772580	-3.730213	-0.733592
105	6	0	-6.047467	-3.878902	-2.242204
106	1	0	-6.520042	-4.848226	-2.438106
107	1	0	-6.724864	-3.102184	-2.614853
108	1	0	-5.123074	-3.836051	-2.829885
109	6	0	-4.878073	-4.912476	-0.289791
110	1	0	-3.893127	-4.868392	-0.766081
111	1	0	-4.715604	-4.915421	0.792748
112	1	0	-5.350838	-5.865972	-0.557155
113	6	0	-7.126303	-3.808242	0.012310
114	1	0	-7.630983	-4.758107	-0.205213
115	1	0	-6.993223	-3.740286	1.097213
116	1	0	-7.790647	-2.991911	-0.294119

Phosphate in *S-anti*

B3LYP/6-31+G(d); E(RB3LYP) = -2547.09578230 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.224126	2.861289	-0.571806
2	6	0	1.801773	1.660156	-0.158853
3	6	0	3.769707	2.177100	-1.441892
4	6	0	3.173101	3.333185	-1.938996
5	6	0	1.890348	3.657817	-1.517432
6	1	0	4.778821	1.920675	-1.748513
7	1	0	3.704164	3.962818	-2.648655
8	6	0	1.021416	4.815501	-1.955222
9	1	0	1.360759	5.764076	-1.515709
10	1	0	1.027556	4.953656	-3.042588
11	6	0	-0.047736	3.574577	-0.122861
12	6	0	-0.362950	4.406892	-1.413029
13	1	0	-0.867581	3.755523	-2.135849
14	1	0	-1.022591	5.256526	-1.212878
15	6	0	0.236420	4.556978	1.061889
16	1	0	0.739103	4.004588	1.863997
17	1	0	0.886011	5.387996	0.770649
18	6	0	-1.164269	5.006210	1.529446
19	1	0	-1.501639	5.900598	0.987311
20	1	0	-1.194072	5.257235	2.596120
21	6	0	-2.018442	3.800710	1.201572
22	6	0	-1.313087	2.894008	0.392814
23	6	0	-3.325210	3.535267	1.591052
24	1	0	-3.886403	4.250658	2.187192
25	6	0	-1.873509	1.645083	0.122631
26	8	0	1.088247	0.838833	0.718651
27	8	0	-1.132724	0.698522	-0.588104
28	15	0	0.000228	-0.231725	0.127460
29	8	0	-0.558610	-0.927577	1.371782
30	8	0	0.581529	-1.108092	-0.952487
31	6	0	3.095640	1.291100	-0.583074
32	6	0	-3.196062	1.342109	0.506983
33	6	0	3.804432	0.024322	-0.198294
34	6	0	4.221519	-0.203930	1.132603
35	6	0	4.187780	-0.898152	-1.209876
36	6	0	5.022938	-1.318749	1.420098
37	6	0	5.000154	-1.980768	-0.865534
38	6	0	5.447640	-2.216689	0.439187
39	1	0	5.340633	-1.459693	2.447348
40	1	0	5.300640	-2.661367	-1.656756
41	6	0	-3.910928	2.332049	1.202754
42	1	0	-4.940996	2.124391	1.475682
43	6	0	-3.865140	0.029517	0.227055
44	6	0	-4.324711	-0.770859	1.302527
45	6	0	-4.127898	-0.384833	-1.103623
46	6	0	-5.026130	-1.953797	1.023038
47	6	0	-4.831696	-1.572359	-1.319516
48	6	0	-5.305579	-2.378385	-0.277671
49	1	0	-5.374600	-2.543768	1.863264
50	1	0	-5.037751	-1.861953	-2.346250
51	6	0	3.764943	-0.766643	-2.677520
52	6	0	4.973952	-0.496476	-3.596320
53	6	0	2.984293	-1.999334	-3.174297
54	1	0	3.086835	0.085478	-2.762993
55	1	0	5.677289	-1.337933	-3.589437
56	1	0	5.528844	0.397175	-3.290319
57	1	0	2.073069	-2.138412	-2.588858
58	1	0	3.584217	-2.915496	-3.117064
59	6	0	3.889526	0.751070	2.279573
60	6	0	3.060202	0.062293	3.380083
61	6	0	5.162035	1.396999	2.863441
62	1	0	3.279266	1.564612	1.881067
63	1	0	3.618608	-0.755003	3.853134
64	1	0	2.130998	-0.345894	2.972073
65	1	0	5.732511	1.919926	2.087525
66	1	0	5.824422	0.650942	3.318308
67	6	0	-3.740447	0.448223	-2.326496
68	6	0	-2.810535	-0.319988	-3.284642
69	6	0	-4.991714	0.967899	-3.063394
70	1	0	-3.191861	1.327672	-1.982556
71	1	0	-3.306490	-1.202026	-3.708412
72	1	0	-1.901464	-0.647464	-2.772257
73	1	0	-5.634351	1.549319	-2.392630
74	1	0	-5.592356	0.145934	-3.470783
75	6	0	-4.123950	-0.399361	2.775781
76	6	0	-5.471447	-0.126429	3.474873
77	6	0	-3.318787	-1.458182	3.548821
78	1	0	-3.541103	0.522433	2.820023
79	1	0	-6.093933	-1.028297	3.514271
80	1	0	-6.049007	0.648282	2.957640
81	1	0	-2.322238	-1.570690	3.114800
82	1	0	-3.812168	-2.436357	3.550623
83	1	0	-2.515394	0.323542	-4.122539
84	1	0	-4.701406	1.613870	-3.901049
85	1	0	-3.198048	-1.149079	4.594564
86	1	0	-5.305404	0.206599	4.506590
87	1	0	4.642465	-0.350135	-4.631582
88	1	0	2.694448	-1.859824	-4.223202
89	1	0	4.899233	2.124784	3.640996
90	1	0	2.799541	0.781598	4.166308
91	6	0	-6.130480	-3.641085	-0.591821
92	6	0	-6.564874	-4.392855	0.680800
93	1	0	-5.706368	-4.717848	1.279433
94	1	0	-7.207217	-3.775096	1.318355
95	1	0	-7.136208	-5.286841	0.405176
96	6	0	-7.408132	-3.234959	-1.365789

97	1	0	-7.170338	-2.736672	-2.311230
98	1	0	-8.013528	-4.120392	-1.596806
99	1	0	-8.022117	-2.548407	-0.772006
100	6	0	-5.299355	-4.609788	-1.464907
101	1	0	-4.976069	-4.142639	-2.400751
102	1	0	-4.401213	-4.944216	-0.931754
103	1	0	-5.889224	-5.498618	-1.720976
104	6	0	6.412779	-3.383057	0.726431
105	6	0	5.861065	-4.703919	0.140764
106	1	0	5.745174	-4.655540	-0.946425
107	1	0	6.546762	-5.531216	0.361612
108	1	0	4.882263	-4.950498	0.565990
109	6	0	6.650359	-3.592033	2.234563
110	1	0	7.121774	-2.719676	2.700262
111	1	0	5.716133	-3.798658	2.769940
112	1	0	7.318727	-4.446816	2.389569
113	6	0	7.775976	-3.071419	0.061635
114	1	0	8.488325	-3.886932	0.240446
115	1	0	7.672964	-2.944776	-1.021399
116	1	0	8.206296	-2.148127	0.466022

Phosphate in *S-si*

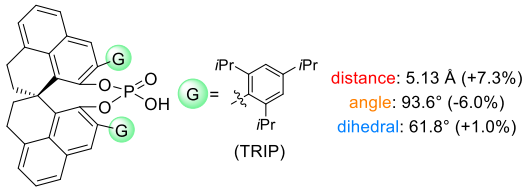
B3LYP/6-31+G(d); E(RB3LYP) = -2547.09833394 Hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.237528	2.829904	-0.540548
2	6	0	1.811290	1.598954	-0.222923
3	6	0	3.780377	2.204907	-1.462486
4	6	0	3.172396	3.382285	-1.895384
5	6	0	1.894788	3.683764	-1.440669
6	1	0	4.795134	1.981337	-1.774674
7	1	0	3.697539	4.052792	-2.571206
8	6	0	1.025802	4.874982	-1.781524
9	1	0	1.396184	5.793527	-1.305074
10	1	0	0.994462	5.072181	-2.859354
11	6	0	-0.002168	3.534357	0.003229
12	6	0	-0.347580	4.458330	-1.212360
13	1	0	-0.896082	3.869457	-1.956362
14	1	0	-0.977075	5.307118	-0.927795
15	6	0	0.367946	4.424759	1.238529
16	1	0	0.916089	3.810140	1.961867
17	1	0	1.006827	5.271015	0.968311
18	6	0	-0.991377	4.845172	1.834389
19	1	0	-1.360454	5.773644	1.376315
20	1	0	-0.943230	5.026072	2.914462
21	6	0	-1.874176	3.667407	1.485545
22	6	0	-1.248023	2.837509	0.541916
23	6	0	-3.138131	3.358349	1.972656
24	1	0	-3.638348	4.012636	2.682425
25	6	0	-1.843527	1.624415	0.195862
26	6	0	-3.760713	2.191358	1.534284
27	1	0	-4.760369	1.953573	1.884393
28	8	0	1.090198	0.697825	0.562400
29	8	0	-1.176064	0.771871	-0.680924
30	15	0	-0.024657	-0.267069	-0.156141
31	8	0	-0.551703	-1.129427	0.988749
32	8	0	0.510956	-0.953340	-1.383035
33	6	0	3.112835	1.268925	-0.654522
34	6	0	-3.125253	1.280006	0.673269
35	6	0	3.832891	0.006754	-0.274168
36	6	0	4.213031	-0.224344	1.068838
37	6	0	4.250276	-0.909739	-1.276754
38	6	0	5.000749	-1.343109	1.378517
39	6	0	5.050117	-1.996752	-0.910273
40	6	0	5.453122	-2.239785	0.409001
41	1	0	5.286962	-1.487358	2.414315
42	1	0	5.380655	-2.671301	-1.695021
43	6	0	-3.850275	0.016567	0.311441
44	6	0	-4.220654	-0.903010	1.324203
45	6	0	-4.276860	-0.217264	-1.020796
46	6	0	-5.021553	-2.005144	0.988356
47	6	0	-5.056297	-1.344012	-1.298189
48	6	0	-5.461007	-2.253391	-0.313952
49	1	0	-5.309184	-2.681753	1.785650
50	1	0	-5.381181	-1.497575	-2.323479
51	6	0	-3.978514	0.745428	-2.171214
52	6	0	-3.169093	0.072361	-3.296001
53	6	0	-5.273593	1.378324	-2.719474
54	1	0	-3.369310	1.564493	-1.783370
55	1	0	-3.728207	-0.748950	-3.760862
56	1	0	-2.223091	-0.324806	-2.916844
57	1	0	-5.831650	1.890054	-1.927215
58	1	0	-5.937174	0.626092	-3.162287
59	6	0	-3.801291	-0.752374	2.790465
60	6	0	-5.015245	-0.480188	3.702194
61	6	0	-3.010735	-1.969969	3.307589
62	1	0	-3.130927	0.106680	2.865501
63	1	0	-5.711643	-1.327458	3.704540
64	1	0	-5.576302	0.404290	3.381332
65	1	0	-2.102083	-2.120988	2.720087
66	1	0	-3.607767	-2.889935	3.278847
67	6	0	3.884700	-0.755899	-2.756316
68	6	0	5.108896	-0.352674	-3.604759
69	6	0	3.247735	-2.028819	-3.345203
70	1	0	3.137751	0.037555	-2.837998
71	1	0	5.879443	-1.133040	-3.579758
72	1	0	5.570582	0.575480	-3.252666
73	1	0	2.384607	-2.350907	-2.760795
74	1	0	3.960657	-2.861231	-3.391117
75	6	0	3.862627	0.732838	2.209565
76	6	0	3.006124	0.054205	3.295326
77	6	0	5.129713	1.368328	2.816949
78	1	0	3.268323	1.551928	1.798838
79	1	0	3.540813	-0.776355	3.772406
80	1	0	2.073082	-0.330622	2.873189
81	1	0	5.720562	1.883093	2.050981
82	1	0	5.775455	0.617684	3.287828
83	1	0	2.908704	-1.835258	-4.369864
84	1	0	4.816600	-0.207510	-4.651874
85	1	0	4.857873	2.101265	3.586394
86	1	0	2.749639	0.774547	4.081941
87	1	0	-4.688430	-0.316362	4.736268
88	1	0	-2.713194	-1.806793	4.350736
89	1	0	-2.939134	0.799876	-4.084060
90	1	0	-5.038630	2.113150	-3.499136
91	6	0	6.392886	-3.418977	0.727009
92	6	0	5.778449	-4.746350	0.224782
93	1	0	5.581384	-4.727866	-0.851807
94	1	0	6.460661	-5.582055	0.423532
95	1	0	4.831431	-4.957609	0.735892
96	6	0	6.666777	-3.563071	2.236184
97	1	0	7.165441	-2.678406	2.647224
98	1	0	5.743772	-3.727795	2.804412
99	1	0	7.323468	-4.422602	2.413038
100	6	0	7.746184	-3.188444	0.011413
101	1	0	8.437646	-4.014183	0.221244
102	1	0	7.622815	-3.121494	-1.074577
103	1	0	8.213813	-2.257740	0.351991
104	6	0	-6.367879	-3.442086	-0.685428
105	6	0	-5.677507	-4.314359	-1.760334
106	1	0	-6.327255	-5.149505	-2.049758
107	1	0	-5.446971	-3.743025	-2.665161
108	1	0	-4.737952	-4.735200	-1.383068
109	6	0	-6.688385	-4.339661	0.525003
110	1	0	-5.782327	-4.772557	0.964689

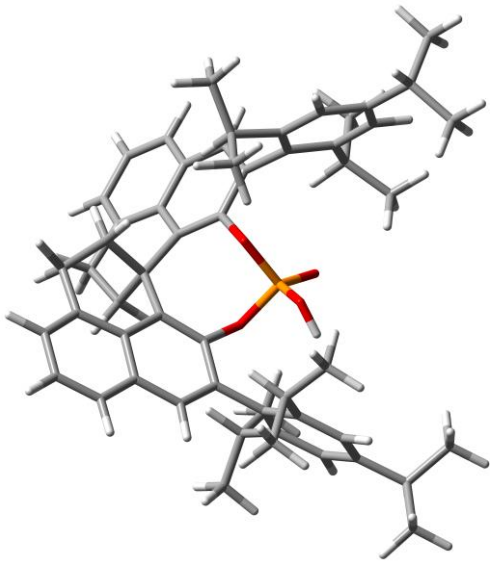
111	1	0	-7.220219	-3.791267	1.310655
112	1	0	-7.330658	-5.169783	0.209554
113	6	0	-7.705011	-2.904829	-1.250389
114	1	0	-8.366763	-3.736066	-1.524007
115	1	0	-8.223204	-2.287497	-0.507735
116	1	0	-7.551143	-2.291847	-2.144424

13. Screening of CPA Candidates by Calculation and their Structural Properties

Optimized structure of SPHENOL-derived CPA (*S*)-1ca



(*S*)-**1ca** (SPHENOL)



B3LYP/6-31G(d); E(RB3LYP) = -2776.21311781 Hartree

Zero-point correction= 1.055886 Hartree

Thermal correction to Energy= 1.113561 Hartree

Thermal correction to Enthalpy= 1.114505 Hartree

Thermal correction to Gibbs Free Energy= 0.964482 Hartree

Sum of electronic and zero-point Energies= -2775.157232 Hartree

Sum of electronic and thermal Energies= -2775.099557 Hartree

Sum of electronic and thermal Enthalpies= -2775.098613 Hartree

Sum of electronic and thermal Free Energies= -2775.248636 Hartree

The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.113194	-3.016592	-1.479905
2	6	0	-1.251833	-2.242915	-0.603885
3	6	0	-1.746675	-1.020179	-0.181513
4	6	0	-3.070687	-0.539833	-0.426848
5	6	0	-3.885517	-1.323620	-1.206324
6	6	0	-3.427933	-2.529894	-1.788182
7	6	0	-1.720828	-4.261820	-2.064496
8	6	0	-0.378390	-4.869579	-1.747808
9	6	0	0.600884	-3.853000	-1.175757
10	6	0	-0.002379	-2.980327	-0.029511
11	6	0	-0.639762	-3.841363	1.110211
12	6	0	0.310776	-4.862284	1.717271
13	6	0	1.613335	-4.234537	2.133026
14	6	0	2.039099	-3.004032	1.540431
15	6	0	1.253730	-2.274113	0.561637
16	6	0	-4.281789	-3.262506	-2.651635
17	6	0	-3.865202	-4.444667	-3.215264
18	6	0	-2.579642	-4.934438	-2.915503
19	6	0	3.325999	-2.501591	1.931532
20	6	0	3.825711	-1.315097	1.346237
21	6	0	3.093921	-0.590712	0.437246
22	6	0	1.811446	-1.108753	0.066477
23	6	0	2.405051	-4.871276	3.071422
24	6	0	3.657508	-4.358215	3.460262
25	6	0	4.110771	-3.193561	2.889665
26	8	0	-0.920005	-0.146843	0.548333
27	8	0	1.127444	-0.378432	-0.909171
28	15	0	0.038678	0.723068	-0.421827
29	8	0	-0.538108	1.412951	-1.588198
30	8	0	0.727688	1.609059	0.722953
31	6	0	-3.584080	0.738214	0.173295
32	6	0	3.625422	0.695748	-0.130660
33	6	0	3.856637	1.819307	0.718225
34	6	0	4.319951	3.011622	0.146075
35	6	0	4.586172	3.138826	-1.219941
36	6	0	4.392118	2.014097	-2.020404
37	6	0	3.921673	0.797402	-1.512673
38	6	0	-3.774938	0.827929	1.573727
39	6	0	-4.306921	2.004259	2.112850
40	6	0	-4.665683	3.094372	1.321030
41	6	0	-4.480101	2.979812	-0.058132
42	6	0	-3.946459	1.832517	-0.655465
43	6	0	-3.477365	-0.328094	2.529306
44	6	0	-4.773500	-0.872808	3.162771
45	6	0	-2.451217	0.059183	3.610941
46	6	0	-5.240195	4.357992	1.947804
47	6	0	-6.672334	4.644559	1.458338
48	6	0	-4.325005	5.576187	1.720726
49	6	0	-3.807689	1.814848	-2.179866
50	6	0	-3.067862	3.050245	-2.727560
51	6	0	-5.187281	1.680544	-2.858175
52	6	0	3.818612	-0.390267	-2.469432
53	6	0	5.223838	-0.860065	-2.899298
54	6	0	2.935018	-0.091459	-3.694948
55	6	0	3.686567	1.776740	2.243475
56	6	0	2.889474	2.962994	2.822656
57	6	0	5.066627	1.701914	2.932121
58	6	0	5.080236	4.448902	-1.818581
59	6	0	4.039879	5.574671	-1.664724
60	6	0	6.442940	4.870665	-1.237108
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62	1	0	-0.515805	-5.695134	-1.034417
63	1	0	0.047647	-5.326970	-2.649648
64	1	0	1.496615	-4.367487	-0.814741
65	1	0	0.930335	-3.166724	-1.965071
66	1	0	-0.980279	-3.147965	1.889122
67	1	0	-1.532200	-4.347312	0.733187
68	1	0	-0.165467	-5.347046	2.578630
69	1	0	0.508140	-5.667101	0.994296
70	1	0	-5.269794	-2.861781	-2.863526
71	1	0	-4.515503	-4.998606	-3.886635
72	1	0	-2.247104	-5.869524	-3.361455
73	1	0	4.816002	-0.974333	1.632159
74	1	0	2.046209	-5.797553	3.515012
75	1	0	4.254839	-4.882865	4.200732
76	1	0	5.077170	-2.777943	3.163804
77	1	0	1.523854	2.067824	0.391840
78	1	0	4.490027	3.865760	0.795606
79	1	0	4.617480	2.086682	-3.081659
80	1	0	-4.456057	2.070072	3.188500
81	1	0	-4.756712	3.814126	-0.697015
82	1	0	-3.042684	-1.149365	1.953002
83	1	0	-5.485489	-1.193379	2.393992
84	1	0	-4.554815	-1.734674	3.805331
85	1	0	-5.268672	-0.113942	3.779906
86	1	0	-1.522822	0.419243	3.157982
87	1	0	-2.214182	-0.808456	4.239359

88	1	0	-2.836346	0.846180	4.270124
89	1	0	-6.692410	4.844039	0.380350
90	1	0	-7.086895	5.523535	1.966827
91	1	0	-7.334650	3.793640	1.652099
92	1	0	-3.315739	5.388833	2.103068
93	1	0	-4.237735	5.814124	0.654021
94	1	0	-4.725463	6.461988	2.228825
95	1	0	-3.207670	0.944707	-2.456480
96	1	0	-2.081654	3.143833	-2.268942
97	1	0	-2.930144	2.946715	-3.810848
98	1	0	-3.630333	3.976573	-2.558822
99	1	0	-5.725288	0.785799	-2.525617
100	1	0	-5.074921	1.621989	-3.947747
101	1	0	-5.822450	2.546289	-2.633766
102	1	0	3.358328	-1.223893	-1.933606
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104	1	0	5.150188	-1.742800	-3.545848
105	1	0	5.753572	-0.079687	-3.458423
106	1	0	1.936899	0.237703	-3.392655
107	1	0	2.827557	-0.993889	-4.308834
108	1	0	3.373537	0.685065	-4.332915
109	1	0	3.134987	0.868971	2.500385
110	1	0	1.882290	3.028265	2.401331
111	1	0	2.782253	2.836541	3.906186
112	1	0	3.393669	3.922049	2.658250
113	1	0	5.661189	0.856453	2.570629
114	1	0	4.948974	1.595752	4.017155
115	1	0	5.646831	2.613344	2.744500
116	1	0	3.860712	5.809927	-0.608746
117	1	0	4.388553	6.491405	-2.154865
118	1	0	3.080662	5.292380	-2.111909
119	1	0	6.371840	5.078980	-0.162881
120	1	0	7.194125	4.085488	-1.376135
121	1	0	6.805669	5.781456	-1.728085
122	1	0	5.221288	4.276666	-2.894260
123	1	0	-5.292781	4.184452	3.031628

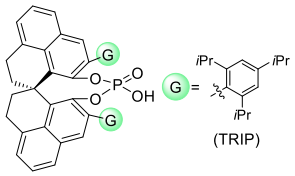
DFT calculation for all conformations of real system using SPHENOL-derived CPA (*S*)-1ca

TS	Orientation I	Orientation II	$G^{\neq}$ (a.u.)	$\Delta\Delta G^{\neq}$ (kcal/mmol)
R-anti	up	up		
	up	down	-3428.311328	-2.30
	down	up		
	down	down	-3428.310477	-1.76
S-anti	up	up	-3428.301208	4.05
	up	down	-3428.302572	3.20
	down	up	-3428.298938	5.48
	down	down	-3428.299655	5.03
S-syn	up	up	-3428.305496	1.36
	up	down	-3428.305311	1.48
	down	down	-3428.30585	1.14
	down	up	-3428.305498	1.36

TS	Orientation I	Orientation II	$G^{\neq}$ (a.u.)	$\Delta\Delta G^{\neq}$ (kcal/mmol)
R-re	up	up	-3428.307665	0.00
	up	down	-3428.307105	0.35
	down	up	-3428.306828	0.53
	down	down	-3428.306622	0.65
S-si	up	up	-3428.303409	2.67
	up	down		
	down	up	-3428.303673	2.51
	down	down		
S-re	up	up	-3428.30801	-0.22
	up	down		
	down	up		
	down	down		

* Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using SPHENOL-derived CPA (*S*)-1ca



(TRIP)

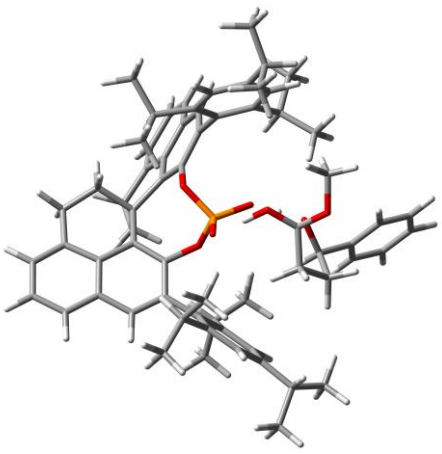
(*S*)-**1ca** (SPHENOL)

1st / 2nd	$\Delta\Delta G^{\neq}$ (kcal/mol)
R-anti* / *R-re	-2.30 / **0.00**
R-syn / *R-si*	-- / --
S-anti* / *S-si	**3.20** / 2.51
S-syn* / *S-re	**1.14** / -0.22

$\Delta\Delta G^{\neq}$ of RDS = **1.14** kcal/mol

B3LYP/6-31G(d); E(RB3LYP) = -3429.49279510 Hartree
Zero-point correction= 1.289302 Hartree
Thermal correction to Energy= 1.360115 Hartree
Thermal correction to Enthalpy= 1.361060 Hartree
Thermal correction to Gibbs Free Energy= 1.181467 Hartree
Sum of electronic and zero-point Energies= -3428.203494 Hartree
Sum of electronic and thermal Energies= -3428.132680 Hartree
Sum of electronic and thermal Enthalpies= -3428.131736 Hartree
Sum of electronic and thermal Free Energies= -3428.311328 Hartree
The number of Imaginary frequencies = 1

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1ca (SPHENOL)



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4	6	0	2.688847	2.127905	-0.670298
5	6	0	3.181138	3.231958	-1.323817
6	6	0	2.427484	4.418521	-1.465350
7	6	0	0.465551	5.777320	-0.944016
8	6	0	-0.840453	5.998794	-0.230714
9	6	0	-1.538040	4.687702	0.096731
10	6	0	-0.621227	3.638531	0.807521
11	6	0	0.050024	4.200570	2.102347
12	6	0	-0.934836	4.799929	3.095972
13	6	0	-2.114206	3.897941	3.348733
14	6	0	-2.445389	2.858562	2.422783
15	6	0	-1.658704	2.559859	1.239897
16	6	0	2.964487	5.508611	-2.197653

17	6	0	2.268231	6.686969	-2.315064
18	6	0	1.018276	6.810933	-1.678202
19	6	0	-3.632291	2.099048	2.690515
20	6	0	-4.045823	1.105019	1.774455
21	6	0	-3.288561	0.757684	0.681781
22	6	0	-2.072495	1.484215	0.469840
23	6	0	-2.892013	4.107156	4.473595
24	6	0	-4.044617	3.341613	4.734866
25	6	0	-4.411681	2.359452	3.846700
26	6	0	3.552193	0.905798	-0.542358
27	6	0	-3.779146	-0.308374	-0.256038
28	6	0	-4.004146	-1.630281	0.210105
29	6	0	-4.534344	-2.576764	-0.676963
30	6	0	-4.855334	-2.275669	-1.999911
31	6	0	-4.638564	-0.966159	-2.432566
32	6	0	-4.116178	0.022931	-1.594549
33	6	0	4.032816	0.506785	0.728588
34	6	0	4.915460	-0.578060	0.820169
35	6	0	5.354054	-1.279521	-0.303100
36	6	0	4.866209	-0.868738	-1.547550
37	6	0	3.983801	0.206438	-1.701995
38	6	0	3.699416	1.262850	2.015859
39	6	0	4.954391	1.947605	2.594861
40	6	0	3.022953	0.364241	3.067937
41	6	0	6.387572	-2.400481	-0.232560
42	6	0	6.423220	-3.149957	1.108096
43	6	0	7.791288	-1.858129	-0.576942
44	6	0	3.576316	0.601462	-3.125504
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46	6	0	4.773528	1.205197	-3.890502
47	6	0	-4.007214	1.441793	-2.155498
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49	6	0	-3.099652	1.511977	-3.397935
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51	6	0	-2.889715	-3.360159	1.740114
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53	6	0	-5.458135	-3.331807	-2.917159
54	6	0	-6.936761	-3.028466	-3.229284
55	6	0	-4.651174	-3.514253	-4.215531
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57	1	0	-0.656520	6.565384	0.693886
58	1	0	-1.500752	6.629958	-0.838783
59	1	0	-2.419124	4.883929	0.713507
60	1	0	-1.901498	4.223435	-0.828288
61	1	0	0.590358	3.368791	2.570518
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67	1	0	0.469186	7.746965	-1.756558
68	1	0	-4.991676	0.603120	1.950316
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74	1	0	5.286724	-0.859058	1.801130
75	1	0	5.204628	-1.398733	-2.435937
76	1	0	2.992643	2.059616	1.774181
77	1	0	5.411014	2.621413	1.861367
78	1	0	4.693698	2.537164	3.482297
79	1	0	5.713707	1.215011	2.893092
80	1	0	2.104117	-0.077925	2.671009
81	1	0	2.759984	0.950622	3.956874
82	1	0	3.687969	-0.444522	3.396292
83	1	0	6.792413	-2.510641	1.918688
84	1	0	7.099074	-4.009965	1.041660
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86	1	0	7.800562	-1.371395	-1.557863
87	1	0	8.111146	-1.117512	0.165937
88	1	0	8.530643	-2.668310	-0.589771
89	1	0	2.800464	1.366839	-3.056261
90	1	0	2.069197	-0.938408	-3.454676
91	1	0	2.698495	-0.209593	-4.937701
92	1	0	3.681255	-1.388341	-4.064510
93	1	0	5.217184	2.053876	-3.358720
94	1	0	4.458015	1.554076	-4.881213
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98	1	0	-5.319205	3.062080	-2.801816
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100	1	0	-2.103401	1.118653	-3.177693
101	1	0	-2.992566	2.551787	-3.731067
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103	1	0	-3.168068	-1.289731	2.150989
104	1	0	-1.946211	-3.255917	1.202081
105	1	0	-2.654654	-3.580099	2.788322
106	1	0	-3.422027	-4.231875	1.339553
107	1	0	-5.686286	-1.386030	2.416458
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123	6	0	1.547976	-3.487360	0.816677
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125	6	0	2.075957	-3.536171	-1.549967
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128	1	0	3.537216	-3.927394	0.035850
129	1	0	2.471390	-4.080460	-2.412267
130	1	0	2.385112	-2.490135	-1.621602
131	8	0	-0.160458	-2.715424	-2.248176
132	8	0	0.127892	-4.868465	-1.723994
133	6	0	-1.288833	-5.057008	-1.897167
134	1	0	-1.439557	-6.136562	-1.855884
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136	1	0	-1.844908	-4.563487	-1.096328
137	6	0	1.311384	-4.301368	2.067373
138	6	0	1.815796	-3.861439	3.294810
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140	6	0	1.640579	-4.627463	4.449628
141	1	0	2.342427	-2.911434	3.349450
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144	6	0	0.948081	-5.836291	4.386777
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148	1	0	-0.078326	-2.215847	0.302389
149	1	0	0.157455	-1.761696	-2.100454
150	1	0	-5.427847	-4.286386	-2.373066
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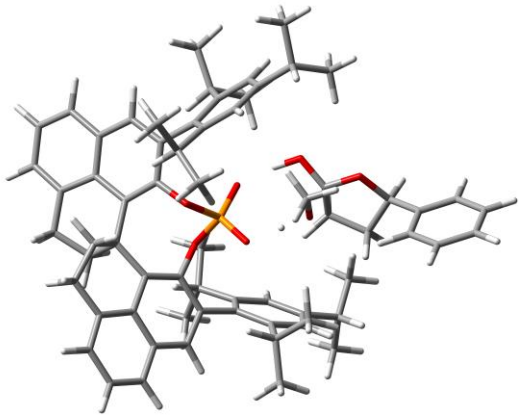
TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1ca (SPHENOL)



B3LYP/6-31G(d); E(RB3LYP) = -3429.48594863

Zero-point correction= 1.290558 (Hartree/Particle)

Thermal correction to Energy= 1.361343

Thermal correction to Enthalpy= 1.362287

Thermal correction to Gibbs Free Energy= 1.183242

Sum of electronic and zero-point Energies= -3428.200349

Sum of electronic and thermal Energies= -3428.129564

Sum of electronic and thermal Enthalpies= -3428.128620

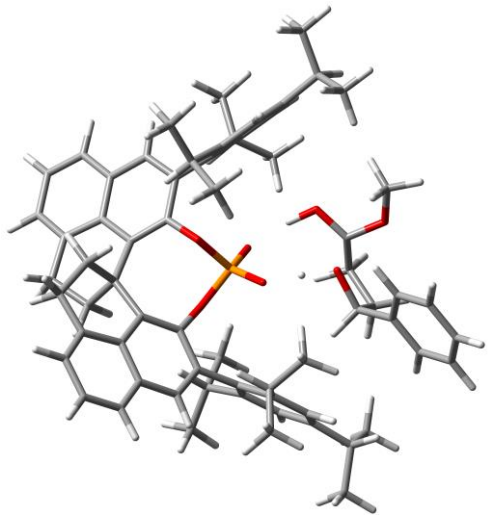
Sum of electronic and thermal Free Energies= -3428.307665

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.446748	-2.642314	-1.998650
2	6	0	3.009279	-1.710322	-0.973710
3	6	0	1.842859	-2.031837	-0.297275
4	6	0	1.139450	-3.271716	-0.442875
5	6	0	1.625734	-4.170490	-1.360719
6	6	0	2.731866	-3.871267	-2.188793
7	6	0	4.582552	-2.413414	-2.838264
8	6	0	5.432705	-1.182431	-2.660599
9	6	0	4.723763	-0.094401	-1.866305
10	6	0	4.036062	-0.611593	-0.561900
11	6	0	5.009862	-1.423964	0.354819
12	6	0	6.282041	-0.676720	0.722782
13	6	0	5.989284	0.699860	1.253700
14	6	0	4.746165	1.340034	0.948385
15	6	0	3.686445	0.714124	0.177432
16	6	0	3.136584	-4.797476	-3.183773
17	6	0	4.215910	-4.533132	-3.992187
18	6	0	4.931601	-3.334488	-3.810117
19	6	0	4.576515	2.684710	1.419607
20	6	0	3.398282	3.394141	1.097638
21	6	0	2.364657	2.816512	0.400505
22	6	0	2.540360	1.464207	-0.037989
23	6	0	6.946342	1.348313	2.012944
24	6	0	6.756512	2.660184	2.488409
25	6	0	5.589623	3.318272	2.184746
26	6	0	-0.066089	-3.623447	0.381393
27	6	0	1.124219	3.614028	0.121817
28	6	0	0.330742	4.097840	1.197916
29	6	0	-0.797623	4.871999	0.908804
30	6	0	-1.184799	5.182059	-0.396094
31	6	0	-0.376518	4.717680	-1.434670
32	6	0	0.774403	3.952291	-1.207871
33	6	0	0.046309	-3.764228	1.789274
34	6	0	-1.075713	-4.147465	2.529936
35	6	0	-2.311455	-4.411072	1.935291
36	6	0	-2.397635	-4.283757	0.549046
37	6	0	-1.309064	-3.901124	-0.247051
38	6	0	1.366945	-3.588352	2.540210
39	6	0	1.858714	-4.934802	3.109928
40	6	0	1.275197	-2.518061	3.643969
41	6	0	-3.513472	-4.863884	2.754418
42	6	0	-3.881527	-3.861587	3.863739
43	6	0	-3.297587	-6.273033	3.340287
44	6	0	-1.519917	-3.852234	-1.763598
45	6	0	-2.736108	-3.006710	-2.183689
46	6	0	-1.657211	-5.274548	-2.347862
47	6	0	1.647379	3.589654	-2.410194
48	6	0	2.287928	4.853707	-3.019657
49	6	0	0.885190	2.786398	-3.480035
50	6	0	0.661625	3.849368	2.673919
51	6	0	-0.504788	3.232868	3.469664
52	6	0	1.131351	5.153080	3.353901
53	6	0	-2.416098	6.030040	-0.688425
54	6	0	-3.675521	5.526501	0.040350
55	6	0	-2.156370	7.516271	-0.370981
56	1	0	1.144488	-5.137025	-1.471266
57	1	0	6.367395	-1.463123	-2.153860
58	1	0	5.734950	-0.790262	-3.640094
59	1	0	5.433821	0.699887	-1.617910
60	1	0	3.940584	0.366404	-2.480286
61	1	0	4.456215	-1.678671	1.267044
62	1	0	5.266946	-2.370556	-0.127588
63	1	0	6.851415	-1.253762	1.462448
64	1	0	6.936082	-0.595300	-0.157676
65	1	0	2.566932	-5.716576	-3.296949
66	1	0	4.518219	-5.236554	-4.763214
67	1	0	5.788677	-3.122345	-4.446081
68	1	0	3.312073	4.427297	1.420308
69	1	0	7.873164	0.825918	2.241003
70	1	0	7.527905	3.141574	3.083275
71	1	0	5.417079	4.335311	2.528003
72	1	0	-1.401600	5.234507	1.735780
73	1	0	-0.641156	4.979877	-2.457380
74	1	0	-0.972049	-4.260206	3.606147
75	1	0	-3.347364	-4.505338	0.066994
76	1	0	2.126508	-3.254614	1.829879
77	1	0	1.969505	-5.684286	2.318128
78	1	0	2.832499	-4.810231	3.599243
79	1	0	1.161111	-5.336583	3.854405
80	1	0	0.944332	-1.559978	3.233792
81	1	0	2.256847	-2.371122	4.110939
82	1	0	0.577437	-2.813427	4.437079
83	1	0	-3.078237	-3.769540	4.603870
84	1	0	-4.784966	-4.185871	4.394149
85	1	0	-4.067179	-2.862788	3.452424
86	1	0	-3.077948	-6.999432	2.550393
87	1	0	-2.457794	-6.283104	4.045185
88	1	0	-4.191077	-6.611958	3.878763
89	1	0	-0.642627	-3.383177	-2.214340
90	1	0	-2.656180	-1.985428	-1.806984
91	1	0	-2.794893	-2.959926	-3.278137
92	1	0	-3.680670	-3.436455	-1.828125
93	1	0	-0.799575	-5.908199	-2.099028
94	1	0	-1.742802	-5.234586	-3.440714
95	1	0	-2.553910	-5.773286	-1.960237
96	1	0	2.468590	2.959257	-2.060831
97	1	0	2.871083	5.401675	-2.271133
98	1	0	2.959494	4.584732	-3.844361
99	1	0	1.528451	5.537720	-3.416688
100	1	0	0.471542	1.866981	-3.055693
101	1	0	1.560403	2.509112	-4.298959
102	1	0	0.065158	3.369321	-3.917312
103	1	0	1.483841	3.132423	2.724516
104	1	0	-0.785323	2.262434	3.056753
105	1	0	-0.199648	3.082758	4.512789
106	1	0	-1.389977	3.879377	3.477104

107	1	0	1.981986	5.605548	2.832066
108	1	0	1.433813	4.958370	4.390126
109	1	0	0.327895	5.899361	3.375504
110	1	0	-3.589590	5.660968	1.125055
111	1	0	-4.557334	6.088912	-0.289955
112	1	0	-3.852178	4.462079	-0.143409
113	1	0	-1.952443	7.657991	0.697258
114	1	0	-1.292914	7.896316	-0.928162
115	1	0	-3.028509	8.128952	-0.630807
116	8	0	1.302142	-1.146903	0.634980
117	8	0	1.492751	0.919469	-0.780583
118	15	0	0.372869	0.055789	0.041487
119	8	0	-0.208402	0.781295	1.225599
120	8	0	-0.586829	-0.449069	-1.032175
121	1	0	-1.839695	0.060718	-1.063656
122	6	0	-3.336435	0.975744	0.438631
123	8	0	-4.593046	1.437983	0.246832
124	8	0	-2.856354	0.476866	-1.128052
125	6	0	-5.589724	0.413689	0.586100
126	6	0	-4.773337	-0.879613	0.782147
127	6	0	-3.388478	-0.356862	1.174680
128	1	0	-6.020629	0.737213	1.540597
129	1	0	-4.718803	-1.445075	-0.151154
130	1	0	-5.224982	-1.523173	1.541640
131	1	0	-2.565042	-1.024106	0.919821
132	1	0	-3.323741	-0.128590	2.244631
133	8	0	-2.504546	1.939183	0.785322
134	6	0	-2.836378	1.558614	-2.086296
135	1	0	-3.860443	1.909366	-2.216770
136	1	0	-2.451478	1.149201	-3.022588
137	1	0	-2.196590	2.372085	-1.735219
138	1	0	-1.586047	1.554158	0.990858
139	6	0	-6.678394	0.369728	-0.458060
140	6	0	-7.999991	0.651793	-0.098889
141	6	0	-6.393081	0.034668	-1.789697
142	6	0	-9.024382	0.593181	-1.046224
143	1	0	-8.230235	0.920992	0.929529
144	6	0	-7.412331	-0.015579	-2.738404
145	1	0	-5.369892	-0.185253	-2.080961
146	6	0	-8.731676	0.261044	-2.368523
147	1	0	-10.046750	0.812713	-0.750899
148	1	0	-7.178658	-0.273828	-3.767803
149	1	0	-9.525584	0.218404	-3.109236
150	1	0	-2.606960	5.955231	-1.768462
151	1	0	-4.368731	-4.922911	2.066672

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1ca (SPHENOL)

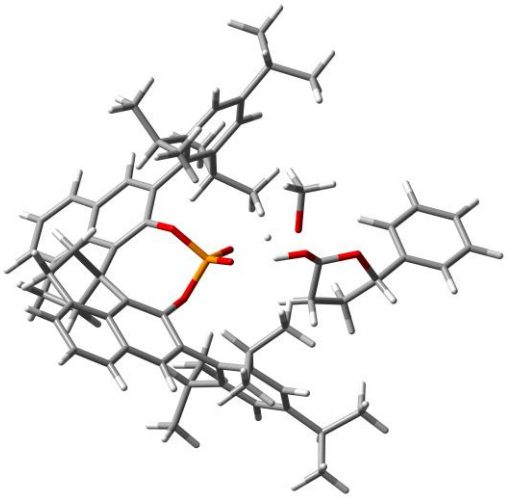


B3LYP/6-31G(d); E(RB3LYP) = -3429.48406763 Hartree
Zero-point correction= 1.289509 Hartree
Thermal correction to Energy= 1.360308 Hartree
Thermal correction to Enthalpy= 1.361252 Hartree
Thermal correction to Gibbs Free Energy= 1.181496 Hartree
Sum of electronic and zero-point Energies= -3428.194558 Hartree
Sum of electronic and thermal Energies= -3428.123759 Hartree
Sum of electronic and thermal Enthalpies= -3428.122815 Hartree
Sum of electronic and thermal Free Energies= -3428.302572 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697916	-4.193685	1.808519
2	6	0	-0.967401	-3.168487	0.812383
3	6	0	0.132142	-2.569005	0.212241
4	6	0	1.487343	-2.970924	0.443647
5	6	0	1.703961	-3.992062	1.337807
6	6	0	0.655534	-4.588842	2.068533
7	6	0	-1.718754	-4.879300	2.541779
8	6	0	-3.171512	-4.600561	2.270674
9	6	0	-3.374133	-3.274459	1.556685
10	6	0	-2.440912	-3.065550	0.317490
11	6	0	-2.512803	-4.242285	-0.710648
12	6	0	-3.923966	-4.583944	-1.163461
13	6	0	-4.710072	-3.361563	-1.554182
14	6	0	-4.296341	-2.061759	-1.121787
15	6	0	-3.092201	-1.816262	-0.345578
16	6	0	0.953542	-5.583991	3.034997
17	6	0	-0.050482	-6.193517	3.746577
18	6	0	-1.386402	-5.832481	3.487681
19	6	0	-5.150309	-0.962809	-1.464568
20	6	0	-4.822860	0.335967	-1.018643
21	6	0	-3.652012	0.611109	-0.353558
22	6	0	-2.792222	-0.494770	-0.050502
23	6	0	-5.857731	-3.517231	-2.311104
24	6	0	-6.677431	-2.425634	-2.655510
25	6	0	-6.329673	-1.168018	-2.225748
26	6	0	2.681422	-2.360044	-0.229505
27	6	0	-3.361600	2.032856	0.031128
28	6	0	-3.293444	3.040120	-0.970586
29	6	0	-3.117678	4.371109	-0.573448
30	6	0	-3.023915	4.756685	0.763935
31	6	0	-3.105642	3.752659	1.729757
32	6	0	-3.274567	2.404785	1.397137
33	6	0	2.871912	-2.484046	-1.627786
34	6	0	4.056795	-2.006905	-2.202355
35	6	0	5.071849	-1.420322	-1.445021
36	6	0	4.861846	-1.304166	-0.067881
37	6	0	3.700167	-1.764838	0.564325
38	6	0	1.876330	-3.201162	-2.540675
39	6	0	2.487210	-4.495226	-3.116529
40	6	0	1.350148	-2.287839	-3.663683
41	6	0	6.410461	-1.002739	-2.045580
42	6	0	6.312420	-0.415308	-3.462508
43	6	0	7.400207	-2.186915	-2.023087
44	6	0	3.622244	-1.636283	2.090766
45	6	0	3.711464	-0.180829	2.581485
46	6	0	4.704271	-2.497100	2.775650
47	6	0	-3.443052	1.407785	2.544889
48	6	0	-4.739581	1.685634	3.332978
49	6	0	-2.219484	1.382497	3.479968
50	6	0	-3.464230	2.767005	-2.470996
51	6	0	-2.295072	3.275340	-3.335556
52	6	0	-4.789853	3.369716	-2.984926
53	6	0	-2.920180	6.232154	1.132792
54	6	0	-4.311273	6.808990	1.467809
55	6	0	-1.929953	6.515178	2.275064

56	1	0	2.716947	-4.344610	1.506267
57	1	0	-3.587967	-5.418687	1.665359
58	1	0	-3.739792	-4.608494	3.209518
59	1	0	-4.419373	-3.179959	1.251121
60	1	0	-3.175395	-2.447060	2.248924
61	1	0	-1.906090	-3.947572	-1.575617
62	1	0	-2.039754	-5.132246	-0.286524
63	1	0	-3.884063	-5.291223	-2.001718
64	1	0	-4.456600	-5.109893	-0.357926
65	1	0	1.995381	-5.845657	3.202257
66	1	0	0.176040	-6.946766	4.496140
67	1	0	-2.187833	-6.319052	4.039798
68	1	0	-5.517683	1.142997	-1.227909
69	1	0	-6.132833	-4.516967	-2.640999
70	1	0	-7.573187	-2.582491	-3.250181
71	1	0	-6.945482	-0.305245	-2.467159
72	1	0	-3.064955	5.142057	-1.339442
73	1	0	-3.057766	4.022795	2.781073
74	1	0	4.194936	-2.127691	-3.272918
75	1	0	5.644490	-0.853986	0.539894
76	1	0	1.015097	-3.502476	-1.940782
77	1	0	2.825913	-5.164033	-2.317234
78	1	0	1.744091	-5.032871	-3.717963
79	1	0	3.347669	-4.284575	-3.762568
80	1	0	0.869872	-1.395571	-3.252124
81	1	0	0.609071	-2.822566	-4.270290
82	1	0	2.155834	-1.969651	-4.336742
83	1	0	5.989003	-1.166584	-4.192122
84	1	0	7.292141	-0.048008	-3.789156
85	1	0	5.605333	0.420505	-3.510073
86	1	0	7.524640	-2.579725	-1.008390
87	1	0	7.037778	-3.005930	-2.655932
88	1	0	8.385380	-1.880267	-2.395589
89	1	0	2.650614	-2.010662	2.416741
90	1	0	2.879439	0.409327	2.189871
91	1	0	3.654572	-0.153707	3.676623
92	1	0	4.651159	0.300786	2.290334
93	1	0	4.651898	-3.546238	2.463335
94	1	0	4.586112	-2.461431	3.865315
95	1	0	5.712149	-2.135395	2.539531
96	1	0	-3.545498	0.406376	2.121614
97	1	0	-5.616239	1.660054	2.675890
98	1	0	-4.879785	0.931321	4.117052
99	1	0	-4.714982	2.668642	3.817963
100	1	0	-1.305556	1.157981	2.923039
101	1	0	-2.347835	0.613860	4.252128
102	1	0	-2.083443	2.342414	3.992916
103	1	0	-3.509678	1.686638	-2.621079
104	1	0	-1.369890	2.751242	-3.091858
105	1	0	-2.515322	3.093028	-4.394635
106	1	0	-2.124167	4.351053	-3.213850
107	1	0	-5.652279	3.024038	-2.404340
108	1	0	-4.954621	3.094937	-4.033912
109	1	0	-4.776332	4.464720	-2.925706
110	1	0	-4.734272	6.314730	2.350732
111	1	0	-4.249506	7.883897	1.678551
112	1	0	-5.010286	6.662347	0.637380
113	1	0	-2.275183	6.090766	3.224924
114	1	0	-0.941180	6.093667	2.064065
115	1	0	-1.817251	7.595573	2.423915
116	8	0	-0.047638	-1.576758	-0.753736
117	8	0	-1.612371	-0.181850	0.634540
118	15	0	-0.277836	-0.030737	-0.294049
119	8	0	-0.502258	0.772700	-1.548239
120	8	0	0.823465	0.453857	0.656159
121	1	0	1.458347	1.527708	0.353258
122	6	0	1.406279	3.374848	-1.138521
123	8	0	2.087211	2.468605	0.104578
124	6	0	3.440353	2.118650	-0.293369
125	6	0	3.571883	2.517054	-1.792125
126	6	0	2.138900	2.706959	-2.288843
127	1	0	3.510309	1.030737	-0.197488
128	1	0	4.131378	3.451273	-1.884708
129	1	0	4.099540	1.743337	-2.355231
130	1	0	2.077935	3.342583	-3.176608
131	1	0	1.646497	1.754415	-2.501927
132	8	0	0.094359	3.258637	-0.997384
133	8	0	1.868365	4.626409	-0.938650
134	6	0	1.190257	5.417382	0.050206
135	1	0	1.757973	6.346382	0.113453
136	1	0	0.160661	5.614902	-0.254457
137	1	0	1.196096	4.906730	1.017347
138	1	0	-0.218243	2.332669	-1.259049
139	6	0	4.467913	2.777729	0.608869
140	6	0	4.107137	3.430305	1.791772
141	6	0	5.826039	2.704494	0.266558
142	6	0	5.081438	4.006900	2.609545
143	1	0	3.060756	3.480647	2.070848
144	6	0	6.799755	3.275621	1.085634
145	1	0	6.127283	2.199157	-0.648083
146	6	0	6.429950	3.932630	2.260983
147	1	0	4.782505	4.512788	3.524005
148	1	0	7.847285	3.209379	0.803352
149	1	0	7.187029	4.380410	2.899051
150	1	0	-2.554818	6.760945	0.240788
151	1	0	6.825406	-0.222091	-1.391492

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1ca (SPHENOL)



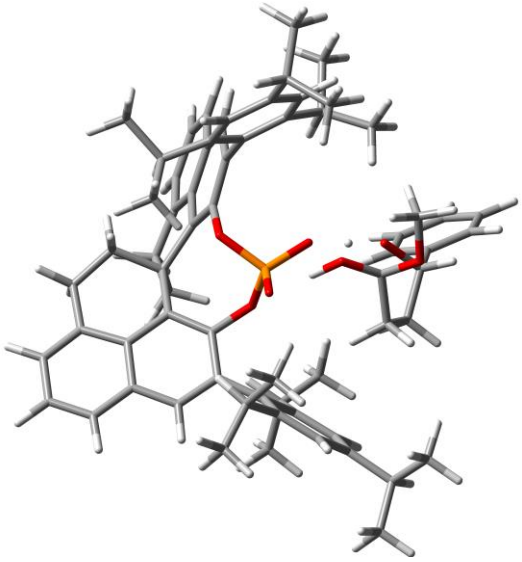
B3LYP/6-31G(d); E(RB3LYP) = -3429.48666090 Hartree
Zero-point correction= 1.290901 Hartree
Thermal correction to Energy= 1.361621 Hartree
Thermal correction to Enthalpy= 1.362565 Hartree
Thermal correction to Gibbs Free Energy= 1.182988 Hartree
Sum of electronic and zero-point Energies= -3428.195760 Hartree
Sum of electronic and thermal Energies= -3428.125040 Hartree
Sum of electronic and thermal Enthalpies= -3428.124096 Hartree
Sum of electronic and thermal Free Energies= -3428.303673 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.724011	-2.347393	1.872492
2	6	0	-3.152569	-1.517508	0.826885
3	6	0	-1.994555	-1.977113	0.214132
4	6	0	-1.390073	-3.245364	0.493026

5	6	0	-1.975072	-4.023257	1.464772	74	1	0	0.738671	-5.015002	-3.277312
6	6	0	-3.099998	-3.595741	2.200821	75	1	0	2.847856	-5.198454	0.430969
7	6	0	-4.915011	-2.013314	2.593515	76	1	0	-2.240188	-3.309153	-1.850926
8	6	0	-5.694020	-0.777860	2.236923	77	1	0	-2.421730	-5.774863	-2.113392
9	6	0	-4.834901	0.237784	1.502134	78	1	0	-3.073682	-4.905668	-3.516523
10	6	0	-4.037424	-0.353953	0.292315	79	1	0	-1.492130	-5.693735	-3.618141
11	6	0	-4.953002	-1.089701	-0.739356	80	1	0	-0.760156	-1.936473	-3.301605
12	6	0	-6.126650	-0.253958	-1.228588	81	1	0	-2.086994	-2.667201	-4.221841
13	6	0	-5.713319	1.138084	-1.627452	82	1	0	-0.458202	-3.343759	-4.343550
14	6	0	-4.469103	1.685274	-1.179677	83	1	0	3.431810	-7.402957	-0.578343
15	6	0	-3.506602	0.945013	-0.383479	84	1	0	3.896703	-7.989948	-2.183545
16	6	0	-3.620752	-4.421931	3.230449	85	1	0	2.184939	-7.938854	-1.714394
17	6	0	-4.739812	-4.046796	3.932562	86	1	0	4.346959	-4.270268	-2.589532
18	6	0	-5.383040	-2.838916	3.599433	87	1	0	4.746465	-5.152128	-1.104322
19	6	0	-4.193367	3.047075	-1.530662	88	1	0	5.161367	-5.841899	-2.679575
20	6	0	-3.010017	3.658147	-1.061259	89	1	0	0.291876	-3.318594	2.349732
21	6	0	-2.043361	2.960535	-0.376706	90	1	0	2.391533	-2.145328	1.827511
22	6	0	-2.310709	1.582638	-0.085852	91	1	0	2.477457	-2.938627	3.405060
23	6	0	-6.569724	1.893939	-2.408118	92	1	0	3.318728	-3.650327	2.024083
24	6	0	-6.277592	3.225463	-2.760887	93	1	0	0.233294	-5.830484	2.649024
25	6	0	-5.108848	3.794102	-2.315532	94	1	0	1.193716	-5.017760	3.897572
26	6	0	-0.197866	-3.807496	-0.228181	95	1	0	1.996294	-5.863468	2.565489
27	6	0	-0.811151	3.697332	0.068901	96	1	0	-2.207042	2.687307	2.092804
28	6	0	0.008810	4.362026	-0.886786	97	1	0	-2.702207	5.046247	2.699042
29	6	0	1.059305	5.170070	-0.433912	98	1	0	-2.790742	3.965202	4.103678
30	6	0	1.346113	5.345265	0.922088	99	1	0	-1.390910	5.027194	3.888438
31	6	0	0.542912	4.668022	1.839313	100	1	0	-0.185326	1.510496	2.925473
32	6	0	-0.535312	3.863268	1.450071	101	1	0	-1.302245	1.906113	4.243674
33	6	0	-0.268044	-4.109200	-1.610675	102	1	0	0.166630	2.864562	4.022278
34	6	0	0.803447	-4.777156	-2.217847	103	1	0	-0.957105	3.505547	-2.596379
35	6	0	1.930826	-5.191216	-1.510249	104	1	0	1.483298	2.948081	-2.806839
36	6	0	1.982289	-4.883466	-0.147496	105	1	0	0.818885	3.748385	-4.236851
37	6	0	0.956063	-4.194765	0.510360	106	1	0	1.834836	4.655563	-3.114671
38	6	0	-1.499322	-3.818664	-2.469758	107	1	0	-1.665551	5.943984	-2.470710
39	6	0	-2.156967	-5.126436	-2.956249	108	1	0	-0.954765	5.520567	-4.037695
40	6	0	-1.175678	-2.885617	-3.651809	109	1	0	-0.006176	6.416566	-2.840842
41	6	0	3.037040	-5.981488	-2.198626	110	1	0	3.783637	6.166689	-0.331806
42	6	0	3.142202	-7.412288	-1.635952	111	1	0	4.572159	6.686552	1.162645
43	6	0	4.400009	-5.267496	-2.138435	112	1	0	4.133976	4.983350	0.938577
44	6	0	1.134217	-3.924344	2.009664	113	1	0	1.906408	7.983597	0.114248
45	6	0	2.408398	-3.117109	2.325040	114	1	0	1.076196	7.982645	1.677261
46	6	0	1.135548	-5.234990	2.824180	115	1	0	2.788306	8.444813	1.581769
47	6	0	-1.414881	3.278267	2.556479	116	8	0	-1.402601	-1.217886	-0.795419
48	6	0	-2.113418	4.396935	3.356699	117	8	0	-1.299030	0.891499	0.584743
49	6	0	-0.631976	2.334847	3.488582	118	15	0	-0.345612	-0.051232	-0.354839
50	6	0	-0.212579	4.280879	-2.401870	119	8	0	0.108734	0.635405	-1.613948
51	6	0	1.058699	3.882769	-3.175335	120	8	0	0.720587	-0.596550	0.592536
52	6	0	-0.745685	5.616085	-2.965350	121	1	0	2.004115	-0.620470	0.115818
53	6	0	2.440432	6.293159	1.398367	122	6	0	3.315826	0.946575	-0.898713
54	6	0	3.809323	6.013625	0.753365	123	8	0	4.654842	0.978088	-1.100598
55	6	0	2.027865	7.763116	1.181539	124	8	0	3.041733	-0.581875	-0.235568
56	1	0	-1.564213	-5.005109	1.676972	125	1	0	1.653005	0.886921	-1.891701
57	1	0	-6.555103	-1.060131	1.613619	126	6	0	5.339304	1.639922	0.015218
58	1	0	-6.118439	-0.322969	3.140909	127	6	0	4.252799	1.808990	1.096014
59	1	0	-5.458869	1.067832	1.161181	128	6	0	2.963725	1.856448	0.270834
60	1	0	-4.098347	0.664789	2.194037	129	1	0	5.641996	2.620648	-0.370061
61	1	0	-4.316769	-1.370701	-1.587254	130	1	0	4.249337	0.949223	1.771449
62	1	0	-5.323341	-2.022464	-0.303971	131	1	0	4.419427	2.708984	1.693690
63	1	0	-6.616146	-0.758055	-2.071658	132	1	0	2.071418	1.538186	0.809731
64	1	0	-6.890326	-0.187924	-0.439955	133	1	0	2.776043	2.854102	-0.139546
65	1	0	-3.110076	-5.356006	3.451079	134	8	0	2.655009	0.965021	-2.047332
66	1	0	-5.133053	-4.672613	4.729002	135	6	0	3.289022	-1.644814	-1.186182
67	1	0	-6.280576	-2.544875	4.139620	136	1	0	3.155759	-2.587170	-0.657745
68	1	0	-2.864087	4.714368	-1.259499	137	1	0	2.594261	-1.579116	-2.025845
69	1	0	-7.498427	1.442220	-2.750852	138	1	0	4.316181	-1.535477	-1.535400
70	1	0	-6.972959	3.791749	-3.374400	139	6	0	6.569454	0.863977	0.417441
71	1	0	-4.858907	4.822774	-2.563066	140	6	0	6.477657	-0.468628	0.844149
72	1	0	1.661990	5.693056	-1.171880	141	6	0	7.823602	1.481480	0.387718
73	1	0	0.740297	4.801270	2.900919	142	6	0	7.620448	-1.164297	1.233273

143	1	0	5.508482	-0.958721	0.867137
144	6	0	8.968874	0.788656	0.785957
145	1	0	7.906083	2.511872	0.049020
146	6	0	8.869234	-0.536653	1.207961
147	1	0	7.537805	-2.197769	1.559083
148	1	0	9.936181	1.282970	0.759269
149	1	0	9.758832	-1.080444	1.514144
150	1	0	2.759144	-6.065689	-3.258157
151	1	0	2.550192	6.140060	2.480961

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1ca (SPHENOL)

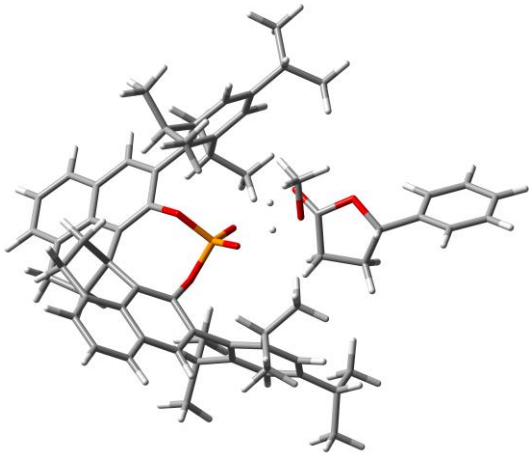


B3LYP/6-31G(d); E(RB3LYP) = -3429.48612444 Hartree
Zero-point correction= 1.289224 Hartree
Thermal correction to Energy= 1.360292 Hartree
Thermal correction to Enthalpy= 1.361236 Hartree
Thermal correction to Gibbs Free Energy= 1.180275 Hartree
Sum of electronic and zero-point Energies= -3428.196900 Hartree
Sum of electronic and thermal Energies= -3428.125833 Hartree
Sum of electronic and thermal Enthalpies= -3428.124888 Hartree
Sum of electronic and thermal Free Energies= -3428.305850 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.056970	4.038254	-0.939631
2	6	0	1.283626	3.048072	-0.212586
3	6	0	1.815811	1.768824	-0.130443
4	6	0	3.095434	1.394589	-0.651432
5	6	0	3.801945	2.352540	-1.338900
6	6	0	3.303445	3.658183	-1.538999
7	6	0	1.663718	5.407625	-1.080895
8	6	0	0.429328	5.910280	-0.386073
9	6	0	-0.549375	4.782014	-0.105675
10	6	0	0.082057	3.557331	0.636513
11	6	0	0.761222	3.955235	1.985658
12	6	0	-0.145671	4.748010	2.918220
13	6	0	-1.520200	4.142032	3.046117
14	6	0	-1.994929	3.201851	2.078007
15	6	0	-1.188569	2.722391	0.972019
16	6	0	4.064868	4.593496	-2.286777
17	6	0	3.631568	5.887447	-2.442086
18	6	0	2.429405	6.285793	-1.825357
19	6	0	-3.343695	2.736126	2.219133
20	6	0	-3.881968	1.855690	1.251878
21	6	0	-3.117048	1.321275	0.242565
22	6	0	-1.749746	1.743905	0.167765
23	6	0	-2.332384	4.530999	4.096670
24	6	0	-3.650471	4.054415	4.234315
25	6	0	-4.148876	3.178309	3.299804
26	6	0	3.745575	0.059138	-0.419610
27	6	0	-3.730779	0.379650	-0.754168
28	6	0	-4.330578	-0.837745	-0.327686
29	6	0	-4.931516	-1.666543	-1.281509
30	6	0	-4.968468	-1.348581	-2.640190
31	6	0	-4.396982	-0.139650	-3.032231
32	6	0	-3.789003	0.735667	-2.125637
33	6	0	4.180625	-0.288295	0.882830
34	6	0	4.911309	-1.469370	1.065088
35	6	0	5.252671	-2.310309	0.005770
36	6	0	4.818171	-1.946233	-1.271648
37	6	0	4.072294	-0.786231	-1.514353
38	6	0	3.983749	0.628032	2.091742
39	6	0	5.328781	1.241213	2.532936
40	6	0	3.286355	-0.076167	3.268710
41	6	0	6.120904	-3.541189	0.238204
42	6	0	7.515941	-3.366920	-0.394187
43	6	0	5.459237	-4.842124	-0.250853
44	6	0	3.695320	-0.466407	-2.964728
45	6	0	2.982302	-1.630862	-3.677974
46	6	0	4.937052	-0.049034	-3.781675
47	6	0	-3.288148	2.075779	-2.666559
48	6	0	-4.468077	2.948913	-3.141385
49	6	0	-2.240122	1.906395	-3.782413
50	6	0	-4.388959	-1.287502	1.135464
51	6	0	-3.932480	-2.744057	1.339991
52	6	0	-5.810512	-1.117106	1.713506
53	6	0	-5.614453	-2.274565	-3.662060
54	6	0	-4.890544	-3.632147	-3.741481
55	6	0	-7.119767	-2.466274	-3.397744
56	1	0	4.786398	2.110798	-1.726748
57	1	0	0.714667	6.402113	0.555644
58	1	0	-0.057798	6.685142	-0.991161
59	1	0	-1.396416	5.163265	0.469976
60	1	0	-0.958444	4.410120	-1.053213
61	1	0	1.076589	3.024560	2.472510
62	1	0	1.672356	4.527443	1.785170
63	1	0	0.321804	4.832720	3.907594
64	1	0	-0.243957	5.779365	2.549128
65	1	0	4.998461	4.260078	-2.733021
66	1	0	4.208897	6.601406	-3.023050
67	1	0	2.092027	7.315129	-1.926888
68	1	0	-4.932310	1.594022	1.322526
69	1	0	-1.938344	5.231232	4.830509
70	1	0	-4.263004	4.382136	5.069854
71	1	0	-5.165766	2.801306	3.375762
72	1	0	-5.386959	-2.594739	-0.946781
73	1	0	-4.437095	0.138106	-4.083119
74	1	0	5.258945	-1.723811	2.064149
75	1	0	5.081249	-2.577682	-2.116436
76	1	0	3.342034	1.459808	1.793393
77	1	0	5.802093	1.787935	1.709875
78	1	0	5.178234	1.941037	3.364120
79	1	0	6.030745	0.468550	2.868380
80	1	0	2.310248	-0.468824	2.968160
81	1	0	3.127730	0.629930	4.092962
82	1	0	3.882230	-0.908267	3.661907
83	1	0	7.446971	-3.278591	-1.484961
84	1	0	8.155968	-4.228341	-0.167604
85	1	0	8.010208	-2.464844	-0.017668
86	1	0	4.491205	-5.003250	0.236347
87	1	0	5.290747	-4.824687	-1.334066
88	1	0	6.097309	-5.706088	-0.029639
89	1	0	2.995525	0.372393	-2.954983
90	1	0	2.072206	-1.919917	-3.150458

91	1	0	2.697478	-1.323510	-4.691404
92	1	0	3.627508	-2.512367	-3.776194
93	1	0	5.461828	0.801410	-3.334295
94	1	0	4.646621	0.232556	-4.801065
95	1	0	5.655357	-0.874711	-3.855745
96	1	0	-2.806938	2.621605	-1.851905
97	1	0	-5.191963	3.110450	-2.334617
98	1	0	-4.108365	3.929248	-3.477699
99	1	0	-5.000701	2.483821	-3.979261
100	1	0	-1.398233	1.298440	-3.440229
101	1	0	-1.854191	2.885827	-4.091223
102	1	0	-2.669444	1.429482	-4.671699
103	1	0	-3.707473	-0.658507	1.713581
104	1	0	-2.950462	-2.922459	0.898901
105	1	0	-3.867000	-2.967078	2.411592
106	1	0	-4.640127	-3.459656	0.903302
107	1	0	-6.179797	-0.090394	1.621966
108	1	0	-5.828277	-1.390198	2.775832
109	1	0	-6.523014	-1.765812	1.189422
110	1	0	-4.972670	-4.180101	-2.794847
111	1	0	-5.326622	-4.259625	-4.528459
112	1	0	-3.825320	-3.497843	-3.959518
113	1	0	-7.295414	-2.959160	-2.434069
114	1	0	-7.643540	-1.504274	-3.379865
115	1	0	-7.574590	-3.089012	-4.177773
116	8	0	-0.982559	1.137870	-0.828913
117	8	0	1.104918	0.771591	0.546442
118	15	0	0.016595	-0.057369	-0.352320
119	8	0	0.619381	-0.670439	-1.585542
120	8	0	-0.675450	-0.986009	0.647867
121	1	0	-0.657826	-2.269008	0.530507
122	6	0	0.143417	-3.881196	-0.933474
123	8	0	-0.657229	-3.416226	0.456340
124	6	0	0.125645	-4.065636	1.513033
125	6	0	1.593973	-3.806824	-0.433015
126	1	0	2.118797	-4.683039	-0.820690
127	1	0	2.069157	-2.916577	-0.846316
128	8	0	-0.285559	-3.085133	-1.905842
129	8	0	-0.234997	-5.172322	-1.101248
130	6	0	-1.540086	-5.387613	-1.668511
131	1	0	-1.705167	-6.464132	-1.605543
132	1	0	-1.565627	-5.059857	-2.709809
133	1	0	-2.301643	-4.852879	-1.094360
134	1	0	0.092261	-2.147377	-1.837091
135	6	0	-0.310052	-3.690807	2.909653
136	6	0	-0.226544	-2.381652	3.406816
137	6	0	-0.782049	-4.704728	3.753819
138	6	0	-0.610657	-2.102183	4.717951
139	1	0	0.102470	-1.574227	2.762132
140	6	0	-1.155810	-4.426807	5.069076
141	1	0	-0.855148	-5.722839	3.377952
142	6	0	-1.071152	-3.121686	5.554087
143	1	0	-0.550440	-1.081549	5.085671
144	1	0	-1.516487	-5.227437	5.709253
145	1	0	-1.365310	-2.898555	6.576243
146	1	0	-0.073067	-5.130035	1.365219
147	6	0	1.577024	-3.763602	1.113324
148	1	0	2.263704	-4.484858	1.565952
149	1	0	1.866977	-2.770381	1.467452
150	1	0	6.262992	-3.634026	1.323838
151	1	0	-5.512453	-1.791606	-4.643647

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1ca (SPHENOL)

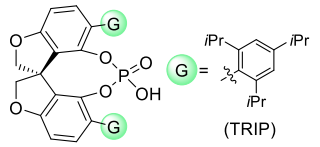


B3LYP/6-31G(d); E(RB3LYP) = -3429.49046166 Hartree
Zero-point correction= 1.290670 Hartree
Thermal correction to Energy= 1.361657 Hartree
Thermal correction to Enthalpy= 1.362601 Hartree
Thermal correction to Gibbs Free Energy= 1.182452 Hartree
Sum of electronic and zero-point Energies= -3428.199791 Hartree
Sum of electronic and thermal Energies= -3428.128804 Hartree
Sum of electronic and thermal Enthalpies= -3428.127860 Hartree
Sum of electronic and thermal Free Energies= -3428.308010 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.019010	-2.279593	-1.673120
2	6	0	3.346099	-1.406348	-0.726958
3	6	0	2.137113	-1.854300	-0.217375
4	6	0	1.595222	-3.160173	-0.451452
5	6	0	2.296132	-3.994588	-1.287553
6	6	0	3.469821	-3.574462	-1.954339
7	6	0	5.232339	-1.927696	-2.345111
8	6	0	5.916487	-0.616974	-2.056718
9	6	0	4.990891	0.386199	-1.383144
10	6	0	4.182417	-0.207004	-0.184495
11	6	0	5.095562	-0.915107	0.870482
12	6	0	6.217260	-0.039046	1.406202
13	6	0	5.710667	1.298837	1.871321
14	6	0	4.462806	1.804660	1.386387
15	6	0	3.593825	1.071389	0.483121
16	6	0	4.104709	-4.445471	-2.876255
17	6	0	5.254113	-4.064217	-3.525720
18	6	0	5.808874	-2.799593	-3.251775
19	6	0	4.088434	3.123288	1.810774
20	6	0	2.897770	3.703448	1.319658
21	6	0	2.037439	3.019335	0.495022
22	6	0	2.415820	1.694932	0.101441
23	6	0	6.478545	2.044143	2.747596
24	6	0	6.087747	3.328396	3.173151
25	6	0	4.912461	3.859798	2.700568
26	6	0	0.335112	-3.648867	0.205127
27	6	0	0.766147	3.676404	0.042700
28	6	0	-0.211003	4.070218	0.997828
29	6	0	-1.369499	4.714301	0.551536
30	6	0	-1.612788	4.978403	-0.797554
31	6	0	-0.628958	4.604746	-1.713889
32	6	0	0.559136	3.972064	-1.326472
33	6	0	0.275798	-3.794054	1.615730
34	6	0	-0.882337	-4.312997	2.202461
35	6	0	-1.990618	-4.708049	1.450675

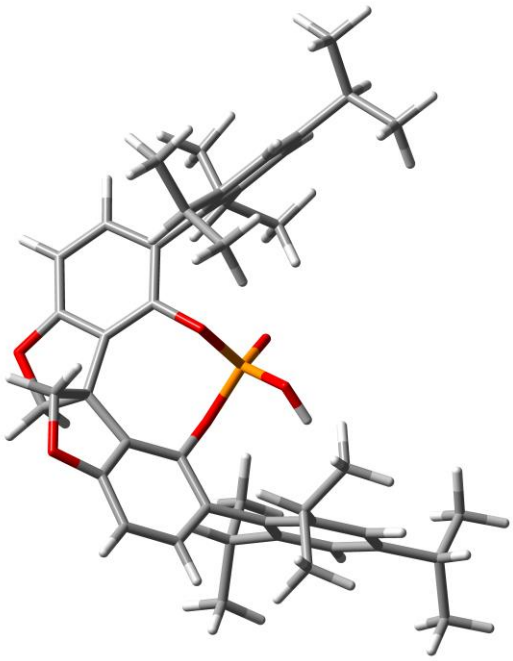
36	6	0	-1.908528	-4.569979	0.064921
37	6	0	-0.775605	-4.055784	-0.581566
38	6	0	1.456022	-3.477885	2.535625
39	6	0	2.015891	-4.765091	3.175092
40	6	0	1.096827	-2.434054	3.609747
41	6	0	-3.225421	-5.317243	2.102973
42	6	0	-3.829955	-4.412285	3.191780
43	6	0	-2.926335	-6.721676	2.663820
44	6	0	-0.788554	-4.014557	-2.113191
45	6	0	-2.034797	-3.324914	-2.698456
46	6	0	-0.670480	-5.436609	-2.703116
47	6	0	1.616229	3.706407	-2.399283
48	6	0	2.189418	5.032714	-2.939625
49	6	0	1.091794	2.823226	-3.546399
50	6	0	-0.054279	3.859676	2.508131
51	6	0	-1.239638	3.113147	3.149461
52	6	0	0.170485	5.207220	3.226410
53	6	0	-2.880111	5.684926	-1.261361
54	6	0	-4.161607	5.035793	-0.707113
55	6	0	-2.836198	7.188234	-0.922271
56	1	0	1.940381	-5.005703	-1.457218
57	1	0	6.791514	-0.802738	-1.417148
58	1	0	6.315576	-0.189270	-2.985338
59	1	0	5.570369	1.250123	-1.044713
60	1	0	4.259128	0.764144	-2.107301
61	1	0	4.447445	-1.229581	1.697898
62	1	0	5.516397	-1.827920	0.440796
63	1	0	6.731519	-0.554425	2.227318
64	1	0	6.978843	0.111695	0.627209
65	1	0	3.655111	-5.417652	-3.062770
66	1	0	5.733517	-4.726119	-4.241773
67	1	0	6.720718	-2.494641	-3.761258
68	1	0	2.658433	4.720767	1.614296
69	1	0	7.413602	1.622282	3.110395
70	1	0	6.713476	3.888150	3.862930
71	1	0	4.587960	4.852593	3.002304
72	1	0	-2.112979	5.009072	1.286823
73	1	0	-0.783502	4.834720	-2.766433
74	1	0	-0.907946	-4.429002	3.282941
75	1	0	-2.754254	-4.893415	-0.538271
76	1	0	2.261475	-3.054646	1.931628
77	1	0	2.314894	-5.490700	2.410226
78	1	0	2.895609	-4.535646	3.788793
79	1	0	1.275419	-5.249135	3.822933
80	1	0	0.720022	-1.515356	3.151801
81	1	0	1.983547	-2.182431	4.204481
82	1	0	0.335316	-2.812144	4.302777
83	1	0	-3.136694	-4.274330	4.029552
84	1	0	-4.749667	-4.854026	3.593676
85	1	0	-4.073609	-3.419921	2.796412
86	1	0	-2.537452	-7.384236	1.883020
87	1	0	-2.178231	-6.674753	3.464096
88	1	0	-3.833882	-7.176743	3.079074
89	1	0	0.075829	-3.434997	-2.444917
90	1	0	-2.139280	-2.303599	-2.327908
91	1	0	-1.952409	-3.279143	-3.791347
92	1	0	-2.956598	-3.872913	-2.467871
93	1	0	0.215665	-5.965186	-2.337114
94	1	0	-0.611620	-5.394827	-3.797639
95	1	0	-1.544390	-6.044285	-2.438183
96	1	0	2.448289	3.170420	-1.936606
97	1	0	2.607229	5.641885	-2.130294
98	1	0	2.987773	4.838384	-3.666475
99	1	0	1.418290	5.629050	-3.441702
100	1	0	0.726197	1.865378	-3.165160
101	1	0	1.894818	2.618828	-4.265280
102	1	0	0.279267	3.313570	-4.096724
103	1	0	0.829148	3.240660	2.677879
104	1	0	-1.351109	2.118352	2.714544
105	1	0	-1.061922	2.995220	4.225656
106	1	0	-2.185086	3.655172	3.031017
107	1	0	1.027237	5.753346	2.816124
108	1	0	0.351303	5.046820	4.296326
109	1	0	-0.707151	5.857928	3.130215
110	1	0	-4.238461	5.168217	0.378542
111	1	0	-5.048935	5.497653	-1.156883
112	1	0	-4.189158	3.960082	-0.907511
113	1	0	-2.796958	7.343493	0.162692
114	1	0	-1.953583	7.668034	-1.359469
115	1	0	-3.728534	7.700371	-1.302988
116	8	0	1.381503	-1.037446	0.622966
117	8	0	1.547900	1.044149	-0.773863
118	15	0	0.421546	0.059363	-0.112249
119	8	0	-0.391280	0.715364	0.974649
120	8	0	-0.313005	-0.539210	-1.304852
121	1	0	-1.627805	-0.186602	-1.513184
122	6	0	-3.360862	0.526688	-0.172223
123	8	0	-4.638791	0.805271	-0.511663
124	8	0	-2.661846	0.090021	-1.696018
125	6	0	-5.397168	-0.439257	-0.555664
126	6	0	-4.755379	-1.279485	0.568188
127	6	0	-3.287670	-0.809513	0.578272
128	1	0	-5.206871	-0.906022	-1.529453
129	1	0	-5.248177	-1.048717	1.517789
130	1	0	-4.861741	-2.351020	0.382354
131	1	0	-2.898234	-0.631981	1.582797
132	1	0	-2.615932	-1.513336	0.086045
133	8	0	-2.715080	1.597341	0.232167
134	6	0	-2.684771	1.159600	-2.664220
135	1	0	-2.189125	2.050130	-2.268768
136	1	0	-2.166292	0.799923	-3.555583
137	1	0	-3.727750	1.378785	-2.895852
138	1	0	-1.786477	1.335775	0.564764
139	6	0	-6.867007	-0.144783	-0.402062
140	6	0	-7.801638	-0.887454	-1.131112
141	6	0	-7.319449	0.829697	0.496931
142	6	0	-9.169813	-0.672524	-0.956965
143	1	0	-7.458024	-1.637376	-1.840467
144	6	0	-8.685679	1.052509	0.662381
145	1	0	-6.597468	1.424137	1.048730
146	6	0	-9.614500	0.299245	-0.060024
147	1	0	-9.885339	-1.257199	-1.528736
148	1	0	-9.026142	1.817196	1.355373
149	1	0	-10.678872	0.473935	0.071621
150	1	0	-3.982081	-5.434757	1.314256
151	1	0	-2.912610	5.597770	-2.356702

Optimized structure of Oxa-SPINOL-derived CPA (*S*)-1da



distance: 4.67 Å (-2.3%)
angle: 101.8° (+2.2%)
dihedral: 55.7° (-9.0%)

(*S*)-**1da** (Oxa-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -2540.72833210 Hartree
Zero-point correction= 0.912841 Hartree
Thermal correction to Energy= 0.965045 Hartree
Thermal correction to Enthalpy= 0.965990 Hartree
Thermal correction to Gibbs Free Energy= 0.826596 Hartree
Sum of electronic and zero-point Energies= -2539.815491 Hartree
Sum of electronic and thermal Energies= -2539.763287 Hartree
Sum of electronic and thermal Enthalpies= -2539.762342 Hartree
Sum of electronic and thermal Free Energies= -2539.901736 Hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.545245	-1.457118	0.753893
2	6	0	1.216625	2.771616	-0.480932
3	6	0	1.773777	1.528077	-0.212392
4	6	0	3.755797	2.176230	-1.396628
5	6	0	3.178965	3.389463	-1.785141
6	6	0	1.895918	3.651833	-1.329395
7	1	0	4.766749	1.950341	-1.720590
8	1	0	3.703951	4.092323	-2.422873
9	6	0	-0.032307	3.493346	-0.017906
10	6	0	-0.204328	4.443966	-1.234417
11	1	0	-0.717897	3.937737	-2.061354
12	1	0	-0.712223	5.378569	-0.989992
13	6	0	0.199492	4.367022	1.250093
14	1	0	0.724609	3.798946	2.027923
15	1	0	0.725925	5.300457	1.045059
16	6	0	-1.914392	3.627046	1.375515
17	6	0	-1.300703	2.801509	0.427240
18	6	0	-3.171284	3.346819	1.891776
19	1	0	-3.648315	4.013737	2.601584
20	6	0	-1.893874	1.592900	0.102217
21	6	0	-3.774221	2.150737	1.488316
22	1	0	-4.754434	1.901984	1.882417
23	8	0	1.010334	0.598787	0.509202
24	8	0	-1.241553	0.745480	-0.790356
25	15	0	-0.070524	-0.286347	-0.317248
26	8	0	-0.666771	-1.074892	0.945873
27	8	0	0.401838	-1.049532	-1.483124
28	6	0	3.075023	1.202952	-0.643434
29	6	0	-3.148162	1.226540	0.635089
30	6	0	-3.756302	-0.115461	0.344100
31	6	0	-3.892268	-1.081350	1.380922
32	6	0	-4.192456	-0.435500	-0.968347
33	6	0	-4.425862	-2.339285	1.062875
34	6	0	-4.722874	-1.704413	-1.219312
35	6	0	-4.841564	-2.678463	-0.224929
36	1	0	-4.530288	-3.079395	1.852369
37	1	0	-5.055312	-1.937105	-2.227473
38	6	0	3.736306	-0.103547	-0.313044
39	6	0	4.119577	-0.382474	1.023595
40	6	0	4.028496	-1.039343	-1.335867
41	6	0	4.775341	-1.584177	1.305750
42	6	0	4.696614	-2.221508	-0.993610
43	6	0	5.076161	-2.520839	0.314056
44	1	0	5.067579	-1.789086	2.332819
45	1	0	4.924153	-2.940447	-1.777019
46	6	0	3.665771	-0.814161	-2.805051
47	6	0	4.923548	-0.515430	-3.647180
48	6	0	2.882948	-1.994394	-3.411814
49	1	0	3.009940	0.058880	-2.862404
50	1	0	5.612173	-1.369113	-3.643838
51	1	0	5.475421	0.352262	-3.268278
52	1	0	1.976693	-2.191969	-2.835797
53	1	0	3.486114	-2.909397	-3.451547
54	6	0	3.888441	0.597417	2.174830
55	6	0	3.009916	-0.009209	3.285645
56	6	0	5.224002	1.116115	2.744582
57	1	0	3.355900	1.468368	1.783178
58	1	0	3.498367	-0.866884	3.763130
59	1	0	2.048722	-0.345839	2.885717
60	1	0	5.831024	1.588295	1.963988
61	1	0	5.817242	0.304667	3.182121
62	6	0	-3.542932	-0.796010	2.846823
63	6	0	-4.829594	-0.578459	3.671831
64	6	0	-2.681531	-1.889672	3.509165
65	1	0	-2.963446	0.130299	2.884536
66	1	0	-5.435561	-1.491945	3.700095
67	1	0	-5.455053	0.216761	3.252686
68	1	0	-1.735221	-2.041486	2.982059
69	1	0	-3.202964	-2.852044	3.563026
70	6	0	-4.161528	0.574541	-2.115580
71	6	0	-3.381389	0.057308	-3.338974
72	6	0	-5.592415	0.996727	-2.507542
73	1	0	-3.651794	1.475046	-1.763785
74	1	0	-3.870758	-0.811223	-3.795559
75	1	0	-2.361257	-0.229426	-3.067628
76	1	0	-6.133715	1.413005	-1.650481
77	1	0	-6.171462	0.146539	-2.887129
78	1	0	4.648392	-0.312455	-4.689385
79	1	0	2.590057	-1.753253	-4.441194
80	1	0	5.043656	1.858531	3.531792
81	1	0	2.815365	0.735590	4.067433
82	1	0	-2.440992	-1.594556	4.537084
83	1	0	-4.582084	-0.307224	4.705043
84	1	0	-3.324308	0.839110	-4.105872
85	1	0	-5.563763	1.759238	-3.295136
86	6	0	-5.409840	-4.059559	-0.522750
87	6	0	-4.537018	-4.831849	-1.530253
88	1	0	-3.503745	-4.918145	-1.177080

89	1	0	-4.930703	-5.843441	-1.684699
90	1	0	-4.515021	-4.330561	-2.505028
91	6	0	-6.872945	-3.987246	-0.999302
92	1	0	-7.503772	-3.469920	-0.268182
93	1	0	-6.956134	-3.450635	-1.951818
94	1	0	-7.279117	-4.994547	-1.149230
95	6	0	5.793337	-3.824687	0.638455
96	6	0	7.204213	-3.580020	1.206223
97	1	0	7.161480	-3.048975	2.164678
98	1	0	7.723642	-4.530951	1.376046
99	1	0	7.808898	-2.978473	0.518677
100	6	0	4.964135	-4.714528	1.583715
101	1	0	5.469429	-5.672622	1.756248
102	1	0	4.820384	-4.233485	2.558590
103	1	0	3.973291	-4.920328	1.164630
104	8	0	1.150151	4.759423	-1.641094
105	8	0	-1.130975	4.692739	1.725466
106	1	0	-5.399218	-4.621959	0.420963
107	1	0	5.910640	-4.371016	-0.307514

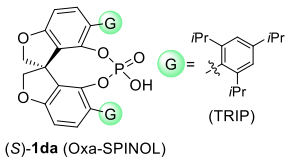
DFT calculation for all conformations of real system using Oxa-SPINOL-derived CPA (*S*)-1da

TS	Orientation I	Orientation II	ΔΔG≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-anti	up	up		
	up	down		
	down	up	-3192.968059	-2.08
	down	down		
S-anti	up	up	-3192.961634	1.95
	up	down	-3192.961495	2.04
	down	up	-3192.960879	2,43
	down	down	-3192.962941	1,13
S-syn	up	up	-3192.961417	2.09
	up	down	-3192.961902	1.79
	down	down	-3192.961517	2.03
	down	up	-3192.961841	1.82

TS	Orientation I	Orientation II	ΔΔG≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-re	up	up	-3192.964749	0.00
	up	down	-3192.964557	0.12
	down	up	-3192.964200	0.34
	down	down	-3192.964032	0.45
S-si	up	up	-3192.962941	1.13
	up	down		
	down	up		
	down	down		
S-re	up	up	-3192.964942	-0.12
	up	down		
	down	up		
	down	down		

* Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using Oxa-SPINOL-derived CPA (*S*)-1da



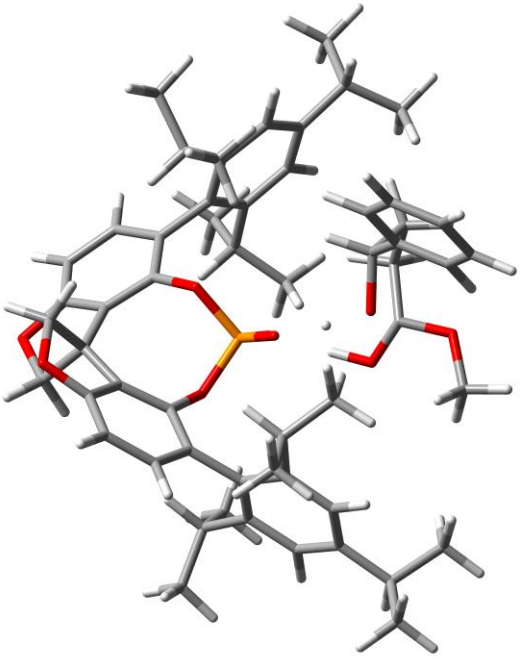
(*S*)-**1da** (Oxa-SPINOL)

1st / 2nd	ΔΔG≠ (kcal/mol)
R-anti / *R-re*	-2.08 / **0.00**
R-syn / *R-si*	-- / --
S-anti / *S-si*	**1.95** / 1.13
S-syn / *S-re*	**1.79** / -0.12

ΔΔG≠ of RDS = **1.79** kcal/mol

B3LYP/6-31G(d); E(RB3LYP) = -3194.01120632 Hartree
Zero-point correction= 1.146457 Hartree
Thermal correction to Energy= 1.211877 Hartree
Thermal correction to Enthalpy= 1.212821 Hartree
Thermal correction to Gibbs Free Energy= 1.043148 Hartree
Sum of electronic and zero-point Energies= -3192.864750 Hartree
Sum of electronic and thermal Energies= -3192.799329 Hartree
Sum of electronic and thermal Enthalpies= -3192.798385 Hartree
Sum of electronic and thermal Free Energies= -3192.968059 Hartree
The number of Imaginary frequencies = 1

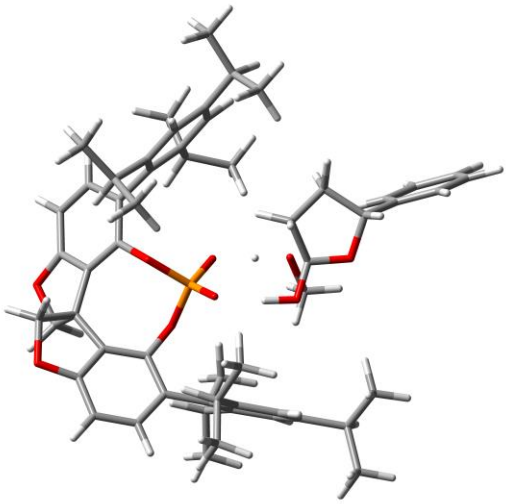
TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1da (Oxa-SPINOL)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.157910	3.007882	-1.631295
2	8	0	0.214615	2.771753	-0.000964
3	6	0	-0.923240	3.187276	0.819763
4	6	0	-1.938584	3.785150	-0.177387
5	6	0	-1.670818	3.053840	-1.492805
6	1	0	-1.336938	2.272593	1.256419
7	1	0	-1.769420	4.859208	-0.295462
8	1	0	-2.959730	3.637670	0.183568
9	1	0	-2.095964	3.563089	-2.361996
10	1	0	-2.052934	2.029225	-1.466261
11	8	0	0.440341	2.032724	-2.303658
12	8	0	0.343063	4.232129	-1.905431
13	6	0	1.759179	4.305095	-2.153489
14	1	0	1.980205	5.369600	-2.240833
15	1	0	2.013913	3.787009	-3.080181
16	1	0	2.316200	3.868969	-1.320054
17	1	0	0.453995	1.682549	0.252612
18	1	0	0.030154	1.127831	-2.107573
19	6	0	-1.198977	-3.709149	0.520731
20	6	0	-1.789644	-2.464449	0.350115
21	6	0	-3.735278	-3.549200	-0.556550
22	6	0	-3.122065	-4.803927	-0.497992
23	6	0	-1.838856	-4.849677	0.024725
24	1	0	-4.747481	-3.480598	-0.942808
25	1	0	-3.618269	-5.700183	-0.854047

26	6	0	0.071004	-4.176484	1.194929
27	6	0	0.280272	-5.491282	0.390928
28	1	0	0.789466	-5.293019	-0.560514
29	1	0	0.811734	-6.263804	0.949231
30	6	0	-0.111318	-4.552728	2.691831
31	1	0	-0.618777	-3.749174	3.240414
32	1	0	-0.631444	-5.500160	2.843786
33	6	0	2.000516	-3.822073	2.463799
34	6	0	1.330992	-3.351584	1.330083
35	6	0	3.294252	-3.427964	2.767407
36	1	0	3.815980	-3.821880	3.632851
37	6	0	1.901254	-2.340397	0.569252
38	6	0	3.889106	-2.498372	1.908681
39	1	0	4.912775	-2.193452	2.100141
40	8	0	-1.085734	-1.334689	0.754916
41	8	0	1.161511	-1.798214	-0.478377
42	15	0	0.037954	-0.638275	-0.218222
43	8	0	0.618030	0.474655	0.654054
44	8	0	-0.523607	-0.272332	-1.564577
45	6	0	-3.093755	-2.355980	-0.179292
46	6	0	3.218973	-1.903880	0.824501
47	6	0	-0.479930	4.120387	1.921790
48	6	0	-0.807553	3.838568	3.251462
49	6	0	0.240693	5.286781	1.629429
50	6	0	-0.433500	4.711959	4.275370
51	1	0	-1.355228	2.929418	3.488488
52	6	0	0.621749	6.154326	2.650727
53	1	0	0.506369	5.504690	0.598694
54	6	0	0.282608	5.870745	3.976991
55	1	0	-0.695532	4.481018	5.304391
56	1	0	1.184386	7.053494	2.413620
57	1	0	0.579456	6.549147	4.772361
58	6	0	3.928499	-0.884888	-0.019809
59	6	0	4.327137	0.358938	0.537556
60	6	0	4.281625	-1.193936	-1.356106
61	6	0	5.078138	1.242353	-0.245130
62	6	0	5.023697	-0.264571	-2.094841
63	6	0	5.442072	0.953915	-1.562803
64	1	0	5.390620	2.186740	0.193437
65	1	0	5.299154	-0.507340	-3.118924
66	6	0	-3.818487	-1.050074	-0.331335
67	6	0	-4.259460	-0.344117	0.814368
68	6	0	-4.147812	-0.560997	-1.622565
69	6	0	-5.013491	0.824163	0.645062
70	6	0	-4.921479	0.600873	-1.730390
71	6	0	-5.372429	1.309837	-0.613667
72	1	0	-5.364623	1.356114	1.527273
73	1	0	-5.189355	0.953150	-2.722997
74	6	0	-3.723737	-1.266600	-2.913269
75	6	0	-4.935267	-1.903202	-3.625243
76	6	0	-2.966226	-0.335406	-3.878661
77	1	0	-3.032809	-2.070518	-2.647461
78	1	0	-5.654263	-1.139303	-3.945453
79	1	0	-5.469522	-2.605055	-2.975472
80	1	0	-2.068821	0.064441	-3.402018
81	1	0	-3.590139	0.499625	-4.219883
82	6	0	-4.007330	-0.840046	2.238878
83	6	0	-3.178215	0.159122	3.067806
84	6	0	-5.329421	-1.188524	2.951935
85	1	0	-3.428171	-1.764921	2.180178
86	1	0	-3.694898	1.121078	3.174500
87	1	0	-2.203751	0.334770	2.600977
88	1	0	-5.903014	-1.927543	2.381599
89	1	0	-5.963844	-0.304298	3.084735
90	6	0	3.986196	0.776569	1.970169
91	6	0	5.230769	0.735394	2.881169
92	6	0	3.334936	2.170642	2.043053
93	1	0	3.255691	0.064954	2.364061
94	1	0	5.991178	1.448345	2.539682
95	1	0	5.695837	-0.255880	2.899625
96	1	0	2.460696	2.236050	1.392544
97	1	0	4.035214	2.965229	1.758014
98	6	0	3.933469	-2.523716	-2.025612
99	6	0	3.050538	-2.327484	-3.272974
100	6	0	5.203135	-3.330598	-2.363961
101	1	0	3.359859	-3.125672	-1.316580
102	1	0	3.575195	-1.763396	-4.053458
103	1	0	2.131306	-1.790251	-3.022188
104	1	0	5.811184	-3.506977	-1.469469
105	1	0	5.830682	-2.808866	-3.096031
106	1	0	-4.610413	-2.450141	-4.518563
107	1	0	-2.656036	-0.895573	-4.769139
108	1	0	-5.129475	-1.606522	3.946039
109	1	0	-3.003180	-0.234448	4.076634
110	1	0	3.008998	2.379250	3.069008
111	1	0	4.962105	1.001209	3.910932
112	1	0	2.773567	-3.299613	-3.699448
113	1	0	4.935059	-4.304843	-2.790876
114	6	0	6.277409	1.920169	-2.392900
115	6	0	7.672729	2.144073	-1.779598
116	1	0	8.204827	1.195071	-1.652322
117	1	0	8.279777	2.793268	-2.422332
118	1	0	7.602784	2.621393	-0.794894
119	6	0	5.555508	3.261128	-2.622051
120	1	0	4.582091	3.105606	-3.100415
121	1	0	5.385779	3.787746	-1.675041
122	1	0	6.152017	3.918724	-3.266106
123	6	0	-6.291561	2.519526	-0.742093
124	6	0	-5.793217	3.567327	-1.752307
125	1	0	-5.768152	3.166422	-2.772209
126	1	0	-6.459597	4.437881	-1.759659
127	1	0	-4.784709	3.916435	-1.505337
128	6	0	-7.728604	2.076219	-1.085215
129	1	0	-8.405803	2.938509	-1.116584
130	1	0	-7.762493	1.584700	-2.064923
131	1	0	-8.111093	1.366979	-0.343342
132	1	0	-6.325915	3.003657	0.244044
133	1	0	6.422857	1.455385	-3.377764
134	8	0	1.238515	-4.692355	3.200077
135	8	0	-1.059028	-5.971970	0.116846

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1da (Oxa-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3194.00903732 Hartree

Zero-point correction= 1.147386 Hartree

Thermal correction to Energy= 1.212762 Hartree

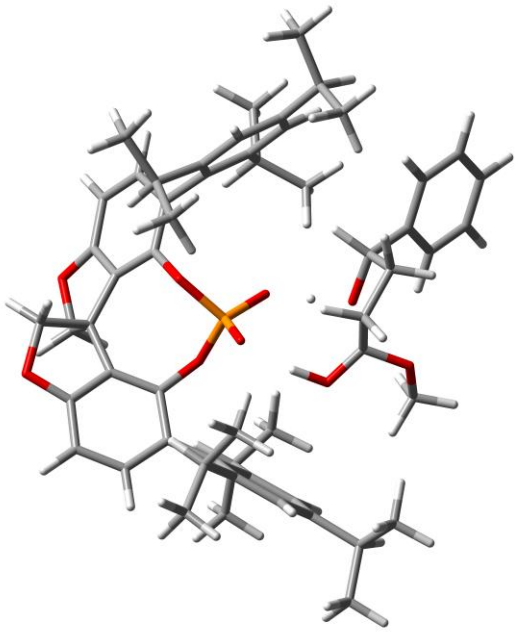
Thermal correction to Enthalpy= 1.213706 Hartree

Thermal correction to Gibbs Free Energy= 1.044288 Hartree
Sum of electronic and zero-point Energies= -3192.861651 Hartree
Sum of electronic and thermal Energies= -3192.796276 Hartree
Sum of electronic and thermal Enthalpies= -3192.795331 Hartree
Sum of electronic and thermal Free Energies= -3192.964749 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625562	2.430322	0.608113
2	8	0	-2.317557	3.589961	0.509965
3	8	0	-1.499834	1.907643	-1.001033
4	6	0	-3.748080	3.373397	0.761468
5	6	0	-3.914460	1.840750	0.797359
6	6	0	-2.521895	1.353207	1.207925
7	1	0	-3.932490	3.796462	1.755665
8	1	0	-4.177779	1.458376	-0.191957
9	1	0	-4.701615	1.543297	1.495047
10	1	0	-2.277243	0.347894	0.864653
11	1	0	-2.377259	1.389757	2.293494
12	8	0	-0.390068	2.633477	1.034451
13	6	0	-0.756157	2.822567	-1.837936
14	1	0	-1.314338	3.757737	-1.888461
15	1	0	-0.687077	2.365172	-2.826828
16	1	0	0.241438	2.996190	-1.427057
17	1	0	-0.988204	0.927698	-1.013583
18	1	0	0.082870	1.747262	1.174112
19	6	0	3.721626	-2.092372	-0.162177
20	6	0	3.312608	-0.767522	-0.211055
21	6	0	5.356912	-0.125380	0.880263
22	6	0	5.748728	-1.459693	1.031078
23	6	0	4.892765	-2.426014	0.525278
24	1	0	6.008035	0.655917	1.260293
25	1	0	6.668715	-1.731062	1.537392
26	6	0	3.161572	-3.375947	-0.731245
27	6	0	3.785420	-4.364277	0.295697
28	1	0	3.170602	-4.427334	1.202394
29	1	0	3.961697	-5.361810	-0.110432
30	6	0	3.710438	-3.738792	-2.138638
31	1	0	3.618079	-2.890574	-2.828473
32	1	0	4.738588	-4.104621	-2.125340
33	6	0	1.632025	-4.582502	-2.022463
34	6	0	1.693899	-3.632166	-0.997680
35	6	0	0.443345	-5.196835	-2.384939
36	1	0	0.414103	-5.954930	-3.160055
37	6	0	0.515615	-3.160482	-0.434653
38	6	0	-0.711795	-4.786013	-1.712098
39	1	0	-1.654335	-5.267048	-1.953248
40	8	0	2.096934	-0.472646	-0.817209
41	8	0	0.578967	-2.124540	0.490947
42	15	0	0.680662	-0.562430	0.009255
43	8	0	-0.369005	-0.261642	-1.056753
44	8	0	0.681407	0.258211	1.269113
45	6	0	4.133311	0.258929	0.305207
46	6	0	-0.725031	-3.749156	-0.763085
47	6	0	-4.582359	4.115610	-0.253814
48	6	0	-5.464314	5.115857	0.166662
49	6	0	-4.502523	3.810801	-1.620417
50	6	0	-6.261688	5.797137	-0.755459
51	1	0	-5.527360	5.365455	1.223471
52	6	0	-5.290706	4.495480	-2.543133
53	1	0	-3.819737	3.036584	-1.958932
54	6	0	-6.174729	5.489075	-2.112655
55	1	0	-6.943942	6.570240	-0.412717
56	1	0	-5.218288	4.252392	-3.599839
57	1	0	-6.790740	6.019845	-2.833459
58	6	0	-2.018285	-3.329966	-0.125758
59	6	0	-3.046813	-2.740825	-0.904463
60	6	0	-2.246809	-3.584838	1.250928
61	6	0	-4.268196	-2.433519	-0.290554
62	6	0	-3.484851	-3.252151	1.810088
63	6	0	-4.514990	-2.680160	1.060397
64	1	0	-5.061790	-1.993230	-0.890441
65	1	0	-3.651512	-3.463605	2.863369
66	6	0	3.722139	1.700857	0.268026
67	6	0	3.623168	2.381504	-0.969270
68	6	0	3.444044	2.396986	1.474028
69	6	0	3.210780	3.720131	-0.977101
70	6	0	3.052801	3.737866	1.405166
71	6	0	2.910191	4.417855	0.193649
72	1	0	3.135956	4.243322	-1.928660
73	1	0	2.838970	4.263925	2.331450
74	6	0	4.012178	1.734736	-2.299440
75	6	0	2.858220	1.730486	-3.319233
76	6	0	5.268465	2.406746	-2.890068
77	1	0	4.273750	0.690918	-2.106801
78	1	0	2.555751	2.749023	-3.592227
79	1	0	1.986466	1.204215	-2.919135
80	1	0	6.105427	2.370734	-2.183846
81	1	0	5.084090	3.459642	-3.134386
82	6	0	3.579187	1.756844	2.858348
83	6	0	4.802455	2.326188	3.606853
84	6	0	2.310419	1.900611	3.720078
85	1	0	3.743696	0.685060	2.722652
86	1	0	4.683506	3.399293	3.799900
87	1	0	5.727886	2.197266	3.034206
88	1	0	1.453051	1.440508	3.224427
89	1	0	2.072005	2.949431	3.932654
90	6	0	-2.896226	-2.446531	-2.398774
91	6	0	-3.727488	-3.429840	-3.249014
92	6	0	-3.269379	-0.997465	-2.764441
93	1	0	-1.843913	-2.576800	-2.663870
94	1	0	-4.798815	-3.323269	-3.039232
95	1	0	-3.457093	-4.472571	-3.052110
96	1	0	-2.685889	-0.283230	-2.179769
97	1	0	-4.334719	-0.793489	-2.601794
98	6	0	-1.212650	-4.257460	2.154534
99	6	0	-0.808457	-3.358671	3.338938
100	6	0	-1.707325	-5.633777	2.643091
101	1	0	-0.310160	-4.439688	1.566291
102	1	0	-1.656672	-3.166188	4.007200
103	1	0	-0.422673	-2.397146	2.987882
104	1	0	-1.954259	-6.288978	1.800108
105	1	0	-2.603451	-5.543056	3.268324
106	1	0	-0.025683	-3.844614	3.934304
107	1	0	-0.932995	-6.127821	3.242599
108	1	0	-3.063528	-0.817010	-3.826682
109	1	0	-3.575190	-3.237877	-4.318204
110	1	0	2.458767	1.397772	4.683829
111	1	0	4.929556	1.824642	4.574040
112	1	0	5.578573	1.899427	-3.811935
113	1	0	3.167738	1.223533	-4.241525
114	6	0	2.473506	5.876135	0.140976
115	6	0	1.165259	6.129891	0.912877
116	1	0	1.306045	5.992541	1.991504
117	1	0	0.822616	7.159863	0.755409
118	1	0	0.371020	5.445801	0.597924
119	6	0	3.593169	6.814398	0.633104
120	1	0	3.288129	7.864441	0.545268
121	1	0	3.831716	6.621514	1.686021
122	1	0	4.511888	6.675288	0.052522
123	6	0	-5.876021	-2.373131	1.672482
124	6	0	-6.649094	-3.667468	1.994037
125	1	0	-6.124264	-4.261410	2.751778
126	1	0	-7.649679	-3.438224	2.380640
127	1	0	-6.761998	-4.291857	1.101182
128	6	0	-5.778648	-1.472666	2.917115

129	1	0	-6.778439	-1.216466	3.287576
130	1	0	-5.242040	-1.970453	3.733139
131	1	0	-5.248337	-0.540225	2.692840
132	1	0	2.286039	6.116312	-0.915202
133	1	0	-6.454080	-1.825798	0.914847
134	8	0	5.067634	-3.781417	0.635320
135	8	0	2.854349	-4.815347	-2.597082

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1da (Oxa-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3194.00631468 Hartree

Zero-point correction= 1.146421 Hartree

Thermal correction to Energy= 1.211682 Hartree

Thermal correction to Enthalpy= 1.212627 Hartree

Thermal correction to Gibbs Free Energy= 1.044681 Hartree

Sum of electronic and zero-point Energies= -3192.859894 Hartree

Sum of electronic and thermal Energies= -3192.794632 Hartree

Sum of electronic and thermal Enthalpies= -3192.793688 Hartree

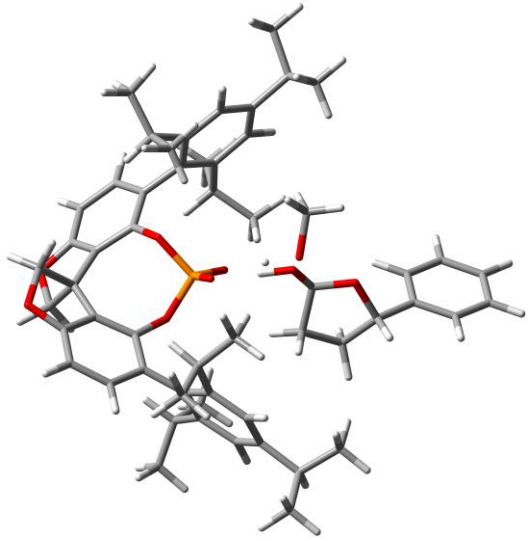
Sum of electronic and thermal Free Energies= -3192.961634 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521974	3.241343	0.563274
2	8	0	-0.695131	2.636512	-0.463089
3	6	0	-1.990815	2.954671	0.106466
4	6	0	-1.690885	3.733670	1.414559
5	6	0	-0.298909	3.272980	1.840154
6	1	0	-2.472630	1.999570	0.346137
7	1	0	-1.688363	4.808738	1.215280
8	1	0	-2.450313	3.530602	2.174651
9	1	0	0.175130	3.947886	2.558303
10	1	0	-0.315494	2.262395	2.259294
11	8	0	1.556617	2.424418	0.441228
12	8	0	0.753875	4.482559	0.092271
13	6	0	1.548722	4.578502	-1.103986
14	1	0	1.569729	5.640943	-1.348958
15	1	0	2.557965	4.201682	-0.931070
16	1	0	1.080272	4.012868	-1.914364
17	1	0	-0.585115	1.503738	-0.666376
18	1	0	1.378849	1.531114	0.878078
19	6	0	2.183075	-3.422954	-0.313929
20	6	0	2.472660	-2.065102	-0.360859
21	6	0	4.658512	-2.543585	0.523456
22	6	0	4.359835	-3.899944	0.670905
23	6	0	3.095210	-4.305029	0.275674
24	1	0	5.640737	-2.190426	0.821462
25	1	0	5.071043	-4.600801	1.094294
26	6	0	1.021904	-4.260876	-0.797701
27	6	0	1.164737	-5.441266	0.205241
28	1	0	0.685048	-5.203254	1.163071
29	1	0	0.787104	-6.389391	-0.181034
30	6	0	1.206926	-4.837940	-2.227451
31	1	0	1.461424	-4.046995	-2.944006
32	1	0	1.937603	-5.646734	-2.280591
33	6	0	-1.001652	-4.594880	-1.905821
34	6	0	-0.403537	-3.776363	-0.940856
35	6	0	-2.368945	-4.588008	-2.131962
36	1	0	-2.825083	-5.255811	-2.854642
37	6	0	-1.160628	-2.794984	-0.313957
38	8	0	1.507947	-1.200070	-0.873327
39	8	0	-0.534979	-1.913736	0.564170
40	15	0	0.307246	-0.603409	0.071350
41	8	0	-0.523244	0.248928	-0.892339
42	8	0	0.829688	0.060552	1.317221
43	6	0	3.733872	-1.589068	0.060940
44	6	0	-2.555846	-2.728599	-0.519189
45	6	0	-2.859159	3.738312	-0.859302
46	6	0	-2.360804	4.270051	-2.051385
47	6	0	-4.202340	3.963023	-0.526087
48	6	0	-3.189024	5.014281	-2.894769
49	1	0	-1.327369	4.088216	-2.322536
50	6	0	-5.028390	4.709056	-1.366007
51	1	0	-4.606450	3.548420	0.394453
52	6	0	-4.523218	5.238301	-2.555921
53	1	0	-2.787889	5.416758	-3.821341
54	1	0	-6.067553	4.873437	-1.093053
55	1	0	-5.166340	5.816499	-3.213803
56	6	0	4.132894	-0.142297	0.073002
57	6	0	4.318098	0.569918	-1.135912
58	6	0	4.423615	0.494093	1.310022
59	6	0	4.791792	1.886692	-1.082695
60	6	0	4.907495	1.805948	1.299332
61	6	0	5.100792	2.525235	0.118562
62	1	0	4.942920	2.428266	-2.014648
63	1	0	5.136165	2.280339	2.249855
64	6	0	-3.123154	-3.669458	-1.397329
65	1	0	-4.199031	-3.644956	-1.540243
66	6	0	-3.432422	-1.701254	0.131810
67	6	0	-4.133790	-0.763160	-0.668852
68	6	0	-3.618360	-1.697136	1.537840
69	6	0	-4.989569	0.152714	-0.041914
70	6	0	-4.487934	-0.761406	2.106882
71	6	0	-5.187612	0.173101	1.339770
72	1	0	-5.529542	0.869996	-0.656075
73	1	0	-4.635492	-0.779046	3.183776
74	6	0	4.240880	-0.186144	2.670567
75	6	0	5.595000	-0.420340	3.370720
76	6	0	3.286955	0.595821	3.594673
77	1	0	3.781437	-1.163501	2.505593
78	1	0	6.095449	0.528298	3.599544
79	1	0	6.278705	-1.010370	2.750178
80	1	0	2.299785	0.689395	3.136291
81	1	0	3.667414	1.598599	3.823383
82	6	0	4.071266	-0.053598	-2.509302
83	6	0	2.989772	0.704338	-3.302543
84	6	0	5.378972	-0.164195	-3.318636
85	1	0	3.705583	-1.072678	-2.360797
86	1	0	3.300555	1.732725	-3.524533
87	1	0	2.048873	0.741326	-2.745805
88	1	0	6.135345	-0.739500	-2.772953
89	1	0	5.804226	0.822630	-3.536698

90	6	0	-2.957451	-2.716957	2.466029
91	6	0	-2.081881	-2.045147	3.540967
92	6	0	-4.007938	-3.646869	3.106535
93	1	0	-2.301054	-3.351622	1.866127
94	1	0	-2.680121	-1.422533	4.217500
95	1	0	-1.311383	-1.416496	3.085372
96	1	0	-4.603603	-4.158830	2.342355
97	1	0	-4.699375	-3.091508	3.751317
98	6	0	-4.028969	-0.717582	-2.196233
99	6	0	-5.367987	-1.104800	-2.857096
100	6	0	-3.542033	0.644205	-2.722211
101	1	0	-3.285251	-1.453286	-2.509010
102	1	0	-6.155630	-0.379830	-2.619328
103	1	0	-5.717206	-2.089191	-2.524792
104	1	0	-2.553386	0.880417	-2.321122
105	1	0	-4.226586	1.459049	-2.462973
106	1	0	-1.582595	-2.806491	4.152768
107	1	0	-3.518030	-4.409712	3.723906
108	1	0	-3.464252	0.614827	-3.816123
109	1	0	-5.261390	-1.133556	-3.948250
110	1	0	5.449617	-0.956014	4.316681
111	1	0	3.170481	0.063642	4.546941
112	1	0	5.195520	-0.665985	-4.276633
113	1	0	2.799765	0.204315	-4.260246
114	6	0	-6.178649	1.144139	1.970084
115	6	0	-7.450028	0.411740	2.443774
116	1	0	-7.215654	-0.309515	3.235751
117	1	0	-8.184161	1.122506	2.842585
118	1	0	-7.918095	-0.138260	1.620349
119	6	0	-5.565811	1.965919	3.118419
120	1	0	-5.268899	1.326288	3.957482
121	1	0	-4.674423	2.512780	2.789050
122	1	0	-6.289642	2.695614	3.500342
123	6	0	5.668432	3.939455	0.123770
124	6	0	4.973068	4.865950	1.137680
125	1	0	5.181583	4.560389	2.169634
126	1	0	5.332147	5.895811	1.024216
127	1	0	3.885684	4.863847	1.006434
128	6	0	7.192486	3.922595	0.357681
129	1	0	7.607101	4.937114	0.309531
130	1	0	7.430764	3.507475	1.344408
131	1	0	7.701239	3.308783	-0.393560
132	1	0	5.496847	4.358179	-0.878230
133	1	0	-6.482632	1.849751	1.184010
134	8	0	2.591795	-5.572260	0.411141
135	8	0	-0.093819	-5.381961	-2.564547

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1da (Oxa-SPINOL)

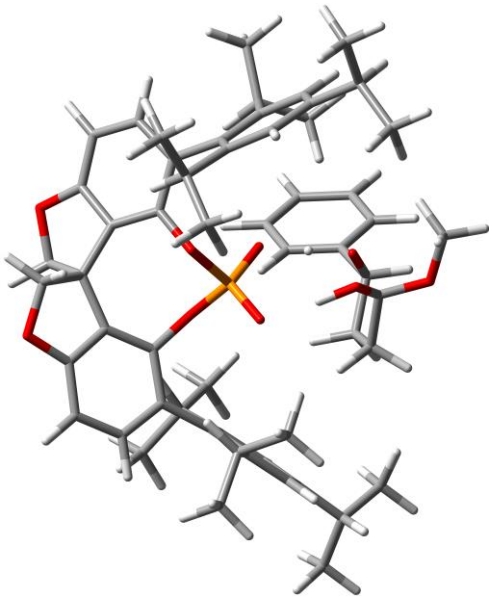


B3LYP/6-31G(d); E(RB3LYP) = -3194.00789230 Hartree
Zero-point correction= 1.147579 Hartree
Thermal correction to Energy= 1.212879 Hartree
Thermal correction to Enthalpy= 1.213824 Hartree
Thermal correction to Gibbs Free Energy= 1.044952 Hartree
Sum of electronic and zero-point Energies= -3192.860313 Hartree
Sum of electronic and thermal Energies= -3192.795013 Hartree
Sum of electronic and thermal Enthalpies= -3192.794069 Hartree
Sum of electronic and thermal Free Energies= -3192.962941 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.443921	-4.125428	-0.025950
2	6	0	1.237903	-2.990809	-0.128412
3	6	0	3.045430	-4.213615	0.881507
4	6	0	2.232021	-5.327329	1.108351
5	6	0	0.922047	-5.244346	0.663605
6	1	0	4.084336	-4.256295	1.191756
7	1	0	2.602371	-6.212835	1.613322
8	6	0	-0.918358	-4.500205	-0.564310
9	6	0	-1.294161	-5.567518	0.500372
10	1	0	-1.702432	-5.097026	1.403564
11	1	0	-1.979143	-6.331981	0.129607
12	6	0	-0.855077	-5.208840	-1.947249
13	1	0	-0.240174	-4.636988	-2.653647
14	1	0	-0.505311	-6.241121	-1.892564
15	6	0	-2.801041	-4.094543	-1.887761
16	6	0	-2.029106	-3.521853	-0.871577
17	6	0	-4.012517	-3.551473	-2.285873
18	1	0	-4.618504	-4.023513	-3.051526
19	6	0	-2.390623	-2.287287	-0.348057
20	6	0	-4.402746	-2.361987	-1.665397
21	1	0	-5.353261	-1.916896	-1.942725
22	8	0	0.692753	-1.845542	-0.701700
23	8	0	-1.561436	-1.697878	0.597870
24	15	0	-0.229248	-0.827490	0.200653
25	8	0	-0.589524	0.284662	-0.781667
26	8	0	0.426774	-0.460678	1.501148
27	6	0	2.580889	-3.016551	0.307149
28	6	0	-3.607068	-1.678445	-0.727928
29	6	0	3.530758	-1.862492	0.161553
30	6	0	3.966957	-1.455627	-1.123457
31	6	0	4.083669	-1.242557	1.314058
32	6	0	4.946046	-0.458798	-1.225618
33	6	0	5.073949	-0.266684	1.150375
34	6	0	5.529119	0.138221	-0.107636
35	1	0	5.288729	-0.158883	-2.213847
36	1	0	5.509405	0.182624	2.039219
37	6	0	-4.085791	-0.362051	-0.189761
38	6	0	-4.269677	0.736670	-1.068295
39	6	0	-4.449761	-0.230609	1.174941
40	6	0	-4.830023	1.918759	-0.565357
41	6	0	-4.987542	0.980556	1.623639
42	6	0	-5.199861	2.067539	0.772095
43	1	0	-4.991019	2.753825	-1.244510
44	1	0	-5.272691	1.065361	2.669356
45	6	0	1.085825	2.689173	0.885636
46	8	0	1.267164	4.020211	1.077436
47	8	0	-0.300190	2.600543	-0.040726
48	1	0	0.693714	1.079390	1.873201
49	6	0	2.221736	4.566590	0.108016
50	6	0	2.449176	3.427329	-0.906087
51	6	0	2.147668	2.174393	-0.079219
52	1	0	3.140341	4.752696	0.676824
53	1	0	1.751144	3.516120	-1.742954
54	1	0	3.465285	3.446372	-1.308852
55	1	0	1.818100	1.318118	-0.667443

56	1	0	3.008109	1.861599	0.521280
57	8	0	0.815599	2.071623	2.030641
58	6	0	-1.479136	3.055651	0.665202
59	1	0	-2.321033	2.956442	-0.019381
60	1	0	-1.646849	2.453328	1.560298
61	1	0	-1.316734	4.099244	0.936353
62	6	0	1.715526	5.871910	-0.455977
63	6	0	0.498845	5.937260	-1.150231
64	6	0	2.473487	7.037235	-0.306254
65	6	0	0.054546	7.145819	-1.682478
66	1	0	-0.099396	5.038322	-1.269422
67	6	0	2.034250	8.247789	-0.846658
68	1	0	3.414049	6.998694	0.238766
69	6	0	0.822596	8.304396	-1.534488
70	1	0	-0.891461	7.184898	-2.215973
71	1	0	2.635691	9.144368	-0.723609
72	1	0	0.475501	9.245476	-1.952464
73	1	0	-0.444244	1.551253	-0.367350
74	6	0	-4.338621	-1.379740	2.177635
75	6	0	-3.408910	-1.034085	3.356447
76	6	0	-5.729745	-1.820040	2.676865
77	1	0	-3.902422	-2.240329	1.665404
78	1	0	-3.796290	-0.192458	3.943470
79	1	0	-2.405640	-0.776195	3.004963
80	1	0	-6.379741	-2.104301	1.841627
81	1	0	-6.232273	-1.019996	3.233193
82	6	0	-3.897959	0.695734	-2.553463
83	6	0	-5.148932	0.780571	-3.451420
84	6	0	-2.887141	1.793341	-2.938371
85	1	0	-3.409867	-0.260457	-2.755645
86	1	0	-5.668421	1.737951	-3.323973
87	1	0	-5.867344	-0.014978	-3.224803
88	1	0	-1.964187	1.689038	-2.362500
89	1	0	-3.293091	2.799719	-2.777489
90	6	0	3.661123	-1.606149	2.739954
91	6	0	4.770933	-2.382804	3.478699
92	6	0	3.250400	-0.373209	3.567122
93	1	0	2.781018	-2.250958	2.676482
94	1	0	5.673352	-1.769439	3.591214
95	1	0	5.059169	-3.296596	2.948591
96	1	0	2.469864	0.200439	3.064325
97	1	0	4.099344	0.294289	3.758614
98	6	0	3.462249	-2.098353	-2.416019
99	6	0	2.755469	-1.080662	-3.331591
100	6	0	4.600096	-2.822097	-3.163872
101	1	0	2.724845	-2.860627	-2.153732
102	1	0	3.437874	-0.284043	-3.652298
103	1	0	1.902599	-0.621705	-2.822431
104	1	0	5.079593	-3.572337	-2.525184
105	1	0	5.375889	-2.122711	-3.497070
106	1	0	2.861133	-0.691665	4.541439
107	1	0	4.434574	-2.667737	4.482918
108	1	0	4.209154	-3.331885	-4.052842
109	1	0	2.382283	-1.577533	-4.235553
110	1	0	-4.868868	0.692198	-4.508082
111	1	0	-2.631619	1.710700	-4.001885
112	1	0	-3.320473	-1.892761	4.033151
113	1	0	-5.639182	-2.683720	3.346778
114	6	0	6.658521	1.149279	-0.266128
115	6	0	6.385422	2.477771	0.461608
116	1	0	6.307079	2.335579	1.545670
117	1	0	7.198606	3.190668	0.280397
118	1	0	5.451395	2.936074	0.116571
119	6	0	8.005661	0.549363	0.183830
120	1	0	8.825152	1.257325	0.009792
121	1	0	7.991374	0.308123	1.253395
122	1	0	8.228504	-0.373288	-0.362706
123	6	0	-5.840297	3.358706	1.266439
124	6	0	-5.043448	4.011858	2.410801
125	1	0	-5.505286	4.960147	2.710539
126	1	0	-5.009633	3.365715	3.295662
127	1	0	-4.010018	4.219587	2.111123
128	6	0	-7.308719	3.136750	1.678667
129	1	0	-7.776629	4.083940	1.973173
130	1	0	-7.890344	2.709459	0.854629
131	1	0	-7.381247	2.449132	2.529626
132	1	0	-5.840174	4.062289	0.422208
133	1	0	6.741805	1.373510	-1.338664
134	8	0	-2.225365	-5.219682	-2.416493
135	8	0	-0.036716	-6.209418	0.829087

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1da (Oxa-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3194.00462938 Hartree

Zero-point correction= 1.146396 Hartree

Thermal correction to Energy= 1.211920 Hartree

Thermal correction to Enthalpy= 1.212864 Hartree

Thermal correction to Gibbs Free Energy= 1.042727 Hartree

Sum of electronic and zero-point Energies= -3192.858233 Hartree

Sum of electronic and thermal Energies= -3192.792710 Hartree

Sum of electronic and thermal Enthalpies= -3192.791766 Hartree

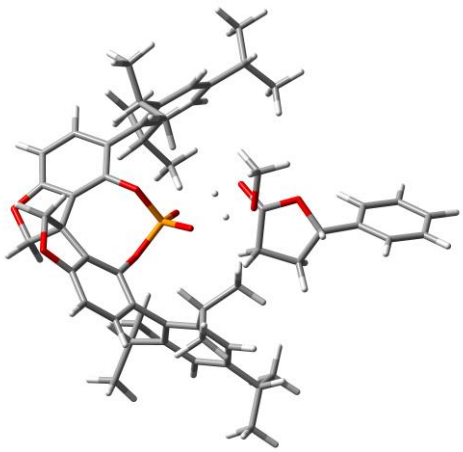
Sum of electronic and thermal Free Energies= -3192.961902 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.355021	3.108208	1.314884
2	6	0	-1.949957	2.086587	0.589279
3	6	0	-3.867264	2.227252	2.027736
4	6	0	-3.237898	3.163945	2.854409
5	6	0	-1.966954	3.573410	2.482292
6	1	0	-4.876853	1.914032	2.272191
7	1	0	-3.719115	3.553755	3.744858
8	6	0	-0.127348	3.962405	1.097798
9	6	0	0.141753	4.346696	2.578806
10	1	0	0.700477	3.556322	3.095915
11	1	0	0.648890	5.305981	2.696435
12	6	0	-0.435974	5.268605	0.310734
13	1	0	-1.012258	5.051496	-0.597384
14	1	0	-0.945541	6.026659	0.907920
15	6	0	1.663802	4.687652	-0.220406
16	6	0	1.102928	3.530477	0.331131
17	6	0	2.897855	4.679867	-0.850819

18	1	0	3.331767	5.589077	-1.252390
19	6	0	1.718501	2.303041	0.119119
20	8	0	-1.254529	1.547562	-0.489734
21	8	0	1.088638	1.154322	0.592450
22	15	0	-0.095114	0.414041	-0.275909
23	8	0	0.375473	0.014355	-1.646027
24	8	0	-0.594449	-0.674896	0.672741
25	6	0	-3.248722	1.636683	0.911169
26	6	0	2.976841	2.234528	-0.517929
27	6	0	-3.981206	0.606275	0.101627
28	6	0	-4.367800	0.895505	-1.232921
29	6	0	-4.352360	-0.633892	0.680243
30	6	0	-5.098948	-0.055003	-1.951563
31	6	0	-5.095560	-1.541287	-0.085142
32	6	0	-5.477026	-1.281120	-1.400566
33	1	0	-5.390885	0.177982	-2.972635
34	1	0	-5.384643	-2.490372	0.360497
35	6	0	3.543571	3.444997	-0.955681
36	1	0	4.520475	3.404874	-1.427196
37	6	0	3.747225	0.960368	-0.721680
38	6	0	3.922408	0.430493	-2.023009
39	6	0	4.403626	0.351403	0.379470
40	6	0	4.755993	-0.684726	-2.189102
41	6	0	5.220284	-0.761326	0.153986
42	6	0	5.419959	-1.292979	-1.124378
43	1	0	4.905755	-1.083602	-3.189804
44	1	0	5.737621	-1.210430	0.997177
45	6	0	0.148109	-3.264950	-1.418275
46	8	0	-0.364748	-3.042381	0.151061
47	6	0	0.681405	-3.702142	0.941386
48	6	0	1.670499	-3.149047	-1.228089
49	1	0	2.129172	-3.971135	-1.783181
50	1	0	2.016157	-2.208583	-1.659884
51	8	0	-0.509532	-2.383851	-2.164953
52	8	0	-0.199103	-4.548634	-1.682954
53	6	0	-1.588633	-4.784535	-1.974176
54	1	0	-1.690253	-5.869348	-2.027913
55	1	0	-1.863792	-4.330030	-2.928489
56	1	0	-2.219792	-4.383221	-1.176477
57	1	0	-0.465094	-1.923102	0.380805
58	1	0	-0.153082	-1.445404	-2.047545
59	6	0	0.527555	-3.494480	2.429166
60	6	0	0.708289	-2.245335	3.041824
61	6	0	0.221706	-4.601918	3.230895
62	6	0	0.581875	-2.116210	4.424636
63	1	0	0.912738	-1.366415	2.440744
64	6	0	0.103006	-4.474204	4.615202
65	1	0	0.076924	-5.574536	2.766076
66	6	0	0.283019	-3.227952	5.215518
67	1	0	0.716237	-1.141112	4.884609
68	1	0	-0.131995	-5.345506	5.220506
69	1	0	0.189353	-3.122015	6.293034
70	1	0	0.540221	-4.764141	0.723493
71	6	0	1.979878	-3.218141	0.284385
72	1	0	2.811000	-3.889577	0.516610
73	1	0	2.247761	-2.226511	0.660008
74	6	0	3.284965	1.053690	-3.267132
75	6	0	4.339248	1.798226	-4.113286
76	6	0	2.538882	0.029237	-4.142244
77	1	0	2.542501	1.783934	-2.934523
78	1	0	5.101593	1.106004	-4.491206
79	1	0	4.854882	2.573825	-3.537321
80	1	0	1.753408	-0.470064	-3.571932
81	1	0	3.214043	-0.728208	-4.558333
82	6	0	4.331253	0.948258	1.786652
83	6	0	4.247545	-0.101423	2.907959
84	6	0	5.524385	1.897618	2.024823
85	1	0	3.421267	1.550516	1.852370
86	1	0	5.171192	-0.684104	3.002888
87	1	0	3.421902	-0.802383	2.746576
88	1	0	5.548973	2.699291	1.279184
89	1	0	6.474395	1.352832	1.964581
90	6	0	-4.068069	2.230022	-1.917505
91	6	0	-3.230861	2.051360	-3.198420
92	6	0	-5.366141	3.011019	-2.205979
93	1	0	-3.479756	2.844532	-1.231832
94	1	0	-3.777115	1.484783	-3.962093
95	1	0	-2.295784	1.525120	-2.986196
96	1	0	-5.941103	3.177767	-1.288057
97	1	0	-6.011988	2.473767	-2.910447
98	6	0	-3.987331	-1.031779	2.112001
99	6	0	-5.215566	-0.975836	3.044276
100	6	0	-3.340534	-2.427470	2.193193
101	1	0	-3.247467	-0.317206	2.482658
102	1	0	-5.983095	-1.690532	2.722970
103	1	0	-5.678672	0.016345	3.060505
104	1	0	-2.502519	-2.518494	1.499648
105	1	0	-4.059642	-3.224119	1.966191
106	1	0	2.065424	0.541388	-4.988538
107	1	0	3.866028	2.278898	-4.978049
108	1	0	5.461105	2.359162	3.018065
109	1	0	4.083318	0.396196	3.871048
110	1	0	-2.983760	3.029336	-3.629865
111	1	0	-5.135539	3.989162	-2.645801
112	1	0	-2.963615	-2.608225	3.206703
113	1	0	-4.929680	-1.231731	4.071982
114	6	0	6.363860	-2.465246	-1.364167
115	6	0	5.942123	-3.731892	-0.597367
116	1	0	6.620567	-4.563769	-0.821638
117	1	0	5.963548	-3.569703	0.486866
118	1	0	4.926877	-4.040317	-0.870764
119	6	0	7.822943	-2.089207	-1.040078
120	1	0	7.945379	-1.854623	0.024040
121	1	0	8.499755	-2.918383	-1.279361
122	1	0	8.141084	-1.211756	-1.613370
123	6	0	-6.278805	-2.301925	-2.197184
124	6	0	-7.666875	-1.762867	-2.591694
125	1	0	-7.582282	-0.899137	-3.261780
126	1	0	-8.248548	-2.532870	-3.113060
127	1	0	-8.233211	-1.445552	-1.709265
128	6	0	-5.507646	-2.797008	-3.435365
129	1	0	-4.531842	-3.208642	-3.154312
130	1	0	-6.073024	-3.577867	-3.958623
131	1	0	-5.329692	-1.981397	-4.146022
132	1	0	6.317339	-2.701018	-2.436263
133	1	0	-6.438395	-3.168876	-1.540936
134	8	0	0.861635	5.787128	-0.068179
135	8	0	-1.177026	4.458497	3.170760

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1da (Oxa-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3194.00864995 Hartree

Zero-point correction= 1.147678 Hartree

Thermal correction to Energy= 1.213227 Hartree

Thermal correction to Enthalpy= 1.214171 Hartree

Thermal correction to Gibbs Free Energy= 1.043708 Hartree

Sum of electronic and zero-point Energies= -3192.860972 Hartree

Sum of electronic and thermal Energies= -3192.795423 Hartree

Sum of electronic and thermal Enthalpies= -3192.794479 Hartree

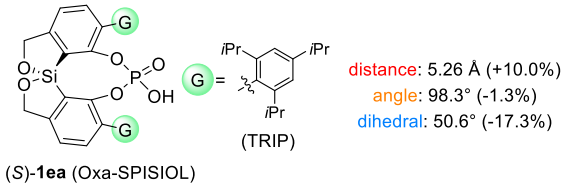
Sum of electronic and thermal Free Energies= -3192.964942 Hartree

The number of Imaginary frequencies = 1

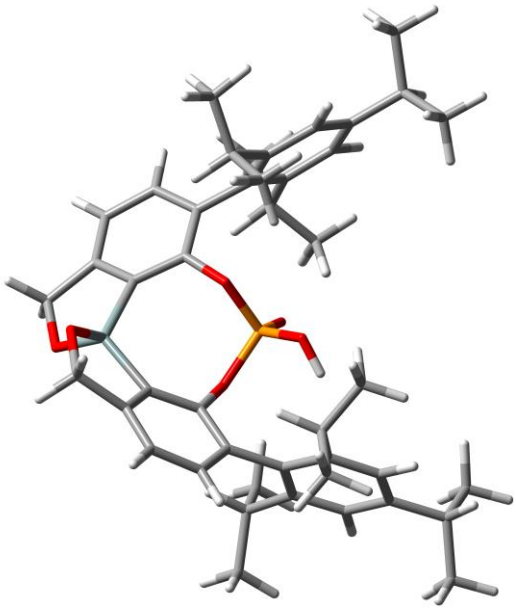
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.662425	1.085327	-0.083240
2	8	0	-3.857391	1.644110	-0.383946
3	8	0	-2.061489	0.640011	-1.627066
4	6	0	-4.859832	0.591121	-0.486675
5	6	0	-4.403146	-0.425887	0.578753
6	6	0	-2.868288	-0.292013	0.565845
7	1	0	-4.775581	0.150674	-1.487648
8	1	0	-4.814129	-0.138172	1.551506
9	1	0	-4.749974	-1.436342	0.348905
10	1	0	-2.424138	-0.289477	1.563157
11	1	0	-2.383669	-1.081495	-0.010378
12	8	0	-1.820466	1.973081	0.405078
13	6	0	-1.846432	1.767072	-2.503989
14	1	0	-1.173443	2.493645	-2.041418
15	1	0	-1.412279	1.378050	-3.427153
16	1	0	-2.816461	2.223535	-2.703346
17	1	0	-0.969714	1.508814	0.716769
18	1	0	-1.112922	0.131784	-1.473967
19	6	0	3.583175	-2.195433	-0.539900
20	6	0	2.258680	-2.425774	-0.191917
21	6	0	2.336255	-4.507734	-1.392668
22	6	0	3.627767	-4.243324	-1.859413
23	6	0	4.218562	-3.063597	-1.434240
24	1	0	1.856997	-5.436830	-1.684106
25	1	0	4.143943	-4.923047	-2.528669
26	6	0	4.613438	-1.165214	-0.129468
27	6	0	5.505288	-1.223060	-1.400220
28	1	0	5.094223	-0.593244	-2.199121
29	1	0	6.548725	-0.963262	-1.213525
30	6	0	5.480752	-1.606071	1.084619
31	1	0	4.849581	-1.959150	1.909863
32	1	0	6.230620	-2.358665	0.834808
33	6	0	5.319694	0.629554	1.196484
34	6	0	4.291317	0.236862	0.334281
35	6	0	5.423309	1.927397	1.673264
36	1	0	6.242220	2.227291	2.318110
37	6	0	3.252345	1.115914	0.065150
38	6	0	4.410906	2.819769	1.305078
39	1	0	4.465612	3.845260	1.657620
40	8	0	1.596313	-1.489041	0.593615
41	8	0	2.195978	0.670454	-0.719127
42	15	0	0.927282	-0.150068	-0.074047
43	8	0	0.276923	0.588762	1.065790
44	8	0	0.086490	-0.513782	-1.290249
45	6	0	1.605602	-3.611697	-0.593277
46	6	0	3.292283	2.444713	0.541070
47	6	0	-6.234872	1.176621	-0.293783
48	6	0	-7.307739	0.686194	-1.045490
49	6	0	-6.468876	2.173013	0.662717
50	6	0	-8.599852	1.171573	-0.837637
51	1	0	-7.132115	-0.078713	-1.798968
52	6	0	-7.757564	2.666098	0.862243
53	1	0	-5.635714	2.572599	1.233007
54	6	0	-8.826968	2.163816	0.116574
55	1	0	-9.424713	0.781197	-1.427491
56	1	0	-7.927172	3.445557	1.600181
57	1	0	-9.830648	2.548898	0.274856
58	6	0	0.203042	-3.949703	-0.176627
59	6	0	-0.081950	-4.242883	1.181541
60	6	0	-0.831345	-4.049354	-1.141895
61	6	0	-1.377614	-4.629851	1.539306
62	6	0	-2.109322	-4.444716	-0.724894
63	6	0	-2.408911	-4.744471	0.604774
64	1	0	-1.579091	-4.864818	2.581419
65	1	0	-2.899493	-4.534583	-1.467316
66	6	0	2.184923	3.419508	0.271397
67	6	0	1.383763	3.904818	1.338785
68	6	0	1.939700	3.873930	-1.046844
69	6	0	0.352536	4.805725	1.054368
70	6	0	0.882532	4.764500	-1.272965
71	6	0	0.068690	5.237905	-0.242941
72	1	0	-0.257769	5.171172	1.875722
73	1	0	0.696267	5.114832	-2.286519
74	6	0	-0.610336	-3.774589	-2.631266
75	6	0	-0.611811	-5.084825	-3.446527
76	6	0	-1.642054	-2.795373	-3.222026
77	1	0	0.370494	-3.306028	-2.745421
78	1	0	-1.586489	-5.584396	-3.386025
79	1	0	0.142229	-5.793026	-3.087647
80	1	0	-1.656025	-1.854615	-2.667972
81	1	0	-2.655610	-3.214443	-3.219870
82	6	0	0.980592	-4.203361	2.280589
83	6	0	0.632307	-3.185708	3.383799
84	6	0	1.226110	-5.605436	2.873340
85	1	0	1.924421	-3.882637	1.833331
86	1	0	-0.287424	-3.463531	3.912974
87	1	0	0.498805	-2.184106	2.964742
88	1	0	1.514959	-6.320400	2.094708
89	1	0	0.330767	-5.997373	3.370242
90	6	0	2.823587	3.483862	-2.232309
91	6	0	2.032819	2.802311	-3.364527
92	6	0	3.603432	4.705074	-2.760793
93	1	0	3.566404	2.763055	-1.880902
94	1	0	1.284504	3.477036	-3.798421
95	1	0	1.523051	1.905855	-2.999275
96	1	0	4.204171	5.164376	-1.967852
97	1	0	2.927941	5.473883	-3.154427
98	6	0	1.608369	3.508585	2.800679
99	6	0	2.176948	4.693752	3.608526
100	6	0	0.340453	2.956210	3.479244
101	1	0	2.349546	2.706098	2.826073
102	1	0	1.463442	5.525884	3.646521
103	1	0	3.104951	5.078122	3.170189
104	1	0	-0.027115	2.074784	2.949374
105	1	0	-0.463095	3.700975	3.521589
106	1	0	0.569836	2.663926	4.511526
107	1	0	2.390130	4.389087	4.640459
108	1	0	2.709999	2.502395	-4.173780
109	1	0	4.279795	4.407888	-3.571699
110	1	0	-1.386702	-2.571709	-4.265065
111	1	0	-0.405898	-4.879936	-4.504266
112	1	0	2.030372	-5.570235	3.618311
113	1	0	1.437757	-3.140886	4.127174
114	6	0	-3.799110	-5.228104	0.998748
115	6	0	-4.407415	-4.422918	2.160815
116	1	0	-3.830898	-4.550415	3.084350
117	1	0	-4.435437	-3.351440	1.933469
118	1	0	-5.432391	-4.754991	2.364570
119	6	0	-3.791031	-6.734975	1.324869
120	1	0	-4.803690	-7.090626	1.551293
121	1	0	-3.403124	-7.319011	0.483303
122	1	0	-3.158423	-6.944633	2.195646
123	6	0	-1.065077	6.213168	-0.531638
124	6	0	-2.413350	5.737065	0.040431

125	1	0	-2.649607	4.717514	-0.280288
126	1	0	-2.404478	5.741468	1.136841
127	1	0	-3.222796	6.402327	-0.284033
128	6	0	-0.725920	7.631562	-0.032604
129	1	0	-1.526341	8.336581	-0.288817
130	1	0	-0.603288	7.645093	1.057118
131	1	0	0.206589	7.996409	-0.477246
132	1	0	-1.170623	6.267246	-1.624433
133	1	0	-4.449267	-5.086390	0.123870
134	8	0	6.170487	-0.401652	1.500841
135	8	0	5.453472	-2.610111	-1.818804

Optimized structure of Oxa-SPISIOL-derived CPA (*S*)-1ea



(*S*)-**1ea** (Oxa-SPISIOL)



B3LYP/6-31G(d); E(RB3LYP) = -2792.22153413 Hartree

Zero-point correction= 0.907065 Hartree

Thermal correction to Energy= 0.960420 Hartree

Thermal correction to Enthalpy= 0.961364 Hartree

Thermal correction to Gibbs Free Energy= 0.819374 Hartree

Sum of electronic and zero-point Energies= -2791.314469 Hartree

Sum of electronic and thermal Energies= -2791.261115 Hartree

Sum of electronic and thermal Enthalpies= -2791.260170 Hartree

Sum of electronic and thermal Free Energies= -2791.402160 Hartree

The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.489627	-1.380882	0.661246
2	6	0	1.462112	2.870128	-0.488274
3	6	0	1.907226	1.578233	-0.219132
4	6	0	3.932058	2.024353	-1.396316
5	6	0	3.445701	3.263169	-1.814761
6	6	0	2.190555	3.678763	-1.371026
7	1	0	4.922038	1.709293	-1.711605
8	1	0	4.040545	3.881194	-2.483185
9	6	0	1.422966	4.911144	-1.829010
10	1	0	1.904127	5.844560	-1.505910
11	1	0	1.358325	4.930872	-2.923620
12	6	0	-1.415434	4.800102	1.983697
13	1	0	-1.899365	5.759514	1.752423
14	1	0	-1.295697	4.743161	3.072535
15	6	0	-2.225036	3.613573	1.482875
16	6	0	-1.581771	2.895092	0.466265
17	6	0	-3.431434	3.149878	2.007134
18	1	0	-3.965006	3.709210	2.771917
19	6	0	-2.046544	1.628049	0.127837
20	6	0	-3.935762	1.927828	1.561489
21	1	0	-4.877856	1.565974	1.961798
22	8	0	1.025933	0.728764	0.475874
23	8	0	-1.292888	0.882401	-0.780631
24	15	0	-0.067232	-0.117928	-0.375831
25	8	0	-0.615560	-0.988037	0.854790
26	8	0	0.404536	-0.797213	-1.593877
27	6	0	3.167646	1.121406	-0.628272
28	6	0	-3.237060	1.103335	0.657697
29	6	0	-3.723276	-0.277520	0.323983
30	6	0	-3.789557	-1.280250	1.332997
31	6	0	-4.123845	-0.592992	-1.001824
32	6	0	-4.221539	-2.566083	0.975417
33	6	0	-4.551910	-1.892069	-1.290697
34	6	0	-4.602097	-2.899708	-0.324407
35	1	0	-4.270781	-3.334450	1.742914
36	1	0	-4.857902	-2.121614	-2.307795
37	6	0	3.711700	-0.232100	-0.278225
38	6	0	4.026062	-0.536567	1.071196
39	6	0	3.964845	-1.189972	-1.291593
40	6	0	4.576842	-1.785182	1.373743
41	6	0	4.525339	-2.420123	-0.926795
42	6	0	4.836383	-2.744958	0.392859
43	1	0	4.817586	-2.009581	2.409932
44	1	0	4.721226	-3.156983	-1.702037
45	6	0	3.669074	-0.944175	-2.772662
46	6	0	4.973393	-0.758977	-3.575850
47	6	0	2.809741	-2.059184	-3.399199
48	1	0	3.088895	-0.021297	-2.855365
49	1	0	5.584551	-1.669298	-3.550405
50	1	0	5.587940	0.058390	-3.181621
51	1	0	1.871255	-2.173083	-2.853217
52	1	0	3.333946	-3.022313	-3.413335
53	6	0	3.834555	0.458649	2.216774
54	6	0	2.877595	-0.079657	3.297649
55	6	0	5.187563	0.872667	2.829591
56	1	0	3.382832	1.368622	1.813743
57	1	0	3.286215	-0.969080	3.792029
58	1	0	1.908446	-0.346109	2.865511
59	1	0	5.853953	1.296542	2.069914
60	1	0	5.702377	0.018267	3.284527
61	6	0	-3.461906	-1.017305	2.808357
62	6	0	-4.758003	-0.955509	3.644619
63	6	0	-2.494951	-2.048736	3.423821
64	1	0	-2.971933	-0.042773	2.881430
65	1	0	-5.272776	-1.923619	3.641248
66	1	0	-5.460809	-0.210008	3.257561
67	1	0	-1.542887	-2.087336	2.886982
68	1	0	-2.921919	-3.057890	3.439367
69	6	0	-4.165248	0.445029	-2.123725
70	6	0	-3.333273	0.022498	-3.349596
71	6	0	-5.622371	0.757421	-2.522263
72	1	0	-3.735089	1.376136	-1.747594
73	1	0	-3.748145	-0.869672	-3.833775
74	1	0	-2.296323	-0.189208	-3.073350
75	1	0	-6.205309	1.106019	-1.662225
76	1	0	-6.125567	-0.127222	-2.930265
77	1	0	4.748850	-0.537201	-4.626326
78	1	0	2.572556	-1.802417	-4.439056
79	1	0	5.039104	1.627522	3.611379
80	1	0	2.711789	0.680608	4.070813
81	1	0	-2.277243	-1.773304	4.462254
82	1	0	-4.530639	-0.699968	4.686396
83	1	0	-3.330433	0.826837	-4.094699
84	1	0	-5.647700	1.539853	-3.289960
85	6	0	-5.059206	-4.311615	-0.665449
86	6	0	-4.118589	-4.986418	-1.681966
87	1	0	-3.085622	-5.002838	-1.317996
88	1	0	-4.431639	-6.020530	-1.868364
89	1	0	-4.124849	-4.458066	-2.642538
90	6	0	-6.518503	-4.338867	-1.158182
91	1	0	-7.195014	-3.891185	-0.421943
92	1	0	-6.633055	-3.785285	-2.097638

93	1	0	-6.844118	-5.370059	-1.338928
94	6	0	5.437157	-4.100373	0.741360
95	6	0	6.842088	-3.966129	1.358586
96	1	0	6.807676	-3.431322	2.315258
97	1	0	7.278822	-4.954599	1.545949
98	1	0	7.516002	-3.415452	0.693148
99	6	0	4.507668	-4.919959	1.656426
100	1	0	4.929789	-5.914260	1.846751
101	1	0	4.367503	-4.426404	2.625525
102	1	0	3.519203	-5.048514	1.202305
103	14	0	-0.045824	3.819870	0.001377
104	8	0	0.091216	4.868589	-1.298576
105	8	0	-0.118623	4.773511	1.381449
106	1	0	-5.015073	-4.897069	0.263175
107	1	0	5.544212	-4.656409	-0.200205

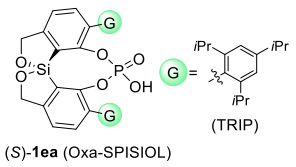
DFT calculation for all conformations of real system using Oxa-SPISIOL-derived CPA (*S*)-1ea

TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-anti	up	up		
	up	down		
	down	up		
	down	down	-3444.465681	-2.08
S-anti	up	up	-3444.460132	1.40
	up	down	-3444.458679	2.31
	down	up	-3444.456643	3.59
	down	down	-3444.455752	4.15
S-syn	up	up	-3444.459471	1.81
	up	down	-3444.45906	2.07
	down	down	-3444.459477	1.81
	down	up	-3444.459111	2.04

TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-re	up	up	-3444.462362	0.00
	up	down	-3444.461982	0.24
	down	up	-3444.461695	0.42
	down	down	-3444.461386	0.61
S-si	up	up	-3444.460073	1.44
	up	down	-3444.460224	1.34
	down	up	-3444.459617	1.72
	down	down	-3444.45952	1.78
S-re	up	up	-3444.463046	-0.43
	up	down		
	down	up		
	down	down		

* Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using Oxa-SPISIOL-derived CPA (*S*)-1ea

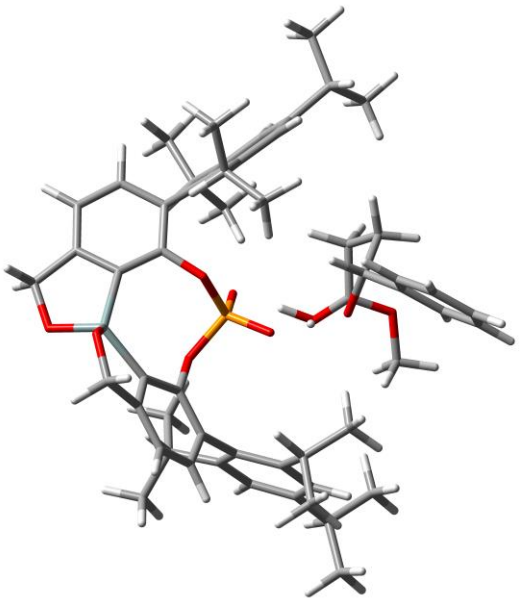


(*S*)-**1ea** (Oxa-SPISIOL)

1st / 2nd	ΔΔG≠ (kcal/mol)
R-anti / *R-re*	-2.08 / **0.00**
R-syn / *R-si*	-- / --
S-anti / *S-si*	**1.40** / 1.34
S-syn / *S-re*	**1.81** / -0.43

ΔΔG≠ of RDS = **1.40** kcal/mol

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1ea (Oxa-SPISIOL)



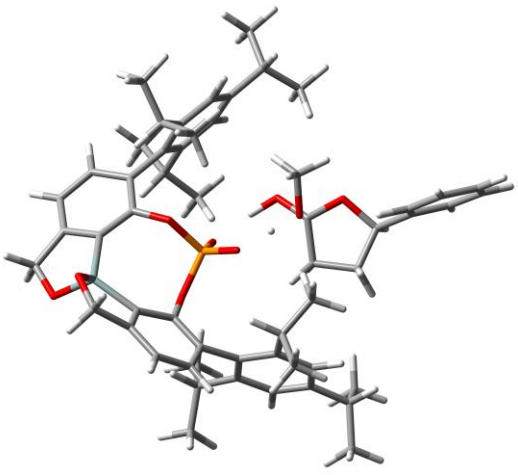
B3LYP/6-31G(d); E(RB3LYP) = -3445.50188311 Hartree
Zero-point correction= 1.140584 Hartree
Thermal correction to Energy= 1.207165 Hartree
Thermal correction to Enthalpy= 1.208109 Hartree
Thermal correction to Gibbs Free Energy= 1.036203 Hartree

Sum of electronic and zero-point Energies= -3444.361299 Hartree
Sum of electronic and thermal Energies= -3444.294718 Hartree
Sum of electronic and thermal Enthalpies= -3444.293774 Hartree
Sum of electronic and thermal Free Energies= -3444.465681 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.131522	-3.009178	-1.428467
2	8	0	-0.236441	-2.704319	0.195390
3	6	0	0.886575	-3.129230	1.031012
4	6	0	1.893596	-3.773388	0.053763
5	6	0	1.642029	-3.075460	-1.282673
6	1	0	1.319327	-2.215330	1.449650
7	1	0	1.706111	-4.847300	-0.034012
8	1	0	2.916441	-3.632535	0.412104
9	1	0	2.062239	-3.615451	-2.135502
10	1	0	2.041418	-2.057485	-1.283831
11	8	0	-0.451852	-2.052183	-2.137311
12	8	0	-0.388930	-4.234762	-1.655274
13	6	0	-1.801913	-4.292504	-1.923484
14	1	0	-2.044686	-5.355467	-1.953703
15	1	0	-2.028414	-3.823743	-2.883055
16	1	0	-2.364430	-3.796296	-1.128381
17	1	0	-0.439948	-1.598337	0.412235
18	1	0	-0.037921	-1.141245	-1.973412
19	6	0	1.490943	3.746813	0.425656
20	6	0	1.964706	2.445810	0.263414
21	6	0	3.917266	3.318288	-0.811086
22	6	0	3.389005	4.608063	-0.799505
23	6	0	2.152653	4.816420	-0.190829
24	1	0	4.897043	3.151744	-1.248464
25	1	0	3.936499	5.424758	-1.264121
26	6	0	1.341757	6.103599	-0.198350
27	1	0	1.824311	6.899742	0.386100
28	1	0	1.226297	6.470776	-1.225819
29	6	0	-1.460208	4.717281	3.360228
30	1	0	-1.922154	5.710553	3.447977
31	1	0	-1.392481	4.292140	4.369345
32	6	0	-2.258874	3.791153	2.453387

33	6	0	-1.547670	3.382280	1.318573
34	6	0	-3.534089	3.279923	2.688276
35	1	0	-4.123963	3.597806	3.544842
36	6	0	-2.016609	2.324238	0.543374
37	6	0	-4.052025	2.343242	1.794374
38	1	0	-5.063643	1.978379	1.940884
39	8	0	1.161631	1.408371	0.741347
40	8	0	-1.166106	1.828093	-0.448405
41	15	0	-0.014548	0.698447	-0.163307
42	8	0	-0.575162	-0.374915	0.770674
43	8	0	0.512982	0.280389	-1.509383
44	6	0	3.215025	2.194800	-0.326600
45	6	0	-3.306534	1.799295	0.726528
46	6	0	0.417191	-4.026740	2.151969
47	6	0	0.740351	-3.718271	3.476859
48	6	0	-0.323341	-5.186396	1.883246
49	6	0	0.342214	-4.558535	4.519275
50	1	0	1.303521	-2.814045	3.695623
51	6	0	-0.728451	-6.020746	2.922834
52	1	0	-0.585116	-5.425216	0.856193
53	6	0	-0.393734	-5.710653	4.244298
54	1	0	0.601286	-4.306957	5.544216
55	1	0	-1.306261	-6.914862	2.703706
56	1	0	-0.709149	-6.363353	5.053924
57	6	0	-3.934453	0.754983	-0.149097
58	6	0	-4.361773	-0.482869	0.402332
59	6	0	-4.205961	1.041587	-1.510161
60	6	0	-5.063428	-1.380399	-0.409546
61	6	0	-4.903581	0.098609	-2.274744
62	6	0	-5.355469	-1.110379	-1.748936
63	1	0	-5.401079	-2.317838	0.025527
64	1	0	-5.120521	0.326116	-3.316101
65	6	0	3.853548	0.841327	-0.436172
66	6	0	4.298998	0.174613	0.731615
67	6	0	4.124120	0.277300	-1.710674
68	6	0	5.001323	-1.030289	0.598229
69	6	0	4.848489	-0.918526	-1.781930
70	6	0	5.306375	-1.589061	-0.644308
71	1	0	5.358004	-1.532100	1.495656
72	1	0	5.072528	-1.328999	-2.762911
73	6	0	3.686878	0.933268	-3.023513
74	6	0	4.899602	1.464496	-3.815669
75	6	0	2.848401	-0.009640	-3.907386
76	1	0	3.045902	1.784323	-2.780300
77	1	0	5.563394	0.646646	-4.121289
78	1	0	5.497599	2.169648	-3.228055
79	1	0	1.948569	-0.333433	-3.380863
80	1	0	3.416334	-0.894823	-4.218579
81	6	0	4.113402	0.748575	2.137351
82	6	0	3.246355	-0.160520	3.028666
83	6	0	5.470731	1.047768	2.805220
84	1	0	3.589336	1.703245	2.052117
85	1	0	3.702680	-1.149632	3.160867
86	1	0	2.248946	-0.288160	2.596255
87	1	0	6.076050	1.720267	2.187288
88	1	0	6.052728	0.133768	2.972257
89	6	0	-4.103394	-0.884537	1.857227
90	6	0	-5.406306	-0.894763	2.683653
91	6	0	-3.402917	-2.251215	1.975463
92	1	0	-3.428916	-0.146314	2.298818
93	1	0	-6.109195	-1.644913	2.301412
94	1	0	-5.918230	0.073219	2.661752
95	1	0	-2.477551	-2.276017	1.396991
96	1	0	-4.045230	-3.070429	1.629778
97	6	0	-3.824332	2.359915	-2.184670
98	6	0	-2.858479	2.141676	-3.365271
99	6	0	-5.074290	3.147577	-2.626521
100	1	0	-3.304047	2.985403	-1.456309
101	1	0	-3.325901	1.554092	-4.164789
102	1	0	-1.953117	1.620567	-3.041044
103	1	0	-5.744798	3.335951	-1.780360
104	1	0	-5.645311	2.607456	-3.390882
105	1	0	4.566458	1.979681	-4.724629
106	1	0	2.536006	0.514727	-4.818563
107	1	0	5.317868	1.527129	3.779544
108	1	0	3.126639	0.284449	4.023882
109	1	0	-3.151493	-2.455885	3.022950
110	1	0	-5.193833	-1.140699	3.731265
111	1	0	-2.562032	3.106539	-3.794586
112	1	0	-4.783297	4.115828	-3.051500
113	6	0	-6.162694	-2.077812	-2.605338
114	6	0	-7.595625	-2.253189	-2.066746
115	1	0	-8.108964	-1.288672	-1.989043
116	1	0	-8.182739	-2.901132	-2.728943
117	1	0	-7.592271	-2.710163	-1.069957
118	6	0	-5.465850	-3.441310	-2.765429
119	1	0	-4.466312	-3.322680	-3.197804
120	1	0	-5.358653	-3.949759	-1.799529
121	1	0	-6.046328	-4.098847	-3.423913
122	6	0	6.180636	-2.834915	-0.736955
123	6	0	5.626405	-3.910370	-1.687127
124	1	0	5.589404	-3.555174	-2.723506
125	1	0	6.266128	-4.800518	-1.669863
126	1	0	4.614419	-4.217162	-1.401644
127	6	0	7.623446	-2.456005	-1.129971
128	1	0	8.271202	-3.341123	-1.135178
129	1	0	7.651532	-2.011356	-2.132022
130	1	0	8.045287	-1.726856	-0.429924
131	14	0	-0.029504	4.421585	1.225150
132	8	0	0.042616	5.849336	0.342946
133	8	0	-0.132714	4.865882	2.841227
134	1	0	6.221395	-3.274696	0.269472
135	1	0	-6.241052	-1.632006	-3.606399

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1ea (Oxa-SPISIOL)



B3LYP/6-31G(d); E(RB3LYP) = -3445.50043667 Hartree

Zero-point correction= 1.141675 Hartree

Thermal correction to Energy= 1.208159 Hartree

Thermal correction to Enthalpy= 1.209103 Hartree

Thermal correction to Gibbs Free Energy= 1.038075 Hartree

Sum of electronic and zero-point Energies= -3444.358761 Hartree

Sum of electronic and thermal Energies= -3444.292278 Hartree

Sum of electronic and thermal Enthalpies= -3444.291334 Hartree

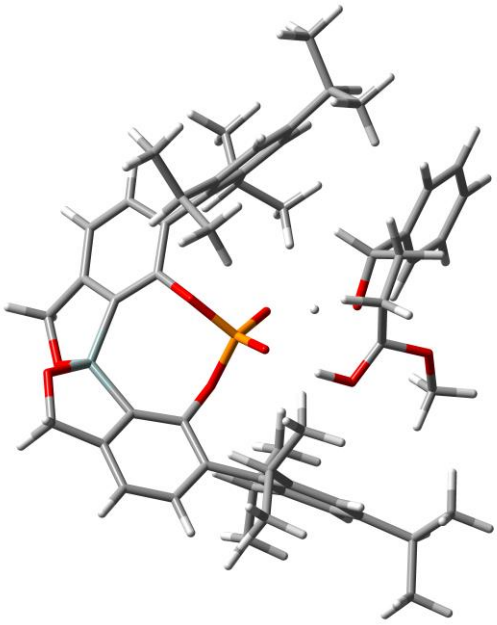
Sum of electronic and thermal Free Energies= -3444.462362 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.107635	1.930863	0.516912
2	8	0	-3.046951	2.899469	0.401292
3	8	0	-1.837244	1.449598	-1.090799
4	6	0	-4.392443	2.359662	0.636227
5	6	0	-4.201548	0.830403	0.673816
6	6	0	-2.740504	0.676259	1.106128
7	1	0	-4.681296	2.728722	1.627116
8	1	0	-4.354031	0.397932	-0.317946
9	1	0	-4.909287	0.358862	1.360187
10	1	0	-2.266442	-0.245942	0.769827
11	1	0	-2.624305	0.744233	2.193649
12	8	0	-0.959936	2.414007	0.959605
13	6	0	-1.342475	2.519827	-1.927690
14	1	0	-2.131426	3.266867	-2.017157
15	1	0	-1.116917	2.083637	-2.902713
16	1	0	-0.444373	2.963889	-1.491825
17	1	0	-1.094472	0.632891	-1.092571
18	1	0	-0.294853	1.662273	1.110464
19	6	0	4.282967	-0.999377	-0.121899
20	6	0	3.476786	0.136362	-0.168517
21	6	0	5.159212	1.355544	1.019297
22	6	0	5.912693	0.196654	1.204881
23	6	0	5.451997	-0.996248	0.650142
24	1	0	5.522774	2.294201	1.426991
25	1	0	6.831605	0.232744	1.785432
26	6	0	6.026469	-2.386821	0.877557
27	1	0	7.015040	-2.508566	0.412543
28	1	0	6.140219	-2.577408	1.951965
29	6	0	3.730007	-4.291179	-2.793682
30	1	0	4.273677	-5.241280	-2.694892
31	1	0	3.558821	-4.116427	-3.863185
32	6	0	2.403173	-4.309473	-2.047148
33	6	0	2.341338	-3.371407	-1.008648
34	6	0	1.280744	-5.076794	-2.354231
35	1	0	1.307919	-5.833311	-3.135052
36	6	0	1.114278	-3.057437	-0.427857
37	6	0	0.103930	-4.855305	-1.639043
38	1	0	-0.761969	-5.477916	-1.841857
39	8	0	2.241400	0.017272	-0.805333
40	8	0	1.071231	-1.980330	0.457045
41	15	0	0.860516	-0.427616	-0.029227
42	8	0	-0.196086	-0.369101	-1.129132
43	8	0	0.638683	0.363429	1.231596
44	6	0	3.903896	1.359028	0.377518
45	6	0	-0.037292	-3.816971	-0.695110
46	6	0	-5.362391	2.891485	-0.390541
47	6	0	-6.448675	3.672323	0.016307
48	6	0	-5.204657	2.605734	-1.754527
49	6	0	-7.369184	4.154955	-0.916419
50	1	0	-6.575277	3.906479	1.070938
51	6	0	-6.116910	3.093710	-2.687899
52	1	0	-4.364265	2.000806	-2.083087
53	6	0	-7.203572	3.867825	-2.270888
54	1	0	-8.209416	4.758423	-0.584039
55	1	0	-5.982654	2.867811	-3.742371
56	1	0	-7.915611	4.244972	-2.999934
57	6	0	-1.361250	-3.596692	-0.024468
58	6	0	-2.507480	-3.257270	-0.789545
59	6	0	-1.494679	-3.811057	1.372014
60	6	0	-3.745120	-3.150248	-0.142192
61	6	0	-2.757313	-3.688520	1.962208
62	6	0	-3.900217	-3.365722	1.228173
63	1	0	-4.625778	-2.902122	-0.731019
64	1	0	-2.847646	-3.870377	3.029829
65	6	0	3.096558	2.619872	0.307288
66	6	0	2.855478	3.236908	-0.944144
67	6	0	2.604918	3.224681	1.494433
68	6	0	2.097597	4.414393	-0.983539
69	6	0	1.867567	4.408303	1.392783
70	6	0	1.584752	5.014952	0.167077
71	1	0	1.914747	4.890506	-1.945114
72	1	0	1.490277	4.863760	2.304132
73	6	0	3.446750	2.712347	-2.253887
74	6	0	2.367461	2.366898	-3.296618
75	6	0	4.474228	3.707457	-2.830911
76	1	0	3.989887	1.788648	-2.039635
77	1	0	1.790627	3.252768	-3.590470
78	1	0	1.676391	1.613610	-2.906941
79	1	0	5.267423	3.922605	-2.106186
80	1	0	4.004405	4.660148	-3.102917
81	6	0	2.865213	2.658726	2.893670
82	6	0	3.840661	3.562094	3.677003
83	6	0	1.576162	2.434496	3.707084
84	1	0	3.336486	1.678969	2.783629
85	1	0	3.406923	4.553911	3.852961
86	1	0	4.784185	3.708981	3.139168
87	1	0	0.915540	1.730310	3.197540
88	1	0	1.028506	3.368589	3.878492
89	6	0	-2.466213	-3.022977	-2.302130
90	6	0	-3.172118	-4.162962	-3.065626
91	6	0	-3.071217	-1.667423	-2.712823
92	1	0	-1.419329	-3.004781	-2.614794
93	1	0	-4.239651	-4.202344	-2.817309
94	1	0	-2.745243	-5.143199	-2.828078
95	1	0	-2.566990	-0.843004	-2.204600
96	1	0	-4.143438	-1.611469	-2.488175
97	6	0	-0.328406	-4.225754	2.270297
98	6	0	-0.067964	-3.196510	3.387117
99	6	0	-0.544781	-5.637187	2.852603
100	1	0	0.577019	-4.274911	1.662057
101	1	0	-0.917173	-3.127938	4.078215
102	1	0	0.118241	-2.202613	2.970096
103	1	0	-0.690518	-6.377255	2.057573
104	1	0	-1.422361	-5.675321	3.508881
105	1	0	0.810633	-3.490551	3.973998
106	1	0	0.326394	-5.941986	3.444840
107	1	0	-2.957791	-1.520683	-3.793978
108	1	0	-3.086726	-4.010569	-4.148471
109	1	0	1.827161	2.016711	4.690000
110	1	0	4.072391	3.121138	4.654232
111	1	0	4.940964	3.295403	-3.733880
112	1	0	2.832719	1.962724	-4.203869
113	6	0	0.777853	6.303888	0.078770
114	6	0	-0.567123	6.214962	0.823358
115	1	0	-0.418506	6.134389	1.906671
116	1	0	-1.163937	7.116937	0.640853
117	1	0	-1.147939	5.342830	0.507420
118	6	0	1.599889	7.511589	0.570982
119	1	0	1.030733	8.442480	0.457632
120	1	0	1.858482	7.403479	1.631276
121	1	0	2.534848	7.611569	0.008553
122	6	0	-5.280730	-3.307215	1.870819
123	6	0	-5.818858	-4.725589	2.148254
124	1	0	-5.183959	-5.249794	2.872521
125	1	0	-6.835419	-4.684313	2.558300
126	1	0	-5.843423	-5.324946	1.231791
127	6	0	-5.318640	-2.453278	3.150331
128	1	0	-6.345133	-2.371468	3.526819
129	1	0	-4.711322	-2.894316	3.949055
130	1	0	-4.940299	-1.441039	2.968470
131	8	0	5.132626	-3.364142	0.334889
132	8	0	4.548039	-3.230793	-2.286284
133	14	0	4.048043	-2.710694	-0.769385
134	1	0	-5.955755	-2.838106	1.141203
135	1	0	0.556367	6.470712	-0.984914

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1ea (Oxa-SPISIOL)



B3LYP/6-31G(d); E(RB3LYP) = -3445.49532186 Hartree

Zero-point correction= 1.140788 Hartree

Thermal correction to Energy= 1.207317 Hartree

Thermal correction to Enthalpy= 1.208261 Hartree

Thermal correction to Gibbs Free Energy= 1.035190 Hartree

Sum of electronic and zero-point Energies= -3444.354534 Hartree

Sum of electronic and thermal Energies= -3444.288005 Hartree

Sum of electronic and thermal Enthalpies= -3444.287061 Hartree

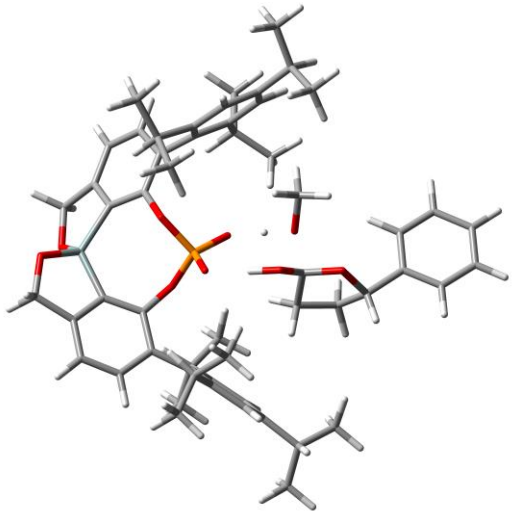
Sum of electronic and thermal Free Energies= -3444.460132 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.340300	-3.131716	0.639205
2	8	0	0.760397	-2.513837	-0.489939
3	6	0	2.104169	-2.830102	-0.034434
4	6	0	1.942603	-3.446838	1.383131
5	6	0	0.554917	-3.019241	1.859188
6	1	0	2.630919	-1.872333	0.039997
7	1	0	2.003305	-4.536698	1.326167
8	1	0	2.730456	-3.095672	2.054297
9	1	0	0.164487	-3.657678	2.656628
10	1	0	0.540511	-1.979628	2.198118
11	8	0	-1.436418	-2.397123	0.528052
12	8	0	-0.498428	-4.417355	0.268294
13	6	0	-1.332540	-4.663237	-0.878113
14	1	0	-1.335848	-5.746624	-1.002430
15	1	0	-2.343368	-4.289039	-0.710158
16	1	0	-0.903484	-4.185270	-1.763020
17	1	0	0.618180	-1.393931	-0.670896
18	1	0	-1.300585	-1.476387	0.919754
19	6	0	-2.515235	3.365482	-0.262748
20	6	0	-2.646991	1.977131	-0.314500
21	6	0	-4.841415	2.189157	0.620710
22	6	0	-4.671261	3.557479	0.813556
23	6	0	-3.477990	4.142180	0.395820
24	1	0	-5.775211	1.724906	0.922867
25	1	0	-5.451509	4.141947	1.295459
26	6	0	-3.024504	5.567703	0.673050
27	1	0	-3.624662	6.307699	0.124613
28	1	0	-3.118652	5.791907	1.742812
29	6	0	0.267888	5.565553	-2.639791
30	1	0	0.431578	6.641348	-2.484710
31	1	0	0.405719	5.359132	-3.708359
32	6	0	1.224664	4.714905	-1.815470
33	6	0	0.578464	3.919139	-0.860253
34	6	0	2.603506	4.608564	-1.986052
35	1	0	3.139239	5.241657	-2.689458
36	6	0	1.260904	2.871537	-0.243461
37	8	0	-1.570997	1.250765	-0.835517
38	8	0	0.528129	2.011241	0.576925
39	15	0	-0.321133	0.702377	0.080658
40	8	0	0.517259	-0.123425	-0.899121
41	8	0	-0.808800	0.025389	1.335254
42	6	0	-3.829022	1.346431	0.112244
43	6	0	2.648493	2.717694	-0.403308
44	6	0	2.826706	-3.733740	-1.016598
45	6	0	2.303824	-4.029572	-2.278938
46	6	0	4.073784	-4.267603	-0.660289
47	6	0	3.006698	-4.851444	-3.162863
48	1	0	1.348257	-3.607828	-2.569263
49	6	0	4.777801	-5.084667	-1.544375
50	1	0	4.499680	-4.044609	0.315235
51	6	0	4.244277	-5.382439	-2.800167
52	1	0	2.584251	-5.072754	-4.139574
53	1	0	5.742457	-5.490279	-1.250712
54	1	0	4.790619	-6.020595	-3.489370
55	6	0	-4.101846	-0.128517	0.083494
56	6	0	-4.225231	-0.817101	-1.147722
57	6	0	-4.371079	-0.814741	1.298371
58	6	0	-4.630627	-2.157039	-1.135627
59	6	0	-4.785257	-2.149514	1.245296
60	6	0	-4.930991	-2.842363	0.042540
61	1	0	-4.738031	-2.680254	-2.083990
62	1	0	-4.997907	-2.661188	2.179636
63	6	0	3.292051	3.652079	-1.243007
64	1	0	4.369890	3.574661	-1.350848
65	6	0	3.464380	1.629883	0.226424
66	6	0	4.168715	0.714269	-0.599999
67	6	0	3.610367	1.555989	1.634198
68	6	0	4.988637	-0.245970	0.005752
69	6	0	4.450830	0.578990	2.181309
70	6	0	5.156454	-0.329804	1.390491
71	1	0	5.531209	-0.945862	-0.626611
72	1	0	4.569572	0.547258	3.260764
73	6	0	-4.232243	-0.169223	2.681488
74	6	0	-5.592762	-0.067015	3.400645
75	6	0	-3.211674	-0.907484	3.570145
76	1	0	-3.850485	0.845941	2.550435
77	1	0	-6.012458	-1.059067	3.605913
78	1	0	-6.329860	0.483528	2.805458
79	1	0	-2.220647	-0.892650	3.111255
80	1	0	-3.502711	-1.949404	3.749218
81	6	0	-3.986926	-0.148924	-2.501751
82	6	0	-2.837446	-0.819081	-3.278434
83	6	0	-5.277383	-0.107127	-3.344552
84	1	0	-3.692273	0.888279	-2.327269
85	1	0	-3.072161	-1.862626	-3.522550
86	1	0	-1.909226	-0.800650	-2.699918
87	1	0	-6.085476	0.402572	-2.807785
88	1	0	-5.629034	-1.114220	-3.598328
89	6	0	2.943438	2.543692	2.592416
90	6	0	2.015859	1.839361	3.600855
91	6	0	3.993480	3.411963	3.315075
92	1	0	2.322279	3.225336	2.007517
93	1	0	2.574018	1.159243	4.256241
94	1	0	1.238484	1.265583	3.088047
95	1	0	4.629168	3.945252	2.599187
96	1	0	4.646826	2.808109	3.956069
97	6	0	4.102130	0.735689	-2.130894
98	6	0	5.474800	1.078326	-2.745396

99	6	0	3.558596	-0.576894	-2.721856
100	1	0	3.404683	1.519105	-2.432927
101	1	0	6.217361	0.301764	-2.526825
102	1	0	5.868806	2.026178	-2.360970
103	1	0	2.542198	-0.765575	-2.366771
104	1	0	4.184638	-1.438288	-2.465309
105	1	0	1.522929	2.581056	4.240926
106	1	0	3.499404	4.156302	3.951020
107	1	0	3.525225	-0.508622	-3.816215
108	1	0	5.394227	1.162033	-3.835890
109	1	0	-5.479603	0.450154	4.361141
110	1	0	-3.139558	-0.412135	4.546317
111	1	0	-5.102038	0.430333	-4.284310
112	1	0	-2.659491	-0.290794	-4.222962
113	6	0	6.147686	-1.327142	1.980212
114	6	0	7.514463	-0.652019	2.219192
115	1	0	7.427318	0.147667	2.964499
116	1	0	8.250485	-1.378182	2.585592
117	1	0	7.902219	-0.206954	1.296658
118	6	0	5.654840	-2.012157	3.265496
119	1	0	5.548226	-1.299128	4.090955
120	1	0	4.683352	-2.497735	3.119053
121	1	0	6.370470	-2.777468	3.587764
122	6	0	-5.452267	-4.274061	-0.011186
123	6	0	-4.870435	-5.184874	1.083706
124	1	0	-5.223536	-4.894581	2.080069
125	1	0	-5.181704	-6.223290	0.919978
126	1	0	-3.775650	-5.152951	1.097811
127	6	0	-6.994266	-4.294051	0.030095
128	1	0	-7.375250	-5.318518	-0.063762
129	1	0	-7.362212	-3.881635	0.977368
130	1	0	-7.419820	-3.694630	-0.781945
131	14	0	-1.164552	4.510167	-0.775128
132	8	0	-1.081106	5.240236	-2.285631
133	8	0	-1.650783	5.707259	0.298401
134	1	0	6.300037	-2.111758	1.225173
135	1	0	-5.147912	-4.689618	-0.982648

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1ea (Oxa-SPISIOL)

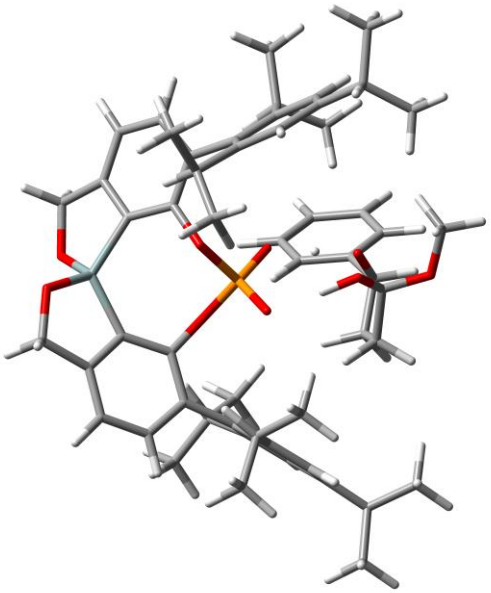


B3LYP/6-31G(d); E(RB3LYP) = -3445.49705483 Hartree
Zero-point correction= 1.141688 Hartree
Thermal correction to Energy= 1.208234 Hartree
Thermal correction to Enthalpy= 1.209178 Hartree
Thermal correction to Gibbs Free Energy= 1.036831 Hartree
Sum of electronic and zero-point Energies= -3444.355367 Hartree
Sum of electronic and thermal Energies= -3444.288821 Hartree
Sum of electronic and thermal Enthalpies= -3444.287877 Hartree
Sum of electronic and thermal Free Energies= -3444.460224 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.059876	-4.104716	0.059629
2	6	0	1.656121	-2.846808	-0.026334
3	6	0	3.587236	-3.731671	1.076755
4	6	0	2.943001	-4.942714	1.319626
5	6	0	1.654178	-5.119077	0.821143
6	1	0	4.608707	-3.600416	1.418556
7	1	0	3.444719	-5.722870	1.887258
8	6	0	0.728572	-6.297865	1.086048
9	1	0	1.106721	-7.228941	0.640913
10	1	0	0.628500	-6.462971	2.166046
11	6	0	-1.942034	-5.369245	-2.675753
12	1	0	-2.496293	-6.313304	-2.576435
13	1	0	-1.823392	-5.166020	-3.747426
14	6	0	-2.659698	-4.210253	-1.999609
15	6	0	-1.942513	-3.659513	-0.930320
16	6	0	-3.864199	-3.631560	-2.394320
17	1	0	-4.461930	-4.055493	-3.197813
18	6	0	-2.309727	-2.424777	-0.396017
19	6	0	-4.291624	-2.479051	-1.739191
20	1	0	-5.245029	-2.038450	-2.014645
21	8	0	0.918369	-1.824684	-0.630456
22	8	0	-1.457020	-1.859224	0.551409
23	15	0	-0.160528	-0.906503	0.211246
24	8	0	-0.570974	0.171054	-0.790588
25	8	0	0.402533	-0.488250	1.540883
26	6	0	2.961228	-2.632572	0.449929
27	6	0	-3.518181	-1.808779	-0.766344
28	6	0	3.750013	-1.362521	0.311727
29	6	0	4.172497	-0.922550	-0.969559
30	6	0	4.209854	-0.683069	1.469790
31	6	0	5.060180	0.156242	-1.060088
32	6	0	5.109094	0.380453	1.316182
33	6	0	5.565267	0.807769	0.068325
34	1	0	5.395640	0.469321	-2.045920
35	1	0	5.483388	0.882304	2.205764
36	6	0	-4.048260	-0.521701	-0.208315
37	6	0	-4.314923	0.567081	-1.079497
38	6	0	-4.411299	-0.424916	1.160002
39	6	0	-4.962273	1.699568	-0.568001
40	6	0	-5.034627	0.742012	1.616806
41	6	0	-5.337448	1.812251	0.771618
42	1	0	-5.185610	2.525245	-1.240992
43	1	0	-5.318368	0.800251	2.664591
44	6	0	0.818450	2.719275	0.926037
45	8	0	0.861840	4.059852	1.132316
46	8	0	-0.547358	2.499658	-0.009937
47	1	0	0.557792	1.068503	1.897753
48	6	0	1.753025	4.711405	0.167256
49	6	0	2.094817	3.611060	-0.857483
50	6	0	1.929645	2.327709	-0.038932
51	1	0	2.648419	4.986018	0.737428
52	1	0	1.385990	3.632734	-1.689808
53	1	0	3.100279	3.739416	-1.264658
54	1	0	1.694014	1.443958	-0.631507
55	1	0	2.819255	2.106976	0.560386
56	8	0	0.602138	2.067087	2.063044
57	6	0	-1.764243	2.820900	0.706107
58	1	0	-2.583155	2.757828	-0.008243
59	1	0	-1.925235	2.120801	1.527864
60	1	0	-1.657663	3.836513	1.088224
61	6	0	1.114166	5.963175	-0.383223
62	6	0	-0.105979	5.910523	-1.072380
63	6	0	1.751061	7.198029	-0.226697

64	6	0	-0.672320	7.072083	-1.593292
65	1	0	-0.610888	4.956695	-1.196303
66	6	0	1.189479	8.362119	-0.755725
67	1	0	2.693160	7.250572	0.314517
68	6	0	-0.024638	8.301200	-1.438813
69	1	0	-1.619796	7.019506	-2.123028
70	1	0	1.697790	9.313925	-0.627578
71	1	0	-0.466853	9.205545	-1.848004
72	1	0	-0.577305	1.450762	-0.353112
73	6	0	-4.213065	-1.565986	2.158859
74	6	0	-3.282903	-1.163389	3.319273
75	6	0	-5.565044	-2.089111	2.685214
76	1	0	-3.735760	-2.400006	1.640775
77	1	0	-3.704917	-0.339836	3.908328
78	1	0	-2.299814	-0.856705	2.950178
79	1	0	-6.215593	-2.407623	1.862827
80	1	0	-6.101924	-1.323968	3.258352
81	6	0	-3.930646	0.573550	-2.562866
82	6	0	-5.172754	0.634131	-3.474660
83	6	0	-2.957284	1.717531	-2.908720
84	1	0	-3.403084	-0.356983	-2.783650
85	1	0	-5.726031	1.570856	-3.337483
86	1	0	-5.867389	-0.188893	-3.273262
87	1	0	-2.032923	1.628945	-2.332417
88	1	0	-3.399945	2.703033	-2.717892
89	6	0	3.788856	-1.067303	2.891290
90	6	0	4.954683	-1.696200	3.682880
91	6	0	3.220672	0.128608	3.679033
92	1	0	2.987417	-1.806943	2.818310
93	1	0	5.776002	-0.980465	3.809653
94	1	0	5.364891	-2.581976	3.187199
95	1	0	2.398670	0.607341	3.144681
96	1	0	3.986649	0.887950	3.878286
97	6	0	3.754873	-1.617225	-2.267021
98	6	0	2.945407	-0.682459	-3.185983
99	6	0	4.970855	-2.209356	-3.007512
100	1	0	3.104337	-2.457010	-2.014240
101	1	0	3.532614	0.192941	-3.489860
102	1	0	2.035354	-0.334410	-2.687795
103	1	0	5.529984	-2.898026	-2.364224
104	1	0	5.664013	-1.428854	-3.342866
105	1	0	2.839825	-0.212159	4.649058
106	1	0	4.617898	-1.995932	4.682590
107	1	0	4.642235	-2.764260	-3.894369
108	1	0	2.646906	-1.213069	-4.098208
109	1	0	-4.876124	0.575765	-4.528811
110	1	0	-2.694294	1.677041	-3.972793
111	1	0	-3.137522	-2.012634	3.997681
112	1	0	-5.407519	-2.949518	3.346488
113	6	0	6.619991	1.902863	-0.039538
114	6	0	7.945967	1.347053	-0.595633
115	1	0	7.824393	0.985931	-1.623729
116	1	0	8.719793	2.124217	-0.602901
117	1	0	8.307737	0.509756	0.010722
118	6	0	6.147096	3.112678	-0.864851
119	1	0	6.926941	3.882526	-0.905362
120	1	0	5.909160	2.827444	-1.896510
121	1	0	5.251130	3.564554	-0.424702
122	6	0	-6.073745	3.047266	1.275781
123	6	0	-5.318806	3.760049	2.412996
124	1	0	-5.852842	4.666679	2.721470
125	1	0	-5.222021	3.116386	3.294990
126	1	0	-4.309600	4.052437	2.101756
127	6	0	-7.515133	2.707806	1.703127
128	1	0	-8.053938	3.614338	2.004169
129	1	0	-8.069607	2.236171	0.884569
130	1	0	-7.523446	2.015949	2.553668
131	8	0	-0.643243	-5.525615	-2.096067
132	8	0	-0.567673	-6.015376	0.547919
133	14	0	-0.522927	-4.784136	-0.592973
134	1	0	6.817683	2.260185	0.980469
135	1	0	-6.138957	3.749826	0.433249

TS-1st-(*S*)-reaction pathway: *S*-*syn*/(*S*)-1ea (Oxa-SPISIOL)



B3LYP/6-31G(d); E(RB3LYP) = -3445.49527041 Hartree

Zero-point correction= 1.140506 Hartree

Thermal correction to Energy= 1.207239 Hartree

Thermal correction to Enthalpy= 1.208184 Hartree

Thermal correction to Gibbs Free Energy= 1.035793 Hartree

Sum of electronic and zero-point Energies= -3444.354764 Hartree

Sum of electronic and thermal Energies= -3444.288031 Hartree

Sum of electronic and thermal Enthalpies= -3444.287087 Hartree

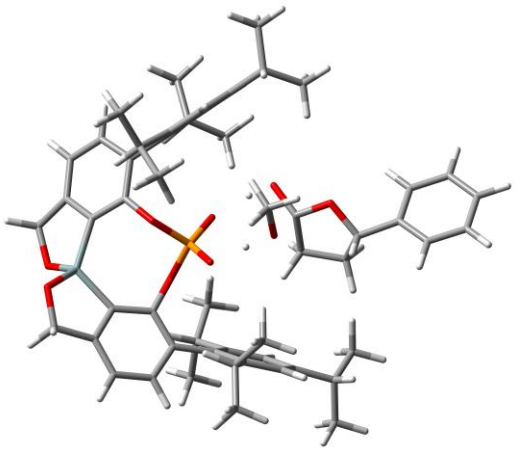
Sum of electronic and thermal Free Energies= -3444.459477 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.559823	3.278446	1.021508
2	6	0	-2.040747	2.181450	0.312555
3	6	0	-4.091281	2.330292	1.527374
4	6	0	-3.563606	3.312552	2.365797
5	6	0	-2.273715	3.778512	2.116807
6	1	0	-5.113453	2.000578	1.682362
7	1	0	-4.158510	3.700040	3.189622
8	6	0	-1.461520	4.747679	2.965948
9	1	0	-1.902925	5.753848	2.982862
10	1	0	-1.408522	4.390616	4.001967
11	6	0	1.312957	5.872209	-0.699320
12	1	0	1.815714	6.702691	-0.183623
13	1	0	1.171135	6.170100	-1.745801
14	6	0	2.117801	4.584013	-0.626784
15	6	0	1.473166	3.560507	0.080507
16	6	0	3.334444	4.332576	-1.257391
17	1	0	3.865866	5.114117	-1.795289
18	6	0	1.944004	2.249646	-0.002593
19	8	0	-1.185217	1.603004	-0.629365
20	8	0	1.154572	1.249625	0.572104
21	15	0	-0.053749	0.482747	-0.245862
22	8	0	0.448612	-0.079621	-1.547289
23	8	0	-0.626717	-0.473845	0.799495
24	6	0	-3.344857	1.697771	0.509975
25	6	0	3.179384	1.959162	-0.607021

26	6	0	-3.973526	0.605282	-0.303390
27	6	0	-4.182028	0.786797	-1.693762
28	6	0	-4.445984	-0.579406	0.323866
29	6	0	-4.847131	-0.211751	-2.415223
30	6	0	-5.112495	-1.535779	-0.448924
31	6	0	-5.326766	-1.376817	-1.819983
32	1	0	-5.009968	-0.067351	-3.480951
33	1	0	-5.477528	-2.435061	0.040724
34	6	0	3.863536	3.045157	-1.192835
35	1	0	4.829730	2.846421	-1.646493
36	6	0	3.839456	0.609838	-0.631977
37	6	0	4.018025	-0.080527	-1.858096
38	6	0	4.417056	0.095321	0.556014
39	6	0	4.776468	-1.257842	-1.864996
40	6	0	5.160162	-1.089522	0.487795
41	6	0	5.363304	-1.778933	-0.709324
42	1	0	4.924233	-1.773805	-2.810247
43	1	0	5.620691	-1.477400	1.392664
44	6	0	0.113599	-3.311158	-0.948847
45	8	0	-0.469761	-2.893090	0.560198
46	6	0	0.503189	-3.502317	1.473467
47	6	0	1.624664	-3.216241	-0.687144
48	1	0	2.088427	-4.095480	-1.140367
49	1	0	2.018828	-2.328710	-1.183460
50	8	0	-0.475677	-2.503492	-1.823560
51	8	0	-0.263541	-4.605773	-1.082591
52	6	0	-1.639799	-4.835973	-1.434725
53	1	0	-1.779456	-5.915020	-1.355853
54	1	0	-1.835286	-4.501945	-2.455853
55	1	0	-2.305713	-4.314709	-0.741976
56	1	0	-0.530676	-1.753913	0.659237
57	1	0	-0.100953	-1.564406	-1.791224
58	6	0	0.287335	-3.120418	2.918622
59	6	0	0.485684	-1.815348	3.394179
60	6	0	-0.094919	-4.118562	3.824414
61	6	0	0.302796	-1.525002	4.745919
62	1	0	0.749165	-1.017600	2.708692
63	6	0	-0.270271	-3.829446	5.178098
64	1	0	-0.254293	-5.133036	3.465913
65	6	0	-0.071109	-2.529003	5.641874
66	1	0	0.452382	-0.508225	5.098387
67	1	0	-0.563742	-4.617940	5.865855
68	1	0	-0.208261	-2.297642	6.694850
69	1	0	0.322444	-4.575220	1.367604
70	6	0	1.855210	-3.149729	0.839631
71	1	0	2.637873	-3.833448	1.180757
72	1	0	2.156557	-2.139550	1.129653
73	6	0	3.458312	0.430830	-3.188509
74	6	0	4.584844	0.975001	-4.092269
75	6	0	2.647359	-0.634058	-3.950676
76	1	0	2.770788	1.252584	-2.971548
77	1	0	5.291175	0.180799	-4.363167
78	1	0	5.156947	1.771089	-3.604308
79	1	0	1.811969	-0.994281	-3.347925
80	1	0	3.266100	-1.489412	-4.247901
81	6	0	4.351152	0.857239	1.881807
82	6	0	4.198603	-0.045658	3.117867
83	6	0	5.587285	1.768988	2.033317
84	1	0	3.471497	1.505429	1.858955
85	1	0	5.091888	-0.653471	3.303130
86	1	0	3.342748	-0.722364	3.024825
87	1	0	5.666704	2.474691	1.199740
88	1	0	6.508733	1.174599	2.060568
89	6	0	-3.768534	2.050047	-2.450226
90	6	0	-2.773774	1.743178	-3.586221
91	6	0	-5.000818	2.810851	-2.980487
92	1	0	-3.263467	2.723285	-1.754539
93	1	0	-3.227939	1.113139	-4.360628
94	1	0	-1.886308	1.230704	-3.204159
95	1	0	-5.690327	3.065716	-2.167646
96	1	0	-5.557106	2.218082	-3.716187
97	6	0	-4.271883	-0.864991	1.818265
98	6	0	-5.614047	-0.769719	2.573534
99	6	0	-3.624685	-2.236884	2.086156
100	1	0	-3.595782	-0.112466	2.232492
101	1	0	-6.319966	-1.528883	2.215436
102	1	0	-6.093916	0.206585	2.446866
103	1	0	-2.688471	-2.349415	1.536425
104	1	0	-4.288876	-3.062787	1.802905
105	1	0	2.234498	-0.197699	-4.868092
106	1	0	4.167014	1.381073	-5.021376
107	1	0	5.529080	2.347826	2.963139
108	1	0	4.041453	0.572651	4.009271
109	1	0	-2.450728	2.674642	-4.067074
110	1	0	-4.691985	3.743023	-3.468930
111	1	0	-3.405775	-2.346848	3.154953
112	1	0	-5.462564	-0.935082	3.647295
113	6	0	6.236973	-3.027219	-0.747566
114	6	0	7.532053	-2.780560	-1.546172
115	1	0	8.182526	-3.662977	-1.513293
116	1	0	7.313122	-2.565470	-2.598838
117	1	0	8.089780	-1.929205	-1.141227
118	6	0	5.489257	-4.260344	-1.286427
119	1	0	5.169694	-4.113859	-2.324893
120	1	0	6.135923	-5.145568	-1.260783
121	1	0	4.596612	-4.476220	-0.688776
122	6	0	-6.065931	-2.424361	-2.642226
123	6	0	-5.319430	-3.771301	-2.666116
124	1	0	-5.257394	-4.208276	-1.661983
125	1	0	-5.837752	-4.491457	-3.310928
126	1	0	-4.298166	-3.647101	-3.042830
127	6	0	-7.519306	-2.607979	-2.165827
128	1	0	-8.064288	-1.657925	-2.185019
129	1	0	-8.051052	-3.320471	-2.808178
130	1	0	-7.556567	-2.992858	-1.139706
131	14	0	-0.032370	4.292034	0.861503
132	8	0	-0.126656	4.834233	2.448539
133	8	0	0.029466	5.663083	-0.106716
134	1	0	-6.103851	-2.053731	-3.675774
135	1	0	6.528471	-3.247686	0.288646

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1ea (Oxa-SPISIOL)



B3LYP/6-31G(d); E(RB3LYP) = -3445.50002732 Hartree

Zero-point correction= 1.141781 Hartree

Thermal correction to Energy= 1.208492 Hartree

Thermal correction to Enthalpy= 1.209436 Hartree

Thermal correction to Gibbs Free Energy= 1.036981 Hartree

Sum of electronic and zero-point Energies= -3444.358246 Hartree

Sum of electronic and thermal Energies= -3444.291535 Hartree

Sum of electronic and thermal Enthalpies= -3444.290591 Hartree

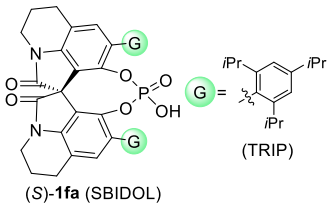
Sum of electronic and thermal Free Energies= -3444.463046 Hartree

The number of Imaginary frequencies = 1

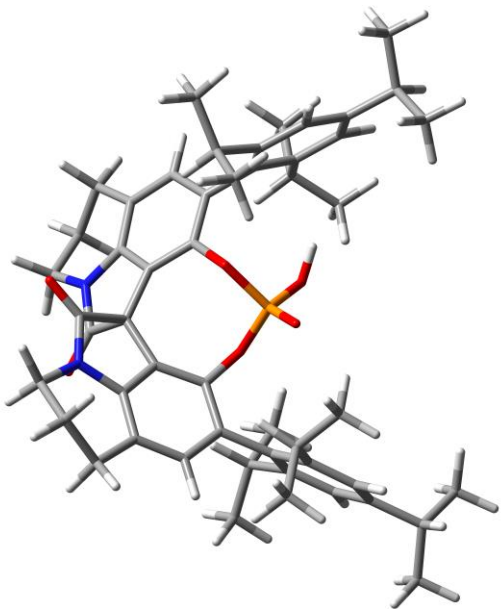
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.585444	1.064566	-0.114366
2	8	0	-3.777734	1.626586	-0.419079
3	8	0	-1.970568	0.638378	-1.662081
4	6	0	-4.771526	0.571319	-0.570017
5	6	0	-4.328337	-0.476940	0.471466
6	6	0	-2.795777	-0.320442	0.513309
7	1	0	-4.667326	0.162363	-1.582257
8	1	0	-4.774680	-0.233849	1.440779
9	1	0	-4.648558	-1.483520	0.192458
10	1	0	-2.389602	-0.318324	1.526780
11	1	0	-2.278440	-1.099487	-0.047695
12	8	0	-1.747549	1.945487	0.390227
13	6	0	-1.774440	1.773384	-2.532524
14	1	0	-1.142908	2.524023	-2.050552
15	1	0	-1.298718	1.402862	-3.442733
16	1	0	-2.754730	2.193161	-2.760651
17	1	0	-0.896608	1.478615	0.698816
18	1	0	-1.014057	0.141630	-1.511547
19	6	0	3.494308	-2.483913	-0.591706
20	6	0	2.155301	-2.569954	-0.215128
21	6	0	1.979318	-4.645684	-1.390357
22	6	0	3.263145	-4.494501	-1.914063
23	6	0	4.017192	-3.388896	-1.524495
24	1	0	1.402576	-5.526739	-1.653766
25	1	0	3.654813	-5.229415	-2.613520
26	6	0	5.369206	-2.963830	-2.080601
27	1	0	6.165139	-3.676990	-1.823774
28	1	0	5.323195	-2.897815	-3.174773
29	6	0	6.324206	-0.257336	1.679006
30	1	0	7.359210	-0.065634	1.362197
31	1	0	6.324720	-0.352854	2.771928
32	6	0	5.377202	0.854055	1.250546
33	6	0	4.407664	0.431452	0.331980
34	6	0	5.337220	2.154610	1.750597
35	1	0	6.093116	2.518048	2.442899
36	6	0	3.296734	1.232285	0.074212
37	6	0	4.289252	2.988807	1.361701
38	1	0	4.262821	4.010931	1.727860
39	8	0	1.629688	-1.533490	0.555574
40	8	0	2.283643	0.685106	-0.711553
41	15	0	1.011673	-0.161378	-0.100079
42	8	0	0.353551	0.564288	1.045000
43	8	0	0.187332	-0.499586	-1.335857
44	6	0	1.365098	-3.676261	-0.570838
45	6	0	3.215828	2.548502	0.560658
46	6	0	-6.153324	1.143011	-0.383753
47	6	0	-7.209878	0.669907	-1.168926
48	6	0	-6.410310	2.108447	0.598266
49	6	0	-8.508386	1.141597	-0.969484
50	1	0	-7.016362	-0.070637	-1.942107
51	6	0	-7.705247	2.588190	0.789698
52	1	0	-5.589793	2.494958	1.195284
53	6	0	-8.758322	2.103036	0.010204
54	1	0	-9.320340	0.764881	-1.585567
55	1	0	-7.892528	3.343872	1.547831
56	1	0	-9.766939	2.477627	0.162189
57	6	0	-0.047942	-3.881592	-0.108973
58	6	0	-0.321357	-4.084694	1.268312
59	6	0	-1.108640	-3.963293	-1.048929
60	6	0	-1.631385	-4.371104	1.668300
61	6	0	-2.399341	-4.253176	-0.587716
62	6	0	-2.687822	-4.469666	0.761184
63	1	0	-1.822781	-4.540839	2.724367
64	1	0	-3.209529	-4.330145	-1.310015
65	6	0	2.063930	3.463517	0.273955
66	6	0	1.232011	3.921580	1.330093
67	6	0	1.823578	3.908331	-1.048714
68	6	0	0.175561	4.787038	1.030069
69	6	0	0.740606	4.763741	-1.289210
70	6	0	-0.102597	5.210843	-0.271232
71	1	0	-0.459166	5.130989	1.842092
72	1	0	0.558440	5.108674	-2.305335
73	6	0	-0.908455	-3.778975	-2.555879
74	6	0	-1.056882	-5.118371	-3.308001
75	6	0	-1.863684	-2.735674	-3.165223
76	1	0	0.106434	-3.408345	-2.720087
77	1	0	-2.073990	-5.516032	-3.206397
78	1	0	-0.368642	-5.882064	-2.930900
79	1	0	-1.766733	-1.769455	-2.666252
80	1	0	-2.911775	-3.053099	-3.103604
81	6	0	0.761207	-4.060445	2.348423
82	6	0	0.499641	-2.965919	3.401030
83	6	0	0.922574	-5.443578	3.010893
84	1	0	1.717365	-3.827813	1.875337
85	1	0	-0.425813	-3.155489	3.958790
86	1	0	0.424517	-1.980475	2.932247
87	1	0	1.146983	-6.216665	2.267272
88	1	0	0.013678	-5.747079	3.543892
89	6	0	2.737517	3.551511	-2.222294
90	6	0	1.990662	2.825147	-3.356423
91	6	0	3.465268	4.803526	-2.753083
92	1	0	3.509946	2.868447	-1.860744
93	1	0	1.213125	3.459630	-3.800000
94	1	0	1.524587	1.905746	-2.990018
95	1	0	4.033355	5.298754	-1.957637
96	1	0	2.760276	5.535837	-3.164255
97	6	0	1.447468	3.534710	2.796406
98	6	0	1.942354	4.744763	3.616043
99	6	0	0.194467	2.922624	3.451367
100	1	0	2.224136	2.767216	2.837183
101	1	0	1.187113	5.539476	3.644529
102	1	0	2.856512	5.178015	3.194498
103	1	0	-0.113268	2.017476	2.923883
104	1	0	-0.647910	3.624104	3.466147
105	1	0	0.414687	2.652885	4.491731
106	1	0	2.153488	4.447908	4.650648
107	1	0	2.689323	2.554665	-4.157436
108	1	0	4.165699	4.529527	-3.551378
109	1	0	-1.629979	-2.593581	-4.227425
110	1	0	-0.856964	-4.982189	-4.377831
111	1	0	1.743042	-5.423537	3.738221
112	1	0	1.321083	-2.936351	4.127109
113	6	0	-4.093236	-4.867138	1.197113
114	6	0	-4.594833	-4.094267	2.429164
115	1	0	-4.006243	-4.331822	3.322727
116	1	0	-4.541522	-3.011149	2.274463
117	1	0	-5.637105	-4.356116	2.646129
118	6	0	-4.179741	-6.388194	1.438547
119	1	0	-5.203983	-6.685241	1.695331
120	1	0	-3.873606	-6.948021	0.548243
121	1	0	-3.523602	-6.689544	2.263880
122	6	0	-1.259534	6.153419	-0.576284
123	6	0	-2.600977	5.646020	-0.015512
124	1	0	-2.810491	4.620707	-0.336108
125	1	0	-2.602590	5.653449	1.080929
126	1	0	-3.422792	6.291222	-0.349201
127	6	0	-0.962036	7.582649	-0.081256
128	1	0	-1.777559	8.265478	-0.349566
129	1	0	-0.851311	7.604740	1.009618
130	1	0	-0.034567	7.969127	-0.518091
131	14	0	4.838673	-1.286950	-0.182012
132	8	0	5.886229	-1.497752	1.114783

133	8	0	5.713718	-1.674002	-1.562592
134	1	0	-4.768094	-4.630856	0.361895
135	1	0	-1.355172	6.199517	-1.670345

Optimized structure of SBIDOL-derived CPA (*S*)-1fa



distance: 4.68 Å (-2.1%)
angle: 101.3° (+1.7%)
dihedral: 57.2° (-6.5%)



B3LYP/6-31G(d); E(RB3LYP) = -2882.55683454 Hartree
Zero-point correction= 1.029830 Hartree
Thermal correction to Energy= 1.088754 Hartree
Thermal correction to Enthalpy= 1.089698 Hartree
Thermal correction to Gibbs Free Energy= 0.936293 Hartree
Sum of electronic and zero-point Energies= -2881.527005 Hartree
Sum of electronic and thermal Energies= -2881.468080 Hartree
Sum of electronic and thermal Enthalpies= -2881.467136 Hartree
Sum of electronic and thermal Free Energies= -2881.620542 Hartree
The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.636943	-2.076821	-0.604809
2	6	0	-1.262762	2.110213	0.381577
3	6	0	-1.780930	0.860519	0.076327
4	6	0	-3.817672	1.426234	1.233420
5	6	0	-3.270862	2.628531	1.698016
6	6	0	-1.992640	2.922349	1.250377
7	1	0	-4.831318	1.162288	1.521099
8	6	0	0.006747	2.837648	0.043290
9	6	0	1.963299	2.951414	-1.243097
10	6	0	1.309456	2.172711	-0.287078
11	6	0	3.223508	2.667932	-1.748803
12	6	0	1.884744	0.963971	0.064411
13	6	0	3.818330	1.489959	-1.281525
14	1	0	4.808909	1.224464	-1.639409
15	8	0	-0.955528	-0.054885	-0.594609
16	8	0	1.178073	0.106613	0.904872
17	15	0	0.055966	-0.929855	0.329043
18	8	0	0.766951	-1.720418	-0.871724
19	8	0	-0.514955	-1.692801	1.450340
20	6	0	-3.095130	0.504734	0.453480
21	6	0	3.164102	0.596671	-0.414665
22	6	0	3.774672	-0.727468	-0.053578
23	6	0	3.997093	-1.719284	-1.051466
24	6	0	4.132303	-1.003426	1.293139
25	6	0	4.531378	-2.957224	-0.663317
26	6	0	4.667254	-2.254551	1.613475
27	6	0	4.867275	-3.253417	0.657617
28	1	0	4.700796	-3.716431	-1.422806
29	1	0	4.938417	-2.452268	2.647125
30	6	0	-3.727035	-0.791272	0.034825
31	6	0	-4.024899	-1.015969	-1.334291
32	6	0	-4.079529	-1.770410	0.997251
33	6	0	-4.653547	-2.207646	-1.706530
34	6	0	-4.717137	-2.939616	0.564161
35	6	0	-5.010329	-3.186317	-0.776179
36	1	0	-4.879439	-2.369830	-2.757646
37	1	0	-4.989450	-3.691488	1.301035
38	6	0	-3.733791	0.011961	-2.429216
39	6	0	-2.783669	-0.543001	-3.507722
40	6	0	-5.037732	0.542107	-3.058572
41	1	0	-3.235757	0.871885	-1.974350
42	1	0	-3.233646	-1.384023	-4.048737
43	1	0	-1.845449	-0.888710	-3.063303
44	1	0	-5.696470	0.975632	-2.297787
45	1	0	-5.593951	-0.254820	-3.566207
46	6	0	-3.814922	-1.609555	2.495819
47	6	0	-5.126483	-1.348842	3.265867
48	6	0	-3.073869	-2.816374	3.102936
49	1	0	-3.164808	-0.741477	2.633568
50	1	0	-5.808549	-2.203686	3.182409
51	1	0	-5.658996	-0.468595	2.888146
52	1	0	-2.131805	-2.991961	2.580273
53	1	0	-3.678700	-3.730382	3.065676
54	6	0	3.742779	-1.485308	-2.546267
55	6	0	5.078931	-1.271085	-3.289783
56	6	0	2.947806	-2.614594	-3.232087
57	1	0	3.151516	-0.571773	-2.651432
58	1	0	5.696364	-2.176443	-3.252107
59	1	0	5.666511	-0.457052	-2.852306
60	1	0	1.969722	-2.769010	-2.767915
61	1	0	3.488209	-3.567846	-3.220016
62	6	0	4.015545	0.036577	2.408094
63	6	0	3.168246	-0.460241	3.594665
64	6	0	5.413522	0.490343	2.876320
65	1	0	3.517358	0.920608	2.003279
66	1	0	3.640081	-1.308515	4.104921
67	1	0	2.171269	-0.769631	3.267940
68	1	0	6.001834	0.890799	2.043048
69	1	0	5.978967	-0.339924	3.316103
70	1	0	3.052179	0.341666	4.333427
71	1	0	5.324447	1.274760	3.637223
72	1	0	2.774664	-2.354906	-4.282974
73	1	0	4.898045	-1.032356	-4.344797
74	1	0	-2.848523	-2.618753	4.158345
75	1	0	-4.921032	-1.189405	4.331650
76	1	0	-4.816693	1.319788	-3.799739
77	1	0	-2.549096	0.235329	-4.244389
78	6	0	-5.696142	-4.478704	-1.199300
79	6	0	-7.069865	-4.217194	-1.845321
80	1	0	-6.970124	-3.646515	-2.776318
81	1	0	-7.570725	-5.162589	-2.086972
82	1	0	-7.721209	-3.647358	-1.173543
83	6	0	-4.802172	-5.324517	-2.125759
84	1	0	-5.288657	-6.276705	-2.370320
85	1	0	-4.599664	-4.802078	-3.068337
86	1	0	-3.838690	-5.543454	-1.652941
87	6	0	5.438308	-4.614710	1.031377
88	6	0	6.865418	-4.501722	1.600293
89	1	0	6.876587	-3.937068	2.540057
90	1	0	7.277879	-5.496615	1.805836
91	1	0	7.534199	-3.993216	0.897230
92	6	0	4.514263	-5.375158	2.001517

93	1	0	4.914223	-6.374337	2.211077
94	1	0	4.419163	-4.847059	2.957553
95	1	0	3.508261	-5.490882	1.583923
96	6	0	-0.134558	3.867652	-1.168596
97	6	0	0.065985	3.931206	1.200986
98	8	0	1.005236	4.638297	1.498948
99	8	0	-1.113699	4.510383	-1.480038
100	7	0	-1.216500	3.996130	1.695239
101	7	0	1.128986	3.967593	-1.709307
102	6	0	-3.912397	3.598690	2.667102
103	6	0	-2.828056	4.290332	3.524769
104	1	0	-4.625443	3.078811	3.316622
105	1	0	-4.486654	4.360661	2.119960
106	6	0	-1.732790	4.952204	2.670251
107	1	0	-3.281718	5.056427	4.162886
108	1	0	-2.365912	3.547706	4.186615
109	1	0	-2.136738	5.821931	2.134792
110	1	0	-0.894439	5.296488	3.281591
111	6	0	3.781254	3.603957	-2.799739
112	6	0	2.631016	4.206711	-3.638672
113	1	0	4.482779	3.074651	-3.454284
114	1	0	4.350324	4.416069	-2.324128
115	6	0	1.556335	4.879190	-2.766836
116	1	0	3.024016	4.949159	-4.341595
117	1	0	2.164545	3.411315	-4.232770
118	1	0	0.673711	5.153525	-3.350528
119	1	0	1.952257	5.794817	-2.307654
120	1	0	-5.869387	-5.064655	-0.286132
121	1	0	5.499442	-5.203146	0.105557

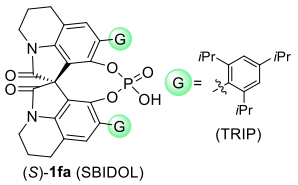
DFT calculation for all conformations of real system using SBIDOL-derived CPA (*S*)-1fa

TS	Orientation I	Orientation II	ΔΔG≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-anti	up	up	-3534.687278	-2.84
	up	down		
	down	up	-3534.687176	-2.77
	down	down		
S-anti	up	up	-3534.681598	0.73
	up	down	-3534.681219	0.97
	down	up	-3534.679384	2.12
	down	down	-3534.679369	2.13
S-syn	up	up	-3534.680196	1.61
	up	down	-3534.680501	1.42
	down	down	-3534.679993	1.73
	down	up	-3534.680469	1.44

TS	Orientation I	Orientation II	ΔΔG≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-re	up	up	-3534.682597	0.10
	up	down	-3534.682757	0.00
	down	up	-3534.682026	0.46
	down	down	-3534.682257	0.31
S-si	up	up	-3534.682354	0.25
	up	down		
	down	up		
	down	down		
S-re	up	up	-3534.683429	-0.42
	up	down		
	down	up		
	down	down		

* Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using SBIDOL-derived CPA (*S*)-1fa

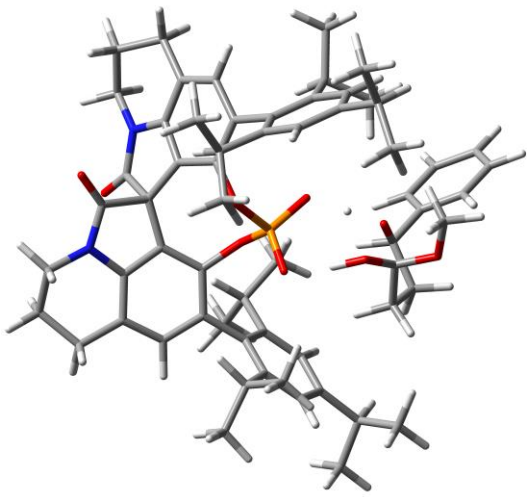


(*S*)-**1fa** (SBIDOL)

1st / 2nd	ΔΔG≠ (kcal/mol)
R-anti / ***R-re***	-2.84 / **0.00**
R-syn / *R-si*	-- / --
S-anti / ***S-si***	**0.73** / 0.25
S-syn / ***S-re***	**1.42** / -0.42

ΔΔG≠ of RDS = **0.73** kcal/mol

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1fa (SBIDOL)



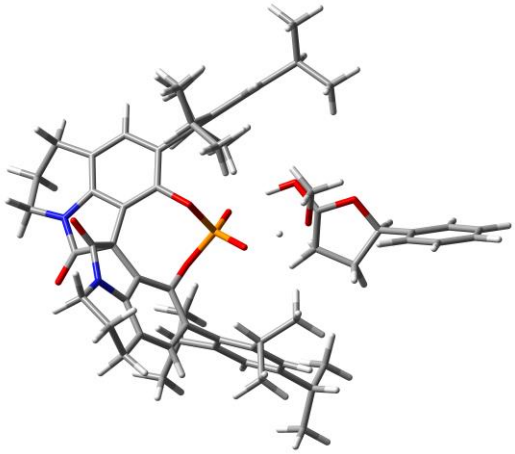
B3LYP/6-31G(d); E(RB3LYP) = -3535.83963680 Hartree

Zero-point correction= 1.263229 Hartree
Thermal correction to Energy= 1.335446 Hartree
Thermal correction to Enthalpy= 1.336390 Hartree
Thermal correction to Gibbs Free Energy= 1.152359 Hartree
Sum of electronic and zero-point Energies= -3534.576408 Hartree
Sum of electronic and thermal Energies= -3534.504191 Hartree
Sum of electronic and thermal Enthalpies= -3534.503247 Hartree
Sum of electronic and thermal Free Energies= -3534.687278 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.444499	-3.805891	-1.336587
2	8	0	-0.011625	-3.401012	0.248866
3	6	0	1.113066	-3.640852	1.150808
4	6	0	2.192189	-4.309267	0.273235
5	6	0	1.949513	-3.756868	-1.131106
6	1	0	1.466003	-2.656196	1.474819
7	1	0	2.071404	-5.396345	0.283312
8	1	0	3.190704	-4.072614	0.649719
9	1	0	2.437773	-4.343513	-1.914193
10	1	0	2.280954	-2.717764	-1.213810
11	8	0	-0.167630	-2.946027	-2.138295
12	8	0	0.010823	-5.076043	-1.480782
13	6	0	-1.387418	-5.247488	-1.777984
14	1	0	-1.558094	-6.324064	-1.738572
15	1	0	-1.618430	-4.862206	-2.773354
16	1	0	-2.002320	-4.737670	-1.031361
17	1	0	-0.327851	-2.310299	0.358699
18	1	0	0.186897	-2.002073	-2.028381
19	6	0	0.998188	3.163355	0.080986
20	6	0	1.664856	1.948175	0.066736
21	6	0	3.555440	3.025897	-0.985759

22	6	0	2.850426	4.226321	-1.134258
23	6	0	1.573475	4.237843	-0.598210
24	1	0	4.580015	2.969164	-1.343112
25	6	0	-0.323132	3.619534	0.623755
26	6	0	-2.262952	3.223194	1.863598
27	6	0	-1.534376	2.748357	0.773219
28	6	0	-3.518618	2.761363	2.218984
29	6	0	-2.001266	1.621661	0.116370
30	6	0	-4.033524	1.735292	1.415923
31	1	0	-5.039428	1.372911	1.606949
32	8	0	1.014467	0.828290	0.574955
33	8	0	-1.179774	1.014042	-0.830086
34	15	0	-0.014658	-0.039588	-0.367313
35	8	0	-0.588697	-1.074131	0.599632
36	8	0	0.646261	-0.529857	-1.627117
37	6	0	2.985937	1.863150	-0.435509
38	6	0	-3.294184	1.114416	0.392910
39	6	0	0.678608	-4.445608	2.353226
40	6	0	0.967430	-3.988753	3.642638
41	6	0	0.007792	-5.666409	2.196291
42	6	0	0.603912	-4.742804	4.760850
43	1	0	1.476147	-3.036491	3.773580
44	6	0	-0.362984	-6.415166	3.311146
45	1	0	-0.227775	-6.020126	1.196345
46	6	0	-0.062829	-5.956648	4.597241
47	1	0	0.835343	-4.376244	5.757347
48	1	0	-0.887206	-7.357971	3.178421
49	1	0	-0.351584	-6.542444	5.465841
50	6	0	-3.899820	-0.018496	-0.384160
51	6	0	-4.245163	-1.234788	0.258705
52	6	0	-4.195600	0.148933	-1.762372
53	6	0	-4.871766	-2.240120	-0.488970
54	6	0	-4.814080	-0.894160	-2.458156
55	6	0	-5.164569	-2.098609	-1.844873
56	1	0	-5.144073	-3.169719	0.005991
57	1	0	-5.040189	-0.752212	-3.512106
58	6	0	3.801560	0.603920	-0.380795
59	6	0	4.231931	0.091230	0.868017
60	6	0	4.224297	-0.031581	-1.578426
61	6	0	5.065880	-1.033947	0.890341
62	6	0	5.074803	-1.140599	-1.494333
63	6	0	5.514961	-1.659666	-0.273910
64	1	0	5.407458	-1.415720	1.850603
65	1	0	5.412243	-1.604138	-2.417602
66	6	0	3.820170	0.457360	-2.972138
67	6	0	5.023032	1.068570	-3.720439
68	6	0	3.170192	-0.647899	-3.825948
69	1	0	3.068230	1.240786	-2.850332
70	1	0	5.800689	0.316906	-3.902698
71	1	0	5.484418	1.886740	-3.156534
72	1	0	2.276433	-1.037018	-3.334341
73	1	0	3.860182	-1.478100	-4.019951
74	6	0	3.885978	0.756525	2.201176
75	6	0	3.094748	-0.179539	3.134303
76	6	0	5.150568	1.294961	2.900410
77	1	0	3.248252	1.620245	1.999742
78	1	0	3.673432	-1.074927	3.393972
79	1	0	2.156746	-0.492787	2.664757
80	1	0	5.695211	1.989236	2.250978
81	1	0	5.837922	0.486201	3.175783
82	6	0	-3.984814	-1.502064	1.743110
83	6	0	-5.295368	-1.466665	2.557323
84	6	0	-3.258604	-2.837191	1.992893
85	1	0	-3.330812	-0.710772	2.118688
86	1	0	-5.979307	-2.260792	2.233774
87	1	0	-5.825184	-0.514547	2.447119
88	1	0	-2.335908	-2.903246	1.413809
89	1	0	-3.886877	-3.699361	1.738073
90	6	0	-3.919598	1.447121	-2.522988
91	6	0	-2.969115	1.229753	-3.715822
92	6	0	-5.232704	2.118107	-2.974111
93	1	0	-3.429171	2.149085	-1.844893
94	1	0	-3.413923	0.572632	-4.472966
95	1	0	-2.025105	0.784324	-3.388802
96	1	0	-5.892534	2.311076	-2.120765
97	1	0	-5.782954	1.492019	-3.686639
98	1	0	4.708107	1.463705	-4.693966
99	1	0	2.870706	-0.239108	-4.798756
100	1	0	4.880029	1.830422	3.818316
101	1	0	2.847525	0.336572	4.069919
102	1	0	-2.998264	-2.929579	3.054102
103	1	0	-5.089477	-1.617918	3.624275
104	1	0	-2.746197	2.187722	-4.201561
105	1	0	-5.022913	3.076442	-3.464407
106	6	0	-5.858510	-3.214798	-2.614656
107	6	0	-5.012253	-3.715919	-3.799658
108	1	0	-4.019897	-4.041011	-3.467713
109	1	0	-5.502726	-4.561824	-4.296614
110	1	0	-4.867962	-2.928586	-4.548655
111	6	0	-7.265110	-2.794799	-3.082935
112	1	0	-7.884614	-2.477518	-2.237004
113	1	0	-7.213730	-1.958561	-3.790270
114	1	0	-7.772489	-3.627158	-3.585930
115	6	0	6.512928	-2.809735	-0.197470
116	6	0	6.135283	-4.013074	-1.078427
117	1	0	6.142694	-3.753418	-2.143379
118	1	0	6.852145	-4.830381	-0.936477
119	1	0	5.137353	-4.393124	-0.834083
120	6	0	7.935996	-2.318070	-0.532966
121	1	0	8.666192	-3.128520	-0.418030
122	1	0	7.991169	-1.958266	-1.567442
123	1	0	8.233754	-1.493006	0.122999
124	6	0	3.340052	5.475094	-1.839596
125	6	0	2.509833	6.710118	-1.424169
126	1	0	3.273254	5.338848	-2.929109
127	1	0	4.399855	5.651073	-1.618582
128	6	0	0.994819	6.463077	-1.525748
129	1	0	2.750370	6.978480	-0.388368
130	1	0	2.771029	7.568002	-2.053097
131	1	0	0.418858	7.308385	-1.139730
132	1	0	0.697299	6.306018	-2.572257
133	6	0	-4.190935	3.384766	3.425564
134	6	0	-3.566699	4.757930	3.761538
135	1	0	-4.094828	2.716460	4.294092
136	1	0	-5.266975	3.502098	3.248561
137	6	0	-2.030514	4.706670	3.835530
138	1	0	-3.853550	5.485161	2.992435
139	1	0	-3.954338	5.123641	4.718540
140	1	0	-1.597765	5.700478	3.978629
141	1	0	-1.704362	4.075923	4.674761
142	7	0	0.660008	5.284697	-0.735111
143	7	0	-1.521077	4.163861	2.582193
144	6	0	-0.573570	4.946624	-0.228286
145	6	0	-0.261278	4.324616	2.053010
146	8	0	-1.599240	5.587107	-0.319682
147	8	0	0.653066	4.967024	2.525083
148	1	0	-5.982617	-4.056918	-1.919422
149	1	0	6.524746	-3.156494	0.845424

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1fa (SBIDOL)



B3LYP/6-31G(d); E(RB3LYP) = -3535.83695266 Hartree

Zero-point correction= 1.264440 Hartree

Thermal correction to Energy= 1.336548 Hartree

Thermal correction to Enthalpy= 1.337492 Hartree

Thermal correction to Gibbs Free Energy= 1.154196 Hartree

Sum of electronic and zero-point Energies= -3534.572512 Hartree

Sum of electronic and thermal Energies= -3534.500405 Hartree

Sum of electronic and thermal Enthalpies= -3534.499460 Hartree

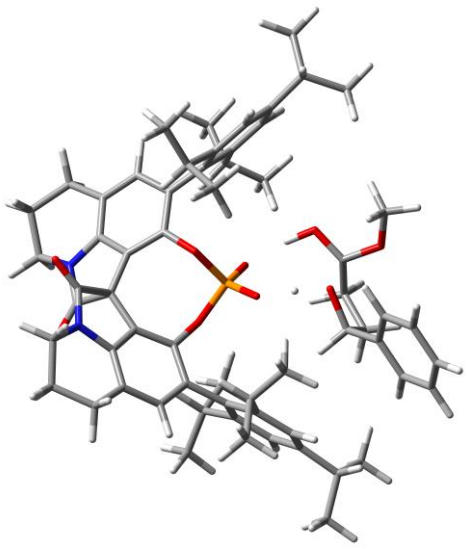
Sum of electronic and thermal Free Energies= -3534.682757 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.398985	1.129833	-0.598271
2	8	0	4.646041	1.629475	-0.437000
3	8	0	2.956781	0.655776	0.977869
4	6	0	5.663961	0.618371	-0.750828
5	6	0	4.876757	-0.698624	-0.906630
6	6	0	3.477978	-0.218426	-1.304433
7	1	0	6.083983	0.923671	-1.716118
8	1	0	4.840546	-1.240159	0.041876
9	1	0	5.339279	-1.351752	-1.651284
10	1	0	2.671896	-0.897915	-1.027491
11	1	0	3.402431	-0.017463	-2.379011
12	8	0	2.538864	2.065270	-0.961208
13	6	0	2.889631	1.761751	1.906066
14	1	0	3.889799	2.186769	1.992918
15	1	0	2.562990	1.354148	2.864908
16	1	0	2.185414	2.518871	1.553187
17	1	0	1.961272	0.182157	0.934179
18	1	0	1.631725	1.650462	-1.150594
19	6	0	-3.596790	0.694595	0.039074
20	6	0	-2.467036	1.493740	0.124054
21	6	0	-3.653749	3.260707	-1.021261
22	6	0	-4.761216	2.434888	-1.246492
23	6	0	-4.676939	1.159456	-0.711492
24	1	0	-3.671605	4.279206	-1.399266
25	6	0	-3.927060	-0.689756	0.510907
26	6	0	-3.404874	-2.615735	1.726039
27	6	0	-2.931081	-1.795727	0.700941
28	6	0	-2.810051	-3.807693	2.105881
29	6	0	-1.698632	-2.097102	0.141819
30	6	0	-1.652657	-4.158819	1.400847
31	1	0	-1.168271	-5.104842	1.624592
32	8	0	-1.329195	0.967500	0.725274
33	8	0	-1.113351	-1.182907	-0.728814
34	15	0	-0.249547	0.080914	-0.141937
35	8	0	0.745513	-0.393371	0.912977
36	8	0	0.276692	0.814321	-1.345142
37	6	0	-2.483232	2.816545	-0.380132
38	6	0	-1.051595	-3.319384	0.445622
39	6	0	6.757610	0.627756	0.289085
40	6	0	8.072384	0.921593	-0.085296
41	6	0	6.483852	0.330503	1.632046
42	6	0	9.101648	0.911521	0.858510
43	1	0	8.293461	1.161770	-1.122884
44	6	0	7.507852	0.328734	2.576923
45	1	0	5.465759	0.102497	1.934680
46	6	0	8.820483	0.616739	2.192112
47	1	0	10.118662	1.139661	0.551456
48	1	0	7.283204	0.099715	3.615220
49	1	0	9.618113	0.612052	2.930032
50	6	0	0.222206	-3.742571	-0.227244
51	6	0	1.409043	-3.942598	0.524502
52	6	0	0.229567	-4.011654	-1.621206
53	6	0	2.558121	-4.401097	-0.133329
54	6	0	1.408803	-4.461969	-2.223227
55	6	0	2.586745	-4.668096	-1.502165
56	1	0	3.464752	-4.564545	0.445341
57	1	0	1.397670	-4.673914	-3.289500
58	6	0	-1.293530	3.723757	-0.269598
59	6	0	-0.858924	4.173626	1.003430
60	6	0	-0.613220	4.162835	-1.434527
61	6	0	0.256946	5.014073	1.085744
62	6	0	0.488608	5.014144	-1.289980
63	6	0	0.952744	5.443922	-0.047555
64	1	0	0.579089	5.356758	2.066414
65	1	0	1.013454	5.348801	-2.181603
66	6	0	-1.606050	3.835804	2.295174
67	6	0	-0.716342	3.114274	3.324424
68	6	0	-2.245238	5.099008	2.907036
69	1	0	-2.426174	3.156604	2.050004
70	1	0	0.119733	3.745200	3.650952
71	1	0	-0.310492	2.187985	2.906750
72	1	0	-2.913352	5.590325	2.190960
73	1	0	-1.485272	5.829620	3.209008
74	6	0	-1.040011	3.779554	-2.854351
75	6	0	-1.657853	4.990195	-3.585359
76	6	0	0.104954	3.181932	-3.694231
77	1	0	-1.809091	3.006775	-2.780830
78	1	0	-0.918724	5.789175	-3.720078
79	1	0	-2.501794	5.416697	-3.031467
80	1	0	0.503116	2.283009	-3.219924
81	1	0	0.924750	3.894750	-3.841756
82	6	0	1.494083	-3.708746	2.034956
83	6	0	1.579835	-5.044681	2.802865
84	6	0	2.674326	-2.804866	2.438051
85	1	0	0.582488	-3.194178	2.348641
86	1	0	2.498819	-5.586249	2.547602
87	1	0	0.737652	-5.706331	2.574294
88	1	0	2.632014	-1.847811	1.914657
89	1	0	3.642919	-3.274490	2.227562
90	6	0	-1.015487	-3.887239	-2.501162
91	6	0	-0.816074	-2.878856	-3.648765
92	6	0	-1.455590	-5.263436	-3.040061
93	1	0	-1.838503	-3.516229	-1.886641
94	1	0	-0.036641	-3.208887	-4.346524
95	1	0	-0.536292	-1.894722	-3.261816
96	1	0	-1.637907	-5.969467	-2.222111
97	1	0	-0.695866	-5.702835	-3.697562
98	1	0	-1.744955	-2.769942	-4.221849
99	1	0	-2.382362	-5.167747	-3.618491
100	1	0	2.639135	-2.605161	3.516239
101	1	0	1.586923	-4.867059	3.885483
102	1	0	-0.270364	2.906059	-4.687685
103	1	0	-2.017128	4.697271	-4.579696
104	1	0	-2.832177	4.839161	3.796387

105	1	0	-1.300571	2.856902	4.216344
106	6	0	2.178328	6.342605	0.052307
107	6	0	1.877809	7.667418	0.776926
108	1	0	1.595482	7.497487	1.822784
109	1	0	2.761074	8.317604	0.774853
110	1	0	1.055754	8.206688	0.293414
111	6	0	3.364937	5.608218	0.706018
112	1	0	4.261878	6.239917	0.702792
113	1	0	3.142064	5.354618	1.750178
114	1	0	3.594159	4.679232	0.173614
115	6	0	3.849813	-5.200284	-2.167241
116	6	0	3.672337	-6.661487	-2.624348
117	1	0	2.893837	-6.742894	-3.392196
118	1	0	4.604780	-7.052791	-3.049369
119	1	0	3.381812	-7.304477	-1.786492
120	6	0	4.318136	-4.315212	-3.336677
121	1	0	5.261834	-4.689371	-3.751538
122	1	0	3.582134	-4.300726	-4.148918
123	1	0	4.474070	-3.279767	-3.013143
124	6	0	-4.750674	-0.765846	1.872714
125	6	0	-5.147378	-1.067397	-0.448511
126	8	0	-5.648456	-2.160206	-0.610630
127	8	0	-5.537936	0.047512	2.308685
128	7	0	-5.593645	0.132707	-0.951644
129	7	0	-4.483344	-2.017205	2.381369
130	6	0	-5.990806	2.772953	-2.062302
131	6	0	-6.530113	1.504041	-2.761534
132	1	0	-5.758436	3.539805	-2.809874
133	1	0	-6.775226	3.194521	-1.416571
134	6	0	-6.778575	0.349082	-1.775528
135	1	0	-7.468820	1.726772	-3.280590
136	1	0	-5.808091	1.178012	-3.520255
137	1	0	-7.629513	0.581059	-1.120798
138	1	0	-7.003120	-0.586401	-2.294841
139	6	0	-3.437409	-4.567855	3.255046
140	6	0	-4.116273	-3.584116	4.235684
141	1	0	-2.682057	-5.159379	3.784811
142	1	0	-4.185030	-5.281791	2.879128
143	6	0	-5.116563	-2.648239	3.534294
144	1	0	-4.646374	-4.135754	5.019823
145	1	0	-3.345140	-2.978928	4.728078
146	1	0	-5.467763	-1.857010	4.202065
147	1	0	-5.995035	-3.212761	3.193279
148	1	0	2.476147	6.591450	-0.975538
149	1	0	4.643819	-5.188657	-1.407491

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1fa (SBIDOL)

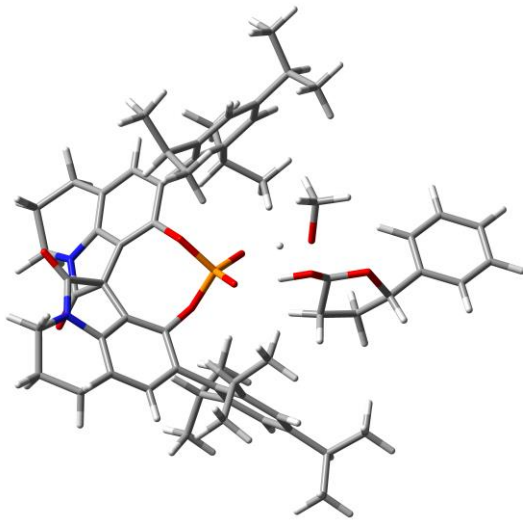


B3LYP/6-31G(d); E(RB3LYP) = -3535.83374456 Hartree
Zero-point correction= 1.263191 Hartree)
Thermal correction to Energy= 1.335448 Hartree
Thermal correction to Enthalpy= 1.336393 Hartree
Thermal correction to Gibbs Free Energy= 1.152146 Hartree
Sum of electronic and zero-point Energies= -3534.570554 Hartree
Sum of electronic and thermal Energies= -3534.498296 Hartree
Sum of electronic and thermal Enthalpies= -3534.497352 Hartree
Sum of electronic and thermal Free Energies= -3534.681598 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.218037	3.671545	-0.976209
2	8	0	1.959635	2.763670	0.231546
3	6	0	3.316980	2.465624	-0.193897
4	6	0	3.424923	2.954034	-1.666429
5	6	0	1.982354	3.091348	-2.153578
6	1	0	3.410990	1.374681	-0.161442
7	1	0	3.930642	3.922239	-1.704630
8	1	0	3.993887	2.244505	-2.272365
9	1	0	1.886808	3.760279	-3.013371
10	1	0	1.538965	2.124773	-2.407837
11	8	0	-0.086383	3.474894	-0.837777
12	8	0	1.605720	4.940084	-0.731578
13	6	0	0.907806	5.642741	0.308929
14	1	0	1.423716	6.598709	0.405785
15	1	0	-0.136993	5.797218	0.033656
16	1	0	0.965017	5.087782	1.249562
17	1	0	1.387021	1.780936	0.464924
18	1	0	-0.344616	2.539529	-1.121220
19	6	0	-2.847683	-1.955377	-0.115809
20	6	0	-2.701958	-0.598410	0.127653
21	6	0	-4.883938	-0.227488	-0.842550
22	6	0	-4.983148	-1.559198	-1.260461
23	6	0	-3.931772	-2.377271	-0.885711
24	1	0	-5.703261	0.452537	-1.056402
25	6	0	-2.043042	-3.170945	0.227968
26	6	0	-0.294713	-4.191193	1.388512
27	6	0	-0.561479	-3.193791	0.449411
28	6	0	0.976868	-4.614123	1.736486
29	6	0	0.500200	-2.437906	-0.025882
30	8	0	-1.513932	-0.150074	0.708023
31	8	0	0.232733	-1.335428	-0.831501
32	15	0	-0.208474	0.129849	-0.244927
33	8	0	0.852506	0.657124	0.727004
34	8	0	-0.530742	0.971249	-1.450029
35	6	0	-3.748174	0.298824	-0.198163
36	6	0	1.831014	-2.820655	0.270550
37	6	0	4.336035	3.091688	0.741158
38	6	0	3.967196	3.659401	1.964715
39	6	0	5.692933	3.074954	0.387243
40	6	0	4.932488	4.207821	2.812155
41	1	0	2.921755	3.667038	2.251789
42	6	0	6.657547	3.618673	1.235216
43	1	0	6.000634	2.635244	-0.558267
44	6	0	6.279847	4.190227	2.452067
45	1	0	4.627315	4.647444	3.758254
46	1	0	7.704275	3.598194	0.943028
47	1	0	7.029948	4.616394	3.112794
48	6	0	-3.725309	1.763540	0.129025
49	6	0	-3.730971	2.191410	1.480007
50	6	0	-3.819849	2.731099	-0.909049
51	6	0	-3.848759	3.558398	1.758712
52	6	0	-3.940822	4.082063	-0.566901
53	6	0	-3.972084	4.521553	0.758685
54	1	0	-3.871975	3.881328	2.797395
55	1	0	-4.028276	4.813338	-1.366689

56	6	0	2.025909	-3.934680	1.108739
57	1	0	3.048016	-4.246874	1.305460
58	6	0	3.037291	-2.104137	-0.259326
59	6	0	3.952638	-1.498362	0.641617
60	6	0	3.326874	-2.111048	-1.647363
61	6	0	5.125355	-0.927436	0.130445
62	6	0	4.516419	-1.527286	-2.099206
63	6	0	5.438811	-0.939141	-1.230956
64	1	0	5.830325	-0.470040	0.821569
65	1	0	4.736638	-1.562064	-3.162777
66	6	0	-3.834700	2.368329	-2.398242
67	6	0	-5.216943	2.641901	-3.027833
68	6	0	-2.743314	3.096075	-3.205969
69	1	0	-3.629839	1.298989	-2.490054
70	1	0	-5.456255	3.711955	-3.007424
71	1	0	-6.021415	2.118120	-2.500285
72	1	0	-1.748345	2.857680	-2.827141
73	1	0	-2.869290	4.184851	-3.180721
74	6	0	-3.680023	1.225607	2.664644
75	6	0	-2.440673	1.465489	3.547926
76	6	0	-4.976502	1.287515	3.497182
77	1	0	-3.607763	0.206564	2.278772
78	1	0	-2.459244	2.461974	4.006082
79	1	0	-1.519768	1.372923	2.964775
80	1	0	-5.855715	1.080897	2.876681
81	1	0	-5.116766	2.272444	3.958168
82	6	0	2.429014	-2.795613	-2.679130
83	6	0	1.906359	-1.808627	-3.740170
84	6	0	3.146753	-3.990993	-3.338091
85	1	0	1.557418	-3.202293	-2.161783
86	1	0	2.725539	-1.371490	-4.324433
87	1	0	1.340368	-0.995841	-3.275428
88	1	0	3.487127	-4.711997	-2.586450
89	1	0	4.022654	-3.671284	-3.915229
90	6	0	3.741257	-1.462499	2.158788
91	6	0	4.814490	-2.292643	2.892655
92	6	0	3.693049	-0.029874	2.719847
93	1	0	2.771270	-1.913906	2.377517
94	1	0	5.814729	-1.864710	2.755940
95	1	0	4.848147	-3.326841	2.531355
96	1	0	2.861508	0.527171	2.280969
97	1	0	4.621155	0.520853	2.531427
98	1	0	1.240895	-2.325513	-4.442178
99	1	0	2.467757	-4.511290	-4.024156
100	1	0	3.541929	-0.058852	3.806105
101	1	0	4.608821	-2.316020	3.969747
102	1	0	-5.232250	2.318000	-4.075815
103	1	0	-2.788801	2.783778	-4.256603
104	1	0	-4.947678	0.543798	4.302656
105	1	0	-2.405721	0.729269	4.360374
106	6	0	6.785546	-0.408723	-1.710686
107	6	0	7.790706	-1.566910	-1.881501
108	1	0	7.456930	-2.259498	-2.663507
109	1	0	8.780131	-1.187326	-2.164907
110	1	0	7.895979	-2.138394	-0.953140
111	6	0	6.704930	0.426884	-2.999073
112	1	0	6.373654	-0.174236	-3.853548
113	1	0	6.009101	1.267076	-2.894291
114	1	0	7.690689	0.834959	-3.251396
115	6	0	-4.179644	5.988915	1.112713
116	6	0	-3.057330	6.892103	0.571103
117	1	0	-3.009648	6.858647	-0.523799
118	1	0	-3.222080	7.935725	0.865769
119	1	0	-2.081886	6.579724	0.959095
120	6	0	-5.560385	6.491531	0.647969
121	1	0	-5.724426	7.527828	0.967871
122	1	0	-5.646461	6.461947	-0.444760
123	1	0	-6.364920	5.874208	1.062112
124	6	0	-2.572279	-4.220999	-0.852082
125	6	0	-2.570234	-3.962976	1.510415
126	8	0	-2.090557	-5.295781	-1.141803
127	8	0	-3.709118	-4.041139	1.919678
128	7	0	-1.474773	-4.652640	1.974229
129	7	0	-3.772471	-3.706664	-1.282905
130	6	0	1.107224	-5.726393	2.757416
131	6	0	-0.209782	-6.524559	2.880618
132	1	0	1.372524	-5.304277	3.738011
133	1	0	1.925865	-6.403570	2.485087
134	6	0	-1.434305	-5.612857	3.070344
135	1	0	-0.358634	-7.122979	1.973768
136	1	0	-0.151455	-7.219232	3.725466
137	1	0	-2.368794	-6.180226	3.061172
138	1	0	-1.375743	-5.080414	4.030267
139	6	0	-6.101628	-2.165386	-2.083687
140	6	0	-6.111146	-3.705484	-1.958847
141	1	0	-5.982200	-1.884309	-3.140487
142	1	0	-7.072190	-1.763229	-1.768743
143	6	0	-4.723300	-4.325040	-2.198722
144	1	0	-6.448236	-3.986570	-0.953851
145	1	0	-6.819378	-4.136866	-2.674471
146	1	0	-4.722404	-5.402850	-2.015233
147	1	0	-4.400675	-4.162020	-3.236852
148	1	0	7.173612	0.245020	-0.916815
149	1	0	-4.157531	6.061415	2.208895

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1fa (SBIDOL)



B3LYP/6-31G(d); E(RB3LYP) = -3535.83598552 Hartree

Zero-point correction= 1.264271 Hartree

Thermal correction to Energy= 1.336464 Hartree

Thermal correction to Enthalpy= 1.337408 Hartree

Thermal correction to Gibbs Free Energy= 1.153631 Hartree

Sum of electronic and zero-point Energies= -3534.571714 Hartree

Sum of electronic and thermal Energies= -3534.499521 Hartree

Sum of electronic and thermal Enthalpies= -3534.498577 Hartree

Sum of electronic and thermal Free Energies= -3534.682354 Hartree

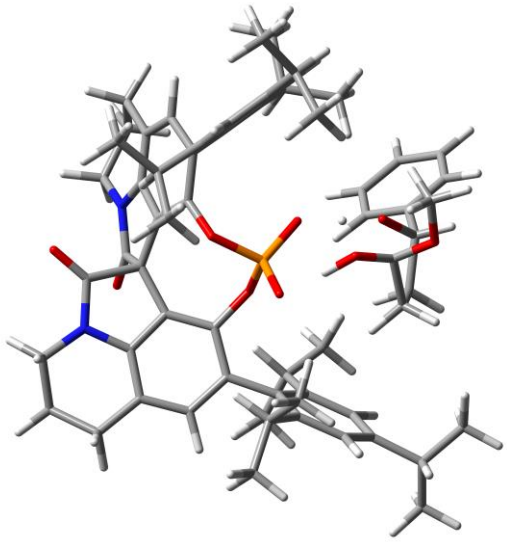
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.205830	-1.450507	-0.108601
2	6	0	1.912761	-1.918140	0.067029
3	6	0	2.564747	-4.007170	-0.959689
4	6	0	3.821440	-3.500477	-1.311770
5	6	0	4.086635	-2.214154	-0.874685
6	1	0	2.320068	-5.032487	-1.220878

7	6	0	3.934838	-0.210157	0.312158	76	6	0	-1.628047	3.435558	2.664593
8	6	0	4.016498	1.757266	1.570002	77	1	0	0.487682	3.375887	2.453907
9	6	0	3.294516	1.122508	0.558976	78	1	0	-0.827412	6.112138	2.907156
10	6	0	3.800372	3.062236	1.979191	79	1	0	0.913359	5.833306	2.798557
11	6	0	2.169547	1.758332	0.055973	80	1	0	-1.784189	2.490693	2.138755
12	6	0	2.752058	3.727596	1.333827	81	1	0	-2.490663	4.088456	2.483062
13	1	0	2.560020	4.768672	1.578585	82	6	0	-0.230615	-4.085321	-2.589546
14	8	0	0.968748	-1.068776	0.638580	83	6	0	0.184443	-5.403635	-3.276060
15	8	0	1.352111	1.062673	-0.826128	84	6	0	-1.376693	-3.429908	-3.382965
16	15	0	0.187620	0.026302	-0.309159	85	1	0	0.617246	-3.397287	-2.632800
17	8	0	-0.756007	0.726912	0.665507	86	1	0	-0.645627	-6.120623	-3.285414
18	8	0	-0.387153	-0.598295	-1.549107	87	1	0	1.027908	-5.886697	-2.771772
19	6	0	1.575077	-3.238628	-0.319245	88	1	0	-1.703068	-2.499277	-2.916286
20	6	0	1.891792	3.100839	0.412835	89	1	0	-2.246032	-4.092688	-3.472151
21	6	0	0.236826	-3.862136	-0.044371	90	6	0	0.672936	-3.721646	2.506262
22	6	0	-0.171802	-4.107042	1.290726	91	6	0	-0.062309	-2.737588	3.435926
23	6	0	-0.584061	-4.307057	-1.116142	92	6	0	1.141196	-4.971125	3.279354
24	6	0	-1.374103	-4.788461	1.520387	93	1	0	1.575267	-3.217303	2.153984
25	6	0	-1.764875	-5.000195	-0.824480	94	1	0	-0.975888	-3.179736	3.852147
26	6	0	-2.180506	-5.259786	0.484449	95	1	0	-0.333491	-1.822079	2.901556
27	1	0	-1.677075	-4.985988	2.546607	96	1	0	1.695654	-5.655133	2.627231
28	1	0	-2.372940	-5.357177	-1.651848	97	1	0	0.296454	-5.525936	3.704751
29	6	0	0.738465	3.882868	-0.143930	98	1	0	-1.039949	-3.197609	-4.400335
30	6	0	-0.263014	4.389658	0.724996	99	1	0	0.474844	-5.217840	-4.317376
31	6	0	0.688659	4.205359	-1.525106	100	1	0	1.800672	-4.681979	4.106391
32	6	0	-1.263754	5.215922	0.195722	101	1	0	0.582273	-2.459433	4.278659
33	6	0	-0.346216	5.019380	-1.998340	102	1	0	-0.016870	5.122345	4.130815
34	6	0	-1.328860	5.548234	-1.158080	103	1	0	-1.601805	3.221391	3.740132
35	1	0	-2.018859	5.621432	0.866522	104	1	0	1.962260	2.557442	-4.329650
36	1	0	-0.366982	5.267558	-3.056624	105	1	0	3.338221	4.618015	-3.750552
37	6	0	-3.572528	-0.375039	-0.815367	106	6	0	-3.433644	-6.074465	0.782224
38	8	0	-4.910682	-0.216674	-0.967910	107	6	0	-4.698931	-5.492255	0.126916
39	8	0	-3.088867	1.022265	-0.024743	108	1	0	-4.625949	-5.498986	-0.966846
40	1	0	-1.952954	-0.495716	-1.858170	109	1	0	-5.582175	-6.080725	0.402674
41	6	0	-5.646775	-0.900786	0.099732	110	1	0	-4.870375	-4.457128	0.444150
42	6	0	-4.565464	-1.326323	1.113534	111	6	0	-3.244022	-7.551323	0.382526
43	6	0	-3.311818	-1.441684	0.241884	112	1	0	-4.124463	-8.145392	0.656450
44	1	0	-6.088803	-1.785970	-0.372460	113	1	0	-3.095213	-7.650685	-0.699316
45	1	0	-4.435458	-0.556085	1.878580	114	1	0	-2.370028	-7.985133	0.880106
46	1	0	-4.832405	-2.260334	1.614983	115	6	0	-2.416066	6.477688	-1.682927
47	1	0	-2.375944	-1.294923	0.780841	116	6	0	-3.275514	5.818849	-2.777786
48	1	0	-3.257893	-2.405310	-0.275476	117	1	0	-4.075188	6.496040	-3.100919
49	8	0	-2.950932	-0.374772	-1.988206	118	1	0	-2.676321	5.568288	-3.660849
50	6	0	-3.237067	2.208326	-0.840833	119	1	0	-3.740886	4.894006	-2.418454
51	1	0	-2.906331	3.055293	-0.240295	120	6	0	-1.826184	7.812447	-2.178613
52	1	0	-2.633197	2.129148	-1.747082	121	1	0	-2.623682	8.495591	-2.495182
53	1	0	-4.293047	2.299749	-1.097181	122	1	0	-1.246401	8.305123	-1.390536
54	6	0	-6.750627	-0.019134	0.631046	123	1	0	-1.159574	7.656963	-3.035119
55	6	0	-6.468200	1.232292	1.197377	124	6	0	5.153793	-0.192154	-0.716695
56	6	0	-8.077781	-0.456221	0.580765	125	6	0	4.816479	-0.388029	1.631799
57	6	0	-7.496096	2.025800	1.702437	126	8	0	5.369705	-1.392953	2.025656
58	1	0	-5.440697	1.582644	1.238125	127	8	0	5.925131	0.717051	-0.938957
59	6	0	-9.108477	0.333769	1.094548	128	7	0	5.229311	-1.479189	-1.196992
60	1	0	-8.307895	-1.421297	0.134804	129	7	0	4.925955	0.877221	2.159641
61	6	0	-8.819290	1.577465	1.654918	130	6	0	4.884750	-4.210953	-2.124752
62	1	0	-7.265616	2.995219	2.136248	131	6	0	6.270246	-3.558577	-1.917963
63	1	0	-10.134668	-0.020755	1.049978	132	1	0	4.621376	-4.180319	-3.192362
64	1	0	-9.619191	2.196860	2.051584	133	1	0	4.932083	-5.272358	-1.852398
65	1	0	-2.031308	0.906273	0.275170	134	6	0	6.235567	-2.030614	-2.096126
66	6	0	1.756115	3.754855	-2.523454	135	1	0	6.629996	-3.782584	-0.906484
67	6	0	1.164462	2.896584	-3.657848	136	1	0	6.993927	-3.980361	-2.623792
68	6	0	2.535026	4.960581	-3.087250	137	1	0	5.991274	-1.767347	-3.135041
69	1	0	2.482650	3.133571	-1.995665	138	1	0	7.197934	-1.571695	-1.854044
70	1	0	0.445158	3.463541	-4.261577	139	6	0	4.678941	3.621182	3.080264
71	1	0	0.658902	2.011838	-3.259961	140	6	0	5.976367	2.795522	3.228816
72	1	0	2.988186	5.551204	-2.283132	141	1	0	4.131226	3.616771	4.034306
73	1	0	1.885943	5.627760	-3.666937	142	1	0	4.929552	4.669494	2.877214
74	6	0	-0.304688	4.092846	2.227284	143	6	0	5.705032	1.284113	3.322672
75	6	0	-0.040939	5.363516	3.061037	144	1	0	6.625473	2.979535	2.364243

145	1	0	6.524292	3.112709	4.122658
146	1	0	6.632214	0.704843	3.332248
147	1	0	5.152847	1.046259	4.243018
148	1	0	-3.079763	6.707156	-0.837533
149	1	0	-3.584975	-6.046458	1.870241

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1fa (SBIDOL)

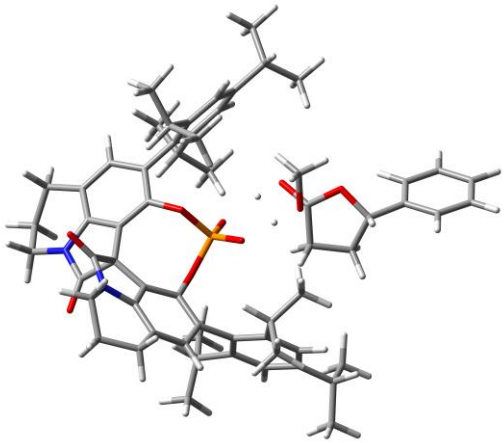


B3LYP/6-31G(d); E(RB3LYP) = -3535.83275672 Hartree
Zero-point correction= 1.263335 Hartree
Thermal correction to Energy= 1.335622 Hartree
Thermal correction to Enthalpy= 1.336567 Hartree
Thermal correction to Gibbs Free Energy= 1.152256 Hartree
Sum of electronic and zero-point Energies= -3534.569422 Hartree
Sum of electronic and thermal Energies= -3534.497134 Hartree
Sum of electronic and thermal Enthalpies= -3534.496190 Hartree
Sum of electronic and thermal Free Energies= -3534.680501 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.316690	2.709810	0.660673
2	6	0	-1.897102	1.618851	0.035141
3	6	0	-3.873477	1.926010	1.386535
4	6	0	-3.250593	2.916492	2.156202
5	6	0	-1.972558	3.268575	1.756800
6	1	0	-4.896595	1.647210	1.619545
7	6	0	-0.038638	3.467498	0.465841
8	6	0	1.839438	3.916209	-0.856086
9	6	0	1.216240	2.900516	-0.129108
10	6	0	3.081599	3.796410	-1.455938
11	6	0	1.786850	1.636148	-0.148381
12	8	0	-1.150016	0.922950	-0.912956
13	8	0	1.078272	0.580324	0.419933
14	15	0	-0.069787	-0.217086	-0.450963
15	8	0	0.495377	-0.811948	-1.710774
16	8	0	-0.700837	-1.152317	0.578991
17	6	0	-3.223174	1.233309	0.348435
18	6	0	3.071050	1.442305	-0.713302
19	6	0	-3.947213	0.152486	-0.400865
20	6	0	-4.231826	0.320411	-1.782030
21	6	0	-4.410968	-1.010247	0.266901
22	6	0	-4.947450	-0.673382	-2.456359
23	6	0	-5.134103	-1.964501	-0.459762
24	6	0	-5.409863	-1.826377	-1.819109
25	1	0	-5.158945	-0.532922	-3.513491
26	1	0	-5.492288	-2.853897	0.053666
27	6	0	3.697703	2.547370	-1.317738
28	1	0	4.694862	2.403940	-1.724589
29	6	0	3.812247	0.135773	-0.666865
30	6	0	4.069314	-0.587785	-1.857284
31	6	0	4.364356	-0.314377	0.561496
32	6	0	4.876122	-1.732653	-1.788880
33	6	0	5.158872	-1.465370	0.568622
34	6	0	5.437079	-2.187878	-0.596305
35	1	0	5.088130	-2.280707	-2.704211
36	1	0	5.596783	-1.792371	1.507567
37	6	0	0.153760	-4.022189	-1.065443
38	8	0	-0.481588	-3.573251	0.415535
39	6	0	0.480090	-4.127414	1.374728
40	6	0	1.657535	-3.911936	-0.760547
41	1	0	2.132124	-4.817411	-1.146949
42	1	0	2.070436	-3.054155	-1.293221
43	8	0	-0.412682	-3.238531	-1.975626
44	8	0	-0.212563	-5.321817	-1.179710
45	6	0	-1.579659	-5.567310	-1.556801
46	1	0	-1.710575	-6.647056	-1.472973
47	1	0	-1.759578	-5.241753	-2.583719
48	1	0	-2.262118	-5.048358	-0.878130
49	1	0	-0.573454	-2.435645	0.478254
50	1	0	-0.041706	-2.297178	-1.951935
51	6	0	0.214733	-3.704269	2.800038
52	6	0	0.390448	-2.384410	3.242186
53	6	0	-0.192255	-4.676997	3.722454
54	6	0	0.161355	-2.054670	4.577721
55	1	0	0.673135	-1.606061	2.542339
56	6	0	-0.415009	-4.348330	5.060053
57	1	0	-0.333779	-5.702840	3.389820
58	6	0	-0.237890	-3.033349	5.490676
59	1	0	0.295935	-1.027221	4.904386
60	1	0	-0.727290	-5.117548	5.761206
61	1	0	-0.410812	-2.771425	6.531174
62	1	0	0.328636	-5.207702	1.299875
63	6	0	1.839311	-3.762104	0.766379
64	1	0	2.631966	-4.402265	1.163067
65	1	0	2.100442	-2.729485	1.014573
66	6	0	3.550674	-0.149057	-3.229259
67	6	0	4.693680	0.422131	-4.095135
68	6	0	2.831350	-1.276011	-3.993821
69	1	0	2.815311	0.644409	-3.072822
70	1	0	5.450159	-0.344073	-4.304331
71	1	0	5.201652	1.259979	-3.605974
72	1	0	1.982932	-1.654445	-3.421100
73	1	0	3.503386	-2.110111	-4.228986
74	6	0	4.211342	0.489733	1.854649
75	6	0	4.012444	-0.376422	3.110213
76	6	0	5.416287	1.436312	2.037711
77	1	0	3.321561	1.117327	1.763617
78	1	0	4.907151	-0.957734	3.362286
79	1	0	3.178034	-1.075893	2.992601
80	1	0	5.521806	2.113179	1.183342
81	1	0	6.349045	0.867130	2.134451
82	6	0	-3.843158	1.572908	-2.570039
83	6	0	-2.934704	1.246837	-3.770826
84	6	0	-5.093811	2.356821	-3.017070
85	1	0	-3.279637	2.237537	-1.911588
86	1	0	-3.451204	0.624876	-4.511988
87	1	0	-2.033536	0.717157	-3.448799
88	1	0	-5.719857	2.626682	-2.159148
89	1	0	-5.710863	1.772227	-3.709838
90	6	0	-4.172059	-1.277607	1.754823
91	6	0	-5.465009	-1.088726	2.576091
92	6	0	-3.595551	-2.680628	2.023315
93	1	0	-3.432197	-0.556991	2.113024
94	1	0	-6.231631	-1.810307	2.268379

95	1	0	-5.892817	-0.087970	2.454527
96	1	0	-2.711489	-2.871612	1.412628
97	1	0	-4.329620	-3.469469	1.817878
98	1	0	2.447427	-0.890459	-4.946070
99	1	0	4.304470	0.777795	-5.056988
100	1	0	5.294624	2.047159	2.940398
101	1	0	3.794612	0.265665	3.971653
102	1	0	-2.627733	2.171620	-4.274765
103	1	0	-4.802052	3.282028	-3.528712
104	1	0	-3.306161	-2.772117	3.076924
105	1	0	-5.268568	-1.245763	3.644067
106	6	0	6.357269	-3.402651	-0.583397
107	6	0	5.837086	-4.530220	0.326707
108	1	0	6.503327	-5.400273	0.284297
109	1	0	5.780397	-4.206624	1.372828
110	1	0	4.836331	-4.855445	0.021151
111	6	0	7.799169	-3.013356	-0.202920
112	1	0	7.848104	-2.624069	0.820984
113	1	0	8.464520	-3.883290	-0.261745
114	1	0	8.188637	-2.238956	-0.872582
115	6	0	-6.188758	-2.897877	-2.570439
116	6	0	-7.517848	-2.358611	-3.132119
117	1	0	-7.345289	-1.574335	-3.878630
118	1	0	-8.087805	-3.160283	-3.617538
119	1	0	-8.138528	-1.930859	-2.337182
120	6	0	-5.342776	-3.545625	-3.683062
121	1	0	-4.410760	-3.958254	-3.280965
122	1	0	-5.896983	-4.357374	-4.170134
123	1	0	-5.074460	-2.814793	-4.454964
124	7	0	1.008954	5.033131	-0.964904
125	7	0	-1.127196	4.141968	2.446006
126	6	0	0.128134	4.179723	1.880995
127	6	0	-0.218346	4.806164	-0.389489
128	8	0	-1.190301	5.529970	-0.435290
129	8	0	1.110682	4.742098	2.317358
130	6	0	3.631446	4.990499	-2.209529
131	6	0	2.928917	6.295026	-1.772560
132	1	0	3.493295	4.844957	-3.291090
133	1	0	4.712695	5.081154	-2.049502
134	6	0	1.395909	6.171272	-1.790300
135	1	0	3.246251	6.556381	-0.755816
136	1	0	3.224559	7.120210	-2.429348
137	1	0	0.911397	7.064832	-1.387769
138	1	0	1.030908	6.027012	-2.817055
139	6	0	-3.812528	3.602854	3.383133
140	6	0	-2.668011	3.983776	4.350742
141	1	0	-4.530737	2.952481	3.895221
142	1	0	-4.363783	4.510155	3.095360
143	6	0	-1.564031	4.810338	3.666920
144	1	0	-3.061782	4.560401	5.194930
145	1	0	-2.225835	3.067450	4.761006
146	1	0	-1.938001	5.810915	3.410571
147	1	0	-0.692532	4.936354	4.315014
148	1	0	6.384569	-3.796062	-1.608931
149	1	0	-6.435375	-3.685262	-1.844452

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1fa (SBIDOL)



B3LYP/6-31G(d); E(RB3LYP) = -3535.83669684 Hartree

Zero-point correction= 1.264518 Hartree

Thermal correction to Energy= 1.336859 Hartree

Thermal correction to Enthalpy= 1.337803 Hartree

Thermal correction to Gibbs Free Energy= 1.153268 Hartree

Sum of electronic and zero-point Energies= -3534.572178 Hartree

Sum of electronic and thermal Energies= -3534.499838 Hartree

Sum of electronic and thermal Enthalpies= -3534.498894 Hartree

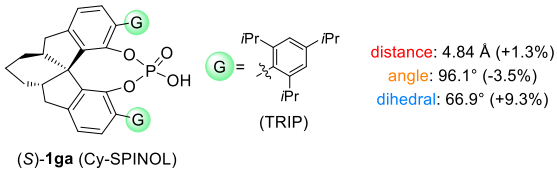
Sum of electronic and thermal Free Energies= -3534.683429 Hartree

The number of Imaginary frequencies = 1

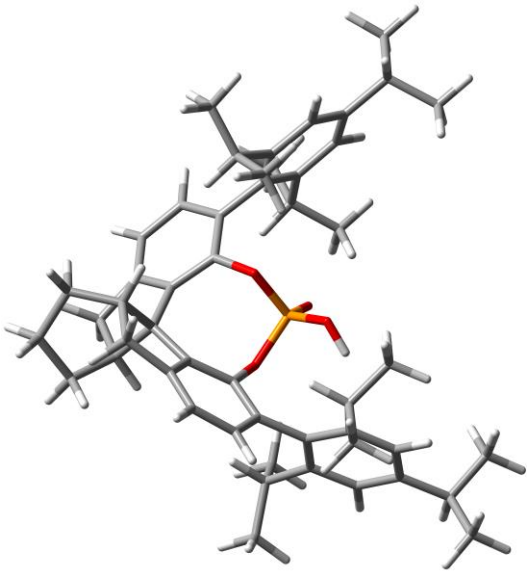
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.502883	0.474277	-0.126999
2	8	0	-4.792251	0.721595	-0.451754
3	8	0	-2.810502	0.062377	-1.648737
4	6	0	-5.525695	-0.537900	-0.468648
5	6	0	-4.852598	-1.345498	0.659704
6	6	0	-3.390025	-0.862343	0.621716
7	1	0	-5.337832	-1.016543	-1.437388
8	1	0	-5.324590	-1.093524	1.614516
9	1	0	-4.955276	-2.422239	0.503812
10	1	0	-2.965883	-0.684067	1.611809
11	1	0	-2.731387	-1.558654	0.100920
12	8	0	-2.885332	1.562923	0.280261
13	6	0	-2.847907	1.143301	-2.605039
14	1	0	-2.355535	2.032721	-2.203244
15	1	0	-2.334340	0.796354	-3.504007
16	1	0	-3.894393	1.357494	-2.824694
17	1	0	-1.948907	1.328018	0.607382
18	1	0	-1.774267	-0.210173	-1.471856
19	6	0	3.322351	-1.323681	-0.438040
20	6	0	2.086426	-1.821751	-0.055764
21	6	0	2.590429	-3.891325	-1.198185
22	6	0	3.763864	-3.357132	-1.745748
23	6	0	4.076335	-2.068705	-1.346093
24	1	0	2.323066	-4.918745	-1.428207
25	6	0	4.085784	-0.065949	-0.141102
26	6	0	4.321769	1.910934	1.088020
27	6	0	3.464100	1.253189	0.206463
28	6	0	4.111368	3.194944	1.564691
29	6	0	2.245569	1.845627	-0.085557
30	6	0	2.933174	3.816216	1.133376
31	1	0	2.725451	4.832199	1.457918
32	8	0	1.229763	-1.008023	0.677617
33	8	0	1.317874	1.119585	-0.822085
34	15	0	0.273295	0.083672	-0.087412
35	8	0	-0.531241	0.745348	1.000765
36	8	0	-0.461602	-0.562477	-1.254009
37	6	0	1.711221	-3.145146	-0.393735

38	6	0	1.965613	3.164186	0.347648
39	6	0	-6.999277	-0.271143	-0.300939
40	6	0	-7.927437	-1.045533	-1.004831
41	6	0	-7.460271	0.709260	0.587169
42	6	0	-9.297429	-0.855913	-0.816335
43	1	0	-7.577376	-1.800444	-1.705699
44	6	0	-8.828641	0.906569	0.766835
45	1	0	-6.743743	1.327951	1.119029
46	6	0	-9.750719	0.121869	0.069721
47	1	0	-10.007890	-1.465074	-1.368515
48	1	0	-9.176070	1.675931	1.451133
49	1	0	-10.816726	0.276764	0.212431
50	6	0	0.439798	-3.770111	0.104164
51	6	0	0.272464	-4.022563	1.490679
52	6	0	-0.573615	-4.174117	-0.803065
53	6	0	-0.890148	-4.662051	1.932717
54	6	0	-1.714966	-4.813916	-0.301255
55	6	0	-1.898397	-5.071520	1.057743
56	1	0	-0.999909	-4.860134	2.996006
57	1	0	-2.486233	-5.135035	-0.998141
58	6	0	0.672042	3.846278	0.014346
59	6	0	-0.239994	4.204765	1.043349
60	6	0	0.358064	4.154469	-1.332192
61	6	0	-1.440263	4.832339	0.694770
62	6	0	-0.867364	4.768170	-1.621203
63	6	0	-1.787683	5.108581	-0.629212
64	1	0	-2.133660	5.101460	1.486892
65	1	0	-1.105995	5.005636	-2.656237
66	6	0	-0.467849	-3.975844	-2.317324
67	6	0	-0.195431	-5.314124	-3.036236
68	6	0	-1.713825	-3.307571	-2.928094
69	1	0	0.375194	-3.307975	-2.511296
70	1	0	-1.030102	-6.011901	-2.896401
71	1	0	0.708016	-5.806539	-2.661734
72	1	0	-1.926764	-2.351618	-2.445883
73	1	0	-2.603859	-3.943270	-2.846526
74	6	0	1.335339	-3.675317	2.534359
75	6	0	0.803441	-2.695782	3.598003
76	6	0	1.911795	-4.947294	3.188175
77	1	0	2.167630	-3.180396	2.029131
78	1	0	-0.008132	-3.140235	4.187191
79	1	0	0.428736	-1.779083	3.133382
80	1	0	2.326981	-5.626596	2.435217
81	1	0	1.146478	-5.497473	3.748684
82	6	0	1.332218	3.910037	-2.485878
83	6	0	0.738802	3.010320	-3.585925
84	6	0	1.829283	5.246244	-3.074571
85	1	0	2.211085	3.394996	-2.090719
86	1	0	-0.130262	3.476553	-4.066634
87	1	0	0.432678	2.043278	-3.175947
88	1	0	2.293111	5.870179	-2.302469
89	1	0	1.007778	5.821015	-3.518866
90	6	0	0.032712	3.962030	2.530881
91	6	0	0.304021	5.293471	3.262239
92	6	0	-1.096034	3.187287	3.237394
93	1	0	0.931808	3.347177	2.616077
94	1	0	-0.579415	5.943065	3.241701
95	1	0	1.129067	5.851091	2.804550
96	1	0	-1.244405	2.211569	2.770449
97	1	0	-2.046414	3.733582	3.219728
98	1	0	-0.831792	3.025538	4.289976
99	1	0	0.558956	5.110760	4.313525
100	1	0	1.485582	2.826329	-4.367913
101	1	0	2.574563	5.065824	-3.858765
102	1	0	-1.548249	-3.119186	-3.996031
103	1	0	-0.071197	-5.153773	-4.114392
104	1	0	2.714268	-4.685738	3.888344
105	1	0	1.604833	-2.423166	4.295532
106	6	0	-3.134136	-5.814335	1.550336
107	6	0	-3.889401	-5.048489	2.651517
108	1	0	-3.279871	-4.940630	3.556174
109	1	0	-4.168308	-4.042481	2.318632
110	1	0	-4.805938	-5.580805	2.932847
111	6	0	-2.779011	-7.238618	2.021213
112	1	0	-3.680862	-7.786721	2.320391
113	1	0	-2.282119	-7.804882	1.226040
114	1	0	-2.101779	-7.210379	2.883118
115	6	0	-3.104936	5.784279	-0.987209
116	6	0	-4.323403	5.059228	-0.386132
117	1	0	-4.320617	3.993135	-0.634338
118	1	0	-4.335762	5.140422	0.707255
119	1	0	-5.254812	5.502719	-0.758800
120	6	0	-3.098822	7.272987	-0.587583
121	1	0	-4.031474	7.762736	-0.893791
122	1	0	-3.001189	7.386988	0.498816
123	1	0	-2.263239	7.805814	-1.054780
124	7	0	5.136217	-1.311195	-1.848941
125	7	0	5.341727	1.057511	1.516708
126	6	0	5.117488	-0.026569	-1.356413
127	6	0	5.178415	-0.213320	1.013689
128	8	0	5.825023	0.896829	-1.699752
129	8	0	5.814151	-1.203420	1.308876
130	6	0	5.124981	3.753951	2.540345
131	6	0	5.742796	2.610266	3.377382
132	1	0	4.656676	4.489768	3.203833
133	1	0	5.924203	4.283968	2.001530
134	6	0	6.328542	1.488714	2.501412
135	1	0	6.538124	2.999314	4.022621
136	1	0	4.970654	2.187151	4.031644
137	1	0	7.225090	1.843132	1.974915
138	1	0	6.614199	0.617005	3.096218
139	6	0	4.690085	-4.042605	-2.730106
140	6	0	6.079793	-3.367464	-2.748047
141	1	0	4.254169	-4.009307	-3.739648
142	1	0	4.798981	-5.104927	-2.479753
143	6	0	5.990680	-1.839559	-2.905037
144	1	0	6.604386	-3.590888	-1.811270
145	1	0	6.684652	-3.772391	-3.566603
146	1	0	6.971825	-1.364701	-2.819938
147	1	0	5.575428	-1.575007	-3.887931
148	1	0	-3.814062	-5.913409	0.692360
149	1	0	-3.200714	5.739662	-2.081330

Optimized structure of Cy-SPINOL-derived CPA (*S*)-1ga



(*S*)-**1ga** (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -2585.65908158 Hartree

Zero-point correction= 1.026655 Hartree

Thermal correction to Energy= 1.081351 Hartree

Thermal correction to Enthalpy= 1.082295 Hartree

Thermal correction to Gibbs Free Energy= 0.938460 Hartree

Sum of electronic and zero-point Energies= -2584.632426 Hartree

Sum of electronic and thermal Energies= -2584.577731 Hartree

Sum of electronic and thermal Enthalpies= -2584.576787 Hartree

Sum of electronic and thermal Free Energies= -2584.720621 Hartree

The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.882367	4.257332	2.118632
2	6	0	0.392185	4.104926	1.241351
3	6	0	-1.245818	2.479244	0.552290
4	6	0	-1.799075	3.162668	1.643456
5	6	0	-0.406016	4.165535	-1.229511
6	6	0	0.895786	4.324440	-2.068671
7	6	0	1.789062	3.205748	-1.598899
8	6	0	1.168696	2.459750	-0.587501
9	6	0	-0.031162	3.217720	-0.012041
10	6	0	-1.857614	1.293743	0.143615
11	6	0	-3.082114	0.853170	0.683498
12	6	0	-3.671130	1.654611	1.674623
13	6	0	-3.022059	2.776760	2.185407
14	6	0	3.044508	2.846727	-2.081564
15	6	0	3.671488	1.711318	-1.571236
16	6	0	3.019351	0.846989	-0.675961
17	6	0	1.740567	1.233656	-0.236178
18	8	0	0.978885	0.330380	0.530538
19	8	0	-1.223190	0.504722	-0.819944
20	15	0	-0.065215	-0.544602	-0.353718
21	8	0	-0.685424	-1.389603	0.861100
22	8	0	0.443181	-1.268548	-1.530770
23	6	0	-3.714898	-0.440506	0.254253
24	6	0	3.690729	-0.413167	-0.211006
25	6	0	4.070204	-0.547779	1.147418
26	6	0	4.739247	-1.708006	1.553898
27	6	0	5.056581	-2.738101	0.670162
28	6	0	4.682534	-2.580288	-0.666016
29	6	0	4.004719	-1.448613	-1.130943
30	6	0	-3.875972	-1.510963	1.184303
31	6	0	-4.433184	-2.716004	0.736564
32	6	0	-4.854797	-2.907563	-0.581693
33	6	0	-4.718709	-1.835525	-1.462351
34	6	0	-4.162233	-0.609142	-1.080630
35	6	0	3.654000	-1.384687	-2.619689
36	6	0	4.916365	-1.156291	-3.477306
37	6	0	2.901141	-2.637084	-3.108310
38	6	0	3.827866	0.538843	2.196022
39	6	0	2.943996	0.038387	3.354593
40	6	0	5.157739	1.115664	2.721747
41	6	0	-3.530003	-1.394514	2.675481
42	6	0	-4.818595	-1.246450	3.513223
43	6	0	-2.696311	-2.571444	3.221309
44	6	0	-4.125656	0.514537	-2.116643
45	6	0	-3.358855	0.118435	-3.392536
46	6	0	-5.554380	0.989418	-2.452837
47	6	0	-5.449773	-4.230292	-1.045733
48	6	0	-4.431684	-5.381827	-0.942111
49	6	0	-6.750663	-4.571682	-0.294682
50	6	0	5.784392	-3.985224	1.154393
51	6	0	4.922417	-5.251230	0.988815
52	6	0	7.153471	-4.156003	0.469427
53	6	0	0.997584	5.460597	0.858675
54	6	0	-0.987611	5.515420	-0.792654
55	6	0	0.011162	6.345241	0.054144
56	1	0	-0.647469	4.143358	3.184461
57	1	0	-1.339319	5.248624	2.013352
58	1	0	1.133094	3.527524	1.806729
59	1	0	-1.147417	3.632728	-1.836418
60	1	0	0.686523	4.233155	-3.142079
61	1	0	1.357582	5.309421	-1.933351
62	1	0	-4.633864	1.359408	2.079100
63	1	0	-3.462562	3.334023	3.008411
64	1	0	3.534366	3.443114	-2.847370
65	1	0	4.670181	1.449966	-1.906029
66	1	0	5.031044	-1.808761	2.597137
67	1	0	4.920107	-3.368537	-1.375348
68	1	0	-4.550590	-3.528446	1.448268
69	1	0	-5.060438	-1.958958	-2.487303
70	1	0	2.981379	-0.537584	-2.774725
71	1	0	4.648659	-1.065278	-4.537194
72	1	0	5.454988	-0.247637	-3.185838
73	1	0	5.615564	-1.995943	-3.380830
74	1	0	2.612296	-2.507230	-4.158618
75	1	0	1.992568	-2.792449	-2.523633
76	1	0	3.522265	-3.539217	-3.051355
77	1	0	3.295223	1.365661	1.718932
78	1	0	3.432287	-0.767491	3.915312
79	1	0	2.741766	0.854329	4.059865
80	1	0	1.986965	-0.338345	2.981786
81	1	0	5.769180	1.511203	1.902928
82	1	0	5.750298	0.353943	3.241819
83	1	0	4.968775	1.931401	3.430598
84	1	0	-2.932673	-0.490530	2.818458
85	1	0	-4.573519	-1.088739	4.570385
86	1	0	-5.432570	-0.404212	3.177575
87	1	0	-5.436147	-2.149843	3.442776
88	1	0	-2.460342	-2.393663	4.276937
89	1	0	-1.747332	-2.685949	2.689958
90	1	0	-3.237091	-3.523117	3.167452
91	1	0	-3.604570	1.368667	-1.677786
92	1	0	-3.298048	0.974840	-4.074982
93	1	0	-2.340601	-0.204249	-3.157856

94	1	0	-3.860320	-0.693453	-3.932599	107	1	0	7.684167	-5.025660	0.875741
95	1	0	-5.521707	1.829751	-3.156767	108	1	0	7.783126	-3.271679	0.617076
96	1	0	-6.086150	1.319656	-1.553366	109	1	0	7.042104	-4.309443	-0.610533
97	1	0	-6.144927	0.189696	-2.915333	110	1	0	1.310633	5.985689	1.770038
98	1	0	-4.859091	-6.311166	-1.336953	111	1	0	1.915175	5.290496	0.284094
99	1	0	-3.520627	-5.158093	-1.507535	112	1	0	-1.287012	6.086045	-1.680809
100	1	0	-4.142346	-5.565301	0.099573	113	1	0	-1.910845	5.337609	-0.228342
101	1	0	-7.192205	-5.494547	-0.689123	114	1	0	0.584456	7.021256	-0.590809
102	1	0	-7.489573	-3.769227	-0.395648	115	1	0	-0.551975	6.997968	0.731395
103	1	0	-6.566072	-4.723477	0.775500	116	1	0	-1.543978	-1.787794	0.619428
104	1	0	5.439472	-6.128373	1.396844	117	1	0	5.969930	-3.852687	2.229379
105	1	0	3.963254	-5.146846	1.507437	118	1	0	-5.705074	-4.111996	-2.107590
106	1	0	4.708985	-5.451145	-0.067857						

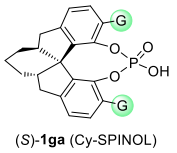
DFT calculation for all conformations of real system using Cy-SPINOL-derived CPA (*S*)-1ga

TS	Orientation I	Orientation II	$\Delta\Delta G^{\neq}$ (a.u.)	$\Delta\Delta G^{\neq}$ (kcal/mmol)
R-anti	up	up	-3237.783695	-1.06
	up	down	-3237.783858	-1.16
	down	up	-3237.784410	-1.51
	down	down	-3237.783176	-0.73
S-anti	up	up	-3237.776556	3.42
	up	down	-3237.777016	3.13
	down	up	-3237.775437	4.12
	down	down	-3237.776137	3.68
S-syn	up	up	-3237.778129	2.43
	up	down	-3237.779085	1.83
	down	down	-3237.778401	2.26
	down	up	-3237.777997	2.52

TS	Orientation I	Orientation II	$\Delta\Delta G^{\neq}$ (a.u.)	$\Delta\Delta G^{\neq}$ (kcal/mmol)
R-re	up	up	-3237.782005	0.00
	up	down	-3237.781048	0.60
	down	up	-3237.780722	0.81
	down	down	-3237.781204	0.50
S-si	up	up	-3237.779510	1.57
	up	down	-3237.778033	2.49
	down	up	-3237.779687	1.45
	down	down	-3237.779924	1.31
S-re	up	up	-3237.782338	-0.21
	up	down	-3237.780577	0.90
	down	up	-3237.781510	0.31
	down	down	-3237.781326	0.43

* Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using Cy-SPINOL-derive CPA (*S*)-1ga



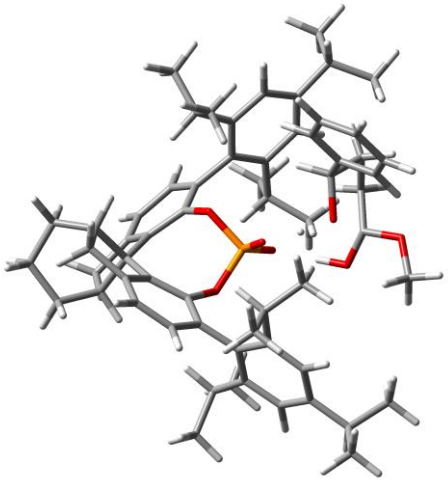
(TRIP)

(*S*)-**1ga** (Cy-SPINOL)

1st / 2nd	$\Delta\Delta G^{\neq}$ (kcal/mol)
R-anti / ***R-re***	-1.51 / **0.00**
R-syn / *R-si*	-- / --
S-anti / ***S-si***	**3.13** / 1.31
S-syn / ***S-re***	**1.83** / -0.21

$\Delta\Delta G^{\neq}$ of RDS = **1.83** kcal/mol

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1ga (Cy-SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3238.940382 hartree

Zero-point Energy Correction = 1.260477 hartree

Thermal Correction to Energy = 1.328243 hartree

Thermal correction to Enthalpy = 1.329188 hartree

Thermal correction to Gibbs Free Energy= 1.155973 hartree

Sum of electronic and Zero-point Energies = -3237.679905 hartree

Sum of electronic and thermal Energies = -3237.612139 hartree

Sum of electronic and thermal Enthalpies = -3237.611195 hartree

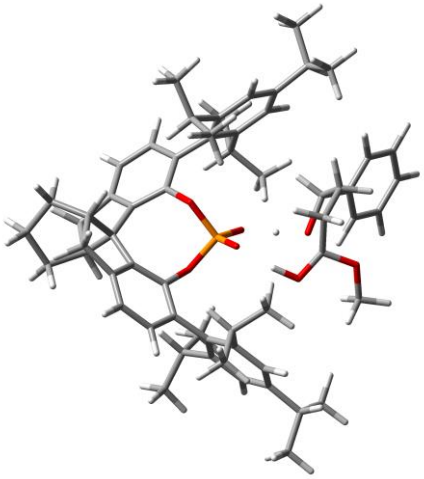
Sum of electronic and thermal Free Energies= -3237.784410 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.316553	4.210154	3.148812
2	6	0	-0.076459	4.459863	2.241101
3	6	0	-1.569506	2.923768	1.142883
4	6	0	-2.164274	3.236824	2.372046
5	6	0	-1.061327	5.142630	-0.061374
6	6	0	0.125179	5.697383	-0.898092
7	6	0	1.167446	4.613262	-0.840579
8	6	0	0.745974	3.546897	-0.035883
9	6	0	-0.476671	3.934773	0.795944
10	6	0	-2.077115	1.842346	0.417689
11	6	0	-3.306336	1.239919	0.750516
12	6	0	-3.952159	1.704243	1.909215
13	6	0	-3.363951	2.643695	2.753528
14	6	0	2.394603	4.572782	-1.495516
15	6	0	3.189325	3.436444	-1.372156
16	6	0	2.741098	2.287327	-0.698081
17	6	0	1.485810	2.360658	-0.063143
18	8	0	0.953318	1.225884	0.551448
19	8	0	-1.333012	1.338813	-0.653291
20	15	0	-0.103432	0.314597	-0.313180
21	8	0	-0.550803	-0.759411	0.678198
22	8	0	0.472826	-0.135085	-1.630052
23	6	0	-3.948404	0.168571	-0.083425
24	6	0	3.620120	1.070227	-0.670001
25	6	0	4.181307	0.625179	0.553036
26	6	0	5.077589	-0.451002	0.539911
27	6	0	5.467408	-1.090796	-0.638065
28	6	0	4.898957	-0.639658	-1.831923
29	6	0	3.981741	0.417624	-1.879183

30	6	0	-4.225047	-1.111074	0.470353
31	6	0	-4.892417	-2.058588	-0.313057
32	6	0	-5.294440	-1.800848	-1.625499
33	6	0	-5.013953	-0.539900	-2.148001
34	6	0	-4.358562	0.453139	-1.410325
35	6	0	3.444736	0.834319	-3.252351
36	6	0	4.553729	1.475968	-4.112680
37	6	0	2.794171	-0.331904	-4.020386
38	6	0	3.916107	1.317933	1.890720
39	6	0	3.263411	0.375419	2.919579
40	6	0	5.204983	1.948120	2.456435
41	6	0	-3.843540	-1.508286	1.899033
42	6	0	-5.086224	-1.596390	2.809728
43	6	0	-3.066245	-2.836367	1.961753
44	6	0	-4.175830	1.820412	-2.070571
45	6	0	-3.320259	1.738806	-3.349005
46	6	0	-5.537463	2.486885	-2.354257
47	6	0	-6.016603	-2.848857	-2.462104
48	6	0	-5.125590	-4.075316	-2.737158
49	6	0	-7.356018	-3.271795	-1.830287
50	6	0	6.540308	-2.173998	-0.607760
51	6	0	6.213160	-3.398914	-1.478377
52	6	0	7.912232	-1.584812	-0.996569
53	6	0	0.369653	5.926860	2.255442
54	6	0	-1.731118	6.231205	0.786234
55	6	0	-0.750753	6.891126	1.789769
56	1	0	-1.018895	3.786026	4.116493
57	1	0	-1.854509	5.137551	3.377758
58	1	0	0.747004	3.829175	2.596237
59	1	0	-1.801692	4.717640	-0.749213
60	1	0	-0.178661	5.899263	-1.933258
61	1	0	0.500576	6.648828	-0.502173
62	1	0	-4.916934	1.280271	2.166815
63	1	0	-3.843332	2.912815	3.691602
64	1	0	2.732904	5.415420	-2.093583
65	1	0	4.168132	3.411201	-1.840266
66	1	0	5.516570	-0.779975	1.480019
67	1	0	5.185365	-1.116043	-2.765544
68	1	0	-5.104749	-3.032555	0.120345
69	1	0	-5.329432	-0.316442	-3.164929
70	1	0	2.662532	1.581154	-3.099019
71	1	0	4.143973	1.820859	-5.069761
72	1	0	5.016958	2.334652	-3.614755
73	1	0	5.351113	0.755680	-4.332462
74	1	0	2.406516	0.027564	-4.981352
75	1	0	1.957586	-0.747723	-3.455927
76	1	0	3.510574	-1.133398	-4.237776
77	1	0	3.215513	2.138319	1.719189
78	1	0	3.911937	-0.478151	3.153783
79	1	0	3.071373	0.909801	3.858151
80	1	0	2.306776	-0.003202	2.545974
81	1	0	5.653955	2.642175	1.737281
82	1	0	5.956252	1.187472	2.699726
83	1	0	4.986658	2.505106	3.375812
84	1	0	-3.181632	-0.736799	2.299673
85	1	0	-4.791187	-1.832569	3.839571
86	1	0	-5.654708	-0.660626	2.828227
87	1	0	-5.767313	-2.385725	2.468728
88	1	0	-2.725404	-3.023723	2.986965
89	1	0	-2.186794	-2.813743	1.316031
90	1	0	-3.689023	-3.690118	1.667314
91	1	0	-3.648849	2.473265	-1.371040
92	1	0	-3.162777	2.741941	-3.764733
93	1	0	-2.341906	1.298587	-3.136852
94	1	0	-3.808212	1.135423	-4.123893
95	1	0	-5.392822	3.489523	-2.775268
96	1	0	-6.129647	2.585402	-1.437367
97	1	0	-6.129197	1.907044	-3.072284
98	1	0	-5.639360	-4.791474	-3.390149
99	1	0	-4.189083	-3.779177	-3.222820
100	1	0	-4.871586	-4.595993	-1.805785
101	1	0	-7.885832	-3.978443	-2.480736
102	1	0	-8.006031	-2.405577	-1.665579
103	1	0	-7.202658	-3.762487	-0.861796
104	1	0	6.987603	-4.166088	-1.362129
105	1	0	5.251761	-3.845012	-1.201662
106	1	0	6.168543	-3.140199	-2.542652
107	1	0	8.699941	-2.344184	-0.917986
108	1	0	8.179960	-0.744544	-0.346975
109	1	0	7.899254	-1.216513	-2.029467
110	1	0	0.696452	6.196850	3.267760
111	1	0	1.255390	6.035017	1.618231
112	1	0	-2.155168	6.995691	0.122623
113	1	0	-2.583727	5.793017	1.317293
114	1	0	-0.292714	7.781434	1.343216
115	1	0	-1.318700	7.258497	2.652586
116	6	0	0.516795	-3.420565	-1.351417
117	8	0	0.155773	-3.044211	0.280152
118	6	0	1.360124	-3.206621	1.087893
119	6	0	2.401984	-3.820999	0.130289
120	6	0	2.026209	-3.283004	-1.249940
121	1	0	1.682547	-2.200243	1.375525
122	1	0	2.337796	-4.912968	0.146890
123	1	0	3.412832	-3.532587	0.429851
124	1	0	2.491341	-3.838938	-2.068849
125	1	0	2.290647	-2.226765	-1.350619
126	8	0	-0.204099	-2.595366	-2.093698
127	8	0	0.149542	-4.712523	-1.468643
128	6	0	-1.251960	-4.969542	-1.675852
129	1	0	-1.350210	-6.055393	-1.645554
130	1	0	-1.574619	-4.585130	-2.645336
131	1	0	-1.845929	-4.512061	-0.880163
132	6	0	1.073447	-4.022299	2.326963
133	6	0	1.448717	-3.541578	3.584912
134	6	0	0.456148	-5.277219	2.232581
135	6	0	1.223560	-4.304939	4.732769
136	1	0	1.915658	-2.562926	3.668295
137	6	0	0.223156	-6.035899	3.377672
138	1	0	0.153292	-5.648992	1.257607
139	6	0	0.609613	-5.552974	4.631432
140	1	0	1.520676	-3.919189	5.704320
141	1	0	-0.260573	-7.005623	3.293895
142	1	0	0.428247	-6.146441	5.523590
143	1	0	-0.221676	-1.978470	0.418319
144	1	0	0.090131	-1.627130	-1.992544
145	1	0	6.617477	-2.520750	0.432460
146	1	0	-6.243262	-2.386028	-3.432460

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1ga (Cy-SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3238.933781 hartree

Zero-point Energy Correction = 1.260586 hartree

Thermal Correction to Energy = 1.328330 hartree

Thermal correction to Enthalpy = 1.329274 hartree

Thermal correction to Gibbs Free Energy= 1.156764 hartree

Sum of electronic and Zero-point Energies = -3237.673194 hartree

Sum of electronic and thermal Energies = -3237.605451 hartree

Sum of electronic and thermal Enthalpies = -3237.604507 hartree

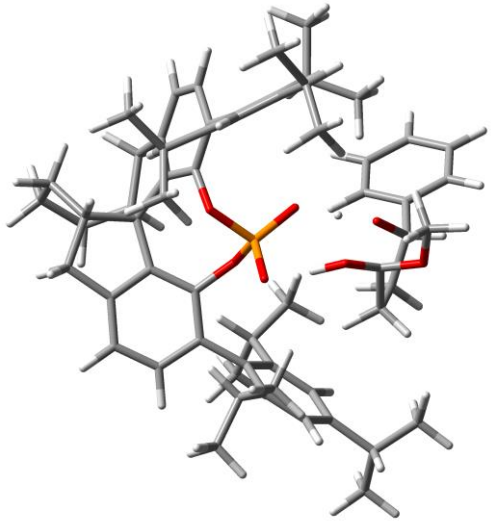
Sum of electronic and thermal Free Energies= -3237.777016 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.345017	4.513194	1.560910
2	6	0	-2.061199	4.814736	0.734586
3	6	0	-2.780867	2.558164	0.292177
4	6	0	-3.697925	3.093056	1.206895
5	6	0	-2.664164	4.176508	-1.705532
6	6	0	-1.528172	4.767407	-2.585849
7	6	0	-0.260396	4.244956	-1.966786
8	6	0	-0.530983	3.454982	-0.840956
9	6	0	-1.968112	3.670835	-0.366281
10	6	0	-2.786458	1.177105	0.074507
11	6	0	-3.831910	0.361070	0.552174
12	6	0	-4.833181	0.985092	1.317117
13	6	0	-4.742454	2.319821	1.702081
14	6	0	1.044152	4.444236	-2.406257
15	6	0	2.081698	3.796168	-1.744529
16	6	0	1.841118	2.857423	-0.725663
17	6	0	0.507002	2.682296	-0.306732
18	8	0	0.214208	1.733645	0.675516
19	8	0	-1.712463	0.597803	-0.613179
20	15	0	-0.372162	0.261696	0.268465
21	8	0	-0.679641	-0.440497	1.565220
22	8	0	0.562658	-0.454753	-0.712522
23	6	0	-3.925769	-1.113373	0.288902
24	6	0	3.007619	2.101069	-0.162073
25	6	0	3.382651	2.252713	1.197048
26	6	0	4.538580	1.614801	1.662659
27	6	0	5.346782	0.832394	0.835348
28	6	0	4.952954	0.686081	-0.496917
29	6	0	3.809952	1.303229	-1.021552
30	6	0	-3.969319	-2.033420	1.371440
31	6	0	-4.129988	-3.396023	1.091905
32	6	0	-4.264200	-3.890920	-0.205144
33	6	0	-4.227324	-2.968975	-1.252377
34	6	0	-4.061960	-1.597005	-1.038588
35	6	0	3.515631	1.105799	-2.513086
36	6	0	4.617121	1.742295	-3.386012
37	6	0	3.318089	-0.371493	-2.896337
38	6	0	2.621482	3.148747	2.175746
39	6	0	2.087805	2.363543	3.388649
40	6	0	3.487175	4.344238	2.623720
41	6	0	-3.903799	-1.614641	2.845351
42	6	0	-5.268726	-1.828283	3.535008
43	6	0	-2.802372	-2.334638	3.645848
44	6	0	-4.108521	-0.680372	-2.262067
45	6	0	-2.988959	-0.999810	-3.271008
46	6	0	-5.494315	-0.724693	-2.937711
47	6	0	-4.509887	-5.375033	-0.448065
48	6	0	-5.994081	-5.641783	-0.771158
49	6	0	-3.602107	-5.968233	-1.539623
50	6	0	6.660249	0.225957	1.316832
51	6	0	7.780392	1.286845	1.310035
52	6	0	6.566621	-0.450433	2.694784
53	6	0	-2.073257	6.231804	0.148126
54	6	0	-3.793640	5.185853	-1.468622
55	6	0	-3.294995	6.479152	-0.774385
56	1	0	-3.153578	4.610138	2.637418
57	1	0	-4.158174	5.213014	1.334817
58	1	0	-1.189371	4.703933	1.389903
59	1	0	-3.072674	3.292623	-2.209246
60	1	0	-1.620903	4.436316	-3.628265
61	1	0	-1.553043	5.863154	-2.613548
62	1	0	-5.670973	0.385432	1.657103
63	1	0	-5.479224	2.746782	2.378185
64	1	0	1.252905	5.094399	-3.252307
65	1	0	3.108370	3.972222	-2.049540
66	1	0	4.825084	1.759848	2.700798
67	1	0	5.569878	0.079309	-1.156726
68	1	0	-4.162233	-4.099537	1.921109
69	1	0	-4.346694	-3.322340	-2.273232
70	1	0	2.577198	1.611840	-2.746959
71	1	0	4.356805	1.660335	-4.448232
72	1	0	4.761577	2.803486	-3.153715
73	1	0	5.581632	1.241065	-3.241408
74	1	0	3.118053	-0.452998	-3.971923
75	1	0	2.463046	-0.795718	-2.364871
76	1	0	4.202674	-0.980318	-2.679944
77	1	0	1.755887	3.566240	1.657153
78	1	0	2.903599	1.931514	3.981160
79	1	0	1.518544	3.028265	4.049998
80	1	0	1.424084	1.554350	3.070592
81	1	0	3.832689	4.927720	1.762870
82	1	0	4.372620	4.017779	3.181813
83	1	0	2.910014	5.010170	3.276751
84	1	0	-3.669051	-0.549126	2.888434
85	1	0	-5.242223	-1.448494	4.563738
86	1	0	-6.082365	-1.319165	3.006954
87	1	0	-5.526308	-2.893451	3.579850
88	1	0	-2.831185	-2.003598	4.691339
89	1	0	-1.813248	-2.103442	3.248711
90	1	0	-2.930183	-3.423235	3.641610
91	1	0	-3.957060	0.348614	-1.929146
92	1	0	-3.017903	-0.290153	-4.107186
93	1	0	-2.005047	-0.930930	-2.798613
94	1	0	-3.099680	-2.006834	-3.691264
95	1	0	-5.533073	-0.021137	-3.778593
96	1	0	-6.288239	-0.455237	-2.231980
97	1	0	-5.721955	-1.723114	-3.329601
98	1	0	-6.181611	-6.715955	-0.891828
99	1	0	-6.644736	-5.267756	0.026694
100	1	0	-6.287091	-5.141438	-1.702064
101	1	0	-3.751255	-7.051884	-1.616584
102	1	0	-2.544484	-5.782413	-1.323459
103	1	0	-3.819408	-5.537147	-2.523831
104	1	0	8.742233	0.841740	1.593182
105	1	0	7.558656	2.092857	2.019904
106	1	0	7.890347	1.737867	0.318031
107	1	0	5.789890	-1.223414	2.714205
108	1	0	7.520950	-0.924412	2.952746
109	1	0	6.337183	0.270986	3.487290
110	1	0	-2.071102	6.962132	0.967297
111	1	0	-1.139200	6.398025	-0.400912
112	1	0	-4.261477	5.435628	-2.429493
113	1	0	-4.578866	4.709157	-0.870854
114	1	0	-3.029066	7.234192	-1.523431
115	1	0	-4.120546	6.917053	-0.201276
116	1	0	1.008798	-1.607000	-0.381794
117	6	0	0.721539	-3.343509	1.226130
118	8	0	1.486993	-2.624002	-0.101099
119	6	0	2.891496	-2.459075	0.225812
120	6	0	3.033941	-2.827633	1.731269
121	6	0	1.618066	-2.757104	2.302319
122	1	0	3.112153	-1.395305	0.087107
123	1	0	3.433692	-3.839748	1.833241
124	1	0	3.712596	-2.137978	2.239471

125	1	0	1.503286	-3.335219	3.223533
126	1	0	1.299693	-1.728120	2.489465
127	8	0	-0.556047	-3.007915	1.135077
128	8	0	0.952854	-4.662617	1.072141
129	6	0	0.091974	-5.369468	0.164923
130	1	0	0.495113	-6.381611	0.116177
131	1	0	-0.933597	-5.381734	0.539442
132	1	0	0.116570	-4.906182	-0.825472
133	1	0	-0.689623	-2.026838	1.352109
134	6	0	3.775297	-3.285250	-0.691150
135	6	0	3.266466	-3.963181	-1.802996
136	6	0	5.152052	-3.352588	-0.431710
137	6	0	4.114299	-4.699941	-2.633253
138	1	0	2.205532	-3.906780	-2.018792
139	6	0	5.999309	-4.084904	-1.262742
140	1	0	5.566901	-2.829391	0.426552
141	6	0	5.481934	-4.764400	-2.367695
142	1	0	3.701498	-5.222225	-3.492554
143	1	0	7.063508	-4.125985	-1.045370
144	1	0	6.140202	-5.336927	-3.015580
145	1	0	-4.280690	-5.897146	0.491549
146	1	0	6.941263	-0.547849	0.588403

TS-1st-(*S*)-reaction pathway: *S*-*syn*/(*S*)-1ga (Cy-SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3238.933745 hartree

Zero-point Energy Correction = 1.260299 hartree

Thermal Correction to Energy = 1.328323 hartree

Thermal correction to Enthalpy = 1.329267 hartree

Thermal correction to Gibbs Free Energy= 1.154660 hartree

Sum of electronic and Zero-point Energies = -3237.673446 hartree

Sum of electronic and thermal Energies = -3237.605422 hartree

Sum of electronic and thermal Enthalpies = -3237.604478 hartree

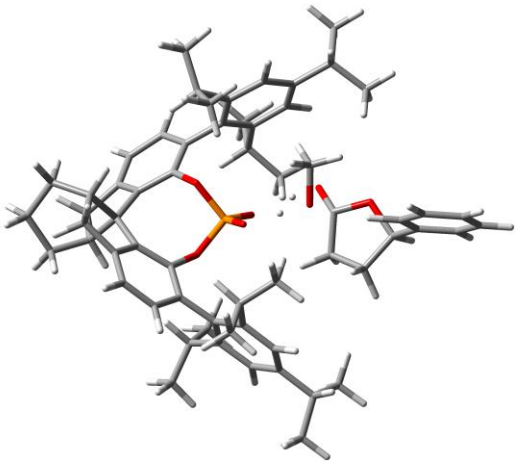
Sum of electronic and thermal Free Energies= -3237.779085 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.240324	5.473378	-1.085127
2	6	0	-0.895756	4.965464	-0.154749
3	6	0	0.867073	3.319905	-0.231826
4	6	0	1.251269	4.359251	-1.089125
5	6	0	0.221197	4.278323	2.086021
6	6	0	-0.969805	4.079913	3.070486
7	6	0	-1.897914	3.131846	2.355423
8	6	0	-1.382015	2.778342	1.102059
9	6	0	-0.283814	3.751213	0.676384
10	6	0	1.578094	2.116540	-0.282323
11	6	0	2.780312	2.001993	-1.008359
12	6	0	3.196681	3.122355	-1.747495
13	6	0	2.420280	4.273949	-1.838299
14	6	0	-3.102124	2.596400	2.802663
15	6	0	-3.775311	1.680519	1.996192
16	6	0	-3.209853	1.172743	0.813599
17	6	0	-1.966857	1.708185	0.420672
18	8	0	-1.290688	1.153740	-0.669913
19	8	0	1.066374	1.010065	0.403368
20	15	0	-0.069141	0.107503	-0.370459
21	8	0	0.417332	-0.396047	-1.701426
22	8	0	-0.489428	-0.921346	0.681161
23	6	0	3.658514	0.783198	-0.996009
24	6	0	-3.948154	0.137652	0.014442
25	6	0	-4.370091	0.430350	-1.310478
26	6	0	-5.107264	-0.523396	-2.018269
27	6	0	-5.464564	-1.755217	-1.467002
28	6	0	-5.056547	-2.016423	-0.160446
29	6	0	-4.304053	-1.107870	0.594564
30	6	0	3.884821	0.043702	-2.185460
31	6	0	4.807479	-1.010884	-2.157866
32	6	0	5.514738	-1.365624	-1.008756
33	6	0	5.271049	-0.627626	0.152396
34	6	0	4.368711	0.441631	0.183700
35	6	0	-3.913286	-1.520610	2.015733
36	6	0	-5.131584	-1.512534	2.962797
37	6	0	-3.235991	-2.903387	2.063619
38	6	0	-4.112903	1.772773	-1.997539
39	6	0	-3.308515	1.614176	-3.301677
40	6	0	-5.433118	2.530427	-2.246632
41	6	0	3.210376	0.375711	-3.519834
42	6	0	4.216088	1.016105	-4.500879
43	6	0	2.547879	-0.844181	-4.187394
44	6	0	4.259743	1.252172	1.476727
45	6	0	3.821252	0.394284	2.676958
46	6	0	5.580412	1.989601	1.778162
47	6	0	6.549065	-2.484391	-1.043906
48	6	0	7.972533	-1.943418	-0.806355
49	6	0	6.224163	-3.620785	-0.057389
50	6	0	-6.267111	-2.781691	-2.255298
51	6	0	-7.643656	-2.238661	-2.682469
52	6	0	-5.479852	-3.306248	-3.471334
53	6	0	-1.469575	6.085605	0.721025
54	6	0	0.714934	5.729562	2.051040
55	6	0	-0.400272	6.725951	1.642298
56	1	0	-0.133995	5.674379	-2.097043
57	1	0	0.674386	6.416025	-0.729766
58	1	0	-1.697278	4.554105	-0.779326
59	1	0	1.044267	3.624834	2.398505
60	1	0	-0.628429	3.651875	4.022003
61	1	0	-1.458569	5.027861	3.323909
62	1	0	4.137054	3.062946	-2.285684
63	1	0	2.729178	5.094457	-2.481313
64	1	0	-3.523629	2.896015	3.759180
65	1	0	-4.748304	1.311047	2.301690
66	1	0	-0.295529	-2.188011	0.522844
67	1	0	-5.423179	-0.287461	-3.031329
68	1	0	-5.331238	-2.968821	0.287266
69	1	0	4.993124	-1.568456	-3.073090
70	1	0	5.822653	-0.869923	1.057879
71	1	0	-3.184904	-0.797766	2.391712
72	1	0	-4.826045	-1.776235	3.982862
73	1	0	-5.623297	-0.534718	2.999973
74	1	0	-5.882747	-2.243515	2.639739
75	1	0	-2.843706	-3.094327	3.069448
76	1	0	-2.403575	-2.964474	1.360168
77	1	0	-3.940633	-3.710843	1.829485
78	1	0	-3.518176	2.396473	-1.326699
79	1	0	-3.866709	1.043772	-4.053868

80	1	0	-3.088287	2.598429	-3.733721
81	1	0	-2.360591	1.101477	-3.116173
82	1	0	-5.985430	2.682795	-1.312416
83	1	0	-6.088464	1.984589	-2.935586
84	1	0	-5.232580	3.514608	-2.687902
85	1	0	2.415006	1.099337	-3.325763
86	1	0	3.713785	1.296563	-5.434685
87	1	0	4.683058	1.915558	-4.086366
88	1	0	5.020897	0.314347	-4.752183
89	1	0	2.041102	-0.530623	-5.108005
90	1	0	1.799675	-1.293962	-3.533057
91	1	0	3.280914	-1.610711	-4.466294
92	1	0	3.495890	2.020626	1.336728
93	1	0	3.714767	1.018521	3.572683
94	1	0	2.857138	-0.085932	2.483664
95	1	0	4.552620	-0.389055	2.908429
96	1	0	5.474558	2.616737	2.671922
97	1	0	5.872216	2.635332	0.942534
98	1	0	6.402249	1.286814	1.959499
99	1	0	8.713608	-2.746776	-0.897932
100	1	0	8.223724	-1.161732	-1.531392
101	1	0	8.070263	-1.511481	0.196695
102	1	0	6.968365	-4.422756	-0.132152
103	1	0	5.238492	-4.053200	-0.262346
104	1	0	6.224504	-3.262908	0.979027
105	1	0	-8.224979	-3.015561	-3.193930
106	1	0	-7.541790	-1.392374	-3.372185
107	1	0	-8.219775	-1.894977	-1.816362
108	1	0	-4.517150	-3.730414	-3.165430
109	1	0	-6.047453	-4.084501	-3.996289
110	1	0	-5.273931	-2.501977	-4.187502
111	1	0	-1.914074	6.854798	0.076510
112	1	0	-2.296599	5.683534	1.317019
113	1	0	1.115131	6.001898	3.035989
114	1	0	1.560763	5.798541	1.356567
115	1	0	-0.894367	7.129394	2.533999
116	1	0	0.057819	7.590536	1.147771
117	6	0	0.507551	-3.640204	-1.097986
118	8	0	-0.130938	-3.317889	0.413316
119	6	0	0.900206	-3.836947	1.317915
120	6	0	1.992313	-3.352452	-0.822068
121	1	0	2.571583	-4.147077	-1.298845
122	1	0	2.265367	-2.405119	-1.288554
123	8	0	-0.179279	-2.908030	-1.966305
124	8	0	0.302939	-4.972285	-1.248507
125	6	0	-1.032014	-5.376510	-1.602474
126	1	0	-1.019640	-6.466809	-1.568007
127	1	0	-1.284995	-5.031153	-2.607090
128	1	0	-1.754237	-4.982809	-0.881873
129	1	0	0.067351	-1.925128	-1.926529
130	6	0	0.634417	-3.539258	2.774600
131	6	0	0.606987	-2.235219	3.291220
132	6	0	0.443288	-4.616457	3.649968
133	6	0	0.389142	-2.023577	4.652290
134	1	0	0.717424	-1.384532	2.628003
135	6	0	0.235297	-4.404765	5.013346
136	1	0	0.458818	-5.631741	3.260037
137	6	0	0.206762	-3.104547	5.517728
138	1	0	0.361143	-1.007615	5.036575
139	1	0	0.091449	-5.253497	5.676573
140	1	0	0.041239	-2.933449	6.578156
141	1	0	0.851013	-4.919233	1.173677
142	6	0	2.204910	-3.305277	0.709206
143	1	0	3.060835	-3.901673	1.037043
144	1	0	2.380723	-2.276380	1.035344
145	1	0	-6.444713	-3.634923	-1.585848
146	1	0	6.526310	-2.912159	-2.055698

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1ga (Cy-SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3238.937809 hartree

Zero-point Energy Correction = 1.261298 hartree

Thermal Correction to Energy = 1.329144 hartree

Thermal correction to Enthalpy = 1.330089 hartree

Thermal correction to Gibbs Free Energy= 1.155780 hartree

Sum of electronic and Zero-point Energies = -3237.676512 hartree

Sum of electronic and thermal Energies = -3237.608665 hartree

Sum of electronic and thermal Enthalpies = -3237.607721 hartree

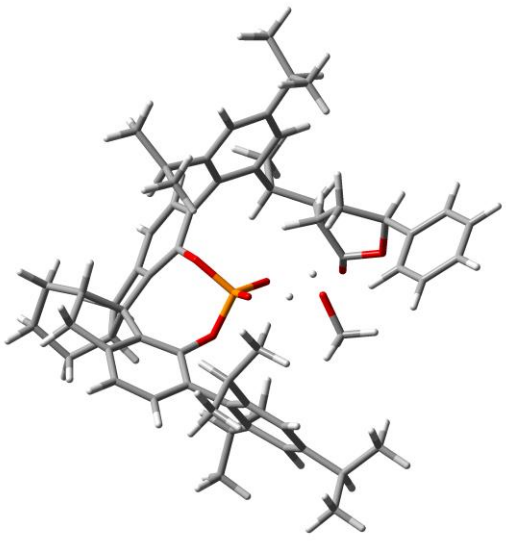
Sum of electronic and thermal Free Energies= -3237.782029 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.896457	0.025821	1.294477
2	6	0	-5.364396	1.224076	0.458414
3	6	0	-3.908075	-0.669540	0.148661
4	6	0	-4.896939	-1.073342	1.055366
5	6	0	-5.047120	0.322788	-1.953471
6	6	0	-4.827074	1.586072	-2.835160
7	6	0	-3.710473	2.333768	-2.155327
8	6	0	-3.284771	1.661767	-1.001435
9	6	0	-4.316098	0.615293	-0.573450
10	6	0	-2.769272	-1.468412	0.010772
11	6	0	-2.682895	-2.744881	0.602291
12	6	0	-3.775418	-3.171027	1.376109
13	6	0	-4.852596	-2.331546	1.648571
14	6	0	-3.091193	3.510176	-2.566495
15	6	0	-2.005241	3.993149	-1.839448
16	6	0	-1.438395	3.260567	-0.783106
17	6	0	-2.083139	2.064132	-0.410449
18	8	0	-1.496499	1.251816	0.560959
19	8	0	-1.690615	-0.974801	-0.723580
20	15	0	-0.600705	-0.020789	0.050151
21	8	0	-0.030241	-0.655597	1.290548
22	8	0	0.366046	0.397479	-1.054501
23	6	0	-1.474983	-3.623443	0.457648
24	6	0	-0.202791	3.767965	-0.096822
25	6	0	-0.244373	4.122222	1.277635
26	6	0	0.903549	4.640694	1.884931
27	6	0	2.097343	4.836141	1.187759
28	6	0	2.115972	4.490632	-0.163227
29	6	0	1.000157	3.961963	-0.825928
30	6	0	-0.713883	-3.988765	1.601669
31	6	0	0.408240	-4.806367	1.434628
32	6	0	0.822311	-5.270217	0.184537
33	6	0	0.045274	-4.921368	-0.920768
34	6	0	-1.098706	-4.120195	-0.814208
35	6	0	1.139984	3.651513	-2.319146
36	6	0	1.222118	4.947450	-3.152853

37	6	0	2.350834	2.754479	-2.637609
38	6	0	-1.510701	4.020526	2.129645
39	6	0	-1.320947	3.090406	3.343106
40	6	0	-1.998493	5.415889	2.569650
41	6	0	-1.073318	-3.555316	3.026678
42	6	0	-1.615468	-4.749586	3.840580
43	6	0	0.095873	-2.892436	3.779173
44	6	0	-1.929975	-3.882117	-2.075889
45	6	0	-1.129619	-3.192159	-3.196024
46	6	0	-2.555903	-5.200394	-2.575497
47	6	0	2.051870	-6.155013	0.024373
48	6	0	3.301891	-5.566744	0.704504
49	6	0	1.777739	-7.586952	0.525633
50	6	0	3.327502	5.432838	1.859669
51	6	0	3.091944	6.898152	2.274715
52	6	0	3.802745	4.594123	3.060438
53	6	0	-6.499719	2.012120	-0.206216
54	6	0	-6.533727	-0.021368	-1.798707
55	6	0	-7.347250	1.136850	-1.164887
56	1	0	-5.955287	0.281111	2.360349
57	1	0	-6.910632	-0.266303	0.996967
58	1	0	-4.807229	1.892324	1.125581
59	1	0	-4.528238	-0.522933	-2.419653
60	1	0	-4.545008	1.308904	-3.859130
61	1	0	-5.736517	2.191538	-2.926378
62	1	0	-3.744330	-4.164844	1.811376
63	1	0	-5.641421	-2.654721	2.323567
64	1	0	-3.448635	4.049608	-3.440283
65	1	0	-1.548269	4.936721	-2.119181
66	1	0	1.593370	-0.166096	-1.066438
67	1	0	0.854766	4.914741	2.935895
68	1	0	3.034214	4.647653	-0.725053
69	1	0	0.987226	-5.075495	2.313552
70	1	0	0.331758	-5.302024	-1.899422
71	1	0	0.251512	3.100562	-2.635876
72	1	0	1.259508	4.713455	-4.223929
73	1	0	0.362323	5.603190	-2.980227
74	1	0	2.124198	5.519907	-2.904591
75	1	0	2.363048	2.512808	-3.707707
76	1	0	2.302158	1.816910	-2.080599
77	1	0	3.302723	3.248395	-2.406942
78	1	0	-2.305753	3.591266	1.515935
79	1	0	-0.570340	3.483243	4.039925
80	1	0	-2.262796	2.993448	3.897397
81	1	0	-1.007064	2.092080	3.025843
82	1	0	-2.177421	6.064821	1.704918
83	1	0	-1.266663	5.915427	3.215488
84	1	0	-2.936156	5.332552	3.132717
85	1	0	-1.865907	-2.806250	2.965793
86	1	0	-1.934711	-4.421814	4.837620
87	1	0	-2.471753	-5.226411	3.350643
88	1	0	-0.845853	-5.519864	3.973683
89	1	0	-0.236526	-2.585604	4.778731
90	1	0	0.441781	-2.003246	3.249401
91	1	0	0.943875	-3.574322	3.912548
92	1	0	-2.758901	-3.218185	-1.818408
93	1	0	-1.775394	-3.002786	-4.062463
94	1	0	-0.730415	-2.232814	-2.854274
95	1	0	-0.295085	-3.815034	-3.541340
96	1	0	-3.199704	-5.015001	-3.444254
97	1	0	-3.164740	-5.669986	-1.794810
98	1	0	-1.787575	-5.922080	-2.877567
99	1	0	4.185275	-6.172590	0.468575
100	1	0	3.490137	-4.536913	0.384914
101	1	0	3.194549	-5.555615	1.795577
102	1	0	2.650931	-8.230948	0.363431
103	1	0	0.922429	-8.032912	0.005991
104	1	0	1.553616	-7.588829	1.599154
105	1	0	4.003101	7.332414	2.704040
106	1	0	2.298778	6.972607	3.028056
107	1	0	2.793686	7.508873	1.415696
108	1	0	4.005330	3.558209	2.765367
109	1	0	4.721842	5.013483	3.487379
110	1	0	3.048538	4.569743	3.855600
111	1	0	-7.143283	2.441198	0.572454
112	1	0	-6.074739	2.867448	-0.744098
113	1	0	-6.950689	-0.273903	-2.781971
114	1	0	-6.627858	-0.930325	-1.193000
115	1	0	-7.771570	1.775028	-1.948788
116	1	0	-8.209483	0.717303	-0.633562
117	6	0	3.085111	-0.933505	0.521485
118	8	0	4.343260	-1.407862	0.378249
119	8	0	2.597470	-0.616412	-1.093530
120	6	0	5.334255	-0.343898	0.585421
121	6	0	4.509682	0.958592	0.632087
122	6	0	3.132051	0.476507	1.096222
123	1	0	5.773506	-0.548043	1.568703
124	1	0	4.443496	1.407480	-0.362001
125	1	0	4.962290	1.691608	1.305045
126	1	0	2.301048	1.102335	0.770852
127	1	0	3.077784	0.375485	2.186135
128	8	0	2.258550	-1.854357	0.978136
129	6	0	2.542599	-1.805200	-1.912115
130	1	0	3.554425	-2.204669	-1.988842
131	1	0	2.178051	-1.501036	-2.895596
132	1	0	1.873186	-2.548684	-1.471752
133	1	0	1.339222	-1.448912	1.141204
134	6	0	6.416074	-0.415971	-0.464151
135	6	0	7.744935	-0.622422	-0.080997
136	6	0	6.117429	-0.262506	-1.825774
137	6	0	8.763511	-0.666600	-1.035342
138	1	0	7.985385	-0.751348	0.971951
139	6	0	7.131095	-0.315619	-2.780307
140	1	0	5.088467	-0.102933	-2.135263
141	6	0	8.457684	-0.515134	-2.387359
142	1	0	9.791611	-0.825421	-0.721561
143	1	0	6.887291	-0.198536	-3.832847
144	1	0	9.247017	-0.553352	-3.133211
145	1	0	2.261277	-6.219849	-1.052811
146	1	0	4.135850	5.428679	1.11518

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1ga (Cy-SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3238.935855 hartree

Zero-point Energy Correction = 1.261444 hartree

Thermal Correction to Energy = 1.329344 hartree

Thermal correction to Enthalpy = 1.330288 hartree

Thermal correction to Gibbs Free Energy= 1.156167 hartree

Sum of electronic and Zero-point Energies = -3237.674410 hartree

Sum of electronic and thermal Energies = -3237.606511 hartree

Sum of electronic and thermal Enthalpies = -3237.605567 hartree

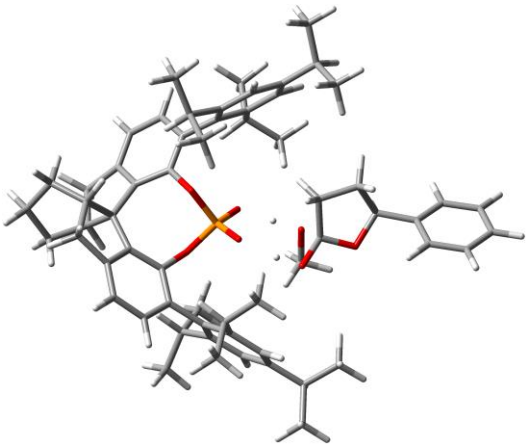
Sum of electronic and thermal Free Energies= -3237.779687 hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.651691	-0.594127	1.642156
2	6	0	-5.337172	0.636492	0.741542
3	6	0	-3.664255	-1.058135	0.384959
4	6	0	-4.553316	-1.578483	1.334278
5	6	0	-5.067973	-0.344257	-1.646373
6	6	0	-5.063552	0.866245	-2.621094
7	6	0	-4.006337	1.786876	-2.074502
8	6	0	-3.444172	1.274984	-0.898154
9	6	0	-4.289834	0.131517	-0.340526
10	6	0	-2.440507	-1.705695	0.190618
11	6	0	-2.201536	-2.993304	0.712053
12	6	0	-3.206182	-3.552960	1.521038
13	6	0	-4.340622	-2.835017	1.891945
14	6	0	-3.560974	2.989143	-2.614592
15	6	0	-2.512701	3.658619	-1.991538
16	6	0	-1.816463	3.104185	-0.902466
17	6	0	-2.290061	1.880178	-0.388809
18	8	0	-1.611357	1.254703	0.656587
19	8	0	-1.433243	-1.045651	-0.518816
20	15	0	-0.541819	0.056590	0.314028
21	8	0	-0.058235	-0.470182	1.637914
22	8	0	0.496283	0.533262	-0.699121
23	6	0	-0.964645	-3.795170	0.424463
24	6	0	-0.638516	3.855950	-0.354079
25	6	0	-0.667233	4.374912	0.966831
26	6	0	0.392609	5.173600	1.409896
27	6	0	1.476077	5.504129	0.592982
28	6	0	1.485549	4.984115	-0.701818
29	6	0	0.463510	4.162137	-1.196111
30	6	0	-0.137925	-4.249483	1.486319
31	6	0	0.940423	-5.094734	1.190893
32	6	0	1.242525	-5.509134	-0.106414
33	6	0	0.428543	-5.035768	-1.137767
34	6	0	-0.668431	-4.199027	-0.904868
35	6	0	0.593946	3.655435	-2.636606
36	6	0	0.494567	4.812028	-3.652585
37	6	0	1.892265	2.859659	-2.873431
38	6	0	-1.844662	4.163884	1.920012
39	6	0	-1.423988	3.445507	3.216088
40	6	0	-2.555617	5.497216	2.228361
41	6	0	-0.377071	-3.892190	2.956580
42	6	0	-0.886427	-5.111943	3.754307
43	6	0	0.875696	-3.320458	3.645913
44	6	0	-1.536744	-3.822849	-2.107102
45	6	0	-0.750538	-3.024706	-3.164734
46	6	0	-2.196587	-5.069761	-2.730408
47	6	0	2.381659	-6.487483	-0.366340
48	6	0	1.845737	-7.862605	-0.812137
49	6	0	3.411478	-5.951034	-1.376152
50	6	0	2.594157	6.418200	1.078207
51	6	0	2.077428	7.841254	1.365784
52	6	0	3.328472	5.843393	2.303901
53	6	0	-6.599848	1.248894	0.124776
54	6	0	-6.486247	-0.855891	-1.365501
55	6	0	-7.393470	0.229808	-0.731813
56	1	0	-5.640622	-0.318427	2.704523
57	1	0	-6.648347	-1.007632	1.447806
58	1	0	-4.829915	1.393564	1.350823
59	1	0	-4.478098	-1.152655	-2.094116
60	1	0	-4.821853	0.551088	-3.644399
61	1	0	-6.043924	1.354516	-2.679519
62	1	0	-3.061797	-4.559040	1.899627
63	1	0	-5.049582	-3.257972	2.599514
64	1	0	-4.025202	3.404444	-3.505768
65	1	0	-2.187477	4.620673	-2.373981
66	1	0	1.772083	0.686841	-0.249118
67	1	0	0.352835	5.573688	2.420031
68	1	0	2.318523	5.234776	-1.355833
69	1	0	1.559924	-5.457802	2.008029
70	1	0	0.632731	-5.349933	-2.158465
71	1	0	-0.231209	2.967187	-2.831445
72	1	0	0.527196	4.424215	-4.677990
73	1	0	-0.434017	5.381109	-3.536338
74	1	0	1.326896	5.517003	-3.537292
75	1	0	1.925957	2.502392	-3.909996
76	1	0	1.941883	1.986949	-2.218658
77	1	0	2.786726	3.473782	-2.711281
78	1	0	-2.578407	3.525921	1.423539
79	1	0	-0.705294	4.039394	3.793892
80	1	0	-2.298972	3.276786	3.855632
81	1	0	-0.972468	2.473485	2.997940
82	1	0	-2.890314	5.990200	1.308671
83	1	0	-1.897778	6.194568	2.760448
84	1	0	-3.434916	5.322902	2.860561
85	1	0	-1.142051	-3.113255	2.996174
86	1	0	-1.103291	-4.826961	4.791034
87	1	0	-1.798063	-5.540583	3.325262
88	1	0	-0.131873	-5.907809	3.778720
89	1	0	0.625826	-3.001787	4.664915
90	1	0	1.268219	-2.454071	3.111670
91	1	0	1.676816	-4.065248	3.726432
92	1	0	-2.348338	-3.181210	-1.758117
93	1	0	-1.410061	-2.741016	-3.994208
94	1	0	-0.334070	-2.109124	-2.734818
95	1	0	0.072024	-3.614883	-3.586672
96	1	0	-2.867431	-4.778533	-3.547997
97	1	0	-2.784965	-5.620358	-1.987852
98	1	0	-1.450952	-5.759459	-3.143046
99	1	0	2.667289	-8.578800	-0.935584
100	1	0	1.144024	-8.269845	-0.076321
101	1	0	1.318112	-7.788877	-1.770495
102	1	0	4.232076	-6.666206	-1.509156
103	1	0	3.841296	-5.002249	-1.035962
104	1	0	2.959291	-5.778981	-2.359788
105	1	0	2.902727	8.502973	1.655311
106	1	0	1.588409	8.269696	0.484164
107	1	0	1.347531	7.839927	2.183956
108	1	0	4.153572	6.500273	2.604471
109	1	0	3.745706	4.852726	2.090588
110	1	0	2.654786	5.742437	3.162823
111	1	0	-7.240881	1.643788	0.923248
112	1	0	-6.311961	2.115253	-0.482368
113	1	0	-6.932690	-1.214656	-2.301792
114	1	0	-6.424754	-1.732287	-0.710513
115	1	0	-7.941271	0.769952	-1.512933
116	1	0	-8.162418	-0.260115	-0.122931
117	6	0	3.157716	-0.616727	1.021678
118	8	0	4.494708	-0.540509	1.221662
119	8	0	2.812289	0.759838	0.095995
120	1	0	1.485750	-0.506262	1.986684
121	6	0	5.221143	-1.341767	0.230667
122	6	0	4.150155	-1.762146	-0.796229
123	6	0	2.860182	-1.733572	0.029188
124	1	0	5.583928	-2.219743	0.777675
125	1	0	4.099892	-1.038035	-1.613719
126	1	0	4.370334	-2.742879	-1.225265
127	1	0	1.956321	-1.559229	-0.554544

128	1	0	2.720361	-2.653241	0.607656
129	8	0	2.488833	-0.470674	2.155018
130	6	0	3.002240	1.985329	0.841000
131	1	0	2.809306	2.812556	0.158888
132	1	0	2.319031	2.029488	1.691658
133	1	0	4.036322	1.999025	1.187405
134	6	0	6.401939	-0.573884	-0.311471
135	6	0	6.227889	0.651458	-0.970822
136	6	0	7.692616	-1.095069	-0.178833
137	6	0	7.326091	1.336384	-1.486754
138	1	0	5.229634	1.066802	-1.075035
139	6	0	8.793578	-0.414313	-0.703084
140	1	0	7.838546	-2.040176	0.339603
141	6	0	8.612020	0.803862	-1.356929
142	1	0	7.179637	2.286609	-1.993416
143	1	0	9.790212	-0.833346	-0.594074
144	1	0	9.466800	1.338521	-1.762345
145	1	0	2.904193	-6.634424	0.589111
146	1	0	3.326121	6.494249	0.261977

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1ga (Cy-SPINOL)



B3LYP/6-31G(d); E(B3LYP) = -3238.937365 hartree

Zero-point Energy Correction = 1.261248 hartree

Thermal Correction to Energy = 1.329408 hartree

Thermal correction to Enthalpy = 1.330352 hartree

Thermal correction to Gibbs Free Energy= 1.155028 hartree

Sum of electronic and Zero-point Energies = -3237.676117 hartree

Sum of electronic and thermal Energies = -3237.607957 hartree

Sum of electronic and thermal Enthalpies = -3237.607013 hartree

Sum of electronic and thermal Free Energies= -3237.782338 hartree

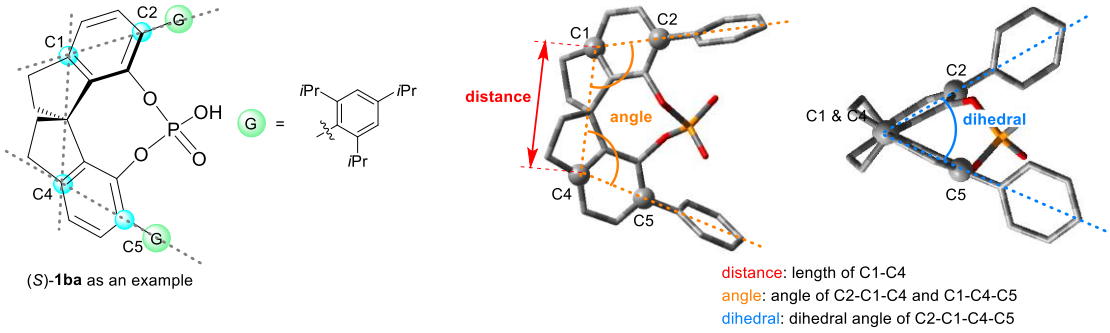
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.696365	-0.491521	1.921284
2	6	0	-5.404832	0.748694	1.029549
3	6	0	-3.838285	-1.001783	0.493893
4	6	0	-4.646113	-1.495097	1.526666
5	6	0	-5.348325	-0.122606	-1.413582
6	6	0	-5.377825	1.156481	-2.300166
7	6	0	-4.246938	2.004011	-1.779099
8	6	0	-3.601628	1.376814	-0.704649
9	6	0	-4.460146	0.239623	-0.146474
10	6	0	-2.664851	-1.693758	0.181525
11	6	0	-2.380597	-2.959004	0.733414
12	6	0	-3.308049	-3.484607	1.648896
13	6	0	-4.404720	-2.746067	2.087029
14	6	0	-3.799039	3.228882	-2.264330
15	6	0	-2.666992	3.809302	-1.695910
16	6	0	-1.892401	3.134915	-0.737476
17	6	0	-2.369010	1.887195	-0.286407
18	8	0	-1.580253	1.132838	0.583088
19	8	0	-1.753222	-1.102068	-0.691595
20	15	0	-0.654580	-0.050105	-0.073010
21	8	0	0.139007	-0.632732	1.068962
22	8	0	0.097132	0.455265	-1.297680
23	6	0	-1.133554	-3.722591	0.397887
24	6	0	-0.623722	3.754682	-0.225295
25	6	0	-0.508414	4.112173	1.144016
26	6	0	0.659752	4.736599	1.592753
27	6	0	1.725119	5.033854	0.740934
28	6	0	1.590046	4.682835	-0.602264
29	6	0	0.445952	4.052684	-1.110628
30	6	0	-0.187362	-4.030193	1.413847
31	6	0	0.967144	-4.740296	1.069456
32	6	0	1.237696	-5.149917	-0.237526
33	6	0	0.283820	-4.859594	-1.213273
34	6	0	-0.899330	-4.166808	-0.926621
35	6	0	0.404745	3.756738	-2.612768
36	6	0	0.232432	5.056060	-3.428595
37	6	0	1.646604	2.999071	-3.118447
38	6	0	-1.632567	3.902429	2.159751
39	6	0	-1.195222	3.004481	3.332843
40	6	0	-2.181465	5.251583	2.666873
41	6	0	-0.372615	-3.646783	2.885997
42	6	0	-0.664233	-4.896108	3.743350
43	6	0	0.824177	-2.872292	3.470649
44	6	0	-1.917346	-3.990449	-2.054328
45	6	0	-1.342159	-3.224774	-3.260301
46	6	0	-2.492900	-5.354076	-2.488798
47	6	0	2.507057	-5.913655	-0.591035
48	6	0	3.781889	-5.198269	-0.106587
49	6	0	2.455499	-7.361553	-0.064405
50	6	0	2.972988	5.752314	1.239305
51	6	0	2.661869	7.209058	1.635326
52	6	0	3.661451	5.006730	2.397178
53	6	0	-6.691584	1.422428	0.538078
54	6	0	-6.756406	-0.610765	-1.051961
55	6	0	-7.579216	0.464471	-0.297305
56	1	0	-5.620222	-0.239655	2.986903
57	1	0	-6.712566	-0.876953	1.774248
58	1	0	-4.824439	1.469677	1.617338
59	1	0	-4.821674	-0.913800	-1.959965
60	1	0	-5.224901	0.907718	-3.358255
61	1	0	-6.342760	1.674222	-2.247692
62	1	0	-3.128657	-4.474316	2.057196
63	1	0	-5.056589	-3.141807	2.862132
64	1	0	-4.324072	3.731282	-3.073188
65	1	0	-2.341559	4.789179	-2.029195
66	1	0	1.393543	0.038013	-1.491319
67	1	0	0.729287	5.012872	2.641992
68	1	0	2.403586	4.921266	-1.284048
69	1	0	1.688033	-4.967732	1.849970
70	1	0	0.460296	-5.200929	-2.231587
71	1	0	-0.456407	3.113812	-2.808554
72	1	0	0.146374	4.829464	-4.498467
73	1	0	-0.658699	5.617692	-3.129922
74	1	0	1.095687	5.719874	-3.296057
75	1	0	1.525079	2.757508	-4.181615
76	1	0	1.791652	2.063111	-2.576004
77	1	0	2.560917	3.598053	-3.026706
78	1	0	-2.460300	3.396809	1.657964
79	1	0	-0.398835	3.472687	3.924021
80	1	0	-2.040962	2.823594	4.007744
81	1	0	-0.833629	2.037734	2.971425
82	1	0	-2.530805	5.875620	1.836485
83	1	0	-1.418358	5.819375	3.212375
84	1	0	-3.025467	5.089583	3.348627
85	1	0	-1.236044	-2.982264	2.960513

86	1	0	-0.857216	-4.611246	4.784939
87	1	0	-1.535253	-5.450542	3.376637
88	1	0	0.187869	-5.586562	3.738528
89	1	0	0.624613	-2.622661	4.520255
90	1	0	0.984882	-1.940087	2.925959
91	1	0	1.750423	-3.458061	3.444255
92	1	0	-2.755062	-3.403252	-1.670777
93	1	0	-2.116553	-3.082145	-4.024278
94	1	0	-0.978770	-2.238331	-2.958012
95	1	0	-0.516200	-3.771926	-3.731553
96	1	0	-3.266891	-5.218754	-3.254451
97	1	0	-2.942621	-5.882140	-1.640473
98	1	0	-1.715921	-6.002781	-2.910565
99	1	0	4.675289	-5.715534	-0.477099
100	1	0	3.814775	-4.158279	-0.446725
101	1	0	3.840286	-5.185338	0.988187
102	1	0	3.350172	-7.919380	-0.367642
103	1	0	1.576145	-7.891445	-0.446995
104	1	0	2.404658	-7.379123	1.031020
105	1	0	3.575760	7.733842	1.939636
106	1	0	2.213560	7.758235	0.800274
107	1	0	1.957894	7.247208	2.475089
108	1	0	4.586523	5.517801	2.689810
109	1	0	3.915052	3.978749	2.114954
110	1	0	3.016392	4.957789	3.282109
111	1	0	-7.256919	1.795838	1.401550
112	1	0	-6.426980	2.308862	-0.049804
113	1	0	-7.283881	-0.908639	-1.967133
114	1	0	-6.672033	-1.521208	-0.447046
115	1	0	-8.172621	1.054578	-1.005638
116	1	0	-8.310421	-0.035042	0.349025
117	6	0	3.108004	-0.578276	-0.081366
118	8	0	4.384394	-0.897233	-0.387269
119	8	0	2.417956	-0.285117	-1.647893
120	6	0	5.144899	0.333180	-0.572487
121	6	0	4.508123	1.296846	0.451268
122	6	0	3.041830	0.828242	0.528894
123	1	0	4.951762	0.687552	-1.591864
124	1	0	5.008924	1.181053	1.417452
125	1	0	4.609514	2.339306	0.139667
126	1	0	2.667381	0.751947	1.551901
127	1	0	2.359261	1.475872	-0.022260
128	8	0	2.452079	-1.598304	0.423359
129	6	0	2.410247	-1.450268	-2.497652
130	1	0	1.866900	-2.272995	-2.025208
131	1	0	1.927647	-1.164889	-3.435007
132	1	0	3.446685	-1.738028	-2.678842
133	1	0	1.523607	-1.296906	0.725638
134	6	0	6.614408	0.053471	-0.391842
135	6	0	7.547536	0.683810	-1.221435
136	6	0	7.068407	-0.794786	0.626507
137	6	0	8.915793	0.483423	-1.030717
138	1	0	7.202738	1.333963	-2.022708
139	6	0	8.434350	-1.004250	0.809818
140	1	0	6.347320	-1.303935	1.259048
141	6	0	9.361822	-0.362353	-0.014817
142	1	0	9.630166	0.980235	-1.681571
143	1	0	8.775731	-1.671378	1.596774
144	1	0	10.426122	-0.526126	0.130780
145	1	0	2.554467	-5.966661	-1.687983
146	1	0	3.682582	5.785774	0.400501

14. Structural Properties of CPA Candidates in Transitions States

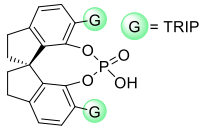
Structural properties in transitions states



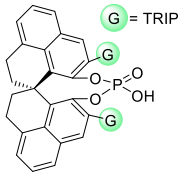
(*S*)-**1ba** as an example

distance: length of C1-C4
angle: angle of C2-C1-C4 and C1-C4-C5
dihedral: dihedral angle of C2-C1-C4-C5

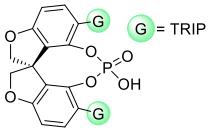
Structural Properties of SPINOL-derived CPA (*S*)-1ba in Transitions States

 (*S*)-**1ba** (SPINOL)	optimized structure	*R-anti*	*R-re*	*S-anti*	*S-si*	*S-syn*	*S-re*
distance (Å)	4.78	4.78	4.78	4.77	4.77	4.78	4.78
angle 1	100.3°	100.0°	99.4°	100.6°	100.2°	100.3°	99.6°
angle 2	99.0°	99.0°	100.0°	100.4°	99.7°	98.7°	99.9°
dihedral angle	61.2°	60.9°	58.8°	58.0°	59.9°	61.4°	58.8°
$\Delta\Delta G^{\neq}$ (kcal/mol)	--	-2.03	**0.00**	1.98	0.55	**1.31**	-0.37

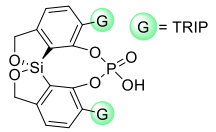
Structural Properties of SPHENOL-derived CPA (*S*)-1ca in Transitions States

 (*S*)-**1ca** (SPHENOL)	optimized structure	*R-anti*	*R-re*	*S-anti*	*S-si*	*S-syn*	*S-re*
distance (Å)	5.13	5.12	5.12	5.10	5.11	5.12	5.12
angle 1	94.2°	93.3°	93.6°	94.4°	94.5°	94.4°	94.5°
angle 2	93.0°	94.4°	94.6°	95.0°	93.5°	92.3°	93.7°
dihedral angle	61.8°	64.7°	62.4°	62.9°	64.9°	66.0°	62.4°
$\Delta\Delta G^{\neq}$ (kcal/mol)	--	-2.30	**0.00**	3.20	2.51	**1.14**	-0.22

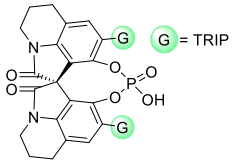
Structural Properties of Oxa-SPINOL-derived CPA (*S*)-1da in Transitions States

 (*S*)-**1da** (Oxa-SPINOL)	optimized structure	*R-anti*	*R-re*	*S-anti*	*S-si*	*S-syn*	*S-re*
distance (Å)	4.67	4.66	4.67	4.65	4.66	4.66	4.67
angle 1	102.2°	101.7°	101.8°	103.0°	102.5°	102.6°	101.9°
angle 2	101.3°	102.2°	102.2°	102.4°	102.0°	101.3°	102.1°
dihedral angle	55.7°	58.5°	56.9°	56.0°	57.8°	59.0°	56.9
$\Delta\Delta G^{\neq}$ (kcal/mol)	--	-2.08	**0.00**	1.95	1.13	**1.79**	-0.12

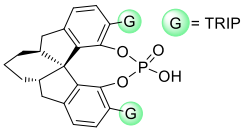
Structural Properties of SPISIOL-derived CPA (*S*)-1ea in Transitions States

 (*S*)-**1ea** (Oxa-SPISIOL)	**optimized structure**	***R-anti***	***R-re***	***S-anti***	***S-si***	***S-syn***	***S-re***
distance (Å)	5.26	5.24	5.25	5.23	5.23	5.24	5.25
angle 1	98.8°	98.1°	99.1°	99.4°	99.3°	99.7°	98.4°
angle 2	97.8°	99.1°	98.4°	100.2°	99.0°	97.6°	99.0°
dihedral angle	50.6°	54.8°	52.7°	50.8°	54.0°	55.3°	52.5°
$\Delta\Delta G^{\neq}$ (kcal/mol)	--	-2.08	**0.00**	**1.40**	1.34	1.81	-0.43

Structural Properties of SBIDOL-derived CPA (*S*)-1fa in Transitions States

 (*S*)-**1fa** (SBIDOL)	**optimized structure**	***R-anti***	***R-re***	***S-anti***	***S-si***	***S-syn***	***S-re***
distance (Å)	4.68	4.67	4.67	4.66	4.66	4.67	4.67
angle 1	101.7°	101.6°	101.3°	101.7°	101.9°	102.2°	101.4°
angle 2	100.9°	101.0°	101.9°	102.1°	101.3°	100.7°	101.6°
dihedral angle	57.2°	60.7°	58.2°	60.4°	60.4°	60.8°	58.7°
$\Delta\Delta G^{\neq}$ (kcal/mol)	--	-2.84	**0.00**	**0.73**	0.25	1.42	-0.42

Structural Properties of Cy-SPINOL-derived CPA (*S*)-1ga in Transitions States

 (*S*)-**1ga** (Cy-SPINOL)	**optimized structure**	***R-anti***	***R-re***	***S-anti***	***S-si***	***S-syn***	***S-re***
distance (Å)	4.84	4.83	4.83	4.82	4.82	4.83	4.83
angle 1	96.7°	96.7°	96.1°	96.5°	96.9°	95.2°	96.1°
angle 2	95.6°	95.7°	96.8°	97.2°	95.8°	97.0°	96.7°
dihedral angle	66.9°	69.7°	67.7°	68.9°	70.0°	70.8°	67.9°
$\Delta\Delta G^{\neq}$ (kcal/mol)	--	-1.51	**0.00**	3.13	1.31	**1.83**	-0.21

Vibrational frequency analysis of carbonyl groups of SBIDOL-derived CPA (*S*)-1fa in transition states

Contrary to our expectations based on the structural similarity of free catalysts, SBIDOL-derived CPA (*S*)-**1fa** exhibited significantly lower $\Delta\Delta G^{\ddagger}$ in the TS of ***S-anti*** and ***S-si*** compared to Oxa-SPINOL-derived CPA (*S*)-**1da** having similar structural parameters. To clarify the structural feature of (*S*)-**1fa**, the following considerations were made regarding the destabilization factors of the TSs. We believed that the distortion energy in the TSs of (*S*)-**1fa** has the most significant impact on the relatively flexible amide bond site of the SBIDOL backbone, rather than aromatic regions. As a result, the extent of this strain should be represented by the frequencies of normal mode vibrations. Specifically, when torsional strain is applied to the amide site, the double bond character of the conjugated carbonyl bond is restored, resulting in a low-wavenumber shift in the vibrational frequency of carbonyl groups. To compare the frequencies of the asymmetric stretching vibration of carbonyl group in the TS structures calculated by vibrational analysis (B3LYP/6-31G(d), scaled by 0.96), we represent the wavenumber shift based on free (*S*)-**1fa** (Table S2 & Figure S1). Thus, the relatively large low-wavenumber shift of ***R-re***, ***S-syn***, and ***S-re*** implied that their TS structures were destabilized due to the torsional strain of amide. On the other hand, ***S-anti*** and ***S-si*** were not significantly influenced in terms of the wavenumber shift. Therefore, these results suggests that the $\Delta\Delta G^{\neq}$ of ***S-anti*** and ***S-si*** are reduced by energetically destabilized ***S-re***, while ***R-re*** and ***S-syn*** are offset by the similar tendency of destabilization. The above discussion is consistent with the calculated values of $\Delta\Delta G^{\neq}$.

Table S2

	shift (cm^{-1})	ir int		freq	scaled by 0.96	$\Delta\Delta G^{\neq}$ (kcal/mol)
free SBIDOL	0.0	561	asym	1823.42	1750.5	--
R-anti	-0.6	563	asym	1822.84	1749.9	-2.84
R-re	**-2.2**	564	asym	1821.12	1748.3	**0.00** (RDS)
S-anti	0.3	570	asym	1823.78	1750.8	**0.73** (RDS)
S-si	-0.3	565	asym	1823.14	1750.2	0.25
S-syn	**-1.5**	559	asym	1821.82	1748.9	1.42
S-re	**-1.8**	539	asym	1821.58	1748.7	-0.42

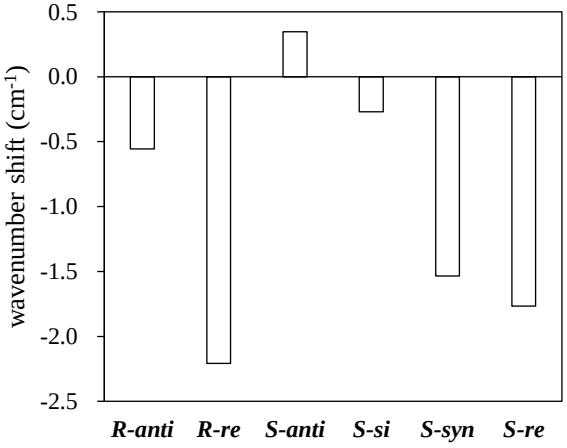
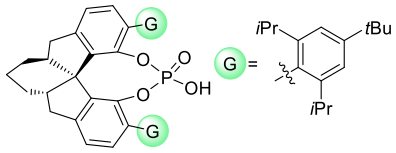


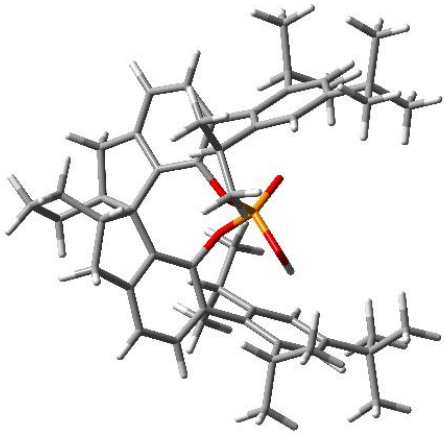
Figure S1

15. DFT Calculation of Cy-SPINOL-derived CPAs Having Bulky Substituents

Optimized structure of Cy-SPINOL-derived CPA (*S*)-1gd



(*S*)-**1gd** (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -2664.27963553 Hartree

Zero-point correction= 1.083112 Hartree

Thermal correction to Energy= 1.140129 Hartree

Thermal correction to Enthalpy= 1.141073 Hartree

Thermal correction to Gibbs Free Energy= 0.993568 Hartree

Sum of electronic and zero-point Energies= -2663.196524 Hartree

Sum of electronic and thermal Energies= -2663.139506 Hartree

Sum of electronic and thermal Enthalpies= -2663.138562 Hartree

Sum of electronic and thermal Free Energies= -2663.286068 Hartree

The number of Imaginary frequencies = 0

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.778903	4.422045	-2.153480
2	6	0	-0.451107	4.267027	-1.215124
3	6	0	1.220773	2.643004	-0.608649
4	6	0	1.719385	3.328438	-1.724576
5	6	0	0.466884	4.325992	1.213860
6	6	0	-0.792339	4.481890	2.116141
7	6	0	-1.705868	3.362297	1.689576
8	6	0	-1.135060	2.618521	0.647782
9	6	0	0.034035	3.379006	0.015001
10	6	0	1.853398	1.457994	-0.231515
11	6	0	3.050728	1.019687	-0.830794
12	6	0	3.589789	1.823057	-1.848477
13	6	0	2.915222	2.944964	-2.325651
14	6	0	-2.935036	3.000453	2.233816
15	6	0	-3.584556	1.864402	1.754170
16	6	0	-2.976306	1.002477	0.826249
17	6	0	-1.721599	1.391709	0.323860
18	8	0	-0.997444	0.490158	-0.480339
19	8	0	1.267624	0.667076	0.760827
20	15	0	0.090438	-0.383995	0.350353
21	8	0	0.651851	-1.226465	-0.894480
22	8	0	-0.358396	-1.110430	1.549933
23	6	0	3.704209	-0.274234	-0.435716
24	6	0	-3.668040	-0.258311	0.394788
25	6	0	-4.116933	-0.396492	-0.939701
26	6	0	-4.805962	-1.557305	-1.315706
27	6	0	-5.080655	-2.592500	-0.421865
28	6	0	-4.634164	-2.425312	0.893792
29	6	0	-3.934929	-1.295664	1.326655
30	6	0	3.822498	-1.343031	-1.373477
31	6	0	4.400237	-2.546951	-0.953954
32	6	0	4.887195	-2.752867	0.342532
33	6	0	4.790307	-1.678529	1.227265
34	6	0	4.214885	-0.450759	0.872898
35	6	0	-3.509416	-1.235351	2.796091
36	6	0	-4.726372	-1.009946	3.717565
37	6	0	-2.731091	-2.487769	3.243072
38	6	0	-3.929134	0.689470	-2.000648
39	6	0	-3.102395	0.190308	-3.201211
40	6	0	-5.283811	1.264972	-2.460414
41	6	0	3.406743	-1.225152	-2.846775
42	6	0	4.653900	-1.076047	-3.744712
43	6	0	2.546821	-2.400414	-3.354185
44	6	0	4.227262	0.667999	1.915338
45	6	0	3.518344	0.267705	3.223086
46	6	0	5.669973	1.140935	2.188676
47	6	0	5.500427	-4.110691	0.730748
48	6	0	4.439858	-5.222640	0.548124
49	6	0	6.716126	-4.407543	-0.179327
50	6	0	-5.835760	-3.872879	-0.823996
51	6	0	-4.926904	-5.101970	-0.584090
52	6	0	-7.116325	-4.008883	0.033552
53	6	0	-1.038807	5.621374	-0.801631
54	6	0	1.024533	5.677250	0.751035
55	6	0	-0.015424	6.506456	-0.045236
56	1	0	0.492354	4.308295	-3.206632
57	1	0	1.239025	5.413995	-2.070148
58	1	0	-1.218057	3.689305	-1.744292
59	1	0	1.237853	3.793362	1.782910
60	1	0	-0.530410	4.389671	3.177853
61	1	0	-1.261907	5.466279	2.005068
62	1	0	4.532060	1.529601	-2.299760
63	1	0	3.314509	3.503813	-3.168375
64	1	0	-3.387073	3.595079	3.023868
65	1	0	-4.564704	1.600605	2.138247
66	1	0	-5.140009	-1.636848	-2.344017
67	1	0	-4.830831	-3.209346	1.618895
68	1	0	4.480295	-3.352005	-1.677895
69	1	0	5.172945	-1.783390	2.235713
70	1	0	-2.830426	-0.387890	2.918367
71	1	0	-4.405048	-0.920643	4.762599
72	1	0	-5.280060	-0.101356	3.455624
73	1	0	-5.428842	-1.850161	3.655374
74	1	0	-2.388440	-2.359460	4.277286
75	1	0	-1.853824	-2.641214	2.611938
76	1	0	-3.353424	-3.390555	3.216916
77	1	0	-3.374753	1.517399	-1.550986
78	1	0	-3.616134	-0.616259	-3.737785
79	1	0	-2.936071	1.006528	-3.915503
80	1	0	-2.127738	-0.184989	-2.875613
81	1	0	-5.854744	1.659577	-1.612409
82	1	0	-5.900610	0.503128	-2.951370
83	1	0	-5.130730	2.081184	-3.177355
84	1	0	2.803816	-0.320605	-2.959895
85	1	0	4.358909	-0.916527	-4.788784
86	1	0	5.283292	-0.234428	-3.437192
87	1	0	5.274101	-1.979566	-3.705365
88	1	0	2.260626	-2.220540	-4.396979
89	1	0	1.624392	-2.515074	-2.778022
90	1	0	3.088632	-3.352713	-3.328284
91	1	0	3.687699	1.524564	1.504329
92	1	0	3.487661	1.122078	3.910109

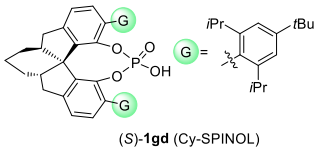
93	1	0	2.490787	-0.054885	3.033146
94	1	0	4.043718	-0.545318	3.738231
95	1	0	5.669704	1.978319	2.896890
96	1	0	6.160784	1.474715	1.267484
97	1	0	6.280627	0.339303	2.620832
98	1	0	4.862086	-6.199125	0.815132
99	1	0	3.568783	-5.042983	1.188418
100	1	0	4.087082	-5.284621	-0.486716
101	1	0	7.159868	-5.375923	0.082258
102	1	0	7.488416	-3.638161	-0.065559
103	1	0	6.435716	-4.445678	-1.237180
104	1	0	-5.451821	-6.025531	-0.858985
105	1	0	-4.013972	-5.036455	-1.186869
106	1	0	-4.626751	-5.187548	0.465286
107	1	0	-7.661624	-4.922221	-0.235415
108	1	0	-7.785212	-3.154833	-0.123643
109	1	0	-6.887167	-4.060458	1.102941
110	1	0	-1.396846	6.147114	-1.695891
111	1	0	-1.926852	5.449189	-0.182978
112	1	0	1.365675	6.247239	1.624428
113	1	0	1.919684	5.501720	0.142504
114	1	0	-0.557481	7.181103	0.627559
115	1	0	0.513163	7.160590	-0.748470
116	1	0	1.522435	-1.622703	-0.696306
117	6	0	-6.252597	-3.869021	-2.307046
118	6	0	5.979098	-4.141210	2.194654
119	1	0	6.401354	-5.126187	2.423315
120	1	0	5.156771	-3.963529	2.896770
121	1	0	6.759835	-3.395951	2.385077
122	1	0	-6.924782	-3.035189	-2.539892
123	1	0	-6.784240	-4.797870	-2.543753
124	1	0	-5.385368	-3.805592	-2.974075

DFT calculation for all conformations of real system using Cy-SPINOL-derived CPA (*S*)-1gd*

TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-anti	up	up		--
	up	down		--
	down	up	-3316.351047	-2.59
	down	down	-3316.350679	-2.36
R-re	up	up	-3316.346916	0.00
	up	down	-3316.346450	0.29
	down	up	-3316.346402	0.32
	down	down	-3316.346083	0.52
S-anti	up	up	-3316.341215	3.58
	up	down	-3316.341395	3.46
	down	up		--
	down	down		--
S-si	up	up	-3316.345109	1.13
	up	down		--
	down	up		--
	down	down	-3316.344528	1.50
S-syn	up	up	-3316.345338	0.99
	up	down	-3316.345224	1.06
	down	up	-3316.345042	1.09
	down	down	-3316.345186	1.18
S-re	up	up	-3316.347215	-0.19
	up	down		--
	down	up		--
	down	down		--

*The TS energies of RDSs, namely, ***S-syn*** and ***R-re***, were fully calculated for conformational isomers, however the TS energies not related to RDSs were partially calculated to reduce computational load. Assignments of "up" and "down" are shown in ESI page S55.

DFT calculation of real system using Cy-SPINOL-derived CPA (*S*)-1gd



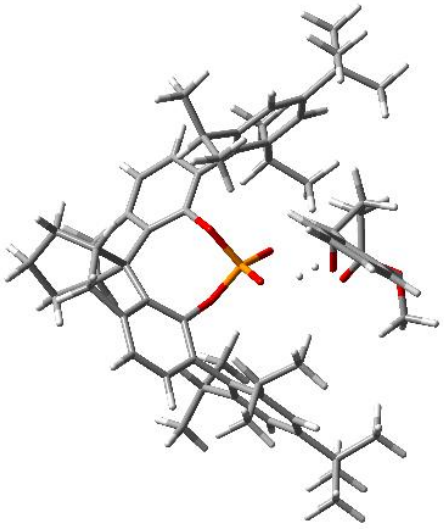
(*S*)-**1gd** (Cy-SPINOL)

1st / 2nd	ΔΔG≠ (kcal/mol)
R-anti* / *R-re	-2.59 / **0.00**
R-syn / *R-si*	-- / --
S-anti* / *S-si	**3.46** / 1.13
S-syn* / *S-re	**0.99** / -0.19

ΔΔG≠ of RDS = **0.99** kcal/mol

B3LYP/6-31G(d); E(RB3LYP) = -3317.56064374 Hartree
Zero-point correction= 1.316490 Hartree
Thermal correction to Energy= 1.386769 Hartree
Thermal correction to Enthalpy= 1.387713 Hartree
Thermal correction to Gibbs Free Energy= 1.209597 Hartree
Sum of electronic and zero-point Energies= -3316.244154 Hartree
Sum of electronic and thermal Energies= -3316.173875 Hartree
Sum of electronic and thermal Enthalpies= -3316.172931 Hartree
Sum of electronic and thermal Free Energies= -3316.351047 Hartree
The number of Imaginary frequencies = 1

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1gd (Cy-SPINOL)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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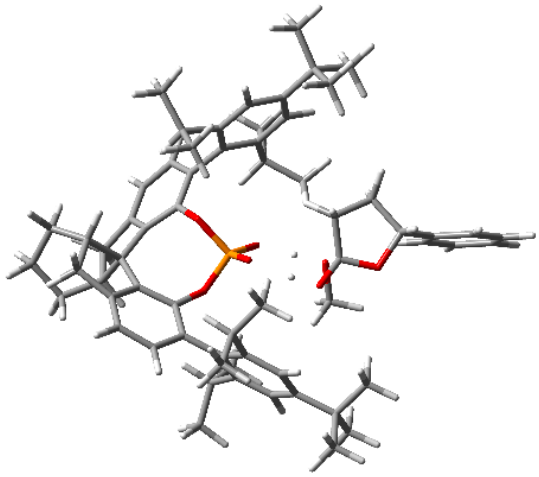
2	6	0	0.065029	4.580376	2.227487
3	6	0	-1.484435	3.041084	1.213375
4	6	0	-2.026245	3.377946	2.460441
5	6	0	-1.001414	5.231121	-0.048704
6	6	0	0.159658	5.762254	-0.935208
7	6	0	1.192629	4.668462	-0.898157
8	6	0	0.790444	3.618831	-0.062076
9	6	0	-0.395725	4.033961	0.808338
10	6	0	-2.032692	1.957282	0.522664
11	6	0	-3.254320	1.373274	0.911397
12	6	0	-3.847878	1.860082	2.088835
13	6	0	-3.216383	2.803566	2.896621
14	6	0	2.393800	4.604778	-1.597751
15	6	0	3.179311	3.461030	-1.487505
16	6	0	2.744123	2.326230	-0.781020
17	6	0	1.515186	2.423261	-0.099184

18	8	0	0.992145	1.303496	0.551286
19	8	0	-1.336013	1.433500	-0.570490
20	15	0	-0.108805	0.396868	-0.261937
21	8	0	-0.539131	-0.658150	0.757287
22	8	0	0.415190	-0.076932	-1.592039
23	6	0	-3.940737	0.299176	0.118118
24	6	0	3.616333	1.103758	-0.773804
25	6	0	4.234585	0.672658	0.423335
26	6	0	5.143331	-0.395540	0.384206
27	6	0	5.493269	-1.046192	-0.800664
28	6	0	4.857479	-0.608053	-1.969159
29	6	0	3.929113	0.437431	-1.989616
30	6	0	-4.217127	-0.968054	0.699126
31	6	0	-4.925108	-1.914828	-0.046179
32	6	0	-5.374558	-1.681640	-1.350784
33	6	0	-5.091305	-0.430306	-1.897348
34	6	0	-4.395266	0.563818	-1.196116
35	6	0	3.324204	0.828723	-3.341975
36	6	0	4.382170	1.467109	-4.266329
37	6	0	2.649105	-0.355734	-4.059351
38	6	0	4.019087	1.371096	1.767391
39	6	0	3.403872	0.431332	2.821446
40	6	0	5.325446	2.006011	2.285589
41	6	0	-3.794701	-1.352229	2.120312
42	6	0	-5.008504	-1.405158	3.072026
43	6	0	-3.038622	-2.692794	2.178502
44	6	0	-4.219318	1.917155	-1.887432
45	6	0	-3.415841	1.802360	-3.196913
46	6	0	-5.580767	2.600407	-2.128999
47	6	0	-6.149694	-2.774885	-2.109342
48	6	0	-5.265934	-4.038130	-2.240466
49	6	0	-7.436535	-3.132116	-1.328102
50	6	0	6.575736	-2.141269	-0.869913
51	6	0	6.033588	-3.401058	-1.583898
52	6	0	7.783288	-1.592314	-1.668835
53	6	0	0.518536	6.045092	2.199134
54	6	0	-1.634220	6.337891	0.803007
55	6	0	-0.613791	7.007959	1.758204
56	1	0	-0.803489	3.936277	4.148254
57	1	0	-1.657565	5.287185	3.430373
58	1	0	0.899767	3.951583	2.558988
59	1	0	-1.767802	4.799990	-0.703462
60	1	0	-0.179187	5.951545	-1.961837
61	1	0	0.557474	6.715746	-0.567340
62	1	0	-4.806586	1.451619	2.390369
63	1	0	-3.655921	3.090392	3.848892
64	1	0	2.718643	5.434813	-2.220370
65	1	0	4.139684	3.417474	-1.991031
66	1	0	5.612775	-0.693581	1.315209
67	1	0	5.104667	-1.085386	-2.913085
68	1	0	-5.132849	-2.874997	0.417333
69	1	0	-5.428161	-0.197635	-2.901124
70	1	0	2.542561	1.570195	-3.161499
71	1	0	3.920763	1.795935	-5.205398
72	1	0	4.862795	2.336145	-3.804436
73	1	0	5.173497	0.750433	-4.518158
74	1	0	2.206701	-0.014811	-5.003286
75	1	0	1.848842	-0.774558	-3.446736
76	1	0	3.363392	-1.151631	-4.303235
77	1	0	3.311341	2.189573	1.617792
78	1	0	4.059321	-0.422541	3.033624
79	1	0	3.245680	0.967596	3.765267
80	1	0	2.434295	0.053394	2.482282
81	1	0	5.744897	2.701899	1.550535
82	1	0	6.088442	1.248756	2.501197
83	1	0	5.138677	2.562057	3.212450
84	1	0	-3.106908	-0.586916	2.488184
85	1	0	-4.684827	-1.633851	4.094949
86	1	0	-5.558985	-0.458815	3.095847
87	1	0	-5.714752	-2.185630	2.763232
88	1	0	-2.664381	-2.868591	3.194090
89	1	0	-2.182970	-2.698140	1.501189
90	1	0	-3.686196	-3.540305	1.921857
91	1	0	-3.655553	2.573829	-1.220941
92	1	0	-3.258195	2.796457	-3.633713
93	1	0	-2.437185	1.348767	-3.016840
94	1	0	-3.943529	1.196405	-3.943341
95	1	0	-5.437302	3.594103	-2.571233
96	1	0	-6.135148	2.722197	-1.191544
97	1	0	-6.209002	2.019639	-2.814669
98	1	0	-5.805785	-4.830792	-2.773677
99	1	0	-4.349521	-3.814591	-2.799107
100	1	0	-4.975124	-4.432962	-1.261124
101	1	0	-7.997684	-3.916476	-1.851484
102	1	0	-8.088352	-2.256656	-1.228505
103	1	0	-7.213280	-3.497315	-0.320252
104	1	0	6.820206	-4.161670	-1.660080
105	1	0	5.196010	-3.839972	-1.030019
106	1	0	5.686825	-3.182958	-2.598994
107	1	0	8.576429	-2.347737	-1.734459
108	1	0	8.199821	-0.701902	-1.184469
109	1	0	7.498083	-1.314224	-2.688973
110	1	0	0.884716	6.331306	3.193361
111	1	0	1.379963	6.136491	1.527000
112	1	0	-2.077416	7.093725	0.142078
113	1	0	-2.469505	5.914441	1.372410
114	1	0	-0.167256	7.887606	1.279877
115	1	0	-1.146953	7.393282	2.635237
116	6	0	0.446295	-3.355818	-1.264204
117	8	0	0.094872	-2.964130	0.365124
118	6	0	1.297274	-3.147502	1.171724
119	6	0	2.335132	-3.762229	0.209042
120	6	0	1.956682	-3.222948	-1.170062
121	1	0	1.626722	-2.146519	1.469828
122	1	0	2.269330	-4.853997	0.224450
123	1	0	3.347569	-3.476666	0.505889
124	1	0	2.417372	-3.781114	-1.989809
125	1	0	2.224044	-2.167560	-1.273323
126	8	0	-0.275898	-2.535654	-2.010190
127	8	0	0.074080	-4.647982	-1.368137
128	6	0	-1.329709	-4.901073	-1.563790
129	1	0	-1.432900	-5.986009	-1.520208
130	1	0	-1.656471	-4.526604	-2.535844
131	1	0	-1.916416	-4.431495	-0.769828
132	6	0	1.003740	-3.971532	2.403684
133	6	0	1.380841	-3.502431	3.665580
134	6	0	0.377917	-5.221476	2.299972
135	6	0	1.148912	-4.272166	4.807868
136	1	0	1.855065	-2.527881	3.756375
137	6	0	0.138213	-5.986502	3.439465
138	1	0	0.073977	-5.585185	1.322357
139	6	0	0.526238	-5.515061	4.697067
140	1	0	1.447637	-3.895398	5.782434
141	1	0	-0.352318	-6.952114	3.348262
142	1	0	0.339530	-6.113391	5.584852
143	1	0	-0.252834	-1.886095	0.497504
144	1	0	0.022821	-1.566555	-1.923652
145	6	0	7.075324	-2.564183	0.524934
146	6	0	-6.558635	-2.330963	-3.526681
147	1	0	-7.102764	-3.141269	-4.025566
148	1	0	-5.687177	-2.087401	-4.144860
149	1	0	-7.217340	-1.455443	-3.505041
150	1	0	7.550553	-1.733974	1.058947
151	1	0	7.822328	-3.359882	0.424925
152	1	0	6.261661	-2.949978	1.150420

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1gd (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3317.55815858 Hartree

Zero-point correction= 1.317542 Hartree

Thermal correction to Energy= 1.387774 Hartree

Thermal correction to Enthalpy= 1.388718 Hartree

Thermal correction to Gibbs Free Energy= 1.211243 Hartree

Sum of electronic and zero-point Energies= -3316.240617 Hartree

Sum of electronic and thermal Energies= -3316.170384 Hartree

Sum of electronic and thermal Enthalpies= -3316.169440 Hartree

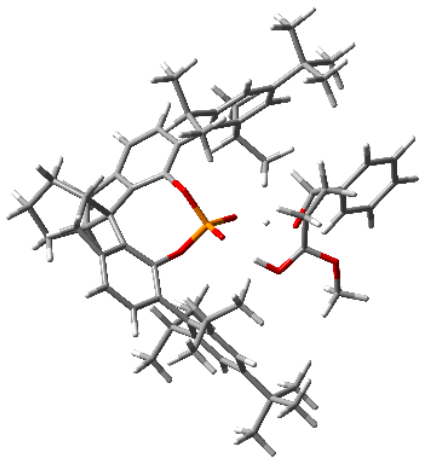
Sum of electronic and thermal Free Energies= -3316.346916 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.973113	-0.522181	1.304145
2	6	0	5.360612	-1.653882	0.431130
3	6	0	4.041992	0.346886	0.178880
4	6	0	5.054672	0.652106	1.097538
5	6	0	5.106463	-0.661366	-1.952962
6	6	0	4.800487	-1.881367	-2.869458
7	6	0	3.631715	-2.565984	-2.210929
8	6	0	3.254370	-1.899589	-1.036983
9	6	0	4.357422	-0.942305	-0.580032
10	6	0	2.965362	1.230313	0.060383
11	6	0	2.971393	2.493957	0.684253
12	6	0	4.088541	2.816880	1.473078
13	6	0	5.099587	1.893158	1.725847
14	6	0	2.928490	-3.680845	-2.656832
15	6	0	1.809105	-4.104714	-1.943822
16	6	0	1.295902	-3.364973	-0.865266
17	6	0	2.025934	-2.230668	-0.456878
18	8	0	1.497650	-1.405620	0.537727
19	8	0	1.856293	0.834886	-0.687891
20	15	0	0.698647	-0.057855	0.059981
21	8	0	0.173165	0.587140	1.315051
22	8	0	-0.293230	-0.377101	-1.055178
23	6	0	1.838453	3.468361	0.552697
24	6	0	0.026879	-3.802614	-0.192795
25	6	0	0.040114	-4.201359	1.169579
26	6	0	-1.141594	-4.656990	1.759043
27	6	0	-2.352581	-4.752588	1.064735
28	6	0	-2.339240	-4.363628	-0.275590
29	6	0	-1.186102	-3.892563	-0.921157
30	6	0	1.103001	3.873904	1.699641
31	6	0	0.061009	4.790957	1.543258
32	6	0	-0.308592	5.327662	0.304955
33	6	0	0.444938	4.931165	-0.801587
34	6	0	1.512117	4.025900	-0.705441
35	6	0	-1.305585	-3.530496	-2.404802
36	6	0	-1.478352	-4.793958	-3.274292
37	6	0	-2.452012	-2.544085	-2.696380
38	6	0	1.309196	-4.217735	2.023708
39	6	0	1.183227	-3.323629	3.271849
40	6	0	1.700998	-5.658803	2.408827
41	6	0	1.411310	3.382683	3.118332
42	6	0	2.027062	4.515514	3.966628
43	6	0	0.187244	2.788182	3.840628
44	6	0	2.324652	3.744445	-1.971033
45	6	0	1.471160	3.153308	-3.108523
46	6	0	3.067738	5.012273	-2.439788
47	6	0	-1.478298	6.325104	0.215232
48	6	0	-2.749450	5.700755	0.839263
49	6	0	-1.109839	7.611649	0.992454
50	6	0	-3.609723	-5.289703	1.774008
51	6	0	-3.931499	-4.407528	3.003334
52	6	0	-3.351545	-6.741109	2.245054
53	6	0	6.438763	-2.496353	-0.261369
54	6	0	6.612238	-0.421900	-1.789546
55	6	0	7.345428	-1.649985	-1.191524
56	1	0	6.009950	-0.813472	2.361741
57	1	0	7.006618	-0.293335	1.017550
58	1	0	4.757897	-2.302788	1.077434
59	1	0	4.645392	0.230117	-2.393951
60	1	0	4.541601	-1.557117	-3.885689
61	1	0	5.665289	-2.546750	-2.976057
62	1	0	4.129581	3.798910	1.933746
63	1	0	5.907376	2.139307	2.410809
64	1	0	3.246494	-4.218548	-3.546805
65	1	0	1.285191	-5.003734	-2.251422
66	1	0	-1.478181	0.267033	-1.054320
67	1	0	-1.104964	-4.963949	2.800600
68	1	0	-3.251211	-4.431351	-0.857533
69	1	0	-0.491145	5.089086	2.429361
70	1	0	0.218423	5.344880	-1.778202
71	1	0	-0.381576	-3.033226	-2.708298
72	1	0	-1.503698	-4.528330	-4.338362
73	1	0	-0.665026	-5.511801	-3.124838
74	1	0	-2.416723	-5.309862	-3.036638
75	1	0	-2.443072	-2.267511	-3.758029
76	1	0	-2.343727	-1.630452	-2.108898
77	1	0	-3.435944	-2.980378	-2.484778
78	1	0	2.131669	-3.820155	1.425053
79	1	0	0.408452	-3.690945	3.955978
80	1	0	2.129859	-3.311197	3.826166
81	1	0	0.936987	-2.295245	2.993141
82	1	0	1.833113	-6.285282	1.519442
83	1	0	0.937773	-6.131106	3.038722
84	1	0	2.643359	-5.661942	2.970350
85	1	0	2.148819	2.580072	3.049002
86	1	0	2.308084	4.143420	4.959567
87	1	0	2.922209	4.939272	3.497777
88	1	0	1.313219	5.336199	4.107829
89	1	0	0.479842	2.446956	4.841536
90	1	0	-0.206639	1.930456	3.292614
91	1	0	-0.616743	3.522522	3.967979
92	1	0	3.090234	3.003766	-1.727556
93	1	0	2.100701	2.929702	-3.978771
94	1	0	0.989893	2.223808	-2.790807
95	1	0	0.694390	3.853847	-3.439274
96	1	0	3.697433	4.789017	-3.309984
97	1	0	3.711562	5.409252	-1.646972
98	1	0	2.368402	5.805674	-2.729268
99	1	0	-3.594455	6.395192	0.750640
100	1	0	-3.019422	4.762204	0.344125
101	1	0	-2.613934	5.478299	1.902353
102	1	0	-1.936463	8.332522	0.956404
103	1	0	-0.222312	8.089737	0.561840
104	1	0	-0.896338	7.399028	2.045331

105	1	0	-4.818528	-4.786641	3.525975
106	1	0	-3.104552	-4.388124	3.720365
107	1	0	-4.132259	-3.372783	2.700807
108	1	0	-2.506973	-6.798448	2.939410
109	1	0	-4.235070	-7.140934	2.758344
110	1	0	-3.128095	-7.393905	1.393580
111	1	0	7.050620	-2.996441	0.500303
112	1	0	5.954032	-3.299932	-0.827691
113	1	0	7.047144	-0.167013	-2.764437
114	1	0	6.764664	0.459648	-1.155962
115	1	0	7.729190	-2.290614	-1.994212
116	1	0	8.231825	-1.305308	-0.646191
117	6	0	-2.904329	1.140530	0.541719
118	8	0	-4.116435	1.722763	0.401533
119	8	0	-2.445958	0.792824	-1.076976
120	6	0	-5.196182	0.745590	0.593357
121	6	0	-4.486320	-0.623045	0.637067
122	6	0	-3.073643	-0.263975	1.106841
123	1	0	-5.624446	0.980613	1.574529
124	1	0	-4.456104	-1.072521	-0.358514
125	1	0	-5.002687	-1.316444	1.306273
126	1	0	-2.298356	-0.956350	0.778755
127	1	0	-3.013329	-0.174769	2.197437
128	8	0	-2.001145	1.982947	1.003713
129	6	0	-2.296375	1.978675	-1.887581
130	1	0	-3.276502	2.448062	-1.978725
131	1	0	-1.936858	1.655375	-2.866770
132	1	0	-1.584282	2.670906	-1.430854
133	1	0	-1.120515	1.498398	1.166707
134	6	0	-6.259294	0.917628	-0.463905
135	6	0	-7.563669	1.256850	-0.091463
136	6	0	-5.968096	0.728529	-1.822724
137	6	0	-8.566167	1.397401	-1.053487
138	1	0	-7.797564	1.413931	0.959137
139	6	0	-6.964866	0.877093	-2.784919
140	1	0	-4.957875	0.466295	-2.123945
141	6	0	-8.267697	1.209425	-2.402574
142	1	0	-9.575563	1.658925	-0.747897
143	1	0	-6.726719	0.730627	-3.835066
144	1	0	-9.044280	1.321829	-3.154282
145	6	0	-1.802941	6.719600	-1.238231
146	6	0	-4.846279	-5.299235	0.855344
147	1	0	-4.701374	-5.945671	-0.017510
148	1	0	-5.096233	-4.294128	0.496177
149	1	0	-5.714085	-5.679303	1.406571
150	1	0	-0.959945	7.222661	-1.725417
151	1	0	-2.651560	7.413103	-1.252259
152	1	0	-2.076893	5.848281	-1.844438

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1gd (Cy-SPINOL)

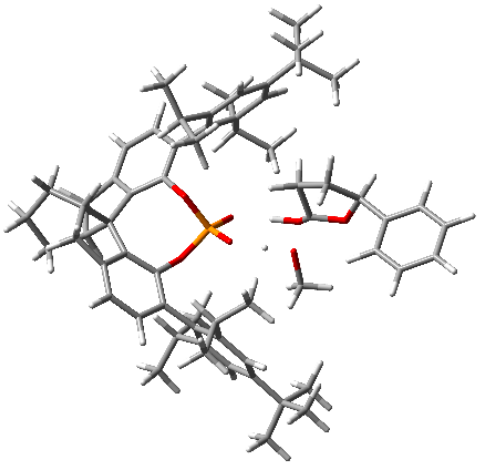


B3LYP/6-31G(d); E(RB3LYP) = -3317.55370348 Hartree
Zero-point correction= 1.316926 Hartree
Thermal correction to Energy= 1.386999 Hartree
Thermal correction to Enthalpy= 1.387943 Hartree
Thermal correction to Gibbs Free Energy= 1.212308 Hartree
Sum of electronic and zero-point Energies= -3316.236777 Hartree
Sum of electronic and thermal Energies= -3316.166705 Hartree
Sum of electronic and thermal Enthalpies= -3316.165760 Hartree
Sum of electronic and thermal Free Energies= -3316.341395 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.716414	5.019744	1.565692
2	6	0	-1.414645	5.148640	0.723221
3	6	0	-2.427212	3.002856	0.301398
4	6	0	-3.255028	3.656095	1.223860
5	6	0	-2.122358	4.581490	-1.706805
6	6	0	-0.928546	5.014564	-2.602567
7	6	0	0.267558	4.337882	-1.990125
8	6	0	-0.091837	3.593961	-0.858098
9	6	0	-1.483580	3.996815	-0.371319
10	6	0	-2.618047	1.634714	0.085586
11	6	0	-3.759565	0.966549	0.572839
12	6	0	-4.659555	1.718795	1.348676
13	6	0	-4.387526	3.028902	1.732132
14	6	0	1.583727	4.368158	-2.439025
15	6	0	2.535569	3.599282	-1.778204
16	6	0	2.186065	2.702204	-0.752622
17	6	0	0.842733	2.696855	-0.326960
18	8	0	0.435867	1.794645	0.658580
19	8	0	-1.636711	0.919525	-0.612908
20	15	0	-0.341185	0.411950	0.254834
21	8	0	-0.727820	-0.248036	1.553168
22	8	0	0.485933	-0.416209	-0.734116
23	6	0	-4.066656	-0.477580	0.304118
24	6	0	3.258653	1.818198	-0.188547
25	6	0	3.654090	1.929631	1.169368
26	6	0	4.744522	1.183111	1.624511
27	6	0	5.484761	0.330263	0.797253
28	6	0	5.061437	0.219439	-0.529176
29	6	0	3.974454	0.942456	-1.044460
30	6	0	-4.248337	-1.386738	1.378425
31	6	0	-4.631742	-2.706318	1.098192
32	6	0	-4.858495	-3.172277	-0.197413
33	6	0	-4.671230	-2.255234	-1.237114
34	6	0	-4.285307	-0.930089	-1.023396
35	6	0	3.651090	0.763193	-2.532701
36	6	0	4.811459	1.252958	-3.423546
37	6	0	3.275910	-0.685894	-2.890124
38	6	0	2.991073	2.893281	2.155226
39	6	0	2.373395	2.156913	3.359030
40	6	0	3.975671	3.986699	2.617364
41	6	0	-4.102214	-0.995577	2.854632
42	6	0	-5.473081	-1.007484	3.564924
43	6	0	-3.109957	-1.879968	3.633058
44	6	0	-4.189157	-0.016119	-2.246574
45	6	0	-3.128950	-0.503747	-3.252196
46	6	0	-5.562959	0.155618	-2.926011
47	6	0	-5.348500	-4.600064	-0.505017
48	6	0	-6.782333	-4.523959	-1.083786
49	6	0	-4.421753	-5.272254	-1.544545
50	6	0	6.737604	-0.381908	1.343221
51	6	0	7.770085	0.685244	1.782327
52	6	0	6.368385	-1.254681	2.564850
53	6	0	-1.249540	6.551883	0.126962
54	6	0	-3.108427	5.730867	-1.465775
55	6	0	-2.438880	6.951558	-0.783801

56	1	0	-2.501521	5.096271	2.639408
57	1	0	-3.434497	5.817946	1.343852
58	1	0	-0.556628	4.928850	1.369198
59	1	0	-2.647435	3.755142	-2.199990
60	1	0	-1.073364	4.689361	-3.640936
61	1	0	-0.812525	6.104158	-2.640771
62	1	0	-5.566680	1.236015	1.696304
63	1	0	-5.054057	3.550330	2.414814
64	1	0	1.867604	4.982757	-3.289785
65	1	0	3.574654	3.645654	-2.088328
66	1	0	5.045130	1.303179	2.661733
67	1	0	5.600196	-0.432346	-1.207756
68	1	0	-4.766684	-3.379762	1.936790
69	1	0	-4.853238	-2.572730	-2.259971
70	1	0	2.777361	1.373110	-2.768875
71	1	0	4.531130	1.191362	-4.482045
72	1	0	5.083921	2.291817	-3.205468
73	1	0	5.711242	0.642020	-3.283841
74	1	0	3.069121	-0.765044	-3.964622
75	1	0	2.374145	-0.990297	-2.353467
76	1	0	4.079169	-1.393716	-2.657213
77	1	0	2.176050	3.405174	1.639414
78	1	0	3.137219	1.633416	3.947272
79	1	0	1.876921	2.871355	4.027108
80	1	0	1.627488	1.427115	3.031266
81	1	0	4.389337	4.534538	1.763195
82	1	0	4.816036	3.565361	3.181688
83	1	0	3.466979	4.707156	3.269529
84	1	0	-3.709713	0.022393	2.901736
85	1	0	-5.373965	-0.646838	4.596118
86	1	0	-6.208136	-0.375619	3.054560
87	1	0	-5.888547	-2.021665	3.605802
88	1	0	-3.068791	-1.553949	4.679710
89	1	0	-2.104348	-1.802351	3.217966
90	1	0	-3.403316	-2.936177	3.628810
91	1	0	-3.881579	0.976825	-1.911977
92	1	0	-3.045893	0.201332	-4.088660
93	1	0	-2.147595	-0.585753	-2.776549
94	1	0	-3.391454	-1.482359	-3.672467
95	1	0	-5.490162	0.860711	-3.763298
96	1	0	-6.308525	0.540669	-2.221165
97	1	0	-5.940176	-0.793773	-3.324209
98	1	0	-7.157640	-5.528452	-1.317178
99	1	0	-7.469274	-4.061975	-0.365602
100	1	0	-6.814076	-3.930871	-2.003889
101	1	0	-4.775211	-6.285877	-1.770780
102	1	0	-3.396096	-5.347028	-1.166280
103	1	0	-4.387737	-4.715737	-2.486433
104	1	0	8.677132	0.204053	2.169113
105	1	0	7.373493	1.334495	2.569772
106	1	0	8.056240	1.321961	0.937604
107	1	0	5.669541	-2.050847	2.282425
108	1	0	7.265400	-1.728772	2.981972
109	1	0	5.901222	-0.667914	3.362451
110	1	0	-1.142554	7.280357	0.940807
111	1	0	-0.308445	6.592030	-0.433755
112	1	0	-3.549135	6.034882	-2.423832
113	1	0	-3.943027	5.363102	-0.858021
114	1	0	-2.085776	7.662529	-1.539945
115	1	0	-3.194509	7.495112	-0.204632
116	1	0	0.775358	-1.626729	-0.408222
117	6	0	0.253751	-3.308651	1.191590
118	8	0	1.097209	-2.701318	-0.144089
119	6	0	2.516142	-2.772221	0.160914
120	6	0	2.620203	-3.121522	1.674178
121	6	0	1.232907	-2.845795	2.255359
122	1	0	2.911473	-1.765225	-0.011699
123	1	0	2.876114	-4.176708	1.798802
124	1	0	3.391069	-2.521316	2.163747
125	1	0	1.047200	-3.394929	3.182765
126	1	0	1.063660	-1.781168	2.436372
127	8	0	-0.967388	-2.804010	1.110185
128	8	0	0.307331	-4.646640	1.039342
129	6	0	-0.628838	-5.232950	0.121103
130	1	0	-0.376205	-6.293365	0.091094
131	1	0	-1.652227	-5.091265	0.474374
132	1	0	-0.515748	-4.790819	-0.872663
133	1	0	-0.964628	-1.814112	1.330890
134	6	0	3.216542	-3.758838	-0.757704
135	6	0	2.626147	-4.196303	-1.948519
136	6	0	4.502936	-4.215775	-0.437853
137	6	0	3.302265	-5.077295	-2.794856
138	1	0	1.634201	-3.844094	-2.208857
139	6	0	5.181874	-5.090792	-1.286515
140	1	0	4.981036	-3.891267	0.482884
141	6	0	4.581796	-5.527532	-2.468791
142	1	0	2.825637	-5.409634	-3.713473
143	1	0	6.177672	-5.434764	-1.019452
144	1	0	5.107361	-6.212138	-3.129021
145	6	0	-5.383956	-5.493417	0.749733
146	6	0	7.407108	-1.286324	0.290850
147	1	0	7.754557	-0.713003	-0.575853
148	1	0	6.729706	-2.068500	-0.069921
149	1	0	8.281574	-1.779811	0.730571
150	1	0	-4.395647	-5.580254	1.216237
151	1	0	-5.713579	-6.502583	0.476891
152	1	0	-6.082325	-5.113001	1.503354

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1gd (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3317.55635221 Hartree

Zero-point correction= 1.317680 Hartree

Thermal correction to Energy= 1.387902 Hartree

Thermal correction to Enthalpy= 1.388847 Hartree

Thermal correction to Gibbs Free Energy= 1.211243 Hartree

Sum of electronic and zero-point Energies= -3316.238672 Hartree

Sum of electronic and thermal Energies= -3316.168450 Hartree

Sum of electronic and thermal Enthalpies= -3316.167506 Hartree

Sum of electronic and thermal Free Energies= -3316.345109 Hartree

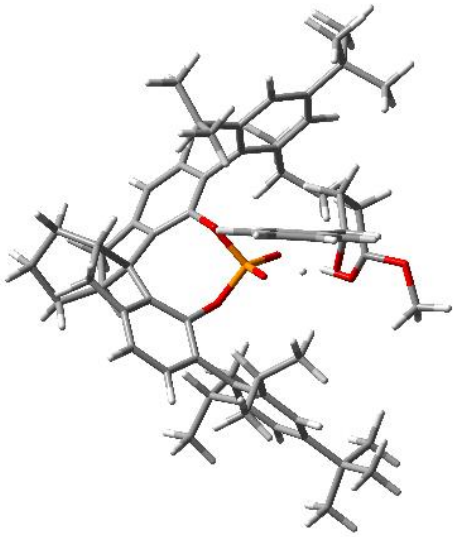
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.176497	-5.704341	1.554376
2	6	0	-2.265902	-5.023830	0.675795
3	6	0	-0.153498	-3.920859	0.320904
4	6	0	0.084925	-4.938787	1.253482
5	6	0	-1.279129	-5.004198	-1.724305

6	6	0	-2.454477	-4.626178	-2.668569	75	1	0	-1.977628	2.500593	-3.913583
7	6	0	-3.012511	-3.356056	-2.086084	76	1	0	-1.421925	2.338565	-2.242548
8	6	0	-2.332369	-2.990729	-0.917260	77	1	0	-2.585917	3.611256	-2.681733
9	6	0	-1.483387	-4.149655	-0.396304	78	1	0	-4.151537	-1.491590	1.484887
10	6	0	0.828981	-2.942627	0.135963	79	1	0	-3.963524	0.447339	3.850594
11	6	0	2.129255	-3.100047	0.657294	80	1	0	-3.724224	-1.303590	3.900805
12	6	0	2.369017	-4.237744	1.447823	81	1	0	-2.589318	-0.286511	2.995929
13	6	0	1.349729	-5.116497	1.804581	82	1	0	-6.593776	-1.022408	1.471079
14	6	0	-4.040805	-2.566443	-2.590734	83	1	0	-6.419671	-0.016598	2.917445
15	6	0	-4.353708	-1.375330	-1.943543	84	1	0	-6.064846	-1.748459	3.001708
16	6	0	-3.590585	-0.889785	-0.866511	85	1	0	2.535781	-2.155752	2.960348
17	6	0	-2.554404	-1.715733	-0.385818	86	1	0	4.156459	-2.665714	4.768589
18	8	0	-1.730795	-1.267755	0.646661	87	1	0	4.643494	-3.524575	3.297121
19	8	0	0.498564	-1.779290	-0.564216	88	1	0	5.494582	-2.055779	3.782338
20	15	0	-0.277267	-0.600889	0.279631	89	1	0	2.934176	-0.462235	4.655256
21	8	0	0.390853	-0.294788	1.592346	90	1	0	2.651478	0.345058	3.107295
22	8	0	-0.439953	0.530629	-0.732967	91	1	0	4.293368	0.221899	3.760705
23	6	0	3.261620	-2.148948	0.394812	92	1	0	2.282881	-3.235274	-1.818985
24	6	0	-3.930005	0.458205	-0.300672	93	1	0	2.151300	-2.150476	-4.027221
25	6	0	-4.382680	0.589243	1.037883	94	1	0	1.853590	-0.972761	-2.736585
26	6	0	-4.795870	1.842516	1.498704	95	1	0	3.417723	-0.999971	-3.581286
27	6	0	-4.810357	2.986096	0.692233	96	1	0	3.664810	-4.154003	-3.625838
28	6	0	-4.360127	2.832322	-0.620728	97	1	0	4.483954	-4.365867	-2.065802
29	6	0	-3.912109	1.605750	-1.134403	98	1	0	5.019140	-3.103344	-3.185436
30	6	0	3.939666	-1.519737	1.475658	99	1	0	7.629222	2.264797	0.183764
31	6	0	5.072082	-0.744506	1.206577	100	1	0	5.897215	2.240532	-0.193146
32	6	0	5.573585	-0.542391	-0.085164	101	1	0	6.472894	1.656979	1.377011
33	6	0	4.875805	-1.150233	-1.129630	102	1	0	8.969432	0.117478	0.272858
34	6	0	3.745026	-1.953782	-0.921696	103	1	0	8.182107	-1.449702	-0.003376
35	6	0	-3.441544	1.584118	-2.593469	104	1	0	7.860829	-0.547701	1.484393
36	6	0	-4.606898	1.857480	-3.566865	105	1	0	-7.192276	5.101507	2.092536
37	6	0	-2.289279	2.570963	-2.864202	106	1	0	-7.431023	3.873852	0.832550
38	6	0	-4.509152	-0.595905	1.996719	107	1	0	-6.920952	3.389988	2.456205
39	6	0	-3.642907	-0.418369	3.258143	108	1	0	-4.859352	5.674086	2.909678
40	6	0	-5.983401	-0.858090	2.366291	109	1	0	-3.433374	4.887241	2.209489
41	6	0	3.511081	-1.663907	2.939929	110	1	0	-4.514145	3.976809	3.274210
42	6	0	4.507281	-2.531787	3.738065	111	1	0	-3.780004	-6.555909	0.845745
43	6	0	3.338886	-0.306820	3.648053	112	1	0	-3.980506	-5.503497	-0.537032
44	6	0	3.137115	-2.639416	-2.147053	113	1	0	-1.002133	-7.026265	-2.429442
45	6	0	2.610714	-1.625593	-3.180507	114	1	0	-0.333481	-6.728029	-0.841352
46	6	0	4.136922	-3.621398	-2.791145	115	1	0	-3.180244	-7.432926	-1.615630
47	6	0	6.862150	0.275341	-0.297015	116	1	0	-2.240226	-7.970207	-0.248742
48	6	0	6.703044	1.690052	0.307271	117	6	0	1.547754	2.694949	0.911915
49	6	0	8.036931	-0.444659	0.408562	118	8	0	1.915860	3.986353	1.088507
50	6	0	-5.327267	4.323477	1.255420	119	8	0	0.115829	2.803142	0.016874
51	6	0	-6.804924	4.159102	1.685665	120	1	0	0.924132	1.161266	1.909872
52	6	0	-4.483656	4.734914	2.485100	121	6	0	2.895728	4.397066	0.077389
53	6	0	-3.226734	-6.041655	0.049595	122	6	0	2.923910	3.236123	-0.937219
54	6	0	-1.199836	-6.515755	-1.478172	123	6	0	2.487259	2.036932	-0.091019
55	6	0	-2.493459	-7.080499	-0.837130	124	1	0	3.853088	4.456183	0.608135
56	1	0	-1.429176	-5.636088	2.620345	125	1	0	2.211223	3.418721	-1.745961
57	1	0	-1.075615	-6.773947	1.335792	126	1	0	3.916203	3.116587	-1.380172
58	1	0	-2.836326	-4.329045	1.303168	127	1	0	2.016220	1.234568	-0.658482
59	1	0	-0.342251	-4.666000	-2.182416	128	1	0	3.320112	1.608929	0.476960
60	1	0	-2.102807	-4.467390	-3.696192	129	8	0	1.216494	2.124179	2.060296
61	1	0	-3.209626	-5.419185	-2.726883	130	6	0	-0.966259	3.391644	0.775215
62	1	0	3.373211	-4.401738	1.823176	131	1	0	-1.830572	3.448837	0.114426
63	1	0	1.545896	-5.930938	2.497664	132	1	0	-1.199820	2.781591	1.650211
64	1	0	-4.594746	-2.872647	-3.474800	133	1	0	-0.644862	4.386914	1.084479
65	1	0	-5.182444	-0.772115	-2.299869	134	6	0	2.549094	5.758631	-0.473689
66	1	0	-0.161304	1.788426	-0.306911	135	6	0	1.323400	5.989420	-1.114767
67	1	0	-5.146119	1.916712	2.524418	136	6	0	3.466161	6.808591	-0.366230
68	1	0	-4.356122	3.689240	-1.285391	137	6	0	1.026796	7.246740	-1.636794
69	1	0	5.588534	-0.291885	2.048229	138	1	0	0.602692	5.181118	-1.200264
70	1	0	5.227548	-1.028842	-2.147969	139	6	0	3.174304	8.067064	-0.896725
71	1	0	-3.051358	0.587711	-2.810826	140	1	0	4.415619	6.641750	0.137678
72	1	0	-4.265776	1.773152	-4.605864	141	6	0	1.952754	8.288687	-1.531666
73	1	0	-5.433898	1.153391	-3.424871	142	1	0	0.072523	7.414887	-2.128905
74	1	0	-5.010958	2.868011	-3.431249	143	1	0	3.898225	8.872461	-0.807112

144	1	0	1.720310	9.267830	-1.941670
145	6	0	7.221308	0.432469	-1.786874
146	6	0	-5.255957	5.464600	0.222854
147	1	0	-5.868110	5.253931	-0.661318
148	1	0	-4.228433	5.651540	-0.110152
149	1	0	-5.631007	6.391973	0.670559
150	1	0	8.132974	1.032662	-1.886747
151	1	0	6.426820	0.939633	-2.346656
152	1	0	7.410327	-0.534718	-2.265560

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1gd (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3317.55416038 Hartree

Zero-point correction= 1.316388 Hartree

Thermal correction to Energy= 1.386826 Hartree

Thermal correction to Enthalpy= 1.387770 Hartree

Thermal correction to Gibbs Free Energy= 1.208823 Hartree

Sum of electronic and zero-point Energies= -3316.237772 Hartree

Sum of electronic and thermal Energies= -3316.167335 Hartree

Sum of electronic and thermal Enthalpies= -3316.166391 Hartree

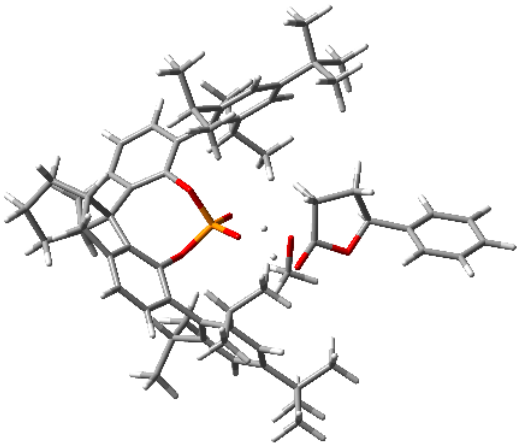
Sum of electronic and thermal Free Energies= -3316.345338 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.340110	5.518988	-1.324766
2	6	0	-0.817610	5.079411	-0.386659
3	6	0	0.922120	3.410601	-0.337522
4	6	0	1.335655	4.393471	-1.246699
5	6	0	0.266410	4.525059	1.906874
6	6	0	-0.930461	4.393855	2.895098
7	6	0	-1.866018	3.417046	2.230771
8	6	0	-1.348231	2.985183	1.003210
9	6	0	-0.232938	3.914217	0.528179
10	6	0	1.612213	2.194200	-0.312206
11	6	0	2.823179	2.020550	-1.011662
12	6	0	3.270271	3.091567	-1.804034
13	6	0	2.514417	4.248324	-1.971042
14	6	0	-3.078782	2.922627	2.701438
15	6	0	-3.758635	1.968296	1.946775
16	6	0	-3.194149	1.387021	0.797933
17	6	0	-1.944815	1.886802	0.379694
18	8	0	-1.272643	1.268040	-0.678038
19	8	0	1.072322	1.132668	0.421389
20	15	0	-0.073840	0.215097	-0.317392
21	8	0	0.410847	-0.361824	-1.619413
22	8	0	-0.523627	-0.753641	0.778002
23	6	0	3.676003	0.787304	-0.922441
24	6	0	-3.935960	0.312518	0.056934
25	6	0	-4.350886	0.528347	-1.284137
26	6	0	-5.083010	-0.464034	-1.939495
27	6	0	-5.446855	-1.670247	-1.331588
28	6	0	-5.045740	-1.850831	-0.008075
29	6	0	-4.299640	-0.897288	0.699443
30	6	0	3.912656	-0.014824	-2.070661
31	6	0	4.812182	-1.081402	-1.974908
32	6	0	5.496364	-1.403214	-0.795879
33	6	0	5.238908	-0.603113	0.318646
34	6	0	4.355601	0.485757	0.280808
35	6	0	-3.931573	-1.226171	2.148988
36	6	0	-5.162448	-1.140183	3.076194
37	6	0	-3.275671	-2.611867	2.299157
38	6	0	-4.092668	1.830928	-2.044544
39	6	0	-3.287377	1.602870	-3.337845
40	6	0	-5.412784	2.573599	-2.335471
41	6	0	3.266981	0.263056	-3.432026
42	6	0	4.301258	0.824162	-4.431128
43	6	0	2.577342	-0.972023	-4.041521
44	6	0	4.248132	1.361787	1.530595
45	6	0	3.843719	0.569011	2.785939
46	6	0	5.560373	2.137568	1.766437
47	6	0	6.512537	-2.561466	-0.781916
48	6	0	5.822388	-3.878373	-1.207764
49	6	0	7.655174	-2.244560	-1.776857
50	6	0	-6.253255	-2.719847	-2.118170
51	6	0	-7.599650	-2.106562	-2.571095
52	6	0	-5.447000	-3.158277	-3.363851
53	6	0	-1.398100	6.254524	0.409002
54	6	0	0.767619	5.969368	1.786461
55	6	0	-0.339651	6.943265	1.307978
56	1	0	-0.014846	5.664167	-2.353099
57	1	0	0.779147	6.476106	-1.018032
58	1	0	-1.610612	4.636142	-1.000319
59	1	0	1.084819	3.888709	2.263768
60	1	0	-0.597172	4.015941	3.870406
61	1	0	-1.410590	5.359183	3.094119
62	1	0	4.216875	2.987000	-2.324321
63	1	0	2.845972	5.026485	-2.654154
64	1	0	-3.501291	3.282631	3.636439
65	1	0	-4.736548	1.627980	2.269641
66	1	0	-0.353275	-2.029972	0.674467
67	1	0	-5.389032	-0.277079	-2.965004
68	1	0	-5.312241	-2.765830	0.507738
69	1	0	4.994453	-1.674046	-2.866871
70	1	0	5.757815	-0.801819	1.249575
71	1	0	-3.197184	-0.491095	2.487934
72	1	0	-4.873872	-1.335362	4.116476
73	1	0	-5.645229	-0.158044	3.038355
74	1	0	-5.916471	-1.885093	2.793759
75	1	0	-2.902193	-2.740215	3.321970
76	1	0	-2.433447	-2.731150	1.615378
77	1	0	-3.988081	-3.424147	2.109059
78	1	0	-3.498691	2.490823	-1.408348
79	1	0	-3.843896	0.991278	-4.058311
80	1	0	-3.068863	2.562474	-3.822902
81	1	0	-2.338303	1.103044	-3.125125
82	1	0	-5.966114	2.775621	-1.411348
83	1	0	-6.067172	1.991126	-2.994742
84	1	0	-5.212365	3.532732	-2.828977
85	1	0	2.489395	1.017178	-3.288657
86	1	0	3.817105	1.074149	-5.382999
87	1	0	4.791210	1.728206	-4.054755
88	1	0	5.087155	0.087978	-4.640195
89	1	0	2.103220	-0.698943	-4.991994
90	1	0	1.798427	-1.352957	-3.379131

91	1	0	3.288102	-1.779862	-4.254332
92	1	0	3.467664	2.106744	1.360409
93	1	0	3.730372	1.246125	3.641423
94	1	0	2.890375	0.053361	2.635336
95	1	0	4.595477	-0.180309	3.060634
96	1	0	5.463104	2.805636	2.631111
97	1	0	5.820735	2.746801	0.893790
98	1	0	6.398456	1.457730	1.961152
99	1	0	6.548054	-4.700841	-1.228047
100	1	0	5.026592	-4.148874	-0.503852
101	1	0	5.376792	-3.803729	-2.205013
102	1	0	8.393186	-3.056433	-1.784517
103	1	0	8.170591	-1.318643	-1.497439
104	1	0	7.281199	-2.122537	-2.798716
105	1	0	-8.182616	-2.840692	-3.141343
106	1	0	-7.453388	-1.229050	-3.209356
107	1	0	-8.197580	-1.794618	-1.707048
108	1	0	-4.488041	-3.601936	-3.072204
109	1	0	-6.007923	-3.904419	-3.940743
110	1	0	-5.232621	-2.314490	-4.027646
111	1	0	-1.826775	6.985616	-0.288331
112	1	0	-2.237499	5.894097	1.014513
113	1	0	1.161127	6.300080	2.756125
114	1	0	1.619115	5.991721	1.096028
115	1	0	-0.844498	7.396162	2.169334
116	1	0	0.127399	7.778329	0.772772
117	6	0	0.373135	-3.575052	-0.904288
118	8	0	-0.218265	-3.166660	0.610521
119	6	0	0.816855	-3.680968	1.511806
120	6	0	1.873698	-3.337143	-0.672003
121	1	0	2.409494	-4.177651	-1.119410
122	1	0	2.175554	-2.425865	-1.189544
123	8	0	-0.303208	-2.849532	-1.785282
124	8	0	0.110473	-4.901764	-0.994096
125	6	0	-1.246840	-5.263257	-1.306972
126	1	0	-1.281770	-6.349888	-1.217111
127	1	0	-1.501374	-4.957921	-2.324169
128	1	0	-1.938703	-4.801509	-0.597117
129	1	0	-0.013319	-1.877268	-1.788654
130	6	0	0.601589	-3.310506	2.960117
131	6	0	0.622758	-1.983755	3.415516
132	6	0	0.411633	-4.340846	3.890314
133	6	0	0.455104	-1.704032	4.771386
134	1	0	0.732634	-1.167458	2.710195
135	6	0	0.254046	-4.061205	5.248235
136	1	0	0.389162	-5.373041	3.547946
137	6	0	0.275115	-2.738925	5.691925
138	1	0	0.464823	-0.671072	5.108282
139	1	0	0.110741	-4.874442	5.954647
140	1	0	0.149124	-2.514958	6.747918
141	1	0	0.727480	-4.766320	1.417434
142	6	0	2.123583	-3.222911	0.849499
143	1	0	2.967371	-3.831524	1.187524
144	1	0	2.339973	-2.185572	1.120432
145	6	0	-6.559591	-3.975795	-1.280397
146	6	0	7.136845	-2.779980	0.609463
147	1	0	-7.130709	-4.691870	-1.882549
148	1	0	-7.157854	-3.738761	-0.393272
149	1	0	-5.643455	-4.478194	-0.949328
150	1	0	7.839872	-3.619976	0.571547
151	1	0	6.378180	-3.016424	1.364476
152	1	0	7.693865	-1.899963	0.949947

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1gd (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3317.55768978 Hartree

Zero-point correction= 1.317656 Hartree

Thermal correction to Energy= 1.388103 Hartree

Thermal correction to Enthalpy= 1.389047 Hartree

Thermal correction to Gibbs Free Energy= 1.210475 Hartree

Sum of electronic and zero-point Energies= -3316.240034 Hartree

Sum of electronic and thermal Energies= -3316.169587 Hartree

Sum of electronic and thermal Enthalpies= -3316.168642 Hartree

Sum of electronic and thermal Free Energies= -3316.347215 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.795307	0.469183	1.940533
2	6	0	5.510349	-0.754870	1.024632
3	6	0	3.932107	0.995748	0.525880
4	6	0	4.737344	1.472891	1.568161
5	6	0	5.447564	0.167609	-1.399923
6	6	0	5.482899	-1.090443	-2.315009
7	6	0	4.358510	-1.956627	-1.811435
8	6	0	3.710474	-1.358015	-0.722294
9	6	0	4.562379	-0.227409	-0.140581
10	6	0	2.753001	1.685126	0.229029
11	6	0	2.461087	2.936899	0.807054
12	6	0	3.385336	3.449132	1.733413
13	6	0	4.487297	2.709619	2.155620
14	6	0	3.919513	-3.173988	-2.322747
15	6	0	2.792841	-3.775057	-1.765814
16	6	0	2.014420	-3.127517	-0.791916
17	6	0	2.482075	-1.886859	-0.313709
18	8	0	1.688181	-1.157666	0.573088
19	8	0	1.844995	1.104653	-0.655460
20	15	0	0.754026	0.032458	-0.056815
21	8	0	-0.040126	0.589873	1.097824
22	8	0	0.002352	-0.451829	-1.289679
23	6	0	1.212085	3.704866	0.489969
24	6	0	0.751773	-3.770631	-0.294945
25	6	0	0.636932	-4.162748	1.064442
26	6	0	-0.521290	-4.817032	1.491181
27	6	0	-1.586116	-5.118613	0.635367
28	6	0	-1.449147	-4.727240	-0.697575
29	6	0	-0.312498	-4.064164	-1.184813
30	6	0	0.269686	3.996546	1.513762
31	6	0	-0.877532	4.723769	1.187792
32	6	0	-1.157785	5.173763	-0.107142
33	6	0	-0.205993	4.893154	-1.089195
34	6	0	0.972382	4.181507	-0.819945
35	6	0	-0.276923	-3.728568	-2.679278

36	6	0	-0.094742	-5.003086	-3.531075
37	6	0	-1.525363	-2.966104	-3.161305
38	6	0	1.753044	-3.959436	2.090821
39	6	0	1.296569	-3.096918	3.282837
40	6	0	2.323777	-5.310502	2.567582
41	6	0	0.454501	3.579652	2.977070
42	6	0	0.744712	4.808694	3.864149
43	6	0	-0.741032	2.789849	3.543122
44	6	0	1.982431	4.020431	-1.957776
45	6	0	1.396132	3.277297	-3.172642
46	6	0	2.564014	5.387158	-2.373841
47	6	0	-2.452882	5.957966	-0.387293
48	6	0	-3.675852	5.132820	0.080098
49	6	0	-2.415733	7.296368	0.388797
50	6	0	-2.815860	-5.876716	1.169469
51	6	0	-2.375267	-7.273685	1.669485
52	6	0	-3.446189	-5.093863	2.345209
53	6	0	6.801132	-1.410514	0.519052
54	6	0	6.853658	0.655123	-1.029949
55	6	0	7.682870	-0.430587	-0.297006
56	1	0	5.724006	0.195597	3.001103
57	1	0	6.808216	0.864464	1.797938
58	1	0	4.934473	-1.490699	1.598195
59	1	0	4.915994	0.967825	-1.928021
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61	1	0	6.451118	-1.603466	-2.276846
62	1	0	3.198092	4.428189	2.163188
63	1	0	5.136619	3.093359	2.938832
64	1	0	4.447207	-3.654441	-3.143118
65	1	0	2.473717	-4.749537	-2.120248
66	1	0	-1.300400	-0.040192	-1.469877
67	1	0	-0.581168	-5.117034	2.533650
68	1	0	-2.243405	-4.949563	-1.400997
69	1	0	-1.586710	4.937417	1.981791
70	1	0	-0.362449	5.248404	-2.101880
71	1	0	0.578690	-3.073715	-2.859374
72	1	0	-0.009030	-4.746210	-4.594134
73	1	0	0.800245	-5.566153	-3.246817
74	1	0	-0.953227	-5.676595	-3.418689
75	1	0	-1.408174	-2.694132	-4.217625
76	1	0	-1.674888	-2.046777	-2.592217
77	1	0	-2.435569	-3.573267	-3.083992
78	1	0	2.574117	-3.427682	1.605184
79	1	0	0.502611	-3.589312	3.857692
80	1	0	2.135741	-2.921676	3.967400
81	1	0	0.924718	-2.126252	2.943018
82	1	0	2.687597	-5.907585	1.723752
83	1	0	1.569070	-5.905289	3.095780
84	1	0	3.161734	-5.149800	3.257036
85	1	0	1.318937	2.914846	3.036213
86	1	0	0.941590	4.499166	4.897973
87	1	0	1.612916	5.375043	3.508949
88	1	0	-0.109591	5.496486	3.879027
89	1	0	-0.540033	2.512598	4.585496
90	1	0	-0.901953	1.872361	2.974178
91	1	0	-1.667644	3.375701	3.533517
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97	1	0	3.022882	5.898286	-1.520090
98	1	0	1.789296	6.048116	-2.780468
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103	1	0	-1.568296	7.912796	0.067093
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105	1	0	-3.235956	-7.830942	2.060254
106	1	0	-1.932370	-7.858224	0.855078
107	1	0	-1.631814	-7.201275	2.470036
108	1	0	-4.316010	-5.632622	2.741078
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122	6	0	-2.956807	-0.833491	0.553893
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129	6	0	-2.314411	1.453478	-2.464385
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133	1	0	-1.411679	1.272288	0.756926
134	6	0	-6.529586	0.007554	-0.311841
135	6	0	-7.486267	-0.652841	-1.089902
136	6	0	-6.953042	0.912345	0.670197
137	6	0	-8.847923	-0.425943	-0.883246
138	1	0	-7.165025	-1.347609	-1.863041
139	6	0	-8.312791	1.147750	0.868747
140	1	0	-6.213574	1.443928	1.261490
141	6	0	-9.263831	0.476200	0.096475
142	1	0	-9.580810	-0.946415	-1.493762
143	1	0	-8.630714	1.858482	1.626833
144	1	0	-10.323059	0.660474	0.254030
145	6	0	-2.634198	6.276574	-1.883618
146	6	0	-3.899259	-6.075521	0.092491
147	1	0	-2.671772	5.365210	-2.491659
148	1	0	-1.827626	6.910531	-2.269030
149	1	0	-3.576426	6.815535	-2.035442
150	1	0	-4.756619	-6.605616	0.522816
151	1	0	-3.532839	-6.671204	-0.751037
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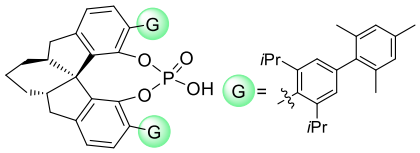
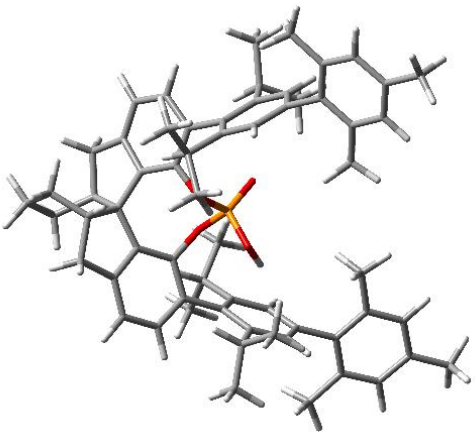
Optimized structure of Cy-SPINOL-derived CPA (*S*)-1gf



(*S*)-**1gf** (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3047.77991365 Hartree

Zero-point correction= 1.184229 Hartree

Thermal correction to Energy= 1.250703 Hartree

Thermal correction to Enthalpy= 1.251647 Hartree

Thermal correction to Gibbs Free Energy= 1.077525 Hartree

Sum of electronic and zero-point Energies= -3046.595685 Hartree

Sum of electronic and thermal Energies= -3046.529211 Hartree

Sum of electronic and thermal Enthalpies= -3046.528266 Hartree

Sum of electronic and thermal Free Energies= -3046.702389 Hartree

The number of Imaginary frequencies = 0

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3	6	0	-1.204258	3.413339	0.702978
4	6	0	-1.611026	4.097436	1.856473
5	6	0	-0.602768	5.100756	-1.172181
6	6	0	0.577967	5.258374	-2.174543
7	6	0	1.523945	4.138722	-1.826370
8	6	0	1.040897	3.393142	-0.742281
9	6	0	-0.073005	4.151520	-0.014544
10	6	0	-1.864000	2.227585	0.378610
11	6	0	-3.008019	1.787916	1.073504
12	6	0	-3.463453	2.589912	2.132069
13	6	0	-2.753324	3.712408	2.553004
14	6	0	2.704771	3.778966	-2.469913
15	6	0	3.392739	2.643107	-2.046556
16	6	0	2.863324	1.780077	-1.072759
17	6	0	1.653466	2.166958	-0.468902
18	8	0	0.999769	1.263985	0.391970
19	8	0	-1.360691	1.436749	-0.658211
20	15	0	-0.151926	0.388018	-0.345640
21	8	0	-0.606907	-0.454425	0.941911
22	8	0	0.197319	-0.339393	-1.577324
23	6	0	-3.691106	0.493818	0.730495
24	6	0	3.589851	0.520262	-0.697703
25	6	0	4.146922	0.391718	0.600279
26	6	0	4.861586	-0.767232	0.922110
27	6	0	5.053902	-1.800429	0.002763
28	6	0	4.507925	-1.650168	-1.273532
29	6	0	3.775590	-0.517189	-1.648171
30	6	0	-3.727761	-0.575341	1.673754
31	6	0	-4.337529	-1.782230	1.301568
32	6	0	-4.925323	-1.969896	0.048357
33	6	0	-4.909488	-0.897856	-0.846461
34	6	0	-4.309077	0.327447	-0.536447
35	6	0	3.230624	-0.457939	-3.077135
36	6	0	4.368450	-0.231594	-4.094635
37	6	0	2.422465	-1.713466	-3.457704
38	6	0	4.048178	1.484737	1.665561
39	6	0	3.321861	0.993397	2.932482
40	6	0	5.437886	2.057552	2.009443
41	6	0	-3.190696	-0.460317	3.107032
42	6	0	-4.359598	-0.311096	4.104960
43	6	0	-2.296313	-1.639970	3.539145
44	6	0	-4.408155	1.453364	-1.566014
45	6	0	-3.814596	1.059534	-2.931816
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49	6	0	1.063802	6.392078	0.716322
50	6	0	-1.119357	6.451996	-0.663352
51	6	0	-0.017052	7.279050	0.046976
52	1	0	-0.269605	5.078929	3.234677
53	1	0	-1.105942	6.183341	2.161011
54	1	0	1.316936	4.458176	1.638687
55	1	0	-1.418331	4.569598	-1.676822
56	1	0	0.229904	5.167894	-3.211339
57	1	0	1.054740	6.242722	-2.100383
58	1	0	-4.365572	2.295541	2.658471
59	1	0	-3.083010	4.270433	3.425795
60	1	0	3.090032	4.375071	-3.293470
61	1	0	4.338472	2.381089	-2.509905
62	1	0	5.290668	-0.869356	1.915705
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64	1	0	-4.366407	-2.603012	2.012603
65	1	0	-5.382147	-1.026220	-1.816465
66	1	0	2.542278	0.388147	-3.143668
67	1	0	3.962615	-0.144636	-5.109946
68	1	0	4.939593	0.678646	-3.880281
69	1	0	5.074659	-1.070867	-4.088726
70	1	0	1.996277	-1.587133	-4.460544
71	1	0	1.599682	-1.868512	-2.757323
72	1	0	3.048027	-2.613866	-3.481333
73	1	0	3.461088	2.311714	1.257804
74	1	0	3.876746	0.188305	3.428593
75	1	0	3.216860	1.813529	3.653783
76	1	0	2.322706	0.619310	2.690251
77	1	0	5.938818	2.445625	1.115399
78	1	0	6.089673	1.295928	2.453168
79	1	0	5.346336	2.878270	2.731580
80	1	0	-2.578214	0.442569	3.171366
81	1	0	-3.978762	-0.154812	5.121290
82	1	0	-5.010584	0.532503	3.852875
83	1	0	-4.982032	-1.213881	4.115049
84	1	0	-1.924954	-1.463605	4.555267
85	1	0	-1.424269	-1.756207	2.889398
86	1	0	-2.842198	-2.589935	3.555062
87	1	0	-3.834647	2.306986	-1.197157
88	1	0	-3.843642	1.917073	-3.614852
89	1	0	-2.774229	0.737115	-2.832772
90	1	0	-4.382390	0.248506	-3.402965
91	1	0	-5.928563	2.769855	-2.411644
92	1	0	-6.279359	2.254931	-0.750020
93	1	0	-6.513735	1.128553	-2.096610
94	1	0	1.493206	6.915939	1.579711
95	1	0	1.899025	6.220984	0.027709
96	1	0	-1.529330	7.023567	-1.505534

97	1	0	-1.962653	6.277022	0.015341
98	1	0	0.468940	7.954448	-0.666604
99	1	0	-0.486057	7.932455	0.791867
100	1	0	-1.490811	-0.850830	0.817084
101	6	0	7.273077	-5.353124	1.077395
102	6	0	5.890282	-5.282906	1.265821
103	6	0	5.153368	-4.144403	0.922989
104	6	0	7.219286	-3.080271	0.179148
105	6	0	7.918195	-4.238423	0.535541
106	6	0	8.043469	-6.606280	1.424692
107	1	0	5.367801	-6.137373	1.692642
108	6	0	3.657566	-4.120485	1.148488
109	6	0	7.967177	-1.901319	-0.403978
110	1	0	8.996145	-4.268433	0.385797
111	6	0	-6.758525	-5.735905	-1.020429
112	6	0	-7.506488	-4.713563	-0.430747
113	6	0	-6.933229	-3.488315	-0.074874
114	6	0	-4.787369	-4.292845	-0.917074
115	6	0	-5.401343	-5.502462	-1.257802
116	6	0	-7.391976	-7.063195	-1.368241
117	1	0	-8.567058	-4.871142	-0.242861
118	6	0	-7.790175	-2.415077	0.560322
119	6	0	-3.313453	-4.094523	-1.195429
120	1	0	-4.801147	-6.282122	-1.723319
121	1	0	-8.822773	-2.758479	0.676344
122	1	0	-7.805055	-1.498351	-0.041018
123	1	0	-7.415574	-2.131376	1.551087
124	1	0	-3.131955	-3.219740	-1.830506
125	1	0	-2.889683	-4.968903	-1.698457
126	1	0	-2.745319	-3.934074	-0.270910
127	1	0	-8.459028	-6.952848	-1.589462
128	1	0	-7.304650	-7.776714	-0.537652
129	1	0	-6.911038	-7.521206	-2.239344
130	1	0	9.037097	-2.118116	-0.483806
131	1	0	7.848592	-1.002006	0.211890
132	1	0	7.598050	-1.643639	-1.403683
133	1	0	3.363578	-3.310778	1.826622
134	1	0	3.312675	-5.065651	1.579591
135	1	0	3.110398	-3.954059	0.213304
136	1	0	8.084852	-7.299174	0.573195
137	1	0	7.578503	-7.145395	2.257346
138	1	0	9.077302	-6.377060	1.705311

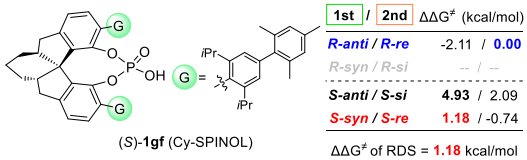
DFT calculation for all conformations of real system using Cy-SPINOL-derived CPA (*S*)-1gf*

TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-anti	--	--	-3699.762322	-2.11
S-anti	--	--	-3699.751096	4.93
S-syn	--	--	-3699.757064	1.18

TS	Orientation I	Orientation II	G≠ (a.u.)	ΔΔG≠ (kcal/mmol)
R-re	--	--	-3699.758952	0.00
S-si	--	--	-3699.755624	2.09
S-re	--	--	-3699.760128	-0.74

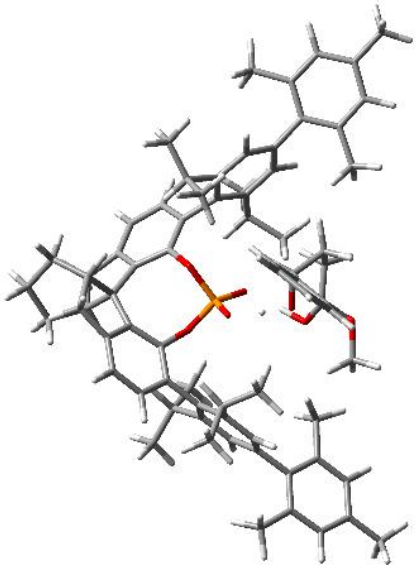
*In all TSs, conformational isomers by changing the orientation of the mesityl group were calculated, however the conformational isomers generated were converged to the single TS.

DFT calculation of real system using Cy-SPINOL-derived CPA (*S*)-1gf



(*S*)-**1gf** (Cy-SPINOL)

TS-1st-(*R*)-reaction pathway: *R-anti*/(*S*)-1gf (Cy-SPINOL)



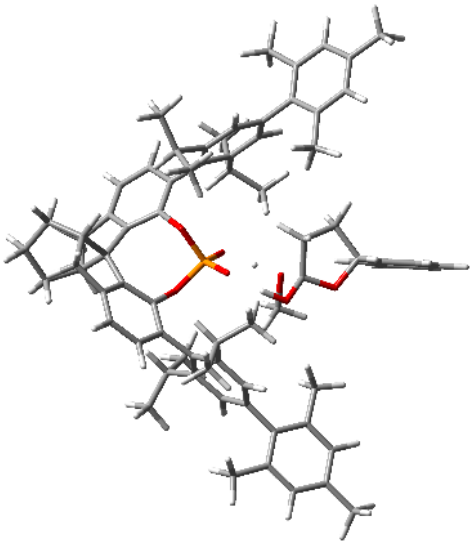
B3LYP/6-31G(d); E(RB3LYP) = -3701.05739287 Hartree
Zero-point correction= 1.418064 Hartree
Thermal correction to Energy= 1.497563 Hartree
Thermal correction to Enthalpy= 1.498507 Hartree
Thermal correction to Gibbs Free Energy= 1.295071 Hartree
Sum of electronic and zero-point Energies= -3699.639329 Hartree
Sum of electronic and thermal Energies= -3699.559830 Hartree
Sum of electronic and thermal Enthalpies= -3699.558886 Hartree
Sum of electronic and thermal Free Energies= -3699.762322 Hartree
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.777003	5.228488	2.671420
2	6	0	0.381560	5.211405	1.628983
3	6	0	-1.322638	3.654651	0.951711
4	6	0	-1.777706	4.232133	2.143800
5	6	0	-0.793767	5.576996	-0.657631
6	6	0	0.322979	5.872483	-1.694744
7	6	0	1.280043	4.720938	-1.554172
8	6	0	0.892229	3.854926	-0.523583
9	6	0	-0.199112	4.487079	0.341354
10	6	0	-1.977170	2.520211	0.469434
11	6	0	-3.227729	2.118630	0.978734
12	6	0	-3.731582	2.839169	2.074972
13	6	0	-2.989954	3.839119	2.702838
14	6	0	2.407667	4.458021	-2.325034
15	6	0	3.134750	3.299102	-2.077739
16	6	0	2.707560	2.333555	-1.147963
17	6	0	1.548018	2.623325	-0.402065
18	8	0	1.029812	1.675523	0.484563
19	8	0	-1.356397	1.755296	-0.524513

20	15	0	-0.193914	0.710021	-0.034709	89	1	0	-5.401613	3.957537	-2.723782
21	8	0	-0.650366	-0.027365	1.223931	90	1	0	-6.100349	3.324347	-1.220125
22	8	0	0.209516	-0.114103	-1.229209	91	1	0	-6.255738	2.406519	-2.726028
23	6	0	-4.018478	0.994710	0.375404	92	1	0	1.381130	7.024301	2.252440
24	6	0	3.561712	1.105041	-1.001115	93	1	0	1.747426	6.530848	0.614293
25	6	0	4.328835	0.907266	0.174457	94	1	0	-1.725445	7.523311	-0.708192
26	6	0	5.296395	-0.105246	0.195264	95	1	0	-2.109375	6.587377	0.717796
27	6	0	5.559291	-0.912284	-0.916010	96	1	0	0.309673	8.334863	0.171895
28	6	0	4.755053	-0.736139	-2.045900	97	1	0	-0.605807	8.141189	1.643491
29	6	0	3.756086	0.242947	-2.113120	98	6	0	6.707684	-1.876642	-0.921922
30	6	0	-4.361430	-0.149424	1.144392	99	6	0	-6.320614	-2.218090	-1.403943
31	6	0	-5.109965	-1.168381	0.543601	100	6	0	8.906235	-3.666174	-0.947977
32	6	0	-5.541629	-1.100003	-0.783425	101	6	0	9.101215	-2.282663	-0.936613
33	6	0	-5.222017	0.047326	-1.511669	102	6	0	8.032503	-1.381152	-0.921787
34	6	0	-4.475383	1.095685	-0.964528	103	6	0	6.493728	-3.270716	-0.955261
35	6	0	2.943762	0.348316	-3.407377	104	6	0	7.592386	-4.137151	-0.962108
36	6	0	3.815128	0.796661	-4.598617	105	6	0	10.078963	-4.618772	-0.925275
37	6	0	2.226532	-0.972234	-3.748485	106	1	0	10.116599	-1.890131	-0.946322
38	6	0	4.203935	1.804170	1.407258	107	6	0	8.327526	0.103997	-0.939692
39	6	0	3.713710	1.020667	2.639381	108	6	0	5.099988	-3.856316	-0.985090
40	6	0	5.521816	2.544895	1.709363	109	1	0	7.412720	-5.210756	-0.979484
41	6	0	-3.984167	-0.314231	2.619154	110	6	0	-7.781756	-4.345817	-2.563891
42	6	0	-5.214781	-0.106570	3.528011	111	6	0	-8.363383	-3.509225	-1.607441
43	6	0	-3.339523	-1.675650	2.935759	112	6	0	-7.659737	-2.452436	-1.021504
44	6	0	-4.247698	2.330174	-1.838727	113	6	0	-5.717620	-3.046856	-2.374502
45	6	0	-3.488645	1.995078	-3.136654	114	6	0	-6.457094	-4.097602	-2.929519
46	6	0	-5.580514	3.044061	-2.143265	115	6	0	-8.571809	-5.464676	-3.202851
47	6	0	0.929656	6.614166	1.340122	116	1	0	-9.396351	-3.680834	-1.309205
48	6	0	-1.289081	6.849239	0.040001	117	6	0	-8.355009	-1.572874	-0.004285
49	6	0	-0.161827	7.580464	0.812593	118	6	0	-4.290514	-2.827192	-2.830127
50	1	0	-0.417327	4.930831	3.664850	119	1	0	-5.981330	-4.739679	-3.669038
51	1	0	-1.209487	6.228361	2.794213	120	1	0	8.104353	0.581838	0.021474
52	1	0	1.190513	4.581278	2.016875	121	1	0	7.728663	0.625050	-1.694363
53	1	0	-1.634440	5.105537	-1.180138	122	1	0	9.384916	0.282954	-1.159195
54	1	0	-0.083584	5.929806	-2.712576	123	1	0	10.412825	-4.816879	0.102342
55	1	0	0.813711	6.835932	-1.510122	124	1	0	10.937639	-4.210906	-1.469980
56	1	0	-4.708138	2.572358	2.464828	125	1	0	9.820869	-5.583882	-1.374181
57	1	0	-3.363855	4.309563	3.608974	126	1	0	4.432601	-3.333442	-0.294767
58	1	0	2.721999	5.148188	-3.104060	127	1	0	5.116984	-4.916674	-0.712774
59	1	0	4.045260	3.105246	-2.635411	128	1	0	4.645618	-3.779471	-1.981130
60	1	0	5.898695	-0.242181	1.089845	129	1	0	-3.613751	-2.616855	-1.995992
61	1	0	4.938669	-1.361184	-2.915804	130	1	0	-4.210513	-1.971970	-3.512858
62	1	0	-5.362683	-2.051453	1.124004	131	1	0	-3.916444	-3.705819	-3.366485
63	1	0	-5.576940	0.127851	-2.535678	132	1	0	-7.915694	-6.266089	-3.559292
64	1	0	2.164151	1.099145	-3.257576	133	1	0	-9.145263	-5.105554	-4.068268
65	1	0	3.199684	0.907079	-5.499569	134	1	0	-9.289515	-5.902272	-2.500047
66	1	0	4.308391	1.755866	-4.409404	135	1	0	-8.223628	-0.510021	-0.235173
67	1	0	4.597891	0.061078	-4.819916	136	1	0	-7.961136	-1.723163	1.008039
68	1	0	1.632328	-0.849159	-4.662084	137	1	0	-9.428284	-1.786663	0.022919
69	1	0	1.547298	-1.261111	-2.944139	138	6	0	-0.042837	-3.212732	-0.128123
70	1	0	2.936161	-1.789605	-3.926241	139	8	0	-0.211039	-2.407286	1.373735
71	1	0	3.454727	2.570718	1.197825	140	6	0	1.041449	-2.508441	2.115415
72	1	0	4.408078	0.215251	2.908394	141	6	0	1.924083	-3.457469	1.278261
73	1	0	3.625030	1.686747	3.506430	142	6	0	1.475223	-3.233729	-0.165237
74	1	0	2.728195	0.583479	2.449169	143	1	0	1.487093	-1.507081	2.116202
75	1	0	5.856911	3.124375	0.841976	144	1	0	1.755243	-4.496467	1.576295
76	1	0	6.326834	1.851635	1.980313	145	1	0	2.982043	-3.226406	1.427908
77	1	0	5.386288	3.237648	2.548849	146	1	0	1.804859	-4.024587	-0.844946
78	1	0	-3.243588	0.449719	2.867900	147	1	0	1.831827	-2.273753	-0.548436
79	1	0	-4.926437	-0.164945	4.584783	148	8	0	-0.745723	-2.514838	-1.007363
80	1	0	-5.695340	0.863224	3.361475	149	8	0	-0.544109	-4.441428	0.110434
81	1	0	-5.970398	-0.880503	3.344764	150	6	0	-1.977731	-4.573591	0.068437
82	1	0	-3.010308	-1.699228	3.981384	151	1	0	-2.178356	-5.598643	0.379480
83	1	0	-2.465573	-1.858889	2.308488	152	1	0	-2.350639	-4.402550	-0.943096
84	1	0	-4.044103	-2.505542	2.800765	153	1	0	-2.446933	-3.867406	0.759356
85	1	0	-3.633379	3.040104	-1.280107	154	6	0	0.793087	-2.954845	3.536948
86	1	0	-3.287783	2.911292	-3.705825	155	6	0	1.330304	-2.228967	4.604112
87	1	0	-2.532701	1.511569	-2.916839	156	6	0	0.049989	-4.112472	3.805751
88	1	0	-4.070493	1.328689	-3.784798	157	6	0	1.139957	-2.654988	5.920536

158	1	0	1.896707	-1.321860	4.404702
159	6	0	-0.148173	-4.534433	5.118792
160	1	0	-0.377852	-4.673667	2.979416
161	6	0	0.399770	-3.808196	6.179644
162	1	0	1.562852	-2.080593	6.739851
163	1	0	-0.730630	-5.431113	5.316072
164	1	0	0.244841	-4.138262	7.203985
165	1	0	-0.468179	-1.302995	1.261021
166	1	0	-0.350120	-1.593432	-1.175201

TS-2nd-(*R*)-reaction pathway: *R-re*/(*S*)-1gf (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3701.05658257 Hartree

Zero-point correction= 1.419138 Hartree

Thermal correction to Energy= 1.498576 Hartree

Thermal correction to Enthalpy= 1.499521 Hartree

Thermal correction to Gibbs Free Energy= 1.297630 Hartree

Sum of electronic and zero-point Energies= -3699.637445 Hartree

Sum of electronic and thermal Energies= -3699.558006 Hartree

Sum of electronic and thermal Enthalpies= -3699.557062 Hartree

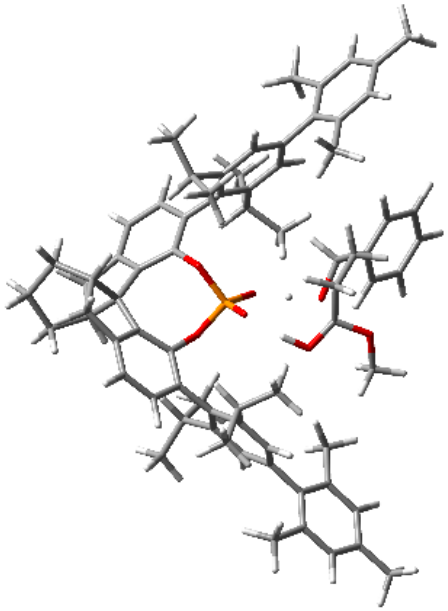
Sum of electronic and thermal Free Energies= -3699.758952 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739705	-6.216055	1.472991
2	6	0	-0.422324	-5.927362	0.481896
3	6	0	1.229082	-4.180606	0.301816
4	6	0	1.676803	-5.051105	1.303189
5	6	0	0.677171	-5.530415	-1.836219
6	6	0	-0.503906	-5.556292	-2.850125
7	6	0	-1.499782	-4.570018	-2.297560
8	6	0	-1.031984	-3.998387	-1.106632
9	6	0	0.118958	-4.821845	-0.529034
10	6	0	1.849140	-2.933849	0.171840
11	6	0	3.025045	-2.618422	0.880938
12	6	0	3.519896	-3.590113	1.768781
13	6	0	2.833649	-4.773425	2.024717
14	6	0	-2.720590	-4.183709	-2.842071
15	6	0	-3.461481	-3.192169	-2.202525
16	6	0	-2.950661	-2.477150	-1.105963
17	6	0	-1.693518	-2.872405	-0.607676
18	8	0	-1.083042	-2.110863	0.393534
19	8	0	1.270118	-1.992571	-0.680814
20	15	0	0.069717	-1.044779	-0.077461
21	8	0	0.504887	-0.294289	1.154098
22	8	0	-0.403703	-0.236836	-1.282687
23	6	0	3.780717	-1.328060	0.736504
24	6	0	-3.764042	-1.370622	-0.498553
25	6	0	-4.256679	-1.500628	0.825897
26	6	0	-5.088624	-0.502891	1.345674
27	6	0	-5.458564	0.622454	0.606093
28	6	0	-4.960587	0.735841	-0.695042
29	6	0	-4.128017	-0.233436	-1.268422
30	6	0	3.954340	-0.475603	1.860448
31	6	0	4.778975	0.648435	1.735040
32	6	0	5.437746	0.967621	0.545144
33	6	0	5.231675	0.133483	-0.556333
34	6	0	4.426569	-1.011312	-0.485401
35	6	0	-3.689381	-0.029576	-2.721670
36	6	0	-4.876960	-0.210722	-3.690657
37	6	0	-3.028087	1.338953	-2.966585
38	6	0	-3.976375	-2.716993	1.709669
39	6	0	-3.244441	-2.329296	3.008693
40	6	0	-5.270813	-3.498904	2.011367
41	6	0	3.324169	-0.744861	3.231345
42	6	0	4.398528	-1.136582	4.268318
43	6	0	2.500702	0.444392	3.761820
44	6	0	4.354900	-1.911820	-1.720019
45	6	0	3.733052	-1.191844	-2.931050
46	6	0	5.740299	-2.491244	-2.070923
47	6	0	-0.924967	-7.200514	-0.208955
48	6	0	1.250541	-6.928081	-1.573090
49	6	0	0.186033	-7.911702	-1.023008
50	1	0	0.373479	-6.283245	2.505471
51	1	0	1.232277	-7.173440	1.263968
52	1	0	-1.248872	-5.472877	1.040837
53	1	0	1.468028	-4.886642	-2.238523
54	1	0	-0.171195	-5.255379	-3.851931
55	1	0	-0.931997	-6.559307	-2.962778
56	1	0	4.444792	-3.380754	2.296235
57	1	0	3.198979	-5.467022	2.778122
58	1	0	-3.099595	-4.653097	-3.746625
59	1	0	-4.443556	-2.927442	-2.580566
60	1	0	-5.482831	-0.614925	2.352279
61	1	0	-5.241698	1.606251	-1.282079
62	1	0	4.929686	1.293336	2.596668
63	1	0	5.747472	0.363008	-1.485670
64	1	0	-2.938481	-0.786566	-2.959131
65	1	0	-4.539955	-0.127336	-4.731181
66	1	0	-5.362362	-1.184859	-3.570296
67	1	0	-5.641346	0.558493	-3.525366
68	1	0	-2.699551	1.411817	-4.010745
69	1	0	-2.151011	1.470054	-2.330092
70	1	0	-3.720240	2.170258	-2.785612
71	1	0	-3.320734	-3.397178	1.161613
72	1	0	-3.861138	-1.678421	3.640514
73	1	0	-3.008853	-3.226745	3.593949
74	1	0	-2.307671	-1.809205	2.789084
75	1	0	-5.770337	-3.810899	1.087190
76	1	0	-5.982642	-2.897698	2.589125
77	1	0	-5.045214	-4.398921	2.596362
78	1	0	2.632595	-1.584427	3.129837
79	1	0	3.930016	-1.391595	5.226728
80	1	0	4.991788	-1.998057	3.943289
81	1	0	5.094492	-0.308283	4.448615
82	1	0	2.075111	0.190541	4.740610
83	1	0	1.675752	0.680073	3.088211
84	1	0	3.112847	1.344148	3.893516
85	1	0	3.709449	-2.761771	-1.487125
86	1	0	3.675260	-1.871341	-3.790382
87	1	0	2.718879	-0.851951	-2.700825
88	1	0	4.331354	-0.324686	-3.236667
89	1	0	5.661351	-3.186976	-2.915352
90	1	0	6.167685	-3.035631	-1.221384

91	1	0	6.449318	-1.704512	-2.354284
92	1	0	-1.329225	-7.885804	0.547040
93	1	0	-1.769444	-6.943228	-0.858518
94	1	0	1.680713	-7.325454	-2.501238
95	1	0	2.087600	-6.840206	-0.870474
96	1	0	-0.276800	-8.469128	-1.845842
97	1	0	0.684782	-8.667144	-0.404580
98	6	0	-6.380870	1.655366	1.178239
99	6	0	6.388395	2.126656	0.483006
100	6	0	-8.133844	3.600975	2.254764
101	6	0	-6.818425	3.485849	2.708974
102	6	0	-5.937215	2.528879	2.193689
103	6	0	-7.711314	1.750076	0.712775
104	6	0	-8.560452	2.716860	1.260297
105	6	0	-9.060516	4.660658	2.804418
106	1	0	-6.464983	4.158377	3.488813
107	6	0	-4.528278	2.452829	2.740958
108	6	0	-8.246642	0.810011	-0.346188
109	1	0	-9.586934	2.775847	0.902406
110	6	0	8.209994	4.289442	0.403560
111	6	0	6.869632	4.462288	0.053227
112	6	0	5.951567	3.405911	0.084459
113	6	0	7.741398	1.929986	0.837356
114	6	0	8.625825	3.011666	0.788283
115	6	0	9.176269	5.451606	0.393768
116	1	0	6.523528	5.447453	-0.254987
117	6	0	4.519849	3.652463	-0.332835
118	6	0	8.248671	0.570130	1.265578
119	1	0	9.667813	2.850625	1.059803
120	1	0	4.317851	3.212862	-1.318507
121	1	0	4.311957	4.724937	-0.404010
122	1	0	3.798714	3.210544	0.360810
123	1	0	8.859389	6.230745	-0.307848
124	1	0	10.185699	5.132281	0.111349
125	1	0	9.251012	5.918100	1.385552
126	1	0	9.321590	0.604223	1.479584
127	1	0	8.080598	-0.186994	0.490823
128	1	0	7.735141	0.211933	2.165567
129	1	0	-4.292030	3.344842	3.330605
130	1	0	-3.788434	2.360260	1.939326
131	1	0	-4.388561	1.581509	3.392449
132	1	0	-8.780510	4.949432	3.823168
133	1	0	-10.099485	4.313579	2.824702
134	1	0	-9.036119	5.570994	2.190005
135	1	0	-7.807131	1.006642	-1.331323
136	1	0	-9.332231	0.913086	-0.441378
137	1	0	-8.021868	-0.235278	-0.107337
138	1	0	-0.038777	1.061374	-1.355142
139	6	0	0.354632	2.763771	0.154824
140	8	0	0.636626	4.069885	-0.056716
141	8	0	0.249750	2.121581	-1.432389
142	6	0	-0.581955	4.886849	-0.004990
143	6	0	-1.739051	3.868531	0.018414
144	6	0	-1.087495	2.621934	0.625024
145	1	0	-0.529749	5.420970	0.951807
146	1	0	-2.089770	3.661323	-0.995582
147	1	0	-2.585825	4.241561	0.600087
148	1	0	-1.547775	1.680252	0.325962
149	1	0	-1.068301	2.660427	1.720180
150	8	0	1.352873	2.131037	0.740083
151	6	0	1.495411	2.202967	-2.159859
152	1	0	1.736708	3.258368	-2.290923
153	1	0	1.332087	1.726357	-3.129743
154	1	0	2.295335	1.694851	-1.616581
155	1	0	1.084178	1.172162	0.948691
156	6	0	-0.594423	5.891144	-1.130843
157	6	0	-0.629945	7.259215	-0.843640
158	6	0	-0.588644	5.477784	-2.471462
159	6	0	-0.666661	8.202641	-1.872706
160	1	0	-0.625096	7.590176	0.191795
161	6	0	-0.616861	6.418564	-3.499648
162	1	0	-0.560620	4.417590	-2.706253
163	6	0	-0.658791	7.784388	-3.202757
164	1	0	-0.697059	9.262856	-1.633082
165	1	0	-0.608444	6.086751	-4.533939
166	1	0	-0.683699	8.515690	-4.005911

TS-1st-(*S*)-reaction pathway: *S-anti*/(*S*)-1gf (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3701.04937008 Hartree

Zero-point correction= 1.418887 Hartree

Thermal correction to Energy= 1.497867 Hartree

Thermal correction to Enthalpy= 1.498811 Hartree

Thermal correction to Gibbs Free Energy= 1.298274 Hartree

Sum of electronic and zero-point Energies= -3699.630483 Hartree

Sum of electronic and thermal Energies= -3699.551503 Hartree

Sum of electronic and thermal Enthalpies= -3699.550559 Hartree

Sum of electronic and thermal Free Energies= -3699.751096 Hartree

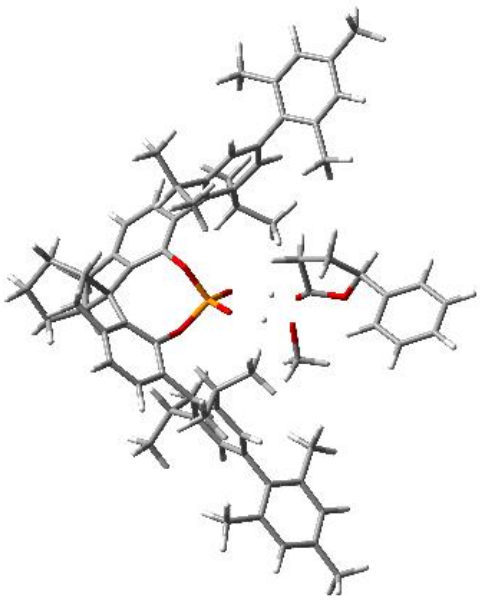
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.363644	5.867951	1.712923
2	6	0	-0.168317	5.704791	0.729695
3	6	0	-1.684878	3.854033	0.453113
4	6	0	-2.238026	4.670897	1.447672
5	6	0	-1.257688	5.338778	-1.597657
6	6	0	-0.110089	5.485807	-2.634514
7	6	0	0.960124	4.546525	-2.148628
8	6	0	0.575949	3.904762	-0.963544
9	6	0	-0.620484	4.612013	-0.332415
10	6	0	-2.210192	2.572367	0.267445
11	6	0	-3.435377	2.195008	0.854531
12	6	0	-4.046562	3.123855	1.715314
13	6	0	-3.430040	4.320098	2.071661
14	6	0	2.186950	4.275716	-2.744963
15	6	0	3.018212	3.325198	-2.162711
16	6	0	2.604223	2.544674	-1.068578
17	6	0	1.342451	2.825474	-0.507848
18	8	0	0.855142	2.037192	0.539404
19	8	0	-1.486264	1.653955	-0.506393
20	15	0	-0.260444	0.869037	0.255671

21	8	0	-0.675540	0.329176	1.599592	90	1	0	-6.265080	2.609190	-1.658444
22	8	0	0.263378	-0.138990	-0.773973	91	1	0	-6.355097	1.294217	-2.840139
23	6	0	-4.132128	0.894675	0.578297	92	1	0	0.611550	7.714127	0.879452
24	6	0	3.544352	1.493936	-0.556679	93	1	0	1.104680	6.862661	-0.566732
25	6	0	4.149218	1.639983	0.716886	94	1	0	-2.378979	7.091039	-2.175662
26	6	0	5.133190	0.727422	1.112331	95	1	0	-2.738659	6.514670	-0.564360
27	6	0	5.530100	-0.345990	0.308574	96	1	0	-0.487343	8.325288	-1.488705
28	6	0	4.897904	-0.487158	-0.933462	97	1	0	-1.449228	8.409098	-0.036766
29	6	0	3.937952	0.420441	-1.399145	98	6	0	6.618631	-1.281718	0.736057
30	6	0	-4.445608	-0.000391	1.638339	99	6	0	-6.431713	-2.698006	-0.208409
31	6	0	-5.169460	-1.162819	1.348842	100	6	0	8.684437	-3.076943	1.504884
32	6	0	-5.626666	-1.465377	0.062716	101	6	0	7.553891	-2.893618	2.299417
33	6	0	-5.322734	-0.562710	-0.958933	102	6	0	6.529335	-2.005656	1.947729
34	6	0	-4.584901	0.603539	-0.734857	103	6	0	7.775478	-1.438350	-0.069891
35	6	0	3.416310	0.246956	-2.830599	104	6	0	8.778154	-2.325078	0.330626
36	6	0	4.548128	0.470336	-3.855833	105	6	0	9.766278	-4.058457	1.890541
37	6	0	2.737729	-1.110008	-3.079447	106	1	0	7.462299	-3.452966	3.229126
38	6	0	3.827736	2.796671	1.664154	107	6	0	5.373137	-1.854471	2.914392
39	6	0	3.235812	2.297925	2.996230	108	6	0	7.995932	-0.642254	-1.340539
40	6	0	5.060048	3.692228	1.902043	109	1	0	9.665791	-2.424198	-0.291998
41	6	0	-4.093239	0.272896	3.106092	110	6	0	-7.956835	-5.036594	-0.707355
42	6	0	-5.361268	0.634490	3.910899	111	6	0	-8.433776	-4.028954	0.135365
43	6	0	-3.370228	-0.892315	3.806780	112	6	0	-7.698768	-2.869490	0.398418
44	6	0	-4.371207	1.539793	-1.925695	113	6	0	-5.946830	-3.694425	-1.084494
45	6	0	-3.567970	0.864262	-3.053434	114	6	0	-6.713113	-4.844147	-1.309656
46	6	0	-5.711979	2.092036	-2.450635	115	6	0	-8.755150	-6.297830	-0.942612
47	6	0	0.248606	7.037304	0.095512	116	1	0	-9.412504	-4.144082	0.598263
48	6	0	-1.915537	6.684089	-1.267857	117	6	0	-8.304732	-1.814885	1.301228
49	6	0	-0.909363	7.709643	-0.685727	118	6	0	-4.620810	-3.558836	-1.803437
50	1	0	-1.019513	5.876619	2.755205	119	1	0	-6.323564	-5.609458	-1.979164
51	1	0	-1.897780	6.813594	1.563211	120	1	0	-8.150133	-0.805682	0.906641
52	1	0	0.682443	5.286546	1.280262	121	1	0	-7.868182	-1.830151	2.307351
53	1	0	-2.014773	4.661053	-2.009210	122	1	0	-9.381626	-1.978876	1.411372
54	1	0	-0.447384	5.210646	-3.642170	123	1	0	-8.582884	-7.034626	-0.146227
55	1	0	0.251753	6.518293	-2.708200	124	1	0	-8.482813	-6.774180	-1.890455
56	1	0	-5.010266	2.871242	2.143387	125	1	0	-9.831463	-6.093273	-0.963853
57	1	0	-3.883463	4.970831	2.815335	126	1	0	-4.215070	-4.546088	-2.051468
58	1	0	2.498534	4.803367	-3.643010	127	1	0	-3.882999	-3.015094	-1.208583
59	1	0	4.002022	3.140745	-2.582392	128	1	0	-4.728351	-3.011309	-2.748978
60	1	0	5.628454	0.872350	2.068164	129	1	0	7.627849	0.383715	-1.249358
61	1	0	5.182885	-1.319872	-1.570051	130	1	0	7.486409	-1.087146	-2.204115
62	1	0	-5.394267	-1.856024	2.154251	131	1	0	9.063281	-0.603244	-1.581676
63	1	0	-5.693167	-0.767152	-1.959602	132	1	0	5.606603	-1.129173	3.705480
64	1	0	2.655774	1.009648	-3.008823	133	1	0	5.157320	-2.806756	3.411708
65	1	0	4.149307	0.437167	-4.876894	134	1	0	4.463902	-1.500671	2.425065
66	1	0	5.043316	1.437917	-3.717000	135	1	0	9.648798	-5.012117	1.358301
67	1	0	5.317967	-0.306608	-3.775457	136	1	0	9.744165	-4.278962	2.962913
68	1	0	2.419150	-1.179731	-4.126769	137	1	0	10.762652	-3.674221	1.644509
69	1	0	1.848178	-1.215450	-2.455102	138	1	0	0.299951	-1.372785	-0.439320
70	1	0	3.407049	-1.954736	-2.884134	139	6	0	-0.434211	-2.885499	1.251215
71	1	0	3.070002	3.425647	1.191403	140	8	0	0.409578	-2.492133	-0.162234
72	1	0	3.950518	1.672999	3.545794	141	6	0	1.804574	-2.837826	0.037397
73	1	0	2.978325	3.147812	3.640190	142	6	0	1.946597	-3.226725	1.537471
74	1	0	2.326195	1.714500	2.825585	143	6	0	0.707805	-2.652230	2.224121
75	1	0	5.458863	4.077245	0.956790	144	1	0	2.375048	-1.923510	-0.159694
76	1	0	5.866883	3.149354	2.408197	145	1	0	1.968789	-4.314365	1.642802
77	1	0	4.791932	4.549070	2.532017	146	1	0	2.870487	-2.822345	1.959502
78	1	0	-3.414000	1.127941	3.139851	147	1	0	0.481374	-3.146878	3.173565
79	1	0	-5.096757	0.915698	4.937611	148	1	0	0.794816	-1.576676	2.398901
80	1	0	-5.916262	1.466255	3.464752	149	8	0	-1.512134	-2.115752	1.257048
81	1	0	-6.046082	-0.220645	3.965793	150	8	0	-0.702060	-4.200720	1.127571
82	1	0	-3.140642	-0.611124	4.841785	151	6	0	-1.838052	-4.556873	0.324401
83	1	0	-2.433176	-1.141886	3.308866	152	1	0	-1.827475	-5.647204	0.279170
84	1	0	-3.985978	-1.798633	3.843731	153	1	0	-2.762233	-4.200984	0.784784
85	1	0	-3.790323	2.400866	-1.588536	154	1	0	-1.742502	-4.137818	-0.680764
86	1	0	-3.385333	1.575408	-3.868635	155	1	0	-1.268223	-1.150596	1.447799
87	1	0	-2.600496	0.510411	-2.686022	156	6	0	2.248206	-3.929166	-0.920093
88	1	0	-4.109247	0.010003	-3.478080	157	6	0	1.430505	-4.385778	-1.958448
89	1	0	-5.538117	2.805574	-3.265493	158	6	0	3.529019	-4.483166	-0.777138

159	6	0	1.880350	-5.380738	-2.829578
160	1	0	0.444300	-3.955977	-2.085182
161	6	0	3.979616	-5.473103	-1.649366
162	1	0	4.181053	-4.137988	0.023103
163	6	0	3.154770	-5.927760	-2.680031
164	1	0	1.230793	-5.724766	-3.631060
165	1	0	4.975985	-5.890669	-1.521628
166	1	0	3.503054	-6.700866	-3.359886

TS-2nd-(*S*)-reaction pathway: *S-si*/(*S*)-1gf (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3701.05231407 Hartree

Zero-point correction= 1.419222 Hartree

Thermal correction to Energy= 1.498718 Hartree

Thermal correction to Enthalpy= 1.499663 Hartree

Thermal correction to Gibbs Free Energy= 1.296690 Hartree

Sum of electronic and zero-point Energies= -3699.633092 Hartree

Sum of electronic and thermal Energies= -3699.553596 Hartree

Sum of electronic and thermal Enthalpies= -3699.552651 Hartree

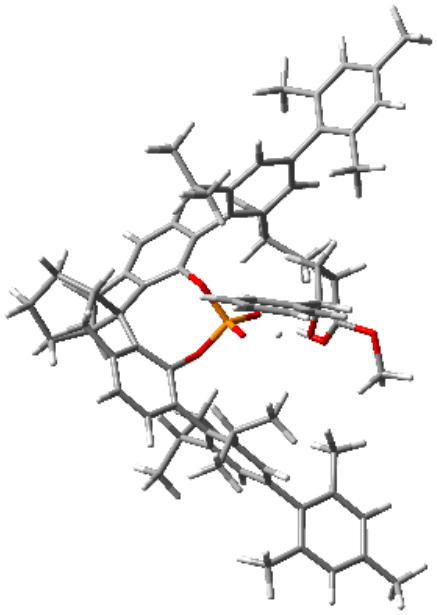
Sum of electronic and thermal Free Energies= -3699.755624 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.714247	-5.983435	1.723829
2	6	0	-0.453661	-5.743094	0.724394
3	6	0	1.183588	-3.992391	0.472137
4	6	0	1.664482	-4.841523	1.476834
5	6	0	0.681927	-5.441338	-1.591636
6	6	0	-0.461111	-5.506363	-2.643309
7	6	0	-1.468384	-4.494282	-2.167953
8	6	0	-1.060663	-3.896253	-0.969524
9	6	0	0.080776	-4.680218	-0.329135
10	6	0	1.799181	-2.748649	0.292373
11	6	0	3.039814	-2.456556	0.893527
12	6	0	3.567297	-3.418201	1.774592
13	6	0	2.863796	-4.566548	2.125309
14	6	0	-2.659541	-4.119195	-2.780834
15	6	0	-3.423819	-3.111796	-2.201061
16	6	0	-2.975975	-2.378945	-1.086376
17	6	0	-1.753779	-2.773393	-0.505870
18	8	0	-1.212577	-2.052321	0.559303
19	8	0	1.151835	-1.783771	-0.488020
20	15	0	-0.050629	-0.932978	0.245345
21	8	0	0.377050	-0.375888	1.576271
22	8	0	-0.541460	0.040133	-0.823758
23	6	0	3.874023	-1.237933	0.612492
24	6	0	-3.852738	-1.268560	-0.581391
25	6	0	-4.459089	-1.362300	0.698006
26	6	0	-5.419145	-0.412989	1.069816
27	6	0	-5.815420	0.624210	0.221886
28	6	0	-5.179490	0.723106	-1.019636
29	6	0	-4.209677	-0.195503	-1.443699
30	6	0	4.266186	-0.379501	1.675345
31	6	0	5.230798	0.607163	1.431602
32	6	0	5.821387	0.782906	0.177550
33	6	0	5.378280	-0.030210	-0.868262
34	6	0	4.425027	-1.039104	-0.680389
35	6	0	-3.618325	-0.009221	-2.846381
36	6	0	-4.687356	-0.214382	-3.940318
37	6	0	-2.940413	1.361240	-3.035889
38	6	0	-4.175353	-2.500708	1.679045
39	6	0	-3.566832	-1.982225	2.995999
40	6	0	-5.437714	-3.346260	1.942848
41	6	0	3.708751	-0.494078	3.097771
42	6	0	4.778276	-0.987004	4.095213
43	6	0	3.116792	0.835292	3.602523
44	6	0	4.085279	-1.921096	-1.882938
45	6	0	3.401990	-1.115649	-3.004497
46	6	0	5.327071	-2.667856	-2.409984
47	6	0	-0.948817	-7.043574	0.080178
48	6	0	1.247007	-6.827757	-1.260538
49	6	0	0.170780	-7.787367	-0.691793
50	1	0	0.355083	-5.976061	2.761000
51	1	0	1.192472	-6.959060	1.576541
52	1	0	-1.282879	-5.271474	1.264500
53	1	0	1.486502	-4.813150	-1.991738
54	1	0	-0.092564	-5.256295	-3.646546
55	1	0	-0.893913	-6.510945	-2.722032
56	1	0	4.539820	-3.229785	2.216125
57	1	0	3.257649	-5.242365	2.880420
58	1	0	-2.996749	-4.609188	-3.690934
59	1	0	-4.382355	-2.848970	-2.636214
60	1	0	-5.909253	-0.507958	2.035363
61	1	0	-5.472449	1.529130	-1.688177
62	1	0	5.556680	1.242198	2.251465
63	1	0	5.824753	0.099921	-1.850926
64	1	0	-2.841056	-0.762755	-2.990319
65	1	0	-4.231415	-0.154177	-4.935950
66	1	0	-5.183002	-1.187151	-3.854931
67	1	0	-5.465704	0.556401	-3.885414
68	1	0	-2.543422	1.441679	-4.055168
69	1	0	-2.104216	1.486020	-2.344914
70	1	0	-3.643300	2.191227	-2.892833
71	1	0	-3.440538	-3.169566	1.227065
72	1	0	-4.258840	-1.315454	3.524906
73	1	0	-3.341090	-2.820938	3.665859
74	1	0	-2.635903	-1.438643	2.810358
75	1	0	-5.851723	-3.742966	1.008903
76	1	0	-6.224036	-2.762939	2.435961
77	1	0	-5.197076	-4.194572	2.595054
78	1	0	2.891774	-1.219722	3.084185
79	1	0	4.341259	-1.103625	5.094292
80	1	0	5.208386	-1.950265	3.802898
81	1	0	5.603397	-0.268830	4.175971
82	1	0	2.665506	0.691302	4.591394
83	1	0	2.338188	1.208074	2.934975
84	1	0	3.883926	1.612582	3.704099
85	1	0	3.375897	-2.685615	-1.560032
86	1	0	3.142123	-1.774051	-3.842528
87	1	0	2.480541	-0.649074	-2.643440
88	1	0	4.059896	-0.329046	-3.393856

89	1	0	5.045893	-3.345230	-3.225575
90	1	0	5.795112	-3.264956	-1.619224
91	1	0	6.083929	-1.977615	-2.800443
92	1	0	-1.364335	-7.698290	0.856759
93	1	0	-1.783980	-6.810358	-0.590733
94	1	0	1.692916	-7.261808	-2.164599
95	1	0	2.071618	-6.713757	-0.547556
96	1	0	-0.282260	-8.372187	-1.500942
97	1	0	0.657812	-8.521910	-0.039749
98	6	0	6.944400	1.757330	-0.023603
99	6	0	-6.939038	1.543331	0.600166
100	6	0	-9.102214	3.232390	1.300207
101	6	0	-9.264037	2.200892	0.371578
102	6	0	-8.211221	1.353282	0.014048
103	6	0	-6.758065	2.577534	1.542031
104	6	0	-7.840036	3.401870	1.871920
105	6	0	-10.264600	4.113146	1.696229
106	1	0	-10.240299	2.044703	-0.084178
107	6	0	-8.464271	0.238746	-0.978626
108	6	0	-5.413020	2.844793	2.180765
109	1	0	-7.688074	4.199775	2.596675
110	6	0	9.091723	3.562624	-0.397672
111	6	0	9.316308	2.256914	0.047208
112	6	0	8.270631	1.348000	0.236758
113	6	0	6.699229	3.071037	-0.468861
114	6	0	7.773368	3.949561	-0.647287
115	6	0	10.242270	4.515345	-0.626781
116	1	0	10.335402	1.933710	0.252483
117	6	0	8.577418	-0.054197	0.715195
118	6	0	5.291300	3.548940	-0.740832
119	1	0	7.572223	4.963225	-0.989660
120	1	0	-9.530488	0.166169	-1.215107
121	1	0	-8.135023	-0.730364	-0.587119
122	1	0	-7.923430	0.394810	-1.919414
123	1	0	-10.941683	4.287660	0.852681
124	1	0	-9.923056	5.086911	2.063138
125	1	0	-10.858880	3.653654	2.497665
126	1	0	-4.942599	1.931204	2.556520
127	1	0	-5.510535	3.544940	3.016266
128	1	0	-4.715700	3.290823	1.460281
129	1	0	8.095520	-0.269007	1.676111
130	1	0	9.655568	-0.196746	0.838164
131	1	0	8.212801	-0.809475	0.009354
132	1	0	5.296282	4.557769	-1.166440
133	1	0	4.695540	3.574472	0.180541
134	1	0	4.767232	2.885193	-1.437583
135	1	0	11.048647	4.352156	0.096762
136	1	0	9.921005	5.559249	-0.545332
137	1	0	10.675410	4.385340	-1.627842
138	1	0	-0.781551	1.320092	-0.424627
139	6	0	0.378872	2.820827	0.856004
140	8	0	0.217349	4.156924	1.006753
141	8	0	-0.929310	2.365651	-0.120451
142	1	0	0.313204	1.175896	1.869440
143	6	0	1.029416	4.898142	0.036099
144	6	0	1.553206	3.823953	-0.937795
145	6	0	1.558011	2.559412	-0.073826
146	1	0	1.860221	5.319542	0.613777
147	1	0	0.870159	3.710200	-1.783618
148	1	0	2.539798	4.085577	-1.330799
149	1	0	1.464148	1.630510	-0.635815
150	1	0	2.455029	2.489818	0.550860
151	8	0	0.215474	2.180650	2.002420
152	6	0	-2.199749	2.503510	0.557982
153	1	0	-2.976114	2.199043	-0.143600
154	1	0	-2.228531	1.875023	1.450092
155	1	0	-2.312273	3.552999	0.831809
156	6	0	0.229947	6.022851	-0.574670
157	6	0	-0.952225	5.768003	-1.285371
158	6	0	0.678426	7.341363	-0.455207
159	6	0	-1.667320	6.815893	-1.862495
160	1	0	-1.311698	4.747538	-1.380340
161	6	0	-0.032285	8.391538	-1.041081
162	1	0	1.589360	7.550195	0.102077
163	6	0	-1.207092	8.131077	-1.743957
164	1	0	-2.583185	6.606851	-2.408132
165	1	0	0.331016	9.410804	-0.940735
166	1	0	-1.764818	8.946199	-2.197871

TS-1st-(*S*)-reaction pathway: *S-syn*/(*S*)-1gf (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3701.05242453 Hartree

Zero-point correction= 1.417893 Hartree

Thermal correction to Energy= 1.497568 Hartree

Thermal correction to Enthalpy= 1.498512 Hartree

Thermal correction to Gibbs Free Energy= 1.295360 Hartree

Sum of electronic and zero-point Energies= -3699.634531 Hartree

Sum of electronic and thermal Energies= -3699.554857 Hartree

Sum of electronic and thermal Enthalpies= -3699.553913 Hartree

Sum of electronic and thermal Free Energies= -3699.757064 Hartree

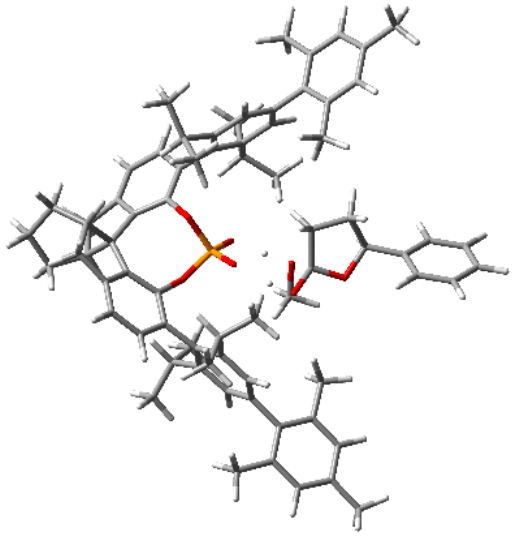
The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.352344	5.560342	-2.178560
2	6	0	-0.760410	5.358512	-1.114805
3	6	0	0.914749	3.641222	-0.849846
4	6	0	1.303083	4.417559	-1.949622
5	6	0	0.425227	5.170241	1.188410
6	6	0	-0.727021	5.280109	2.232420
7	6	0	-1.737411	4.251165	1.792964
8	6	0	-1.293500	3.576911	0.648654
9	6	0	-0.167943	4.348685	-0.033662
10	6	0	1.566585	2.421930	-0.629170
11	6	0	2.727412	2.070485	-1.345687
12	6	0	3.153150	2.950778	-2.356313
13	6	0	2.425764	4.085335	-2.700552
14	6	0	-2.950911	3.914317	2.385303
15	6	0	-3.706585	2.877866	1.838145
16	6	0	-3.216995	2.069235	0.798061

17	6	0	-1.961800	2.415345	0.259419	86	1	0	3.979215	2.130472	3.317629
18	8	0	-1.354436	1.573615	-0.677380	87	1	0	3.138714	0.750441	2.590887
19	8	0	1.041253	1.546060	0.326180	88	1	0	4.883656	0.671184	2.897061
20	15	0	-0.188202	0.559004	-0.140401	89	1	0	5.502437	3.605983	1.920339
21	8	0	0.197170	-0.324994	-1.294441	90	1	0	5.745450	3.269520	0.195190
22	8	0	-0.625889	-0.108567	1.164444	91	1	0	6.487751	2.222857	1.415811
23	6	0	3.593449	0.871243	-1.070571	92	1	0	-1.677842	7.301846	-1.317649
24	6	0	-4.027833	0.919294	0.274430	93	1	0	-2.060894	6.487044	0.180962
25	6	0	-4.464865	0.924030	-1.076579	94	1	0	1.441213	7.019957	1.658531
26	6	0	-5.224719	-0.149755	-1.551905	95	1	0	1.794762	6.393176	0.063811
27	6	0	-5.580293	-1.228194	-0.740327	96	1	0	-0.541430	8.098710	0.971308
28	6	0	-5.172843	-1.199251	0.595031	97	1	0	0.367566	8.166607	-0.515293
29	6	0	-4.408381	-0.153228	1.125133	98	6	0	-6.368320	-2.379747	-1.283995
30	6	0	3.756556	-0.136278	-2.057478	99	6	0	6.754960	-2.064775	-0.675446
31	6	0	4.755565	-1.102541	-1.878721	100	6	0	-7.844674	-4.567156	-2.300001
32	6	0	5.601742	-1.108925	-0.766036	101	6	0	-8.452248	-3.599754	-1.495224
33	6	0	5.385827	-0.143073	0.220492	102	6	0	-7.740685	-2.510323	-0.982537
34	6	0	4.404055	0.848008	0.092479	103	6	0	-5.736388	-3.343898	-2.097861
35	6	0	-4.047375	-0.219580	2.611350	104	6	0	-6.485074	-4.420889	-2.585317
36	6	0	-5.271430	0.105908	3.494229	105	6	0	-8.640846	-5.720024	-2.866968
37	6	0	-3.466666	-1.582096	3.032795	106	1	0	-9.511158	-3.692849	-1.259798
38	6	0	-4.204014	2.081504	-2.042387	107	6	0	-8.456671	-1.487944	-0.126492
39	6	0	-3.444744	1.631174	-3.304913	108	6	0	-4.268551	-3.236716	-2.451731
40	6	0	-5.519869	2.796580	-2.411773	109	1	0	-5.989331	-5.166303	-3.205066
41	6	0	2.927441	-0.185288	-3.344484	110	6	0	8.960526	-3.832680	-0.523003
42	6	0	3.779561	0.180577	-4.578194	111	6	0	9.027179	-2.660195	-1.279985
43	6	0	2.256635	-1.553802	-3.568569	112	6	0	7.949405	-1.773387	-1.370422
44	6	0	4.325784	1.923096	1.177588	113	6	0	6.673217	-3.238544	0.100329
45	6	0	4.068184	1.329014	2.574171	114	6	0	7.773745	-4.099774	0.163155
46	6	0	5.590512	2.805470	1.175577	115	6	0	10.126979	-4.791892	-0.467758
47	6	0	-1.242319	6.686956	-0.519672	116	1	0	9.946074	-2.424326	-1.813933
48	6	0	0.981689	6.540960	0.784585	117	6	0	8.090344	-0.513546	-2.196894
49	6	0	-0.105766	7.469660	0.186183	118	6	0	5.413201	-3.583389	0.860377
50	1	0	-0.059858	5.537948	-3.195443	119	1	0	7.699432	-5.003478	0.765585
51	1	0	0.850575	6.532030	-2.074923	120	1	0	-8.294897	-0.469478	-0.497327
52	1	0	-1.607691	4.852926	-1.592801	121	1	0	-8.101701	-1.501275	0.910927
53	1	0	1.232035	4.567293	1.621523	122	1	0	-9.534462	-1.678850	-0.112702
54	1	0	-0.363022	5.063321	3.245138	123	1	0	-3.644496	-3.029769	-1.575873
55	1	0	-1.152368	6.289571	2.274892	124	1	0	-4.081037	-2.420357	-3.159929
56	1	0	4.063900	2.710675	-2.895267	125	1	0	-3.913859	-4.162247	-2.917488
57	1	0	2.738635	4.705604	-3.536835	126	1	0	-9.453037	-6.016705	-2.194192
58	1	0	-3.317286	4.458293	3.252560	127	1	0	-8.008236	-6.597238	-3.041092
59	1	0	-4.685895	2.656555	2.248230	128	1	0	-9.098869	-5.454584	-3.829562
60	1	0	-5.559889	-0.145440	-2.585761	129	1	0	10.136237	-5.358995	0.469321
61	1	0	-5.453467	-2.028553	1.238254	130	1	0	11.083825	-4.265484	-0.554275
62	1	0	4.905850	-1.856802	-2.646876	131	1	0	10.083585	-5.521124	-1.288144
63	1	0	6.038059	-0.134545	1.090325	132	1	0	5.165651	-2.816207	1.603185
64	1	0	-3.275310	0.528758	2.807733	133	1	0	5.520520	-4.538900	1.383685
65	1	0	-4.990388	0.107785	4.554620	134	1	0	4.551560	-3.659458	0.187182
66	1	0	-5.709448	1.081423	3.258782	135	1	0	9.107028	-0.419158	-2.591068
67	1	0	-6.058656	-0.645970	3.358715	136	1	0	7.869347	0.382697	-1.605886
68	1	0	-3.100288	-1.527965	4.064698	137	1	0	7.397809	-0.504160	-3.046675
69	1	0	-2.631774	-1.876652	2.394672	138	1	0	-0.527599	-1.381845	1.355764
70	1	0	-4.221832	-2.376881	2.998026	139	6	0	0.095969	-3.278993	0.174936
71	1	0	-3.578803	2.820633	-1.536406	140	8	0	-0.445542	-2.508466	1.556305
72	1	0	-4.037978	0.931005	-3.905312	141	6	0	0.590366	-2.841113	2.539965
73	1	0	-3.219394	2.496737	-3.940357	142	6	0	1.607786	-3.044687	0.319447
74	1	0	-2.501603	1.144245	-3.041800	143	1	0	2.108421	-3.982678	0.063534
75	1	0	-6.039039	3.159118	-1.517313	144	1	0	1.921729	-2.285178	-0.397501
76	1	0	-6.204763	2.128840	-2.947498	145	8	0	-0.580831	-2.759134	-0.841383
77	1	0	-5.318568	3.657694	-3.060983	146	8	0	-0.206436	-4.581317	0.401994
78	1	0	2.123322	0.549324	-3.255601	147	6	0	-1.581487	-4.960537	0.211507
79	1	0	3.158563	0.185181	-5.482130	148	1	0	-1.642182	-5.997532	0.543708
80	1	0	4.240462	1.168976	-4.482927	149	1	0	-1.858767	-4.882368	-0.842417
81	1	0	4.585535	-0.547354	-4.732567	150	1	0	-2.239171	-4.329753	0.815232
82	1	0	1.651030	-1.524095	-4.482265	151	1	0	-0.266793	-1.825223	-1.081209
83	1	0	1.592275	-1.806723	-2.740488	152	6	0	0.416292	-2.137715	3.865611
84	1	0	2.992132	-2.358090	-3.690140	153	6	0	0.503308	-0.744584	4.003512
85	1	0	3.482233	2.578636	0.950789	154	6	0	0.194992	-2.917288	5.008121

155	6	0	0.366478	-0.154538	5.259493
156	1	0	0.638702	-0.118602	3.129450
157	6	0	0.068224	-2.327485	6.265744
158	1	0	0.122759	-3.999059	4.912385
159	6	0	0.153437	-0.941107	6.394202
160	1	0	0.426510	0.926819	5.350760
161	1	0	-0.100866	-2.948596	7.141168
162	1	0	0.051165	-0.474503	7.370195
163	1	0	0.460795	-3.914083	2.700612
164	6	0	1.897513	-2.599622	1.771864
165	1	0	2.725727	-3.150350	2.227374
166	1	0	2.158854	-1.537947	1.797150

TS-2nd-(*S*)-reaction pathway: *S-re*/(*S*)-1gf (Cy-SPINOL)



B3LYP/6-31G(d); E(RB3LYP) = -3701.05603065 Hartree

Zero-point correction= 1.419147 Hartree

Thermal correction to Energy= 1.498874 Hartree

Thermal correction to Enthalpy= 1.499818 Hartree

Thermal correction to Gibbs Free Energy= 1.295903 Hartree

Sum of electronic and zero-point Energies= -3699.636884 Hartree

Sum of electronic and thermal Energies= -3699.557157 Hartree

Sum of electronic and thermal Enthalpies= -3699.556212 Hartree

Sum of electronic and thermal Free Energies= -3699.760128 Hartree

The number of Imaginary frequencies = 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.705508	-6.098982	1.957878
2	6	0	-0.449488	-5.914470	0.934396
3	6	0	1.210793	-4.203819	0.577046
4	6	0	1.648500	-4.962430	1.669615
5	6	0	0.662838	-5.772654	-1.407195
6	6	0	-0.514007	-5.903185	-2.417907
7	6	0	-1.507049	-4.857970	-1.980610
8	6	0	-1.042317	-4.164134	-0.855160
9	6	0	0.101862	-4.926035	-0.186403
10	6	0	1.837326	-2.980971	0.316647
11	6	0	3.009164	-2.594016	0.996477
12	6	0	3.494275	-3.465497	1.987729
13	6	0	2.801883	-4.612291	2.364810
14	6	0	-2.721934	-4.525152	-2.571472
15	6	0	-3.460074	-3.466130	-2.047071
16	6	0	-2.951246	-2.640478	-1.030474
17	6	0	-1.699460	-2.987292	-0.484073
18	8	0	-1.088536	-2.125714	0.431756
19	8	0	1.269851	-2.137354	-0.638607
20	15	0	0.069132	-1.122709	-0.155623
21	8	0	0.503075	-0.244925	0.991406
22	8	0	-0.396360	-0.457139	-1.444611
23	6	0	3.768423	-1.327400	0.720378
24	6	0	-3.762039	-1.472204	-0.547020
25	6	0	-4.266394	-1.465449	0.779310
26	6	0	-5.094406	-0.415048	1.190205
27	6	0	-5.448009	0.634963	0.340264
28	6	0	-4.937967	0.614093	-0.961368
29	6	0	-4.111206	-0.414758	-1.429835
30	6	0	3.937848	-0.360926	1.748791
31	6	0	4.763005	0.743917	1.508811
32	6	0	5.426826	0.935731	0.294621
33	6	0	5.225862	-0.010508	-0.712966
34	6	0	4.419340	-1.140873	-0.525377
35	6	0	-3.669696	-0.366084	-2.896022
36	6	0	-4.854419	-0.667157	-3.839113
37	6	0	-3.028261	0.975039	-3.296584
38	6	0	-4.001666	-2.588589	1.783181
39	6	0	-3.270537	-2.077406	3.039228
40	6	0	-5.304532	-3.323985	2.156858
41	6	0	3.299815	-0.482242	3.137015
42	6	0	4.367526	-0.758434	4.217001
43	6	0	2.471632	0.755915	3.530740
44	6	0	4.348818	-2.163087	-1.661104
45	6	0	3.734631	-1.566988	-2.941490
46	6	0	5.733071	-2.780514	-1.945132
47	6	0	-0.953179	-7.253290	0.381825
48	6	0	1.229741	-7.135899	-0.992875
49	6	0	0.159086	-8.051295	-0.345554
50	1	0	0.333156	-6.053713	2.989367
51	1	0	1.195123	-7.075064	1.855721
52	1	0	-1.277490	-5.399757	1.436060
53	1	0	1.457649	-5.178145	-1.872591
54	1	0	-0.175467	-5.714770	-3.444908
55	1	0	-0.946704	-6.910515	-2.422535
56	1	0	4.416228	-3.203227	2.496443
57	1	0	3.159649	-5.221759	3.191081
58	1	0	-3.098743	-5.086720	-3.422856
59	1	0	-4.438472	-3.238917	-2.457249
60	1	0	-5.498029	-0.424536	2.199164
61	1	0	-5.206998	1.423753	-1.634501
62	1	0	4.908898	1.477178	2.297594
63	1	0	5.745473	0.119702	-1.659175
64	1	0	-2.909129	-1.135748	-3.046890
65	1	0	-4.516623	-0.698763	-4.882240
66	1	0	-5.332617	-1.625024	-3.610290
67	1	0	-5.625088	0.109732	-3.761580
68	1	0	-2.701541	0.931182	-4.342850
69	1	0	-2.152291	1.197225	-2.684438
70	1	0	-3.732863	1.811306	-3.213054
71	1	0	-3.350694	-3.326896	1.309902
72	1	0	-3.882300	-1.358201	3.597538
73	1	0	-3.047310	-2.912364	3.714869
74	1	0	-2.327159	-1.592938	2.771650
75	1	0	-5.803562	-3.723789	1.266867
76	1	0	-6.012906	-2.660990	2.667318
77	1	0	-5.089511	-4.161917	2.831226
78	1	0	2.609633	-1.328833	3.122510
79	1	0	3.892986	-0.909443	5.194296
80	1	0	4.963287	-1.649137	3.990249
81	1	0	5.061767	0.085357	4.311619
82	1	0	2.038740	0.608411	4.527945
83	1	0	1.651637	0.915802	2.829240
84	1	0	3.082041	1.665658	3.569216
85	1	0	3.698654	-2.982042	-1.345401
86	1	0	3.672513	-2.331022	-3.726271
87	1	0	2.722981	-1.196733	-2.750037

88	1	0	4.340821	-0.741012	-3.333483
89	1	0	5.654757	-3.557410	-2.715600
90	1	0	6.154205	-3.238279	-1.042987
91	1	0	6.446875	-2.029105	-2.302639
92	1	0	-1.363049	-7.852091	1.205271
93	1	0	-1.793986	-7.065416	-0.295704
94	1	0	1.662400	-7.632011	-1.871002
95	1	0	2.064108	-6.976068	-0.299798
96	1	0	-0.302004	-8.692353	-1.106089
97	1	0	0.652113	-8.737628	0.352828
98	6	0	6.372786	2.085407	0.110898
99	6	0	-6.364152	1.728017	0.798743
100	6	0	-8.101720	3.796578	1.650454
101	6	0	-6.807599	3.685668	2.162265
102	6	0	-5.935785	2.666846	1.761752
103	6	0	-7.672193	1.822409	0.271665
104	6	0	-8.512704	2.851718	0.706479
105	6	0	-9.038799	4.884054	2.122772
106	1	0	-6.462317	4.412749	2.895376
107	6	0	-4.552851	2.602559	2.373588
108	6	0	-8.195030	0.821874	-0.737373
109	1	0	-9.519688	2.913665	0.297263
110	6	0	8.180140	4.240451	-0.192192
111	6	0	6.850693	4.351002	-0.604146
112	6	0	5.940919	3.295982	-0.467174
113	6	0	7.712811	1.954633	0.537277
114	6	0	8.589700	3.031887	0.378105
115	6	0	9.153302	5.381817	-0.378397
116	1	0	6.506501	5.285460	-1.044225
117	6	0	4.520070	3.470718	-0.952723
118	6	0	8.213354	0.671246	1.163639
119	1	0	9.620305	2.923616	0.712048
120	1	0	9.887635	5.420260	0.433950
121	1	0	8.636956	6.347156	-0.413371
122	1	0	9.715302	5.279515	-1.316779
123	1	0	4.346580	2.897452	-1.873027
124	1	0	4.309847	4.521704	-1.176211
125	1	0	3.783192	3.122434	-0.222949
126	1	0	7.682208	0.439804	2.094386
127	1	0	9.281472	0.740340	1.392710
128	1	0	8.062926	-0.187550	0.499157
129	1	0	-7.980177	-0.207783	-0.431998
130	1	0	-7.740628	0.956209	-1.726333
131	1	0	-9.278418	0.924471	-0.855913
132	1	0	-4.482924	1.822286	3.141797
133	1	0	-4.295442	3.554073	2.850514
134	1	0	-3.788041	2.370751	1.626311
135	1	0	-9.702038	5.220486	1.318164
136	1	0	-8.487755	5.754972	2.493520
137	1	0	-9.679063	4.531249	2.942667
138	1	0	-0.063914	0.860425	-1.661062
139	6	0	0.313879	2.667124	-0.283214
140	8	0	0.559006	3.952060	-0.618514
141	8	0	0.192715	1.900010	-1.837014
142	6	0	-0.706810	4.608151	-0.924293
143	6	0	-1.695276	3.935891	0.051717
144	6	0	-1.125422	2.514484	0.225123
145	1	0	-0.968144	4.351273	-1.958408
146	1	0	-1.690486	4.479139	1.001702
147	1	0	-2.715428	3.945405	-0.338267
148	1	0	-1.099339	2.183919	1.265785
149	1	0	-1.677041	1.763721	-0.342385
150	8	0	1.338889	2.110950	0.320752
151	6	0	1.416081	1.951513	-2.598928
152	1	0	2.239122	1.491519	-2.044927
153	1	0	1.239635	1.415142	-3.533107
154	1	0	1.638756	3.000464	-2.801887
155	1	0	1.085913	1.174023	0.639757
156	6	0	-0.551674	6.100008	-0.786252
157	6	0	-1.186026	6.951523	-1.697448
158	6	0	0.180460	6.655125	0.271768
159	6	0	-1.102661	8.336988	-1.550947
160	1	0	-1.745852	6.528245	-2.529409
161	6	0	0.272459	8.038963	0.411959
162	1	0	0.692525	5.999208	0.968840
163	6	0	-0.372686	8.883793	-0.495799
164	1	0	-1.600832	8.986171	-2.265785
165	1	0	0.850549	8.460026	1.230336
166	1	0	-0.300088	9.961906	-0.383068