Supporting Information

1,1'-Binaphthyl-substituted Diphosphene: Synthesis, Structures, and Chiral Optical Properties

Akihiro Tsurusaki,* Rikako Ura, Ken Kamikawa*

Department of Chemistry, Graduate School of Science, Osaka Prefecture University, Sakai, Osaka 599-8531, Japan

E-mail: tsurusaki@c.s.osakafu-u.ac.jp; kamikawa@c.s.osakafu-u.ac.jp

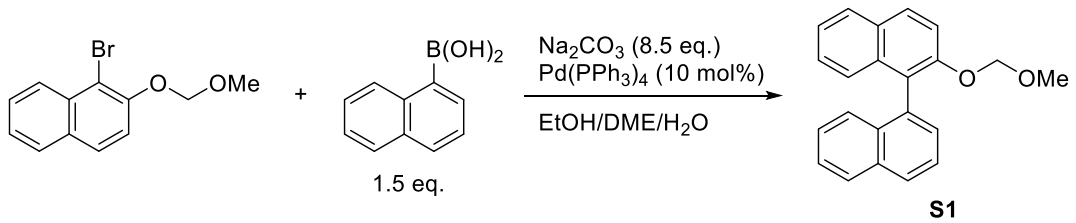
Table of Contents

1. Experimental Details

General. All anaerobic and/or moisture-sensitive manipulations were carried out with standard Schlenk techniques under nitrogen atmosphere or with glovebox techniques under argon atmosphere. The ^{1}H (400 MHz), ^{13}C (100 MHz), ^{19}F NMR (378 MHz), and ^{31}P NMR (162 MHz) spectra were measured in $CDCl_3$ with a JEOL JNM-ECS400 spectrometer. Signals due to tetramethylsilane (0.0 ppm) in ^{1}H NMR and $CDCl_3$ (77.16 ppm) in ^{13}C NMR were used as internal references, and chemical shifts are reported in ppm downfield. ^{31}P NMR chemical shifts are externally referenced to 85% H_3PO_4 (0 ppm), and ^{19}F NMR chemical shifts are externally referenced to $CFCl_3$ (0 ppm). Low- and high-resolution mass spectra were recorded on a JEOL JMS-700 spectrometer at FAB mode using *m*-nitrobenzyl alcohol (NBA) or *o*-nitrophenyl octyl ether (NPOE) as the matrix. Elemental analysis was carried out at the Microanalytical Laboratory of the Institute for Chemical Research, Kyoto University. All melting points were determined on a Yanaco micro melting point apparatus (MP-J3) and were uncorrected. The melting points of diphosphenes *rac*-**1**, (*S*)-(+)-**1**, and (*R*)-(−)-**1** were measured under an argon atmosphere in a sealed tube.

Reagents. Et_2O, THF, dichloromethane, DMSO were purchased (Wako, Super dehydrated grade) and used as received. Toluene, hexane, and $CDCl_3$ used in a glovebox were dried over a potassium mirror (for toluene and hexane) or calcium hydride (for $CDCl_3$), degassed by freeze-pump-thaw cycles, distilled in a vacuum line, and stored in a glovebox. Ethanol (Wako), DME (Kishida), 1,4-dioxane (Wako), sodium carbonate (Kishida), *n*-BuLi (Mitsuwa or Kanto), iodomethane (TCI), conc. H_2SO_4 (Wako), trifluoromethanesulfonic anhydride (TCI), pyridine (Wako), palladium acetate (Wako), 1,4-bis(diphenylphosphino)butane (dppb, Aldrich), diethylphosphite (TCI), lithium aluminum hydride (Wako) were purchased and used as received. *N*,*N*-diisopropylethylamine, chlorotrimethylsilane, and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) were distilled from potassium hydroxide, calcium hydride, and potassium hydroxide prior to use, respectively. 1-bromo-2-(methoxymethoxy)naphthalene,[S1] 1-naphthylbononic acid,[S2] tetrakis(triphenylphosphine)palladium,[S3] and Mes*PCl_2[S4] were synthesized according to the reported procedures.

Synthesis of 2-(Methoxymethoxy)-1,1'-binaphthyl (S1)



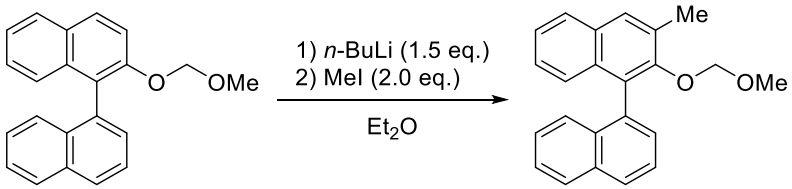
S1

A yellow suspension of 1-bromo-2-(methoxymethoxy)naphthalene (3.30 g, 12.4 mmol), 1-naphthylbononic acid (3.20 g, 18.6 mmol), $Pd(PPh_3)_4$ (1.43 g, 1.24 mmol), and Na_2CO_3 (11.18 g, 105 mmol) in EtOH (60 mL), DME (140 mL), and H_2O (30 mL) was stirred at 95 ˚C for 20 h. The organic layer was separated and then the aqueous layer was extracted with ethyl acetate. The combined organic layer was washed with brine, dried over $MgSO_4$, filtered through a pad of Celite, and then evaporated under reduced pressure. The

residue was chromatographed on silica gel with hexane/AcOEt = 10/1 (R_f = 0.33), followed by recrystallization from MeOH to give **S1** as colorless solid (3.57 g, 11.4 mmol, 92%).

Mp. 136.4-136.9 ˚C. (lit. 157 ˚C for (*R*)-isomer[S5]). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 3.14 (s, 3H), 5.03 (s, 2H), 7.17 (d, *J* = 8.2 Hz, 1H), 7.23 (ddd, *J* = 7.8, 6.8, 1.3 Hz, 1H), 7.27 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.33-7.37 (m, 2H), 7.43-7.48 (m, 2H), 7.56 (d, *J* = 9.2 Hz, 1H), 7.61 (dd, *J* = 8.2, 6.9 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.93-7.96 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 56.1, 95.2, 117.1, 124.2, 125.1, 125.6, 125.9 (×2), 126.0, 126.4, 126.5, 127.89, 127.91, 128.3, 128.5, 129.5, 129.8, 133.1, 133.8, 134.4, 134.6, 152.3. The ^{1}H NMR chemical shifts of **S1** in C_6D_6 are identical to the reported values.[S5]

Synthesis of 2-(Methoxymethoxy)-3-methyl-1,1'-binaphthalene (S2)

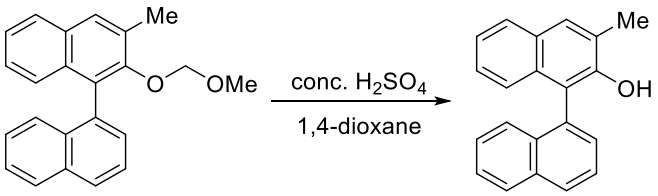


S1 **S2**

This compound was prepared according to the similar method to the reported procedure.[S5] To a solution of **S1** (3.40 g, 10.8 mmol) in THF (100 mL) was added *n*-BuLi in hexane (1.56 M; 10.2 mL, 15.9 mmol) at 0 ˚C. After the reaction mixture was stirred at this temperature for 15 min, iodomethane (1.34 mL, 21.6 mmol) was added. The reaction mixture was stirred at 0 ˚C for 1 h. The reaction was quenched with water, and then the organic layer was separated. The aqueous layer was extracted with ethyl acetate. The combined organic layer was dried over $MgSO_4$, filtered through a pad of Celite, and then evaporated under reduced pressure. The residue was chromatographed on silica gel with hexane/AcOEt = 10/1 (R_f = 0.38) to give **S2** as colorless solid (2.90 g, 8.84 mmol, 82%).

Mp. 74.5-74.9 ˚C. (lit. 89 ˚C for (*R*)-isomer[S5]). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.58 (s, 3H), 2.83 (s, 3H), 4.53 (d, *J* = 5.5 Hz, 1H), 4.55 (d, *J* = 5.5 Hz, 1H), 7.15 (m, 2H), 7.31 (dd, *J* = 7.4, 7.4 Hz, 1H), 7.35-7.39 (m, 2H), 7.47 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.50 (d, *J* = 6.9 Hz, 1H), 7.61 (dd, *J* = 7.3, 7.3 Hz, 1H), 7.80 (s, 1H), 7.81 (d, *J* = 9.6 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 18.0, 56.7, 98.9, 125.1, 125.5 (×2), 126.0, 126.1, 126.3, 126.5, 127.2, 128.1, 128.3, 129.1, 129.2, 129.7, 131.1, 131.7, 133.0, 133.2, 133.7, 134.6, 152.5. The ^{1}H NMR chemical shifts of **S2** in C_6D_6 are identical to the reported values.[S5]

Synthesis of 3-Methyl-(1,1′-binaphthalen)-2-ol (S3).

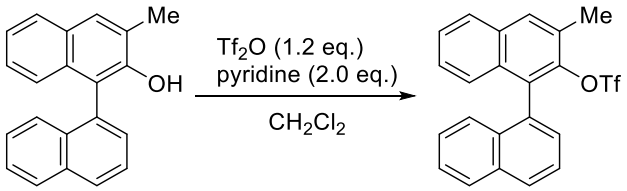


S2 **S3**

To a solution of **S2** (2.70 g, 8.22 mmol) in 1,4-dioxane (16 mL) was added conc. H_2SO_4 (460 μL, 8.63 mmol). After the reaction mixture was stirred at 60 ˚C for 3 h, toluene and water was added. The organic layer was separated, and then the aqueous layer was extracted with toluene. The combined organic layer was dried over $MgSO_4$, filtered through a pad of Celite, and then evaporated under reduced pressure. The residue was chromatographed on silica gel with hexane/AcOEt = 10/1 (R_f = 0.38) to give **S3** as colorless solid (2.30 g, 8.09 mmol, 98%).

Mp. 146.5-147.0 ˚C. (lit. 145 ˚C for (*R*)-isomer[S5]). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.50 (s, 3H), 4.96 (s, 1H), 7.02 (d, *J* = 8.7 Hz, 1H), 7.17 (ddd, *J* = 8.3, 6.5, 1.0 Hz, 1H), 7.29 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.34 (ddd, *J* = 8.2, 6.5, 1.4 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 1H), 7.50-7.56 (m, 2H), 7.66 (dd, *J* = 8.3, 6.9 Hz, 1H), 7.74 (s, 1H), 7.79 (d, *J* = 8.3 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 8.03 (d, *J* = 8.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 17.2, 118.3, 123.4, 124.9, 125.6, 126.0, 126.2, 126.67, 126.75, 127.0, 127.3, 128.6, 129.0, 129.3, 129.4, 129.8, 131.9, 132.8, 133.0, 134.3, 150.3. The ^{1}H NMR chemical shifts of **S3** in C_6D_6 are identical to the reported values.[S5]

Synthesis of 3-Methyl-[1,1′-binaphthalen]-2-yl Trifluoromethanesulfonate (S4)

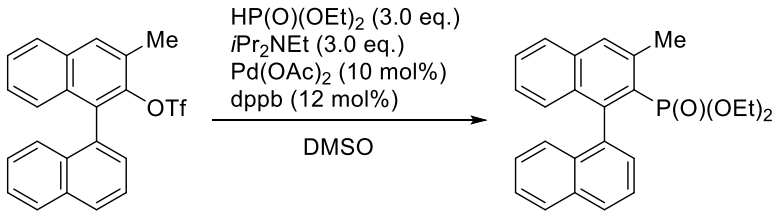


S3 **S4**

To a solution of **S3** (2.30 g, 8.09 mmol) in CH_2Cl_2 (16 mL) was added pyridine (1.30 mL, 16.2 mmol) at 0 °C. After stirring at 0 °C for 10 min, Tf_2O (2.74 g, 9.71 mmol) was added at 0 °C. After the reaction mixture was stirred at rt for 30 min, water and $CHCl_3$ was added. The organic layer was separated, and then the aqueous layer was extracted with $CHCl_3$. The combined organic layer was dried over $MgSO_4$, filtered through a pad of Celite, and then evaporated under reduced pressure. The residue was chromatographed on silica gel with hexane/AcOEt = 20/1 (R_f = 0.35) to give **S4** as colorless solid (2.75 g, 6.60 mmol, 82%).

Mp. 153.0-153.7 ˚C. (lit. 75 ˚C for (*R*)-isomer[S5]). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.67 (s, 3H), 7.24-7.28 (m, 3H), 7.32 (ddd, *J* = 8.3, 6.9, 1.4 Hz, 1H), 7.47-7.53 (m, 3H), 7.62 (dd, *J* = 8.3, 7.4 Hz, 1H), 7.88 (d, *J* = 8.3 Hz, 1H), 7.90 (s, 1H), 7.95 (d, *J* = 8.3 Hz, 1H), 8.02 (d, *J* = 8.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 18.4, 118.0 (q, *J* = 321 Hz), 125.3, 125.9, 126.1, 126.5, 126.7, 127.1, 127.2, 127.4, 128.4, 129.3, 129.4, 129.7, 131.0, 131.1, 131.4, 132.7 (×3), 133.8, 145.1; ^{19}F NMR (378 MHz, $CDCl_3$) δ = −73.8. The ^{1}H NMR chemical shifts of **S4** in C_6D_6 are identical to the reported values.[S5]

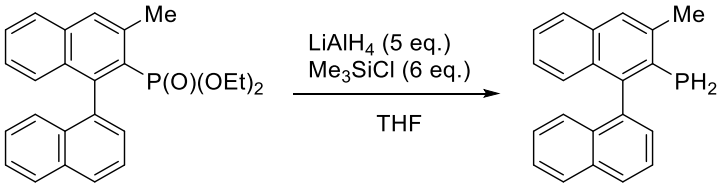
Synthesis of Diethyl 3-Methyl-(1,1'-binaphthylen)-2-ylphosphonate (3)



S4 **3**

A solution of **S4** (480 mg, 1.15 mmol), $Pd(OAc)_2$ (25.9 mg, 0.115 mmol), and dppb (59.0 mg, 0.138 mmol) in DMSO (11 mL) was stirred at rt for 30 min. Diethyl phosphite (446 μL, 3.46 mmol) and *N*,*N*-diisopropylethylamine (588 μL, 3.46 mmol) was added. The mixture was stirred at rt for 10 min and 100 °C for 48 h. Water and ethyl acetate were added. The organic layer was separated, and then the aqueous layer was extracted with ethyl acetate. The combined organic layer was washed with brine, dried over $MgSO_4$, filtered, and then evaporated under reduced pressure. The residue was chromatographed on silica gel with hexane/AcOEt = 1/1 (R_f = 0.35) to give **3** as colorless solid (301 mg, 0.744 mmol, 65%).
Mp. 82.1-82.5 ˚C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 0.82 (t, *J* = 6.9 Hz, 3H), 0.95 (t, *J* = 6.9 Hz, 3H), 2.93 (s, 3H), 3.33 (ddq, *J* = 10.1, 8.3, 6.9 Hz, 1H), 3.49 (ddq, *J* = 10.1, 8.3, 6.9 Hz, 1H), 3.67 (ddq, *J* = 10.1, 6.9, 6.9 Hz, 1H), 3.78 (ddq, *J* = 10.1, 6.9, 6.9 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 1H), 7.14 (ddd, *J* = 8.3, 6.9, 1.0 Hz, 1H), 7.20-7.26 (m, 2H), 7.36 (dd, *J* = 6.9, 1.0 Hz, 1H), 7.44 (ddd, *J* = 8.2, 6.4, 1.4 Hz, 1H), 7.46 (ddd, *J* = 7.8, 6.9, 0.9 Hz, 1H), 7.56 (dd, *J* = 8.3, 6.9 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 1H), 7.83 (d, *J* = 5.0 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 15.8 (d, *J* = 5.8 Hz), 16.0 (d, *J* = 5.8 Hz), 23.7, 61.2 (d, *J* = 5.8 Hz), 61.5 (d, *J* = 5.8 Hz), 125.2, 125.7, 125.89, 125.94, 126.5 (d, *J* = 184 Hz), 126.7, 127.0, 127.7 (×2), 128.0, 128.1 (×2), 130.2 (d, *J* = 14.5 Hz), 131.8 (d, *J* = 15.4 Hz), 133.2, 133.6, 134.6 (d, *J* = 2.4 Hz), 137.5 (d, *J* = 11.5 Hz), 138.3 (d, *J* = 4.8 Hz), 144.4 (d, *J* = 10.6 Hz); ^{31}P {^{1}H} NMR (162 MHz, $CDCl_3$) δ = 18.2. HRMS (FAB, NBA) *m/z* found: 405.1625 ($[M+H]^+$), calcd for $C_{25}H_{26}O_3P$ 405.1620.

Synthesis of 3-Methyl-(1,1'-binaphthylen)-2-ylphosphine (2)



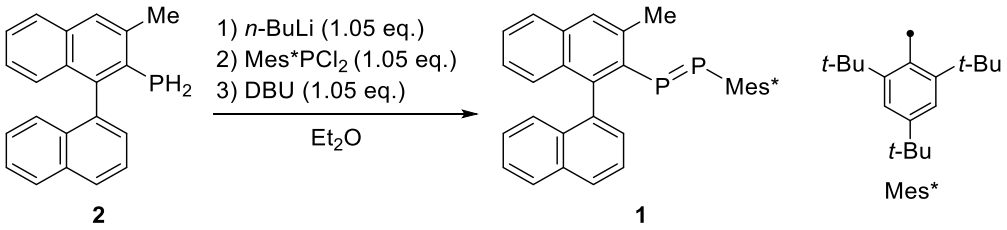
3 **2**

To a suspension of lithium aluminum hydride (276 mg, 7.27 mmol) in THF (4 mL) was added chlorotrimethylsilane (982 μL, 7.77 mmol) at −40 °C. After the mixture was stirred at −40 °C for 30 min, phosphonate **3** (553 mg, 1.36 mmol) in THF (6 mL) was added. The mixture was stirred at −40 °C for 1 h, and then quenched with degassed water at 0 °C. After degassed Et_2O was added and stirred for 30 min, the organic layer was separated. The aqueous layer was extracted with Et_2O. The combined organic layer was dried over $MgSO_4$, filtered through a pad of Celite under nitrogen, and then evaporated under reduced

pressure. The residue was chromatographed on silica gel under nitrogen with hexane/AcOEt = 3/1 (R_f = 0.88) to give **2** as colorless solid (306 mg, 1.02 mmol, 75%).

Mp. 143 ˚C (decomp.). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.63 (s, 3H), 3.32 (dd, *J* = 212, 11.5 Hz, 1H), 3.55 (dd, *J* = 212, 11.5 Hz, 1H), 7.04 (d, *J* = 8.7 Hz, 1H), 7.15-7.19 (m, 1H), 7.20 (d, *J* = 8.7 Hz, 1H), 7.28 (ddd, *J* = 8.3, 6.9, 0.9 Hz, 1H), 7.37 (dd, *J* = 6.9, 0.9 Hz, 1H), 7.40 (dd, *J* = 7.8, 6.9 Hz, 1H), 7.46-7.51 (m, 1H), 7.62 (dd, *J* = 7.8, 6.9 Hz, 1H), 7.77 (d, *J* = 2.3 Hz, 1H), 7.81 (d, *J* = 8.3 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 1H); ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ = 23.4 (d, *J* = 9.6 Hz), 125.6, 125.9, 126.02, 126.05, 126.3, 126.6 (×2), 127.3, 127.7 (d, *J* = 1.9 Hz), 128.0, 128.3, 128.5, 130.2 (d, *J* = 11.5 Hz), 131.9, 132.3, 133.1, 134.0, 137.3 (d, *J* = 10.6 Hz), 138.8 (d, *J* = 2.9 Hz), 141.9 (d, *J* = 10.6 Hz). ^{31}P NMR (162 MHz, $CDCl_3$) δ = −142.8 ($^1J_{PH}$ = 212 Hz). HRMS (FAB, NPOE) *m/z* found: 300.1073 (M^+), calcd for $C_{21}H_{17}P$ 300.1068.

Synthesis of 1-[3-Methyl-(1,1'-binaphthylen)-2-yl]-2-[2,4,6-tri-*tert*-butylphenyl]diphosphene (1)



2 **1**

To a solution of phosphine **2** (120 mg, 0.400 mmol) in Et_2O (10 mL) was added *n*-BuLi (1.55 M in hexane; 270 μL, 0.419 mmol) dropwise at room temperature in a glovebox filled with an argon. After the mixture was stirred for 30 min, Mes*PCl_2 (146 mg, 0.420 mmol) was added in one portion. The mixture was stirred for 1 h. DBU (64.5 mg, 0.424 mmol) in Et_2O (2 mL) was added, and then the reaction mixture was stirred for 1.5 h. The volatiles were removed under reduced pressure. The mixture was filtered through a pad of Celite with hexane. Insoluble yellow solid on a pad of Celite was extracted with toluene, and then the extract was filtered again through a pad of Celite. The solvent of the filtrate was removed under reduced pressure to give **1** as yellow crystals (125 mg, 0.217 mmol, 54%).

Mp. 167 ˚C (decomp.). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.04 (br s, 18H), 1.27 (s, 9H), 2.68 (s, 3H), 6.89 (d, *J* = 8.5 Hz, 1H), 7.13 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.26-7.31 (m, 1H), 7.28 (s, 2H), 7.39-7.46 (m, 4H), 7.50 (dd, *J* = 7.5, 7.5 Hz, 1H), 7.83 (d, *J* = 9.4 Hz, 1H), 7.85 (s, 1H), 7.89 (d, *J* = 5.8 Hz, 1H), 7.91 (d, *J* = 5.8 Hz, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ = 25.3 (br, CH_3), 31.4 (CH_3), 33.8 (br, CH_3), 34.8, 38.3, 122.3 (CH), 125.6 (CH), 125.9 (CH), 126.3 (CH), 126.5 (CH×2), 126.6 (CH), 126.8 (CH), 127.2 (CH), 128.27 (CH), 128.38 (CH), 128.40 (CH), 128.5 (CH), 132.3, 133.1, 133.7, 134.2, 137.2, 137.5 (br dd, *J* = 67, 7.7 Hz),*1) 138.2, 141.5 (br), 142,2 (br dd, *J* = 53.9, 6.8 Hz) 149.6, 153.5 (d, *J* = 6.8 Hz). *1) The partial double signal is superimposed to the singlet signal at δ = 137.2. ^{31}P {^{1}H} NMR (162 MHz, $CDCl_3$) δ = 451.5 (d, $^1J_{PP}$ = 570 Hz), 525.7 (d, $^1J_{PP}$ = 570 Hz). HRMS (FAB, NPOE) *m/z* found: 575.3002 ([M+H]$^+$), calcd for $C_{39}H_{45}P_2$ 575.2996. Anal. Found: C, 82.17; H, 7.89. Calcd for $C_{39}H_{44}P_2$: C, 81.50; H, 7.72. The deviation may be due to the inclusion of the solvated toluene molecule (calcd. for $C_{39}H_{44}P_2 \cdot 0.5(C_7H_8)$: C, 82.23; H, 7.79).

Stability of Diphosphene 1.

Diphosphene **1** was stable in solution at room temperature under argon atmosphere. However, ca. 30% and ca. 15% of **1** decomposed after heating at 80 °C for 21 h in a C_6D_6 solution under argon atmosphere and after standing a C_6D_6 solution with 50 eq. of water for 25 h under air, respectively.

2. Spectral Data

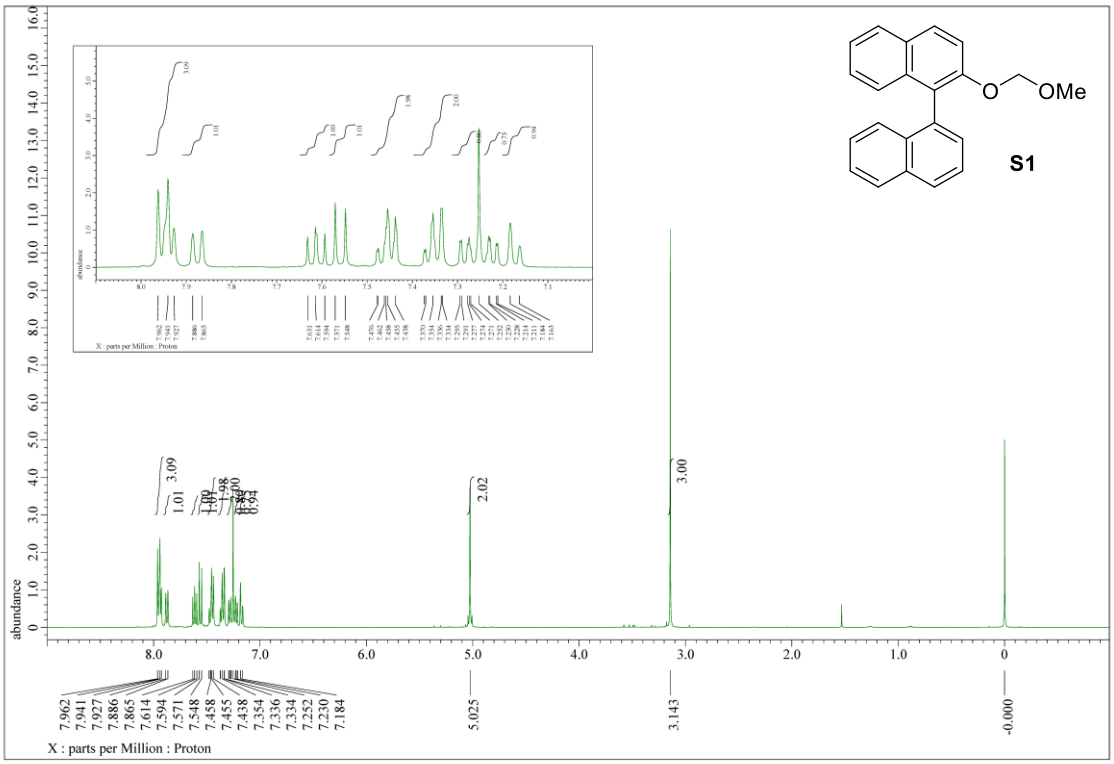


Figure S1. ^{1}H NMR Spectrum of S1.

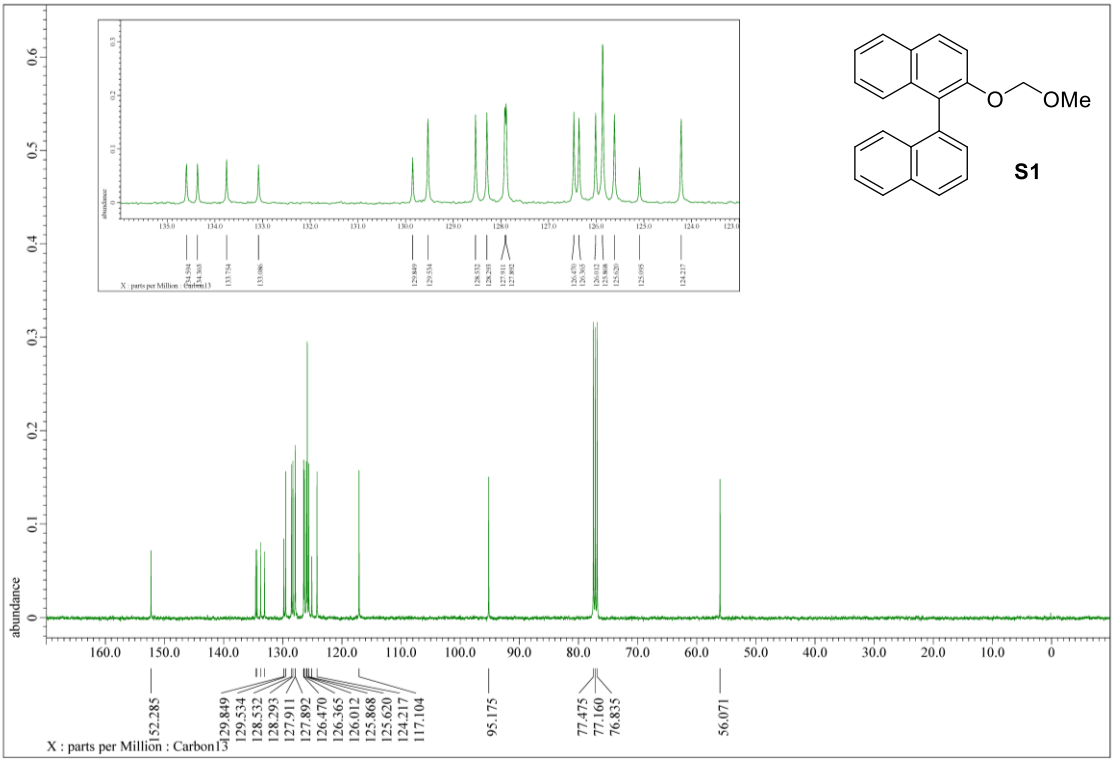


Figure S2. ^{13}C NMR Spectrum of S1.

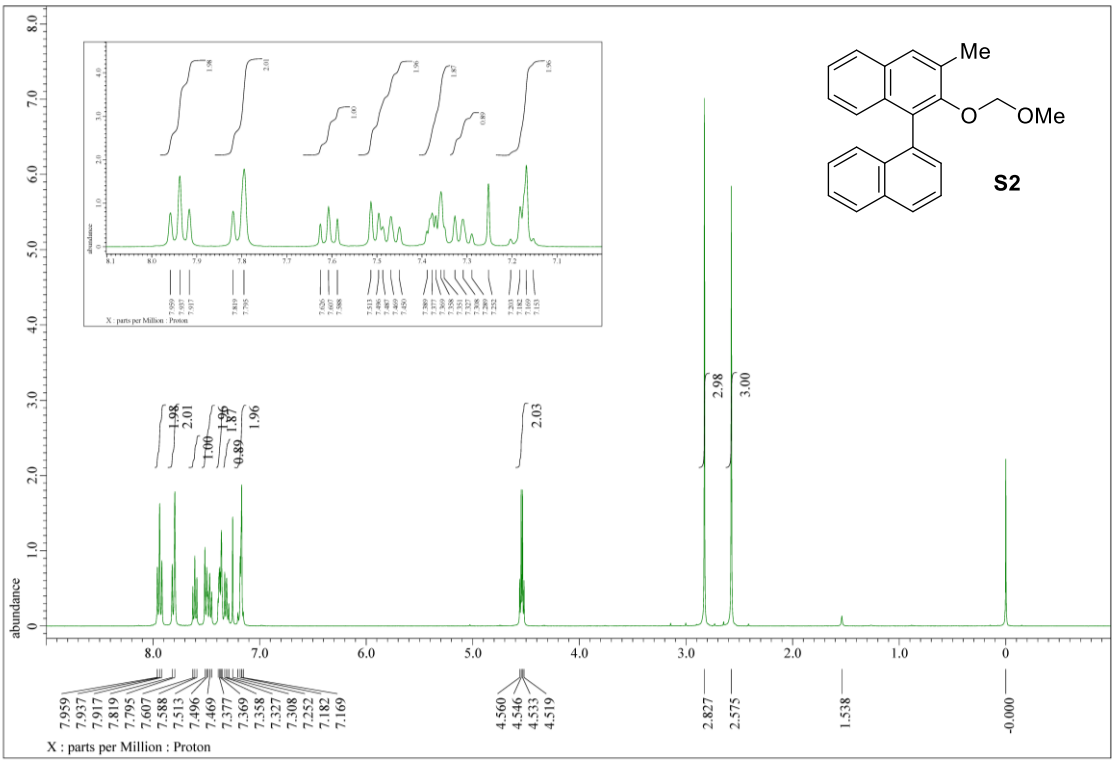


Figure S3. ^{1}H NMR Spectrum of S2.

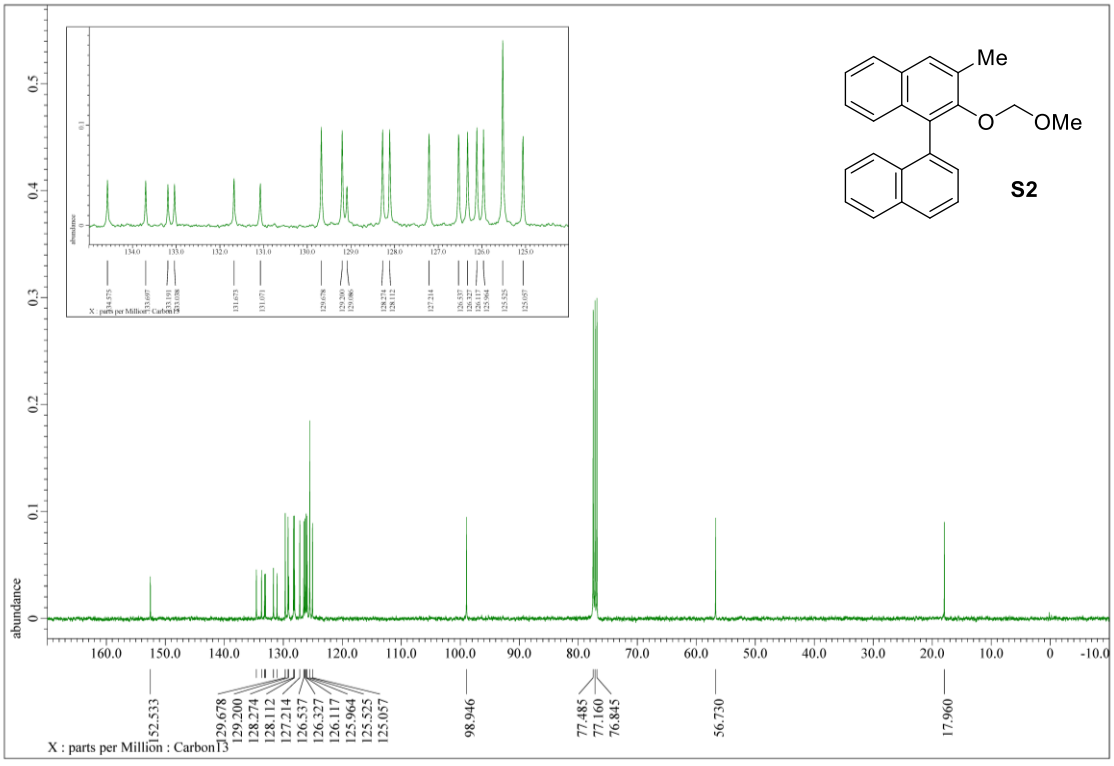


Figure S4. ^{13}C NMR Spectrum of S2.

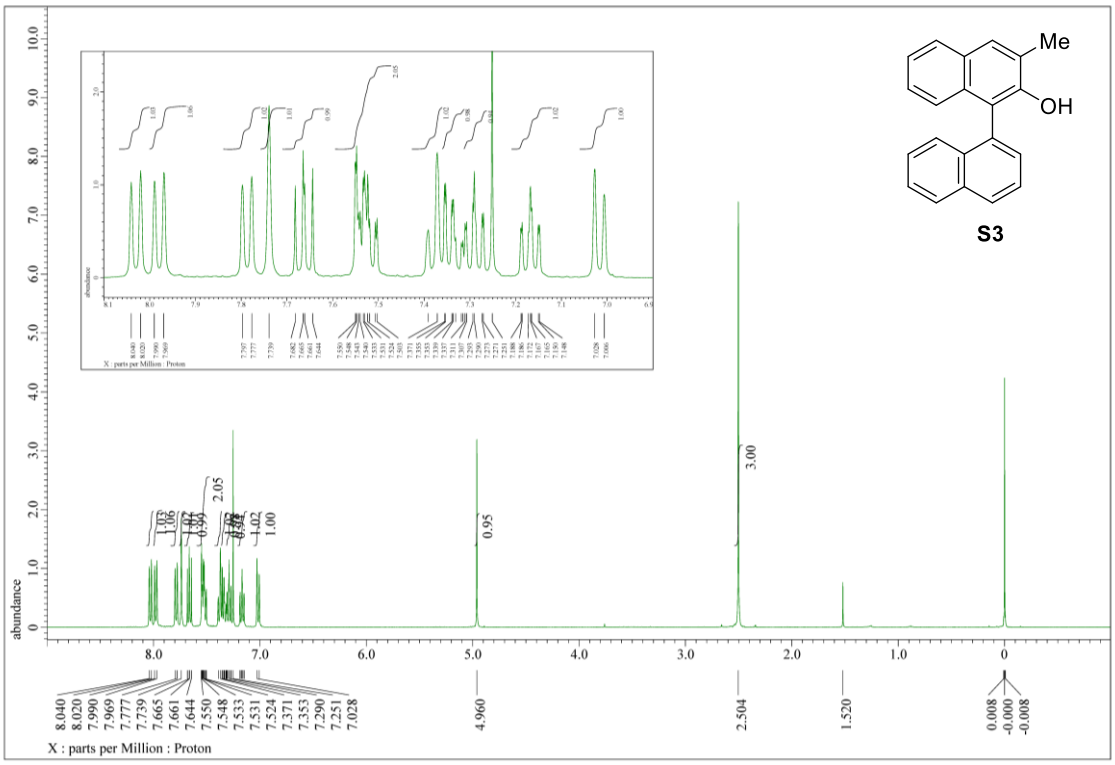


Figure S5. ^{1}H NMR Spectrum of S3.

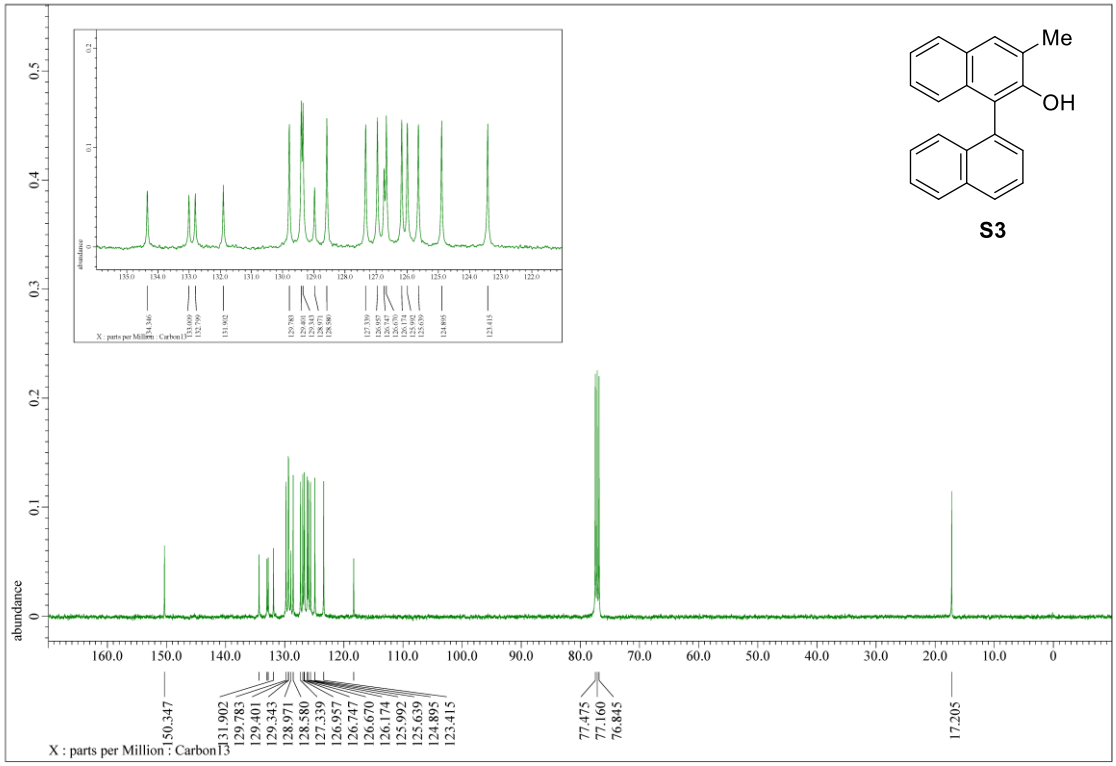


Figure S6. ^{13}C NMR Spectrum of S3.

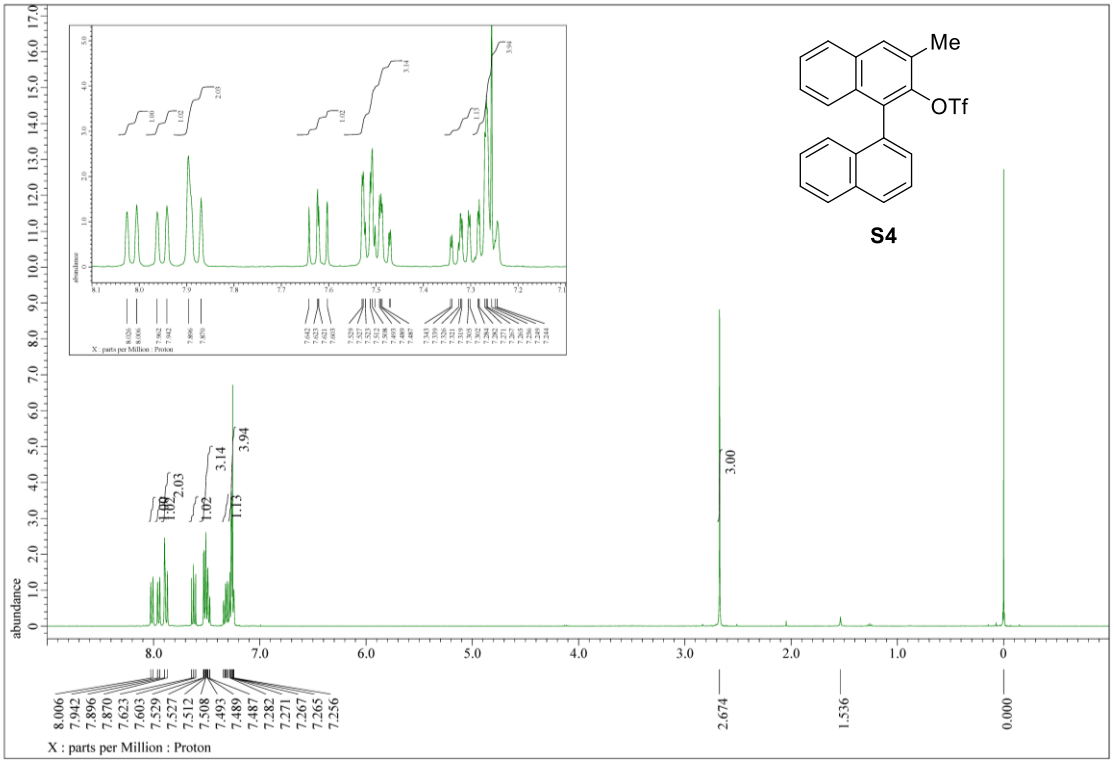


Figure S7. ^{1}H NMR Spectrum of S4.

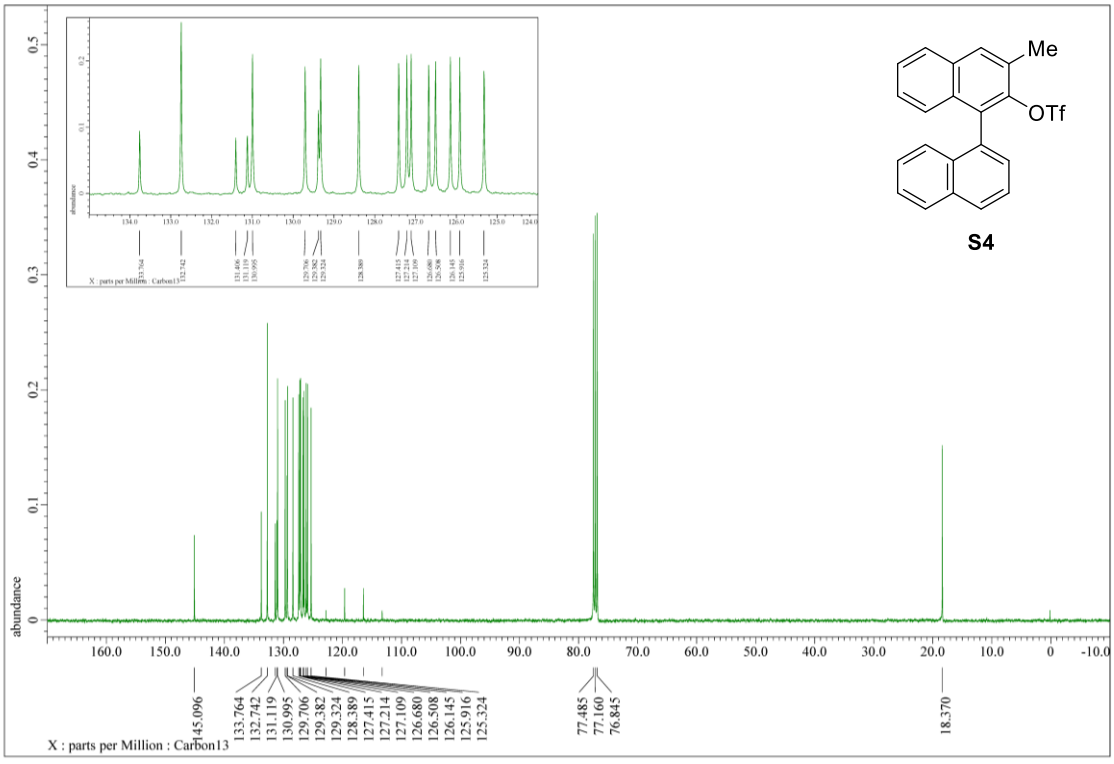


Figure S8. ^{13}C NMR Spectrum of S4.

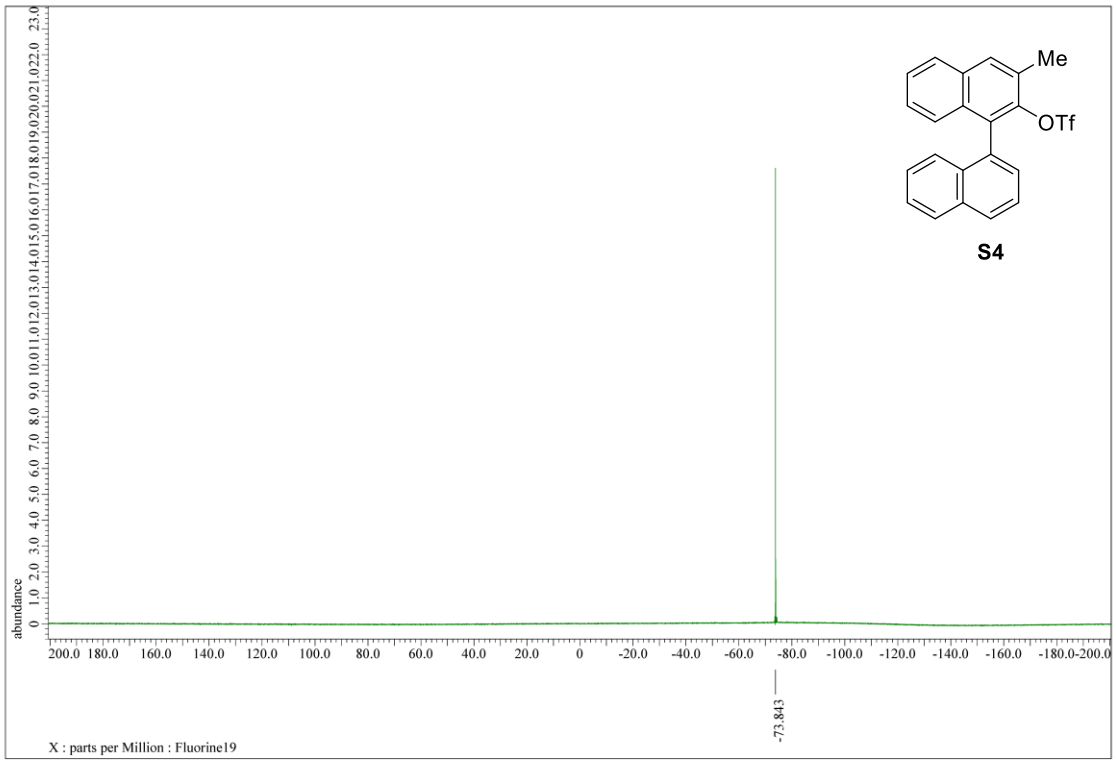


Figure S9. ^{19}F NMR Spectrum of S4.

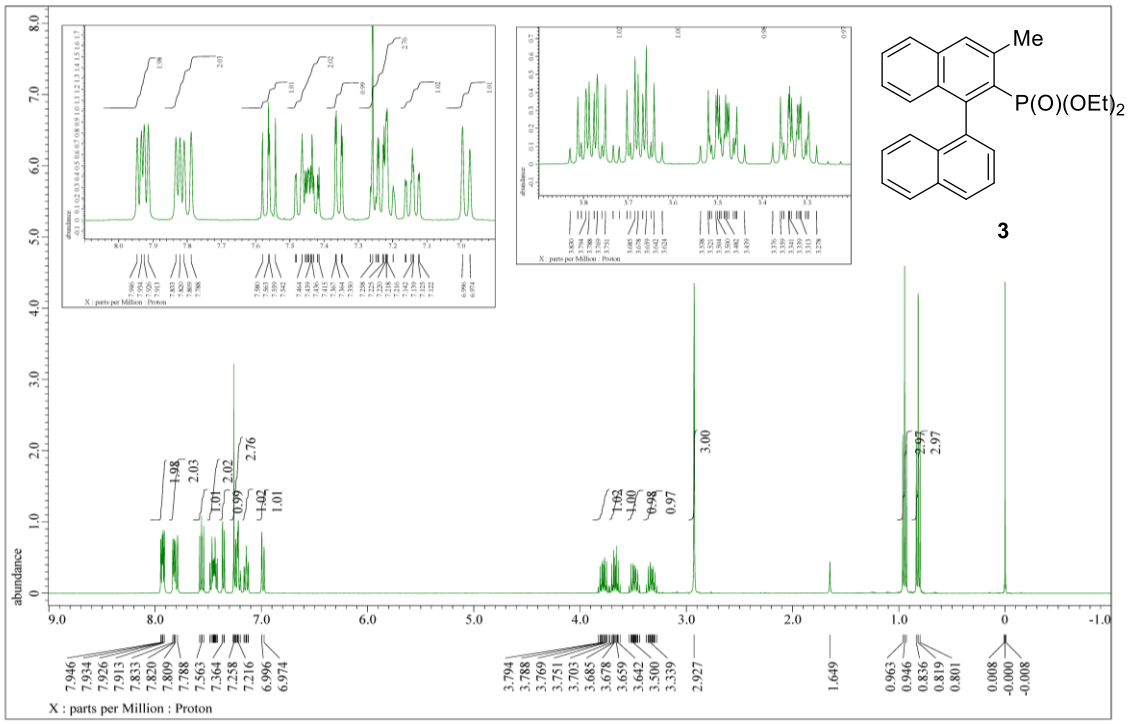


Figure S10. ^{1}H NMR Spectrum of 3.

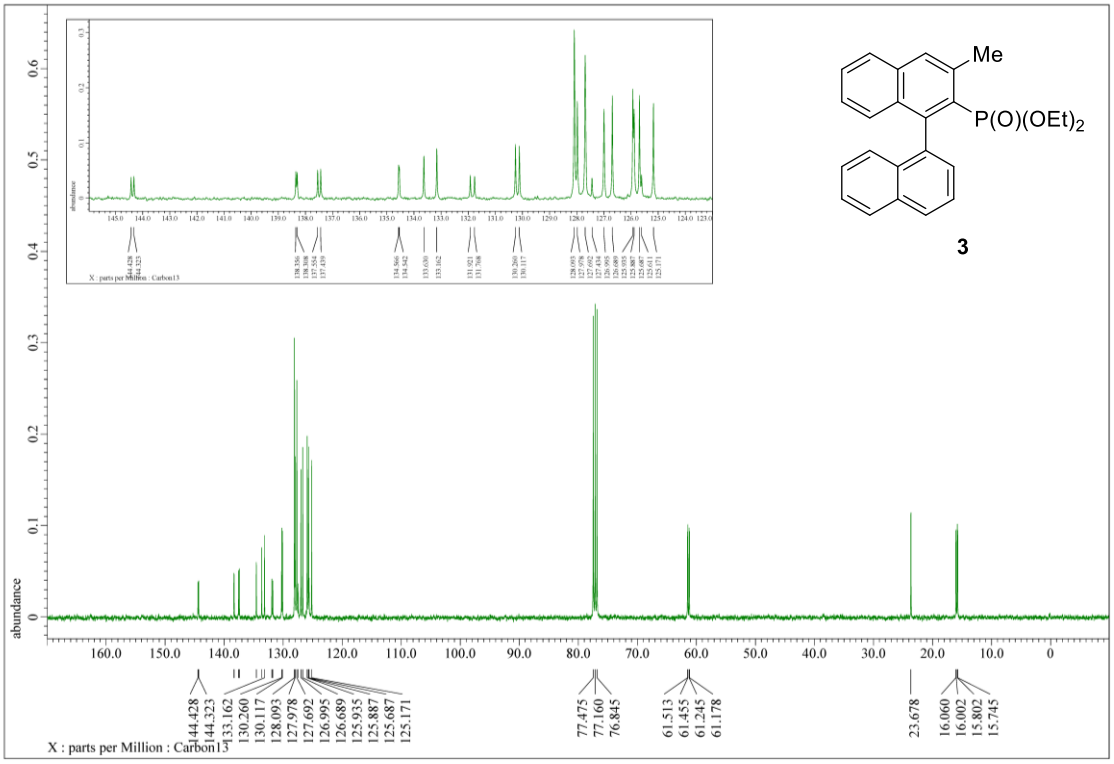


Figure S11. ^{13}C NMR Spectrum of 3.

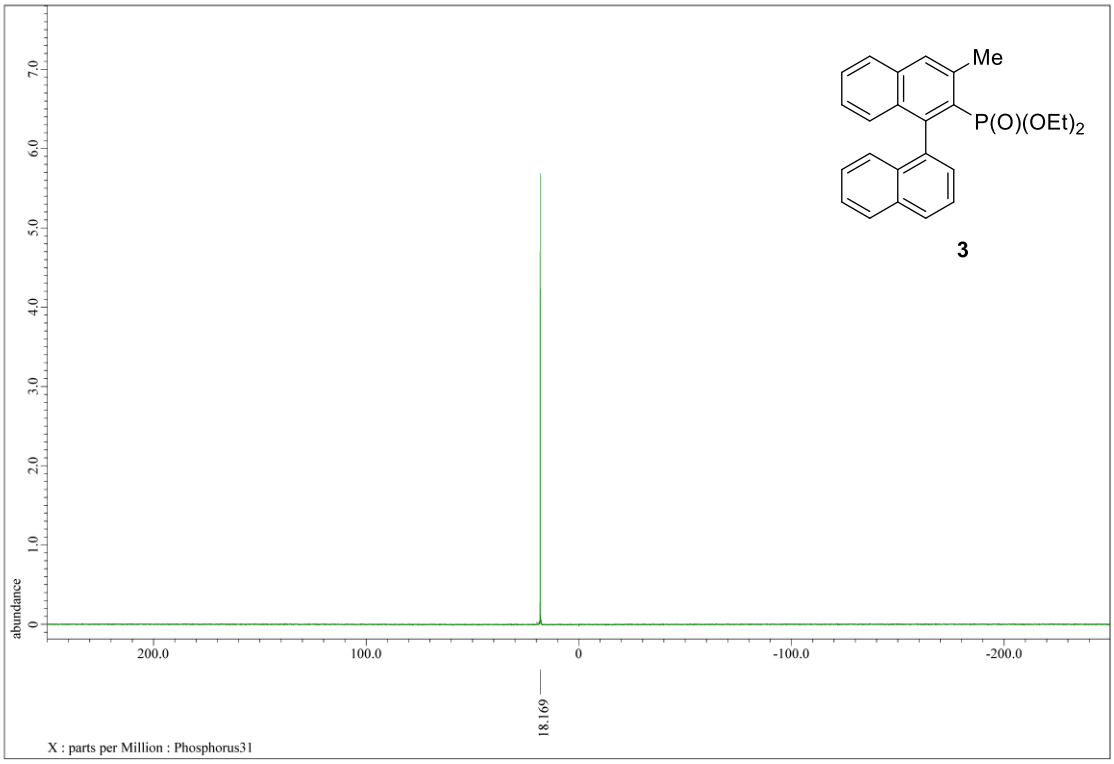


Figure S12. ^{31}P NMR Spectrum of 3.

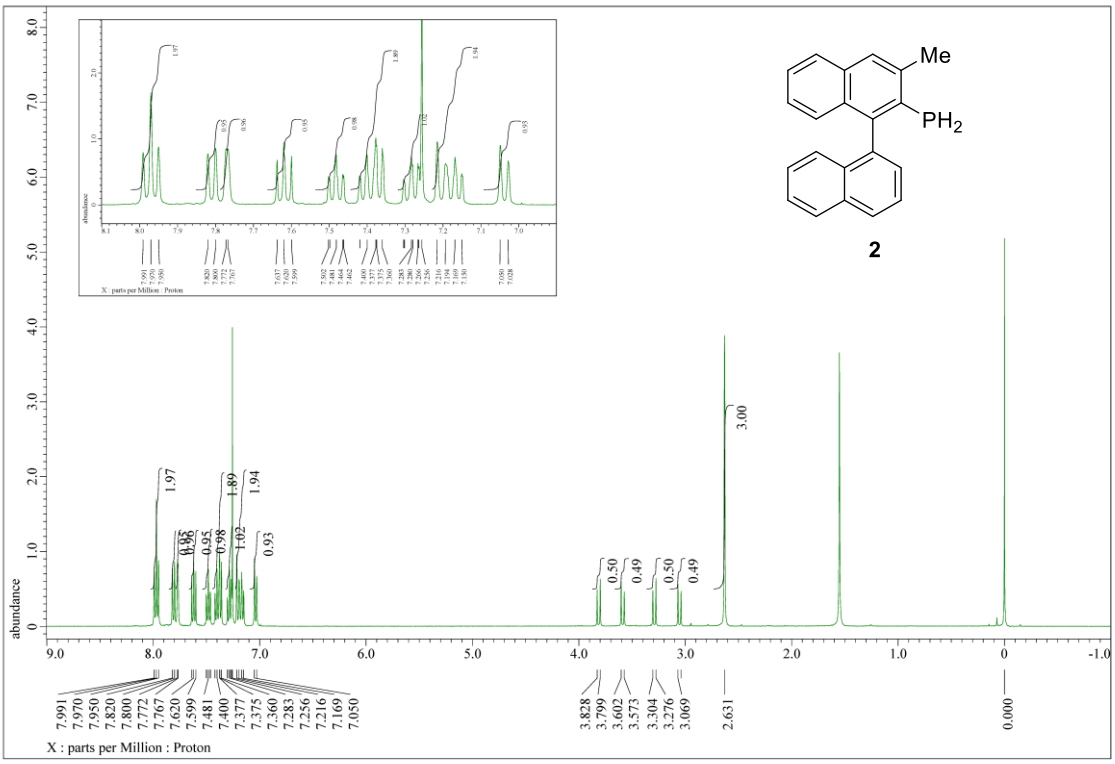


Figure S13. ^{1}H NMR Spectrum of 2.

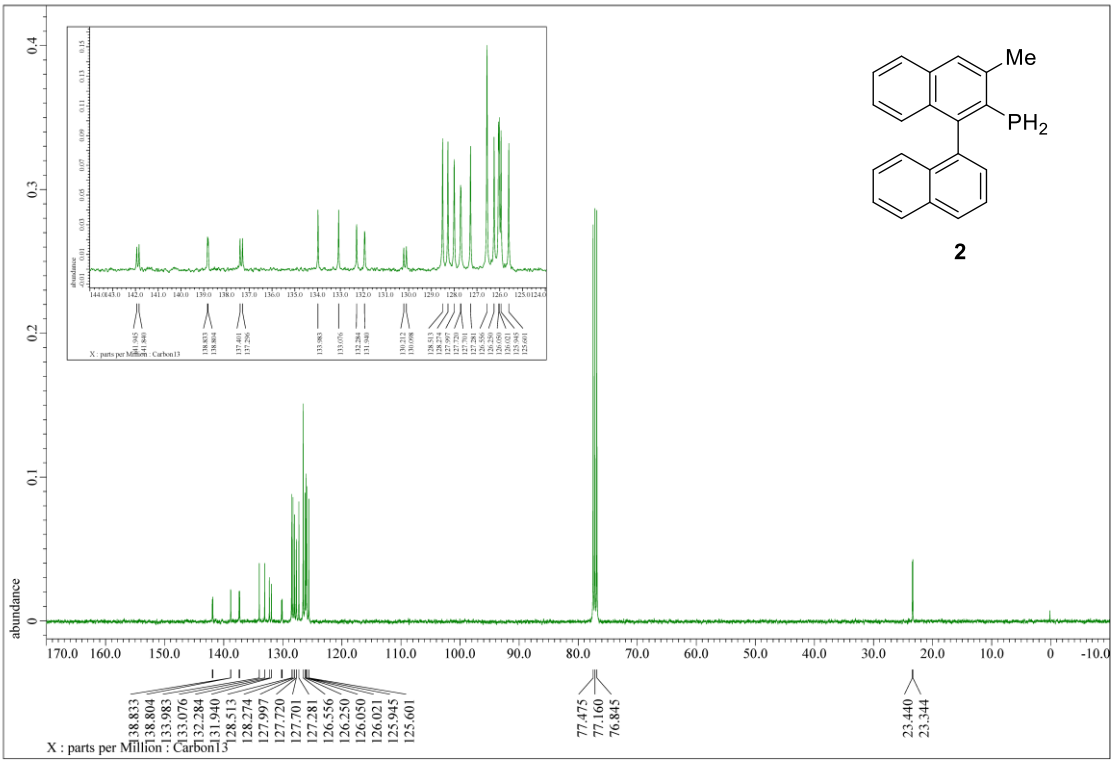


Figure S14. ^{13}C NMR Spectrum of 2.

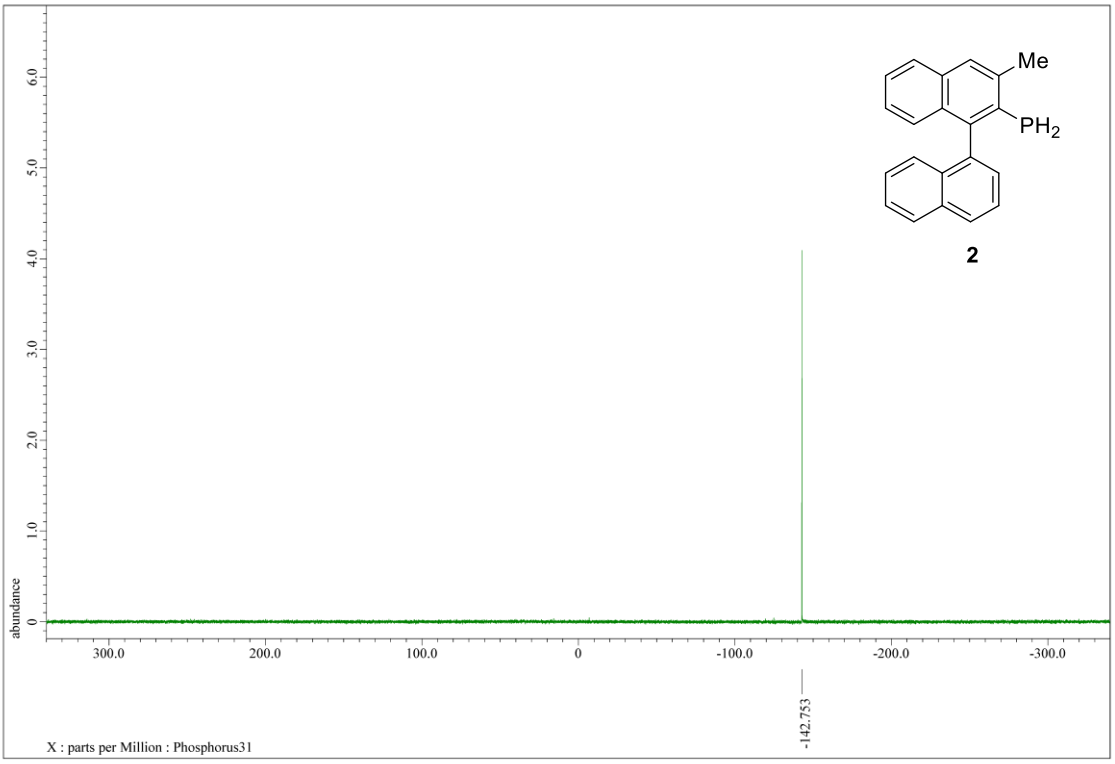


Figure S15. ^{31}P NMR Spectrum of 2.

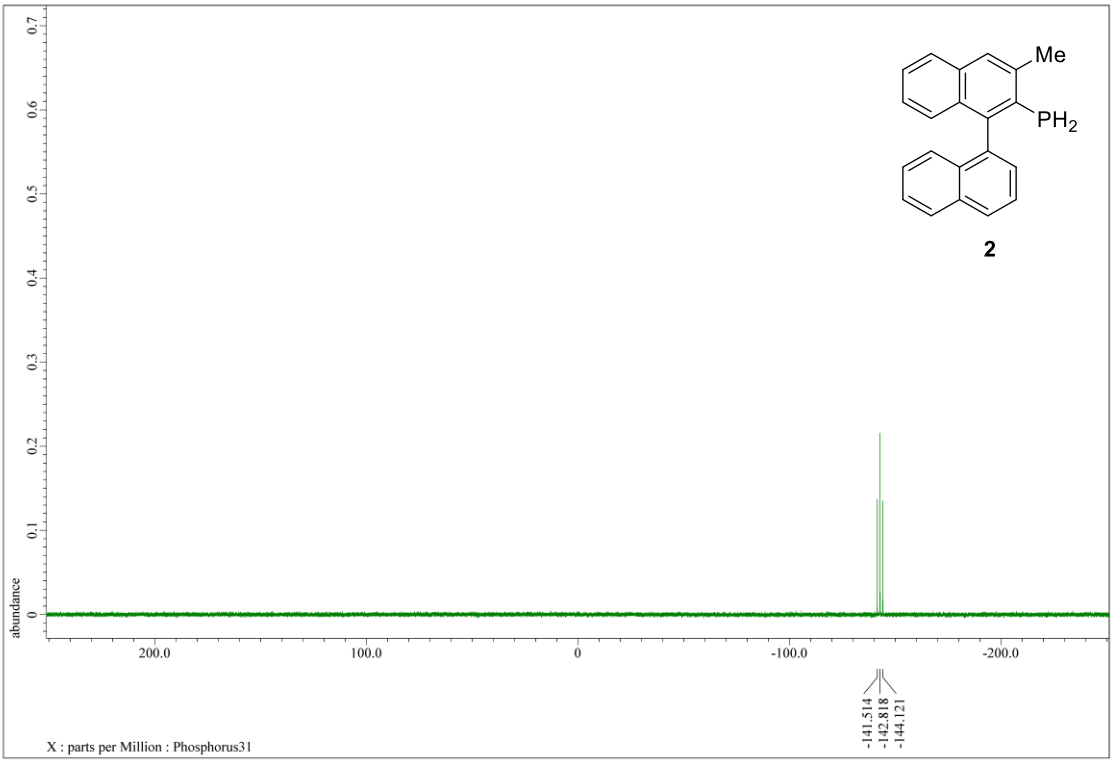


Figure S16. ^{31}P NMR (^{1}H non-decoupling) Spectrum of 2.

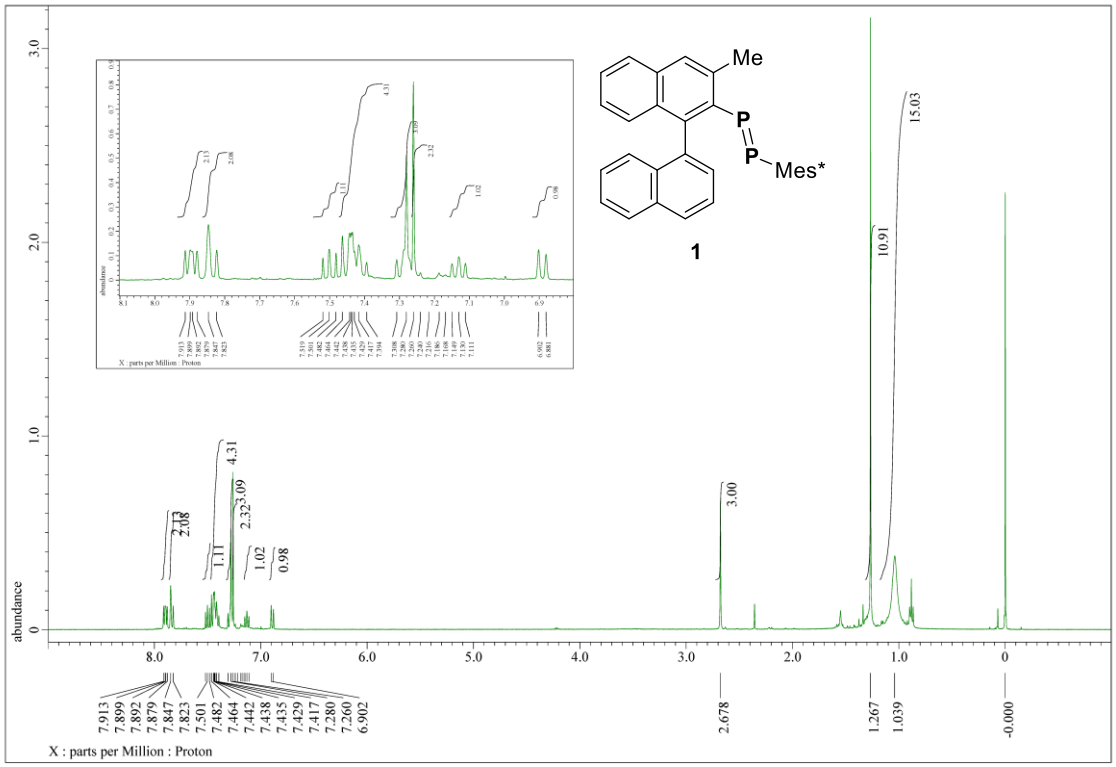


Figure S17. ^{1}H NMR Spectrum of Diphosphene 1.

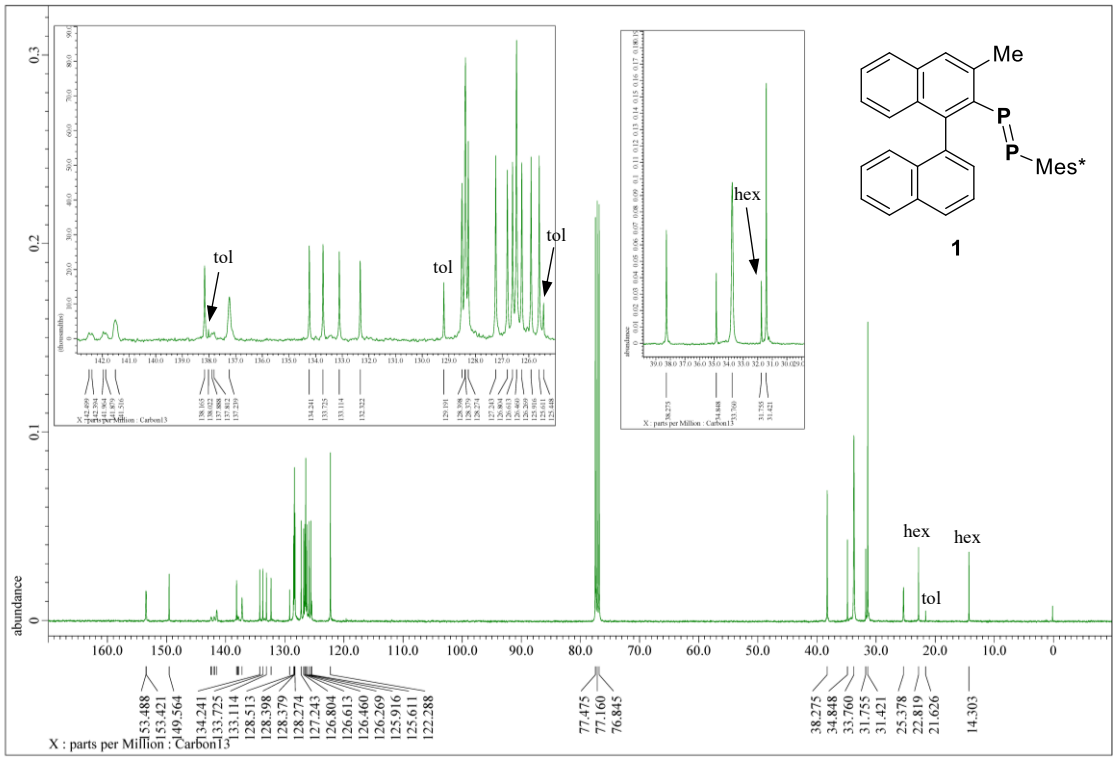


Figure S18. ^{13}C NMR Spectrum of Diphosphene 1.

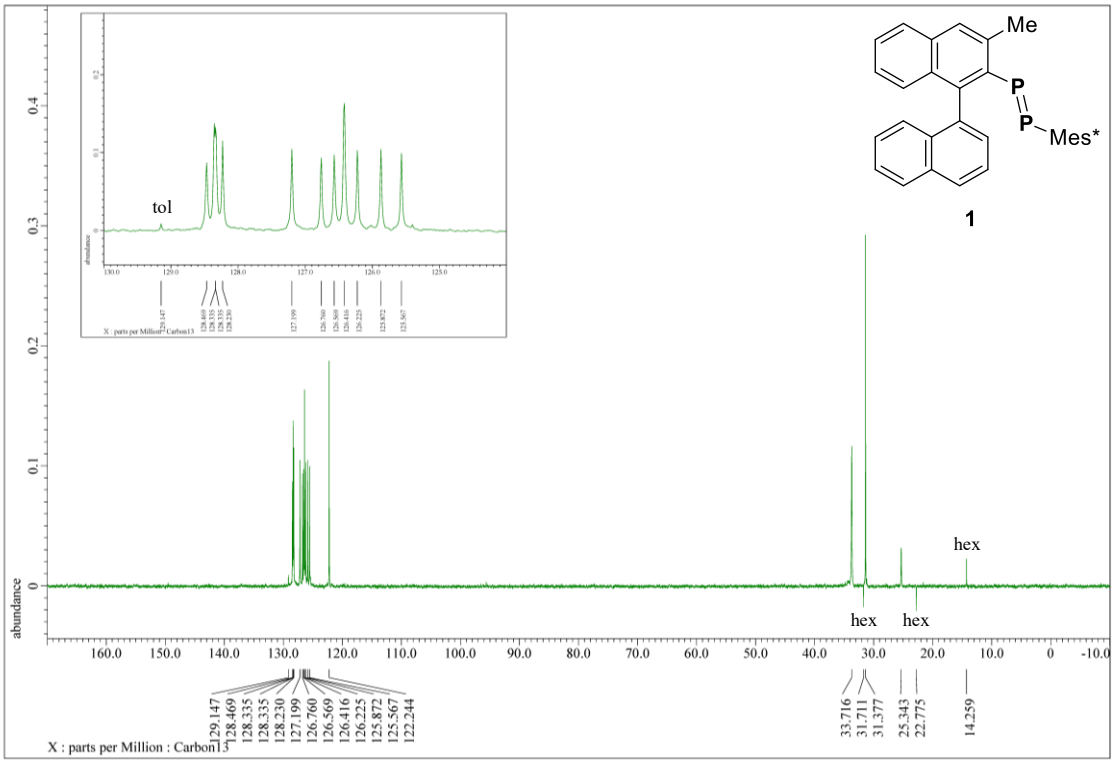


Figure S19. ^{13}C NMR Spectrum (dept135) of Diphosphene 1.

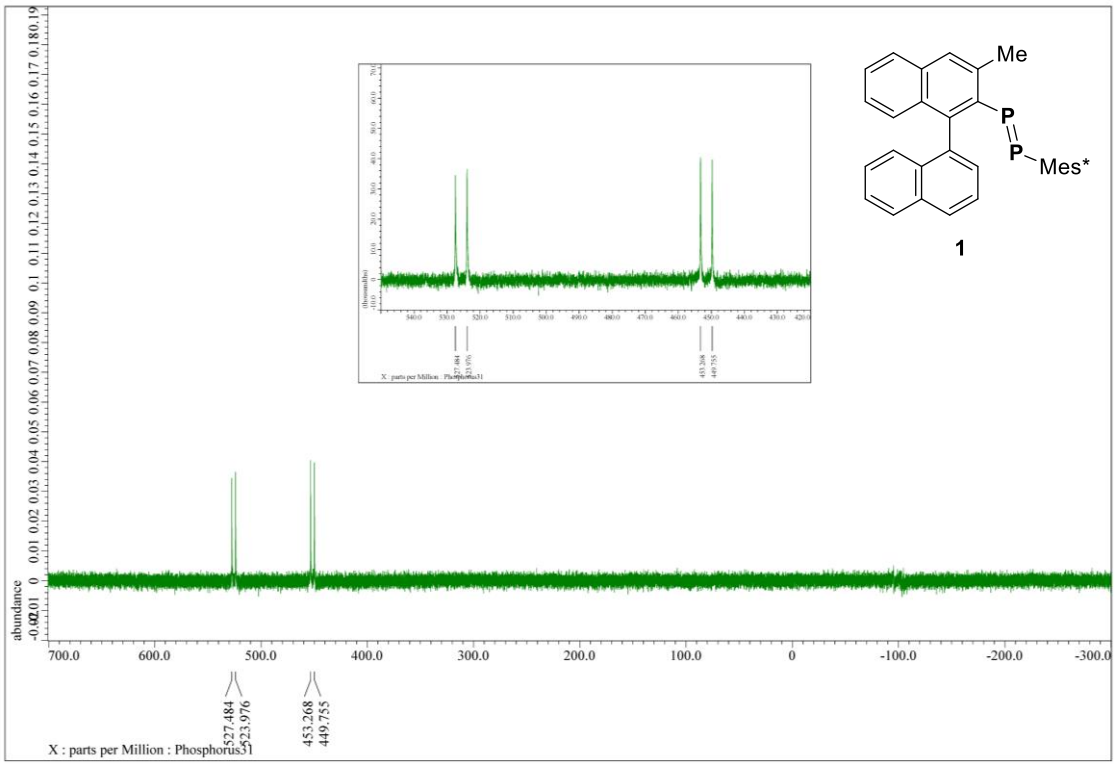


Figure S20. ^{31}P NMR Spectrum of Diphosphene 1.

3. Enantiomer Separation and Synthesis of Enantiomerically pure Diphosphene 1

3-1. Enantiomer Separation of Phosphonate 3.

Enatiomer separation of the racemic mixture of phosphonate **3** was carried out by a YMC Multiple Preparative HPLC LC-Forte/R equipped with CHIRAL ART Cellulose-SB column (20 x 250 mm I.D., S-5 μm) eluted with hexane/^{i}PrOH = 96/4. HPLC analysis of the racemic mixture and both enantiomers of **3** were analyzed by a JASCO LC-2000Plus equipped with DAICEL CHIRALPAK IA (4.6 x 250 mm I.D.) eluted with hexane/^{i}PrOH = 9/1 with the flow rate of 1.0 mL/min at 27 ˚C. The enantiomeric purities of both enantiomers were >99.9% ee. The results are shown in Figure S21. The optical rotations of both enantiomers of **3** were recorded on a JASCO P-2200 Polarimeter at 27 ˚C. The first eluent peak: $[\alpha]_{\mathrm{D}}^{27}$ = +21.6 (c 0.20, $CHCl_3$); the latter eluent peak: $[\alpha]_{\mathrm{D}}^{27}$ = −22.2 (c 0.20, $CHCl_3$).

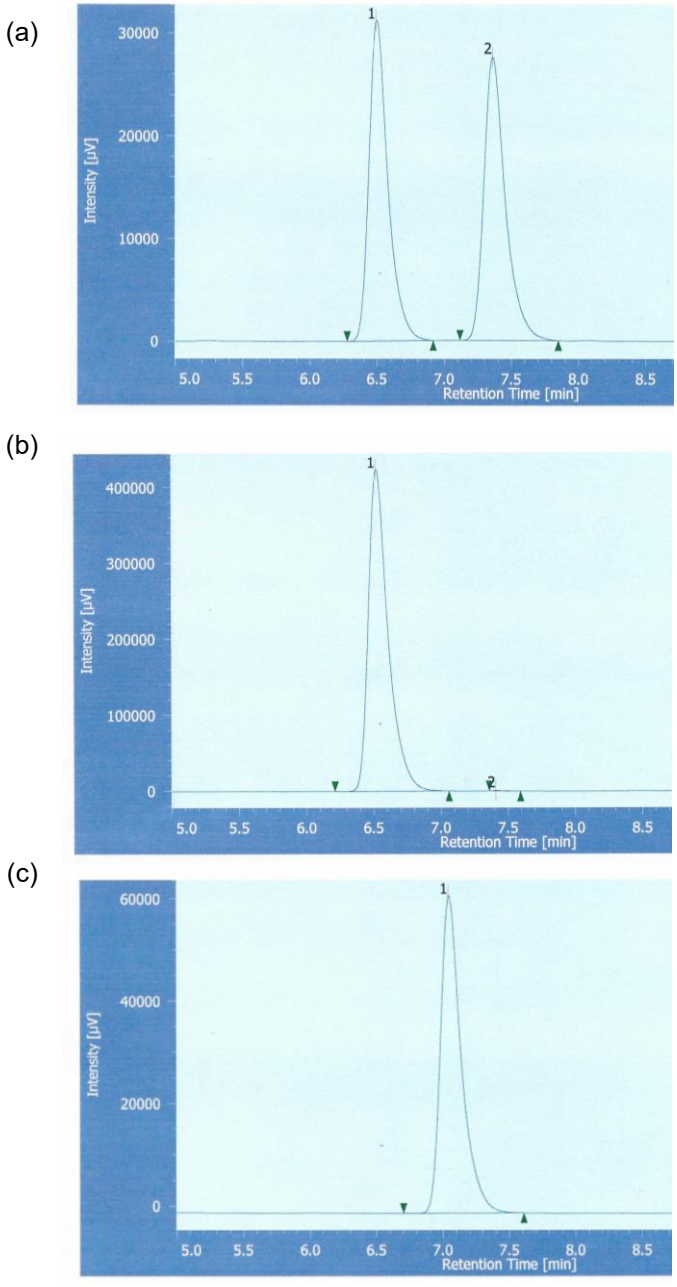


Figure S21. HPLC analysis of (a) the racemic mixture of **3**, (b) the separated (+)-**3**, and (c) (−)-**3**.

3-2. Synthesis of Enantiomerically pure Diphosphene 1.

Enantiomerically pure diphosphene **1** was synthesized from enantiomerically pure phosphonate (+)-**3** and (−)-**3** according to the described procedures for the synthesis of the racemic diphosphene **1**. Phosphine **2** was not isolated and used to next step without further purification. Yield of (*S*)-(+)-**1**; 32.0 mg (0.056 mmol, 32% from 68.9 mg (0.176 mmol) of (+)-**3**). Yield of (*R*)-(−)-**1**; 9.7 mg (0.017 mmol, 14% from 48.0 mg (0.123 mmol) of (−)-**3**). Mp. 179 ˚C (decomp.) for (*S*)-(+)-**1** and 179 ˚C (decomp.) for (*R*)-(−)-**1**.

X-ray crystallographic analysis of (+)-**1** synthesized from (+)-**3** revealed that the absolute configuration was (*S*) (see Section 4). Enantiomeric purities of **1** were confirmed by HPLC with a JASCO LC-2000Plus equipped with DAICEL CHIRALPAK IB (4.6 x 250 mm I.D.) eluted with hexane with the flow rate of 1.5 mL/min at 36 ˚C. The enantiomeric purities of both enantiomers were >99.9% ee although **1** partially decomposed under ambient condition (with wet hexane in air). The results are shown in Figure S22. The optical rotations of both enantiomers of **1** were recorded on a JASCO P-2200 Polarimeter at 27 ˚C under argon atmosphere. (*S*)-**1**: $[\alpha]_{\mathrm{D}}^{27}$ = +158.9 (c 0.014, hexane); (*R*)-**1**: $[\alpha]_{\mathrm{D}}^{22}$ = −158.9 (c 0.014, hexane).

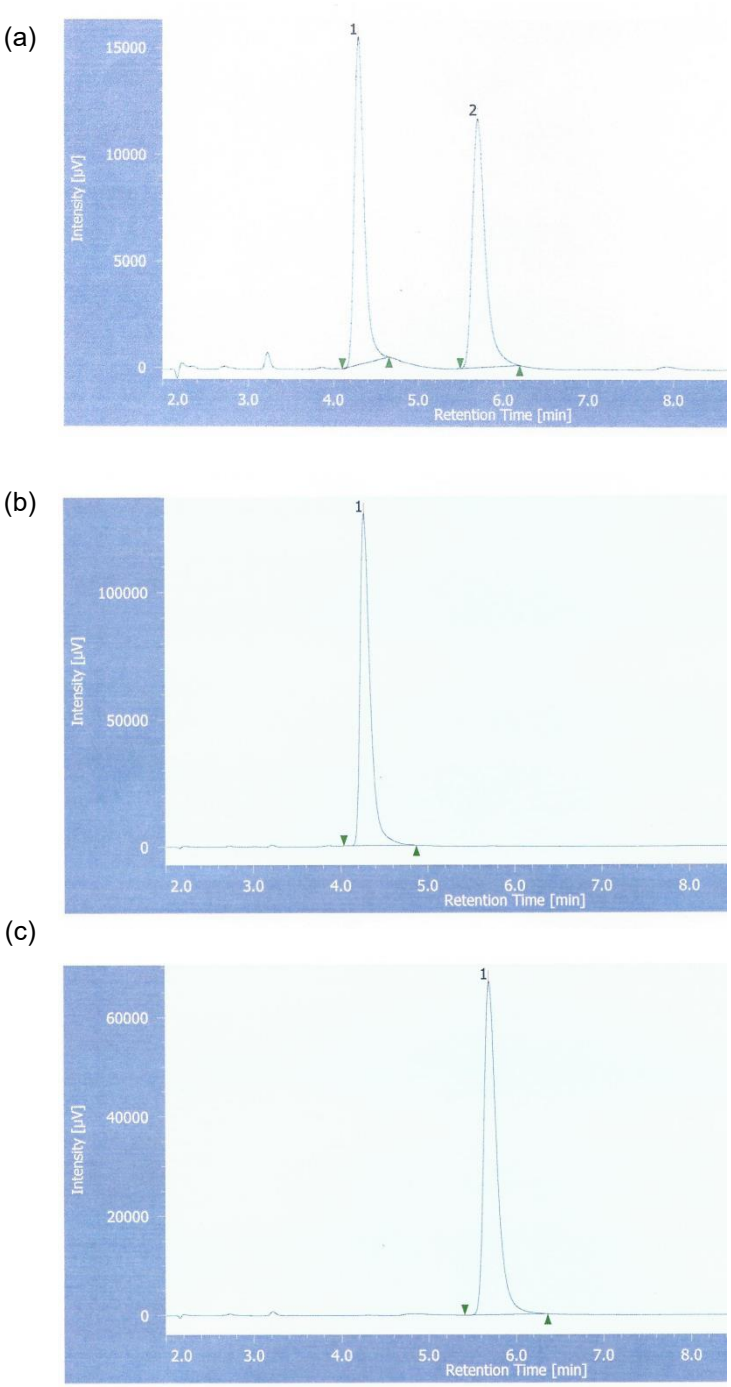


Figure S22. HPLC analysis of (a) the racemic mixture of **1**, (b) the separated (*R*)-(−)-**1**, and (c) (*S*)-(+)-**1**.

3-3. Thermal Stability for Racemization of Diphosphene 1.

Thermal stability for racemization of **1** was confirmed by the enantiomeric purity of (*R*)-(−)-**1** analyzed by the HPLC equipped with DAICEL CHIRALPAK IB (4.6 x 250 mm I.D.) (condition; eluent: hexane, flow rate: 1.5 mL/min at 36 ˚C.). A solution of (*R*)-(−)-**1** in *n*-octane (dried over potassium mirror) charged into a Schleck tube under argon atmosphere was heated by a stainless oil bath (EYELA, OHB-1000S) with a silicon oil (Shinetsu, KF-96-100CS) at 100 °C. After heating for several hours, the reaction mixture was cooled to 0 °C, and then an aliquot of the reaction mixture was directly analyzed by HPLC. Although (*R*)-(−)-**1** partially decomposed after heating, the signal of (*S*)-(+)-**1** was not detected at all.

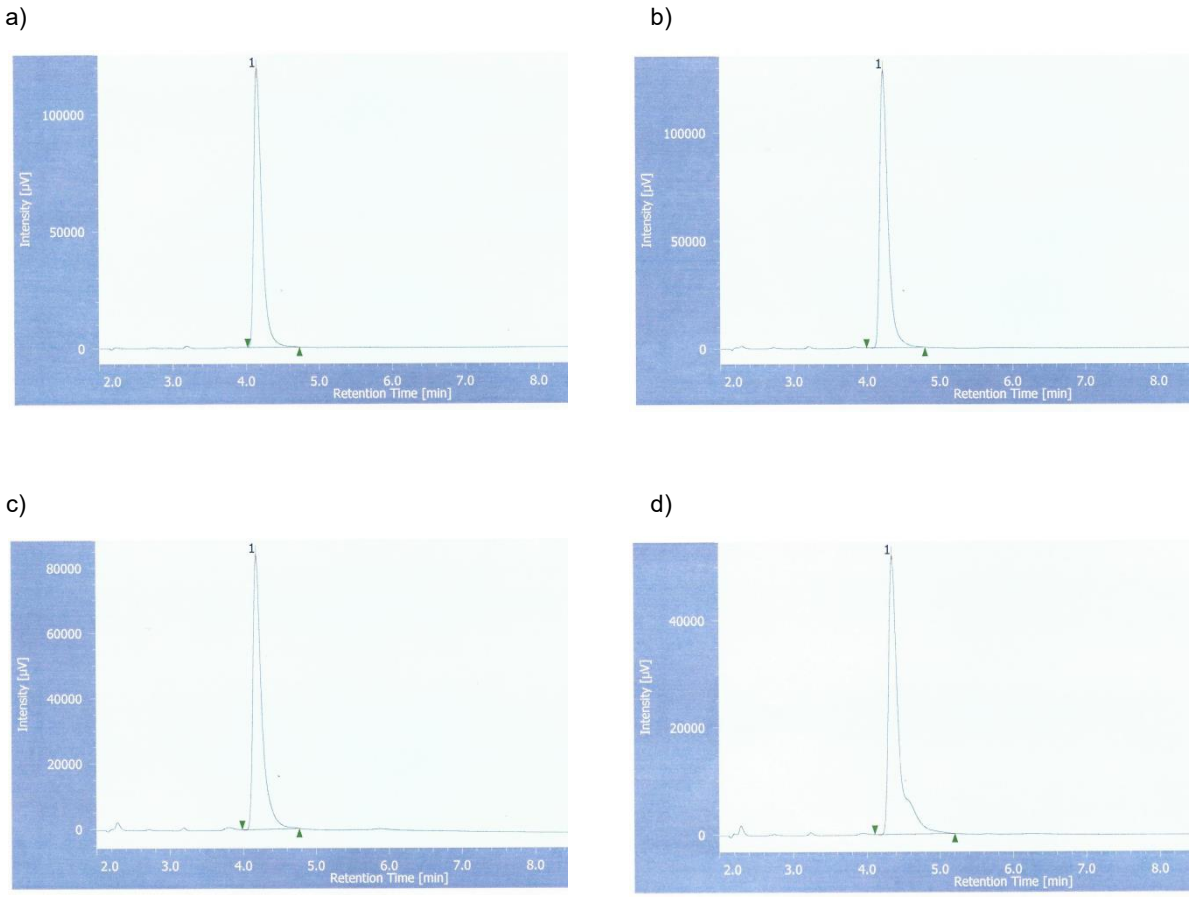


Figure S23. Thermal stability for racemization of (*R*)-(−)-**1** in *n*-octane at 100 °C monitored by HPLC (a) before heating, (b) after heating for 4 h, (c) for 16 h, and (d) for 65 h.

4. X-ray Crystallographic Analysis

Yellow crystals of *rac*-**1** and (*S*)-(+)-**1** were grown by recrystallization from a toluene/hexane solution at room temperature in a glovebox under an argon atmosphere. X-ray data were collected on a Rigaku Saturn diffractometer with VariMax multi-layer mirror monochromated Mo-Kα radiation (λ = 0.71073 Å) at −170 °C. The data were corrected for Lorentz and polarization effects. An empirical absorption correction based on the multiple measurement of equivalent reflections was applied using the REQABS program in CrystalClear software. The structures were solved by direct methods (SIR2014[S6]) and refined by full-matrix least squares against F^2 using all data. Non-hydrogen atoms were refined anisotropically, while all hydrogen atoms were generated by AFIX instructions. All calculations were performed using Yadokari-XG 2009[S7] software package except for refinement, which was performed using SHELXL-2013.[S8] CCDC-1811243 for *rac*-**1** and CCDC-1811244 for (*S*)-(+)-**1** contain the supplementary crystallographic data for this paper.

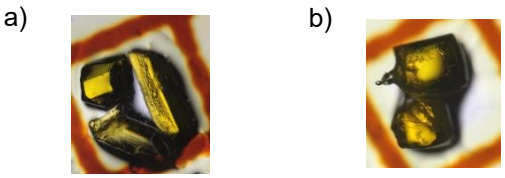
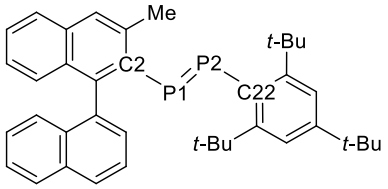


Figure S24. Photographs of a) *rac*-**1** and b) (*S*)-(+)-**1**. Yellow-brown line indicates the scale (1 mm × 1 mm).

Table S1. Crystal Data for *rac*-**1** and (*S*)-(+)-**1**.

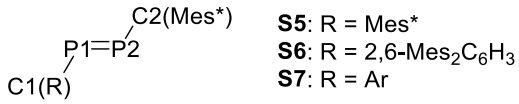
	rac-**1**	(*S*)-(+)-**1**
Formula	$C_{42.5}H_{48}P_2$	$C_{39}H_{44}P_2$
Formula weight	620.75	574.68
Crystal Size/mm	0.21 × 0.19 × 0.11	0.26 × 0.17 × 0.17
Temperature/ °C	−170	−170
Crystal system	triclinic	orthorhombic
Space group	*P*−1 (#2)	$P2_12_12_1$ (#19)
Lattice parameters		
a/Å	11.005(3)	9.8360(5)
b/Å	13.932(3)	10.5827(4)
c/Å	13.967(3)	30.5320(14)
α/°	111.2151(18)	90
β/°	97.790(2)	90
γ/°	113.0868(12)	90
V/Å^3	1737.7(7)	3178.1(2)
Z	2	4
D_{calc} /g cm^{-3}	1.186	1.201
μ (cm^{-1})	1.54	1.63
$2\theta_{max}$/°	55.0	55.0
No. of reflections	21401	43278
Independent reflections	7889	7236
No. of parameters	397	380
R_{int}	0.0229	0.0391
Completeness to θ (%)	99.2	99.3
R_1 [$I>2\sigma(I)$]	0.0378	0.0312
wR_2 (all data)	0.1054	0.0727
Largest diff. peak (e.Å^{-3})	0.763	0.296
Largest diff. hole (e.Å^{-3})	−0.418	−0.257
Goodness-of-fit	1.066	1.061
Absolute Structural Parameter	–	0.02(2)

Table S2. Selected structural parameters of Mes*-substituted diphosphenes.

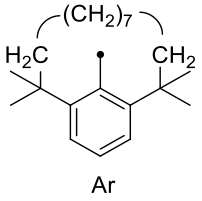


structural parameter	observed		calculated[e]	
	rac-**1**	(*S*)-(+)-**1**	(*S*)-*syn*-**1**	(*S*)-*anti*-**1**
d(P1=P2) /Å	2.0323(6)	2.0351(7)	2.028	2.026
d(P1−C2) /Å	1.8523(13)	1.853(2)	1.861	1.861
d(P2−C22) /Å	1.8565(13)	1.8643(19)	1.870	1.867
deg(C2−P1−P2) /º	98.59(4)	102.64(6)	98.9	98.7
deg(P1−P2−C22) /º	103.07(4)	97.72(6)	98.2	99.5
(Naph)−(Naph) /º [a]	79.41(3)	82.56(3)	81.9	80.7
(CPP)−(Naph) /º [b]	76.96(3)	86.64(5)	85.0	77.8
(CPP)−(Mes*) /º [c]	89.13(4)	81.39(5)	89.7	86.4
P1 /Å [d]	0.09	0.20	0.07	0.14
P2 /Å [d]	0.19	0.64	0.56	0.45

a) Dihedral angles between the two naphthyl rings. b) Dihedral angles between the CPP plane containing the C2 atom and the naphthyl ring. c) Dihedral angles between the CPP plane containing the C22 atom and the benzene ring of the Mes* groups. d) Deviation of phosphorus atom (P1 or P2 atoms) from naphthalene or benzene (Mes*) plane. e) Calculated at M06-2X/6-31G(d) level.



S5: R = Mes*
S6: R = 2,6-$Mes_2C_6H_3$
S7: R = Ar



structural parameter	reported		
	S5[f]	**S6**[g]	**S7**[h]
d(P1=P2) /Å	2.034(2)	2.0240(13)	2.039(2)
d(P1=C1) /Å	1.862(2)	1.846(3)	1.861(4)
d(P2=C2) /Å		1.860(3)	1.861(4)
deg(C1−P1−P2) /º	102.8(1)	101.19(11)	101.4(1)
deg(P1−P2−C2) /º		97.99(11)	97.9(1)

f) Ref S4. g) Ref S9. h) Ref S10.

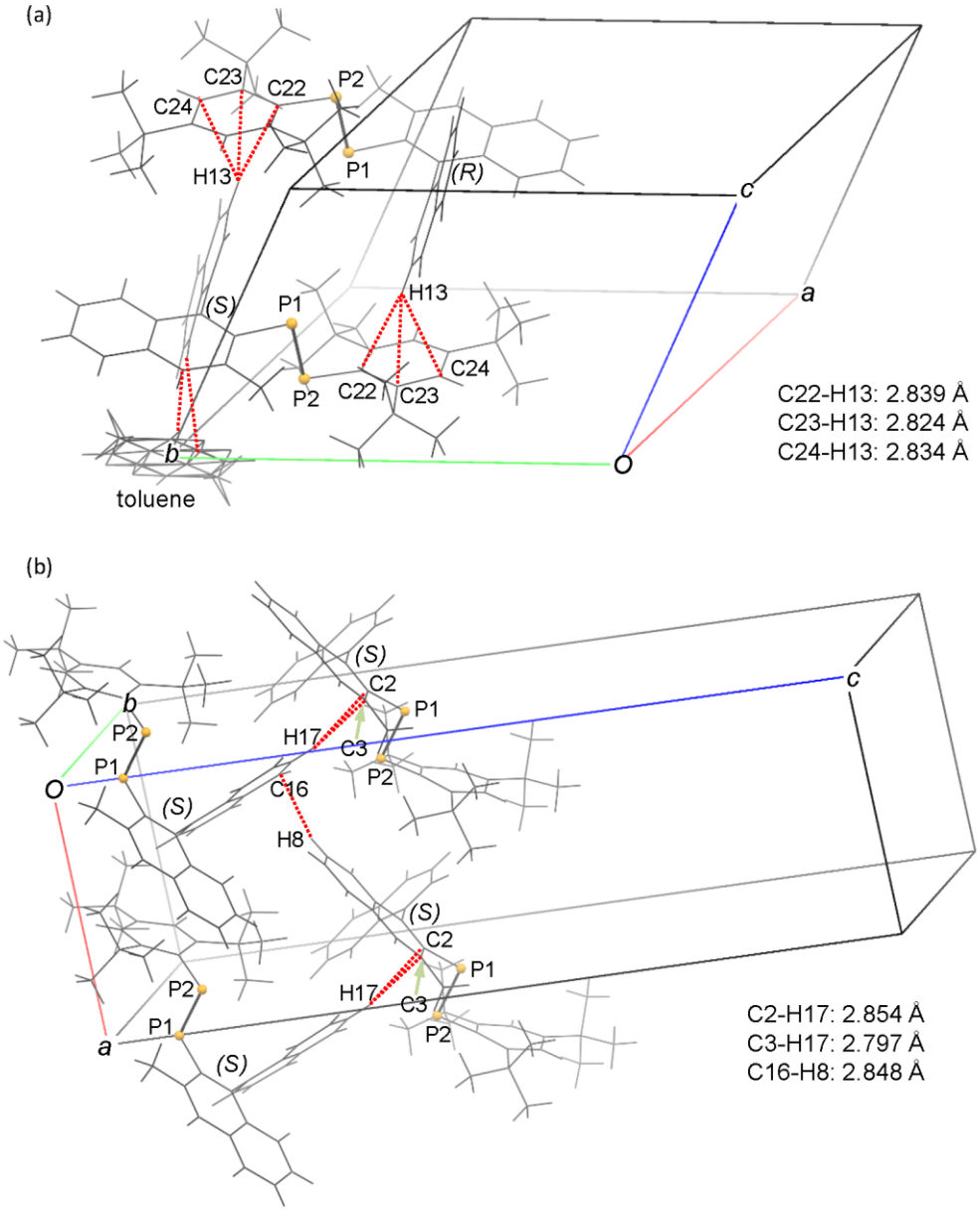


Figure S25. Packing structures of (a) *rac*-**1** and (b) (*S*)-(+)-**1**.

5. UV-vis and CD Spectra

UV-vis spectrum of *rac*-**1** was measured on a JASCO V-670 spectrophotometer with a hexane solution (2.6×10^{-5} M) in a 1 cm quarts cell equipped with J-Young valve filled with argon. The results are shown in Figure 2a and Table S3. Circular dichroism (CD) spectra of (*S*)-(+)-**1** and (*R*)-(−)-**1** were measured on a JASCO J-820 spectrometer at 20 ºC (PTC-423L thermostat, JASCO) with a dilute hexane solution (4.4×10^{-4} M for (*S*)-(+)-**1** and 4.1×10^{-4} M for (*R*)-(−)-**1**) in a 1 mm quartz cell under argon atmosphere. The results are shown in Figure 2b and Table S4.

Table S3. UV-vis spectral parameter of *rac*-**1** in hexane.

Compd.	λ / nm	ε / M^{-1} cm^{-1}
rac-**1**	455	500
	334	7060
	297[a]	17400
	275	22300

a) observed as a shoulder.

Table S4. CD spectral parameters of (*S*)-(+)-**1** and (*R*)-(−)-**1** in hexane.

Compd.	λ / nm	ε / M^{-1} cm^{-1}	$\Delta\varepsilon$ / M^{-1} cm^{-1}	$g^a \times 10^{-3}$
(*S*)-(+)-**1**	480	270	−0.5	−1.8
	433	348	0.7	2.0
	342	6530	6.5	0.99
	290	19200	17.4	0.91
(*R*)-(−)-**1**	480	270	0.5	1.8
	430	319	−0.7	−2.2
	342	6530	−6.4	−0.98
	290	19200	−17.1	−0.89

a) anisotropy factor ($g = \Delta\varepsilon/\varepsilon$)

6. Theoretical Calculations

All theoretical calculations were performed using the Gaussian 09[S11] and GRRM11[S12] programs on a Fujitsu PRIMERGY RX300 system of the Research Center for Computational Science, Japan. All structures were optimized without any symmetry assumptions. Zero-point energy, enthalpy, and Gibbs free energy at 298.15 K and 1 atm were estimated from the gas-phase studies. Harmonic vibration frequency calculations at the same level were performed to verify all stationary points as local minima (with no imaginary frequency) or transition states (with one imaginary). The structures of *syn*-(*S*)-**1** and *anti*-(*S*)-**1** were optimized at B3LYP,[S13] PBE0,[S14] M06-2X,[S15] CAM-B3LYP,[S16] and wB97XD[S17] functionals with the basis set of 6-31G(d). The energies of the obtained structures were recalculated at 6-31+G(d) level in conjunction with PCM model,[S18] where heptane instead of hexane was chosen as solvent item in calculation. The structures of *syn*-(*S*)-**1** obtained from X-ray analysis, described as *rac*-**1** (X-ray) and (*S*)-**1** (X-ray), respectively, were also calculated at M06-2X/6-31G(d) level, where non-hydrogen atoms were fixed, and hydrogen atoms were optimized. Harmonic vibration frequency calculations of *rac*-**1** (X-ray) and (*S*)-**1** (X-ray) at the same level showed four and three imaginary frequencies, respectively.

The TDDFT calculations of *syn*-(*S*)-**1** and *anti*-(*S*)-**1** were performed at five functionals described above with the basis set of 6-311G(d) in conjunction with PCM model[S18] to evaluate solvation effects, where heptane instead of hexane was chosen as solvent item in calculation. The optimized structures obtained at M06-2X/6-31G(d) level were used. UV and ECD spectra were simulated with a half-width at half height of 0.20 eV for each transition and were visualized by using GaussView 5.0.9 software.

Transition states of the rotation of the C(Naph)−P bond and the C1−C1' bond of the binaphthyl moiety of **1** and $\mathbf{1_{Dmp}}$ were optimized at B3LYP/6-31G(d) level. Here, $\mathbf{1_{Dmp}}$ is the model compound with 2,6-dimethylphenyl (Dmp) group instead of Mes* group. **TS-A** and **TS-B** represent the transition states of the rotation of the C(Naph)−P bond via the vicinity of a methyl group at 3-position of naphthyl group and naphthyl group, respectively. **TS-C** and **TS-D** represent the transition states of the rotation of the C1−C1' bond of the binaphthyl moiety via the vicinity of 2- and 2'-substituents/8- and 8'-substituents and of 2- and 8'-substituents/2'- and 8-substituents, respectively. During the course of the optimization, the different transition states were found in **TS-C** and **TS-D**, which represent **TS-C'** and **TS-D'**, respectively. **TS-C** and **TS-D** were lower in energy than **TS-C'** and **TS-D'**, respectively. IRC calculations supported that all transition states connect *syn*-(*S*)-**1** and *anti*-(*S*)-**1** (for the C(Naph)−P bond rotation) or *anti*-(*R*)-**1** (for the C1−C1' bond rotation).

Table S5. Computational Level Dependence of Energies (ΔG: kcal mol^{-1}) for *syn*-(*S*)-**1** and *anti*-(*S*)-**1**.

	B3LYP	PBE0	M06-2X	CAM-B3LYP	wB97XD
syn-(*S*)-**1**[a]	0	0	0	0	0
anti-(*S*)-**1**[a]	−0.5	0.9	1.2	0.3	0.8
syn-(*S*)-**1**[b]	0	0	0	0	0
anti-(*S*)-**1**[b]	2.3	2.6	1.5	0.2	0.3

a) 6-31G(d) level. b) 6-31+G(d) level with PCM model.

Table S6. Uncorrected and thermal-corrected (298 K) energies of stationary points (Hartree).[a]

Molecule	*E*	*E* + *ZPE*	*H*	G	ΔG[d]
Real molecule **1**[b]					
syn-(*S*)-**1**	-2194.63819363	-2193.906084	-2193.865135	-2193.977678	0.0
anti-(*S*)-**1**	-2194.63490914	-2193.903086	-2193.861961	-2193.975837	1.2
rac-**1** (X-ray)	-2194.63417190	-2193.901678	-2193.864033	-2193.965978	7.3
(*S*)-**1** (X-ray)	-2194.63279310	-2193.901640	-2193.862775	-2193.969414	5.2
Real molecule **1**[c]					
syn-(*S*)-**1**	-2195.36613527	-2194.641205	-2194.599417	-2194.714881	0.0
anti-(*S*)-**1**	-2195.36549832	-2194.640646	-2194.598823	-2194.714888	0.0
anti-(*R*)-**1**	-2195.36552004	-2194.640627	-2194.598817	-2194.714675	0.1
TS-A	-2195.36175012	-2194.636616	-2194.595833	-2194.709682	3.3
TS-B	-2195.36021980	-2194.635382	-2194.594493	-2194.707876	4.4
TS-C	-2195.30804724	-2194.583294	-2194.542514	-2194.654812	37.7
TS-C'	-2195.30426700	-2194.579166	-2194.538550	-2194.650983	40.1
TS-D	-2195.30476913	-2194.580268	-2194.539584	-2194.651264	39.9
TS-D'	-2195.29798799	-2194.573839	-2194.533094	-2194.645559	43.5
Model molecule $\mathbf{1_{Dmp}}$[c]					
syn-(*S*)-$\mathbf{1_{Dmp}}$	-1802.27097742	-1801.829169	-1801.800738	-1801.889382	0.0
anti-(*S*)-$\mathbf{1_{Dmp}}$	-1802.26975628	-1801.827790	-1801.799428	-1801.887742	1.0
anti-(*R*)-$\mathbf{1_{Dmp}}$	-1802.26975648	-1801.827789	-1801.799427	-1801.887740	1.0
$\mathbf{TS\text{-}A_{Dmp}}$	-1802.26463554	-1801.822650	-1801.795303	-1801.880305	5.7
$\mathbf{TS\text{-}B_{Dmp}}$	-1802.26259186	-1801.820762	-1801.793356	-1801.878102	7.1
$\mathbf{TS\text{-}C_{Dmp}}$	-1802.21160266	-1801.769955	-1801.742605	-1801.827113	39.1
$\mathbf{TS\text{-}C'_{Dmp}}$	-1802.20848012	-1801.766362	-1801.739199	-1801.823083	41.6
$\mathbf{TS\text{-}D_{Dmp}}$	-1802.21022970	-1801.768933	-1801.741643	-1801.825554	40.1
$\mathbf{TS\text{-}D'_{Dmp}}$	-1802.20154995	-1801.760400	-1801.733116	-1801.817805	44.9

a) *E*: electronic energy; *ZPE*: zero-point energy; *H* (= $E + ZPE + E_{vib} + E_{rot} + E_{trans} + RT$): sum of electronic and thermal enthalpies; *G* (= $H - TS$): sum of electronic and thermal free energies. b) calculated at M06-2X/6-31G(d) level. c) calculated at B3LYP/6-31G(d) level. d) kcal mol^{-1}

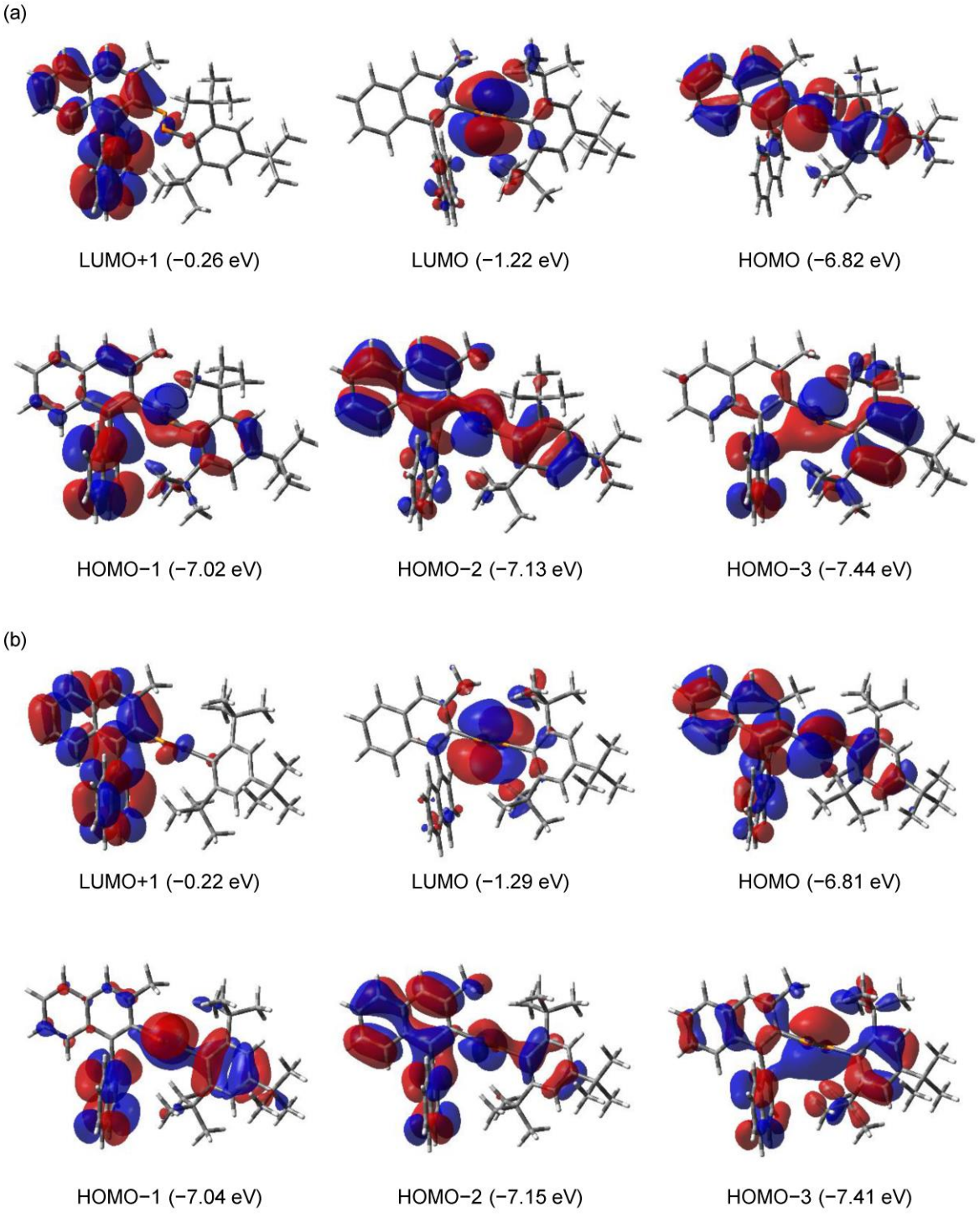


Figure S26. Selected molecular orbitals of (a) *syn*-(*S*)-**1** and (b) *anti*-(*S*)-**1** calculated at M06-2X/6-31G(d) level.

Table S7. Transition energies, wavelengths, and oscillator strengths of the transitions of *syn*-(*S*)-**1** and *anti*-(*S*)-**1**[a]

[a]The 154th orbital is the HOMO, and the 155th orbital is the LUMO.

syn-(*S*)-**1**

Excited State 1: Singlet-A	147 ->155 -0.32737	149 ->155 0.14084
2.6789 eV 462.81 nm f=0.0009	148 ->155 0.14938	150 ->155 0.10450
147 ->155 0.17833	149 ->155 0.25570	152 ->156 -0.24497
152 ->155 0.28008	150 ->155 -0.16829	152 ->157 -0.21514
154 ->155 0.59657	151 ->155 0.33239	153 ->156 0.28931
Excited State 2: Singlet-A	152 ->155 -0.20784	154 ->156 0.36729
3.8319 eV 323.56 nm f=0.0722	153 ->155 -0.12969	154 ->157 0.19935
150 ->155 0.19084	154 ->155 0.27618	154 ->158 0.16763
151 ->155 0.17040	Excited State 5: Singlet-A	Excited State 8: Singlet-A
152 ->155 -0.13774	4.2999 eV 288.34 nm f=0.0421	4.5160 eV 274.54 nm f=0.0872
153 ->155 0.60734	147 ->155 0.18072	149 ->155 -0.10177
154 ->155 0.14588	149 ->155 -0.16459	149 ->156 -0.13259
Excited State 3: Singlet-A	150 ->155 0.28808	150 ->156 0.26013
3.9924 eV 310.55 nm f=0.0335	151 ->155 0.50723	150 ->157 0.18232
149 ->155 0.22334	153 ->155 -0.22023	152 ->156 0.15867
150 ->155 -0.19424	Excited State 6: Singlet-A	152 ->158 0.22073
151 ->155 0.19794	4.4493 eV 278.66 nm f=0.0230	152 ->160 0.10688
152 ->155 0.53607	149 ->155 0.42693	153 ->157 -0.12804
153 ->155 0.18832	150 ->155 0.47847	154 ->156 0.31654
154 ->155 -0.14431	151 ->155 -0.16557	154 ->157 0.18913
Excited State 4: Singlet-A	Excited State 7: Singlet-A	154 ->158 -0.20772
4.1600 eV 298.04 nm f=0.0287	4.4601 eV 277.99 nm f=0.1536	154 ->160 -0.12280

anti-(*S*)-**1**

Excited State 1: Singlet-A	4.1397 eV 299.50 nm f=0.0737	151 ->155 -0.12353
2.6461 eV 468.55 nm f=0.0009	147 ->155 -0.24115	Excited State 7: Singlet-A
147 ->155 -0.19412	149 ->155 0.20265	4.4560 eV 278.24 nm f=0.2068
152 ->155 -0.19965	151 ->155 0.52229	152 ->156 0.22907
153 ->155 -0.41965	152 ->155 -0.11604	152 ->157 -0.13898
154 ->155 0.48034	153 ->155 0.27611	153 ->156 0.10886
Excited State 2: Singlet-A	Excited State 5: Singlet-A	153 ->157 0.15423
3.7279 eV 332.59 nm f=0.0675	4.1736 eV 297.07 nm f=0.0379	154 ->156 0.58221
150 ->155 -0.11268	147 ->155 0.37776	Excited State 8: Singlet-A
151 ->155 -0.24453	148 ->155 0.11484	4.4897 eV 276.15 nm f=0.0081
152 ->155 0.10910	149 ->155 -0.25344	147 ->155 0.30309
153 ->155 0.44009	150 ->155 0.24650	149 ->155 0.31180
154 ->155 0.44751	151 ->155 0.33897	149 ->156 0.15181
Excited State 3: Singlet-A	152 ->155 0.15290	150 ->156 -0.17906
3.9955 eV 310.31 nm f=0.0091	154 ->155 0.22053	151 ->156 -0.11168
149 ->155 0.21626	Excited State 6: Singlet-A	152 ->156 -0.19031
150 ->155 -0.16843	4.4038 eV 281.54 nm f=0.0069	152 ->158 0.17304
152 ->155 0.58547	147 ->155 -0.16331	152 ->160 0.10308
153 ->155 -0.17696	149 ->155 0.24043	154 ->156 0.20191
Excited State 4: Singlet-A	150 ->155 0.60109	154 ->158 0.20678
		154 ->160 0.11175

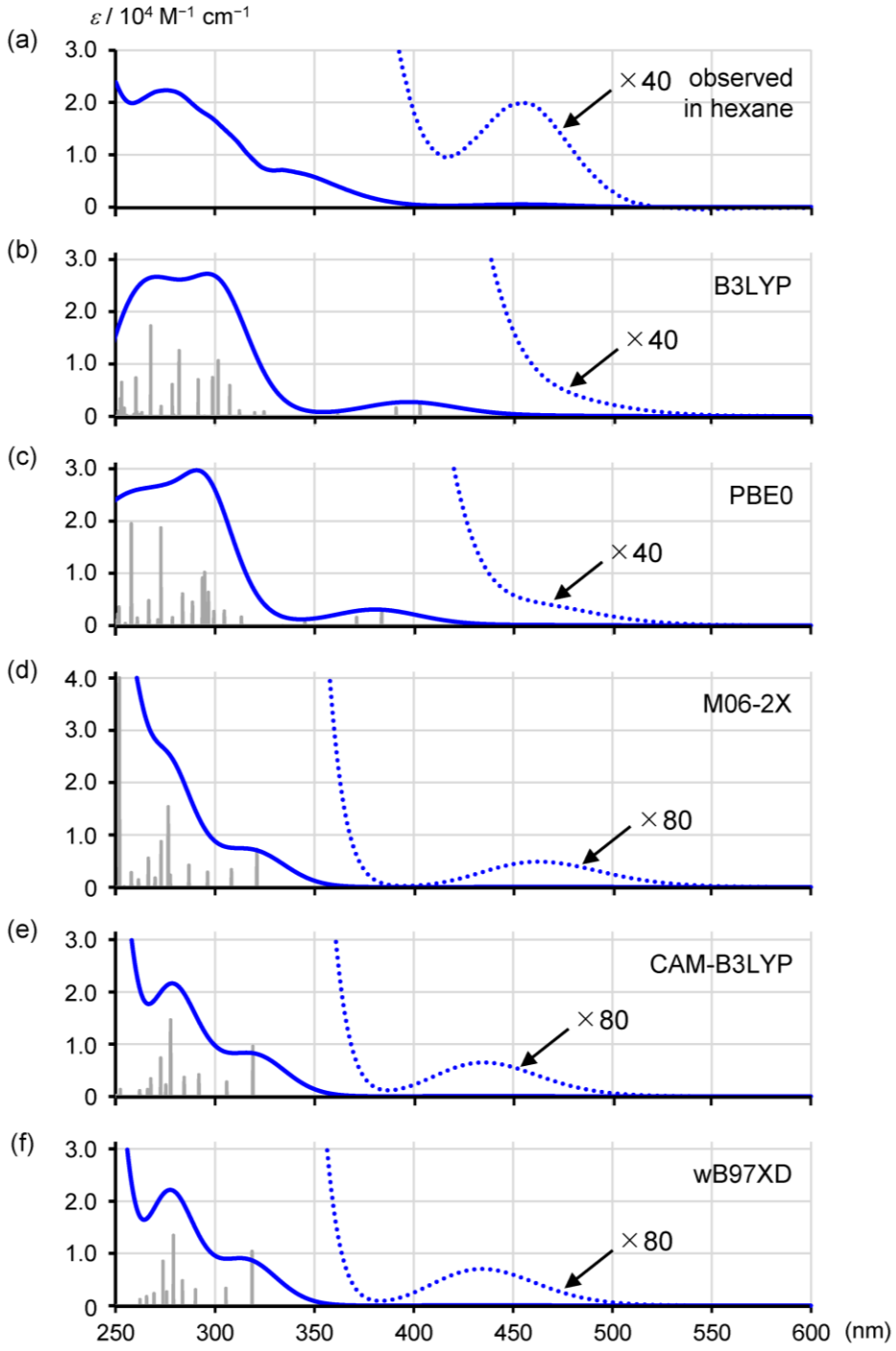


Figure S27. (a) The observed of UV spectrum of *rac*-**1** in hexane. The simulated UV spectra of *syn*-(*S*)-**1** calculated at functionals of (b) B3LYP, (c) PBE0, (d) M06-2X, (e) CAM-B3LYP, and (f) wB97XD with the basis set of 6-311G(d). The calculated oscillator strengths were described as gray bars.

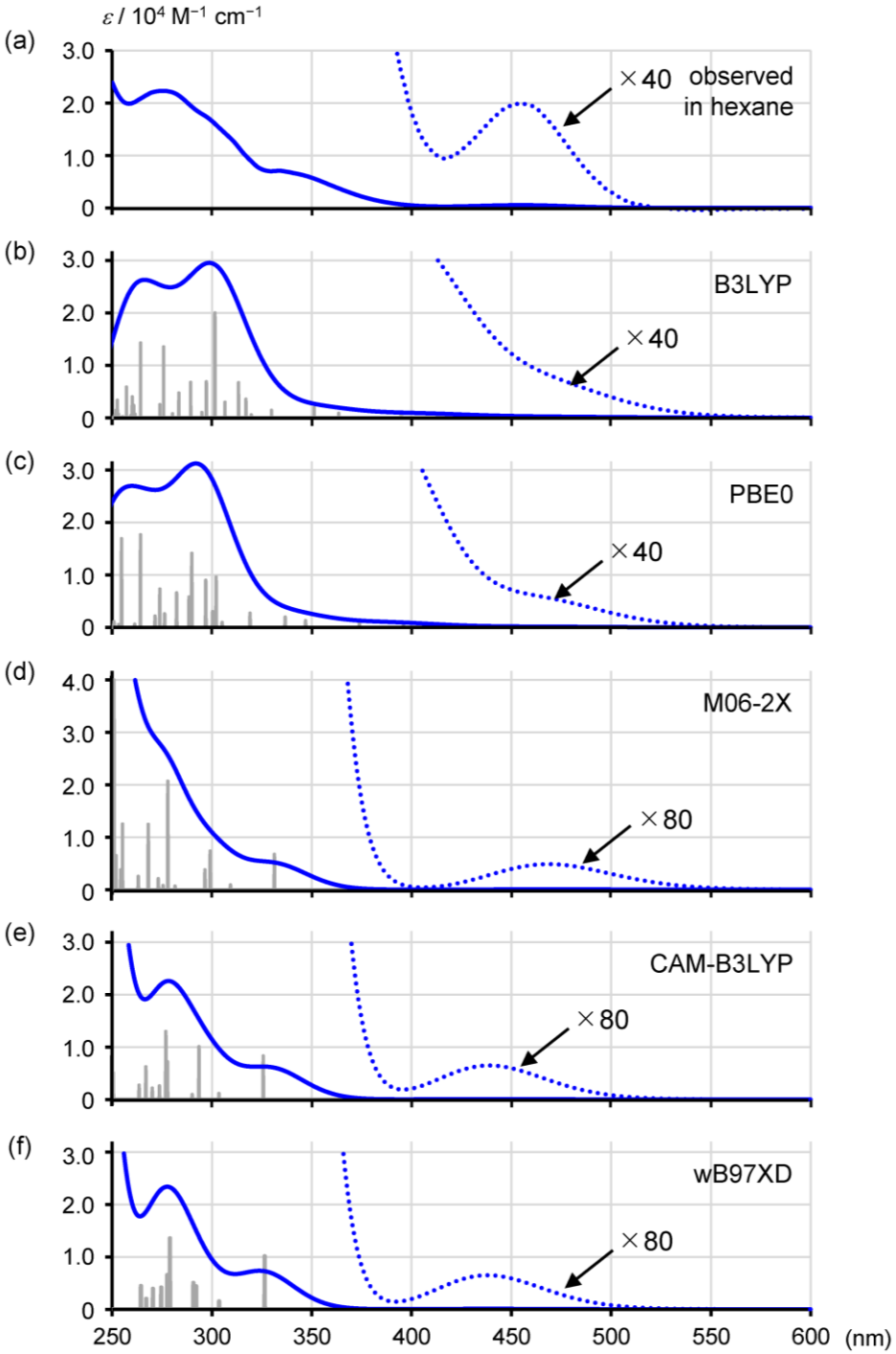


Figure S28. (a) The observed of UV spectrum of *rac*-**1** in hexane. The simulated UV spectra of *anti*-(*S*)-**1** calculated at functionals of (b) B3LYP, (c) PBE0, (d) M06-2X, (e) CAM-B3LYP, and (f) wB97XD with the basis set of 6-311G(d). The calculated oscillator strengths were described as gray bars.

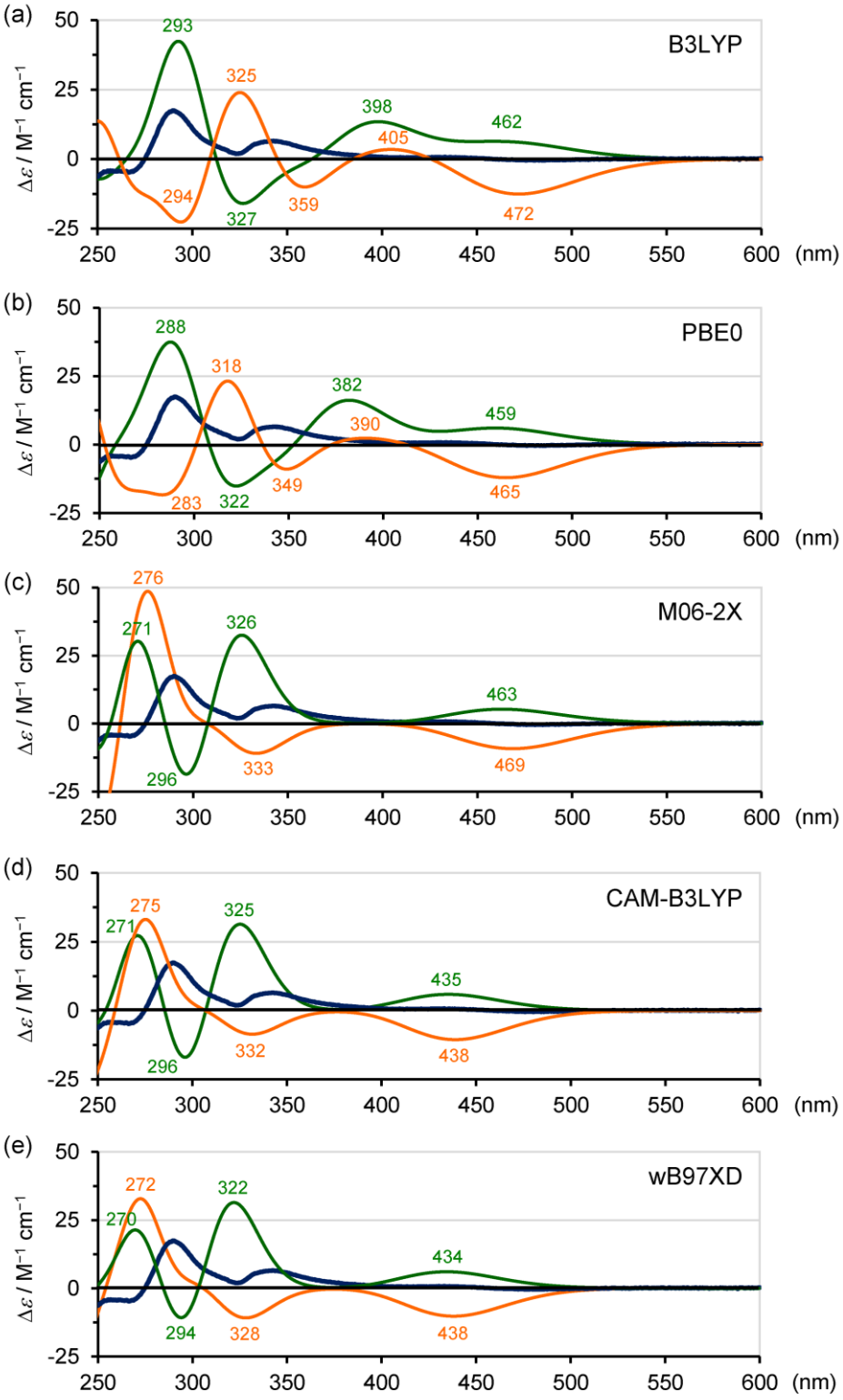


Figure S29. The observed of CD spectrum of (*S*)-**1** (blue), and simulated CD spectra of *syn*-(*S*)-**1** (green) and *anti*-(*S*)-**1** (orange) calculated at functionals of (a) B3LYP, (b) PBE0, (c) M06-2X, (d) CAM-B3LYP, and (e) wB97XD.

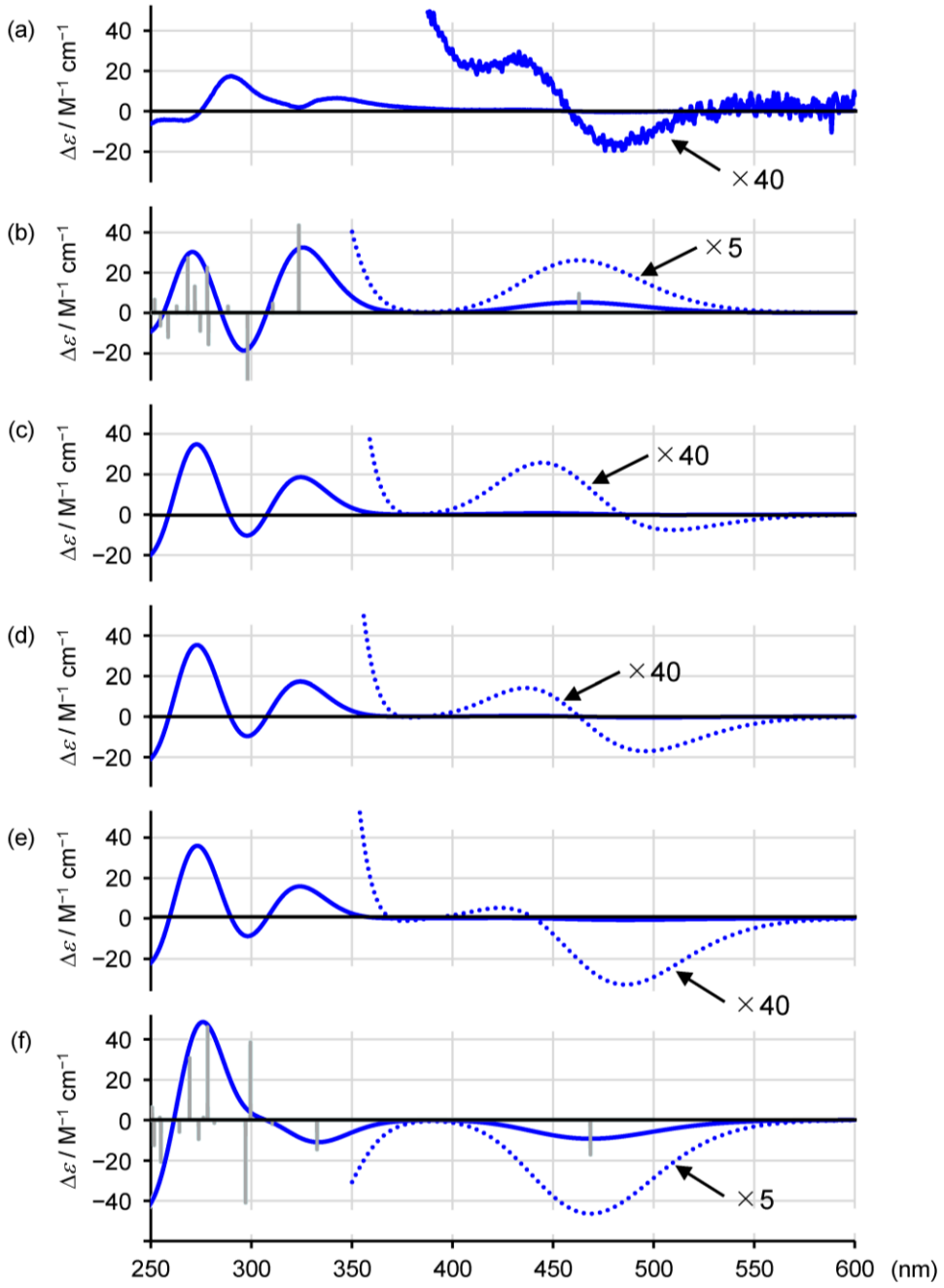
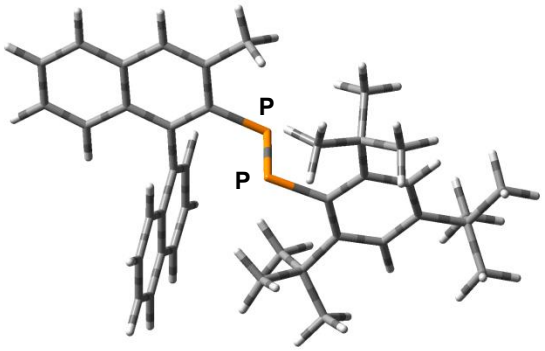


Figure S30. The observed and simulated CD spectra of (*S*)-**1**. Calculated at TD-M06-2X/6-311G(d)//M06-2X/6-31G(d) level. (a) Observed in hexane. Simulated spectra of (b) *syn*-(*S*)-**1**, (c) *syn*-(*S*)-**1**/*anti*-(*S*)-**1** in the ratio of 2/1 (ΔG = 0.40 kcal mol^{-1}) , (d) 1.75/1 (ΔG = 0.33 kcal mol^{-1}), (e) 1.5/1 (ΔG = 0.24 kcal mol^{-1}), and (f) *anti*-(*S*)-**1**. The calculated rotatory strengths were described as gray bars. The ΔG values were estimated from the equation, $\Delta G = -RT\ln([\textit{anti}\text{-}(S)\text{-}\mathbf{1}]/[\textit{syn}\text{-}(R)\text{-}\mathbf{1}])$, where R is the gas constant and T the measured temperature (293 K).

Table S8. Atomic coordinates of the optimized structures.

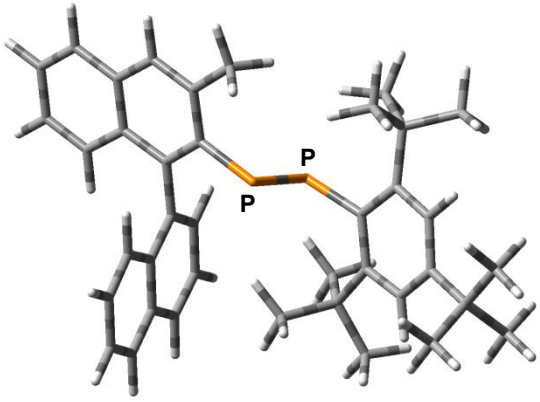
syn-(*S*)-**1**



C	6.74553200	-0.36268000	-0.39282600
C	2.76900500	2.17480100	2.64628700
C	4.38526000	-0.90982600	-0.55857000
C	2.66428700	1.79434300	0.25089300
C	2.70543700	0.92219000	-0.88211200
C	3.01066800	-0.53097500	-0.70747100
C	2.34007900	2.82798200	-2.34810900
C	2.31737000	3.68327000	-1.27909000
C	2.46427000	3.18898600	0.04450200
C	2.41673100	4.05262100	1.16967000
C	2.56534700	3.55955900	2.44132200
H	2.52653100	4.22962600	3.29474200
H	2.25981100	5.11548600	1.00218400
H	2.17360100	4.75109300	-1.42504100
C	7.06332800	-1.73508800	-0.26645900
C	6.06474900	-2.67424100	-0.28711400
C	4.70798500	-2.28643400	-0.43141400
H	8.09909100	-2.04064300	-0.15429900
H	6.29525500	-3.73237100	-0.19240200
C	3.66209600	-3.24187600	-0.45880300
H	3.92111200	-4.29499200	-0.36728600
C	2.81973700	1.31315500	1.57898500
H	2.96997200	0.24955100	1.73828200
C	5.44195500	0.04082000	-0.53707900
H	5.20781000	1.09563700	-0.63781300
H	2.88316600	1.79194000	3.65557800
H	7.54095200	0.37610400	-0.37631800
C	2.01140700	-1.48717800	-0.70724100
C	2.53682000	1.44043500	-2.14569900
P	0.22991000	-1.01931100	-0.97751000
P	-0.28197900	-0.61035600	0.94162100
C	-2.09834700	-0.26481800	0.66384400
C	-3.02263700	-1.33933900	0.66636600
C	-2.53969800	1.03796000	0.29253100
C	-4.27723700	-1.13425600	0.07495500
C	-3.81006500	1.16175300	-0.26865800
C	-4.68002800	0.08771200	-0.43970400
H	-4.95579100	-1.97338300	0.00532700
H	-4.14115700	2.13842100	-0.59978500
C	-1.73093000	2.34692100	0.47158200
C	-2.79695900	-2.75617900	1.25668100
C	2.34704200	-2.87874200	-0.59296100
H	2.21760600	3.20795800	-3.35749000
C	-2.48273700	-3.74073000	0.11883400
H	-3.31373400	-3.78746300	-0.59297900
H	-1.58818700	-3.43273300	-0.43047900
H	-2.31636400	-4.74776300	0.52050400
C	-1.69687100	-2.84615200	2.32929600
H	-0.68542700	-2.84669100	1.91808500
H	-1.77102200	-2.02990700	3.05632100
H	-1.80904300	-3.79062000	2.87244500
C	-4.08352200	-3.22976800	1.97204200
H	-4.39217300	-2.51192800	2.73933000
H	-4.92438000	-3.38666400	1.29359000
H	-3.88969400	-4.19042900	2.45966600
C	-0.90383700	2.65360500	-0.78714100
H	-0.43893500	3.64173700	-0.69059900
H	-0.10344800	1.92463700	-0.94143500
H	-1.54209500	2.65677700	-1.67775300
C	-0.80808800	2.32070600	1.70153000
H	0.07843100	1.69483000	1.57044800
H	-0.43091300	3.33103600	1.89168400
H	-1.34317600	1.97803900	2.59467700
C	-2.68613200	3.53944200	0.69625500
H	-3.23576500	3.81843400	-0.20693700
H	-3.40952400	3.33201700	1.49192000
H	-2.09729800	4.41446400	0.98739400
C	-6.03130900	0.30386900	-1.12388700
C	-6.83709000	-0.99402600	-1.23582100
H	-7.07372000	-1.40920400	-0.25002300
H	-7.78367000	-0.79537500	-1.74884500
H	-6.29679500	-1.75417800	-1.81029900
C	-6.85728000	1.31781100	-0.31441300
H	-6.34936300	2.28455800	-0.23985400
H	-7.82880300	1.48330300	-0.79397600
H	-7.03275400	0.94967900	0.70183300

C	-5.79883000	0.85170300	-2.54191400
H	-5.26189400	1.80526900	-2.52291800
H	-5.21105400	0.14655700	-3.13857500
H	-6.75828500	1.01573100	-3.04555400
H	2.57547000	0.77102200	-3.00079000
C	1.27564900	-3.93851600	-0.60688700
H	0.63515900	-3.87152700	0.28006300
H	0.62103600	-3.83963900	-1.48083400
H	1.72157300	-4.93630200	-0.62665300

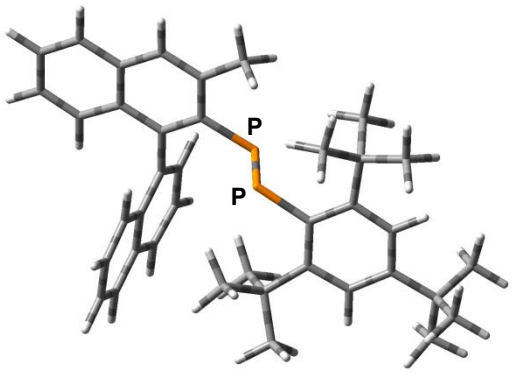
anti-(*S*)-**1**



C	-6.73811500	0.46824600	-0.71593000
C	-2.72825400	-2.68332400	2.93507900
C	-4.41836700	0.89903000	-0.13411200
C	-2.67730200	-1.95698500	0.61908000
C	-2.73265800	-0.93043600	-0.37546800
C	-3.05404400	0.47871000	0.00732300
C	-2.38143200	-2.60308800	-2.10657200
C	-2.34923300	-3.60503000	-1.17304300
C	-2.48185600	-3.30747000	0.20847100
C	-2.40918700	-4.32519200	1.19478600
C	-2.52600100	-4.02261800	2.52682000
H	-2.46282200	-4.80895300	3.27276300
H	-2.25433500	-5.35151700	0.87124000
H	-2.20520700	-4.64036300	-1.47244100
C	-7.07981200	1.79923700	-0.38084300
C	-6.11434700	2.65836300	0.07619600
C	-4.76932700	2.23014900	0.21561400
H	-8.10708600	2.13532400	-0.48294200
H	-6.36330100	3.68243400	0.34268000
C	-3.76357600	3.09765700	0.70745900
H	-4.04255100	4.11559500	0.97277200
C	-2.80557500	-1.67658000	2.00648200
H	-2.96409400	-0.64961000	2.32186400
C	-5.44369800	0.02901300	-0.59731600
H	-5.19281300	-0.99427600	-0.85554000
H	-2.82242400	-2.45329900	3.99180700
H	-7.50769600	-0.21110700	-1.06926500
C	-2.09638500	1.35069200	0.49817300
C	-2.57740400	-1.26111800	-1.70232000
P	-0.34478400	0.82170600	0.83513900
P	0.36276200	0.88337800	-1.06241400
C	2.15597000	0.48096600	-0.73590000
C	3.05289400	1.51331100	-0.36224300
C	2.60968700	-0.87212700	-0.75677900
C	4.28984900	1.14766500	0.18840100
C	3.86671900	-1.14645700	-0.22164700
C	4.70704500	-0.16756500	0.30453800
H	4.94539100	1.92967200	0.54508400
H	4.21556700	-2.17067800	-0.19954100
C	1.81647100	-2.07514600	-1.32917100
C	2.81990800	3.04395500	-0.48890200
C	-2.46362900	2.69141800	0.86121400
H	-2.26462700	-2.82965600	-3.16211400
C	2.40777600	3.61667300	0.87721000
H	3.18609800	3.43262100	1.62530700
H	1.48259300	3.15677500	1.23698900
H	2.25209000	4.70008600	0.80346200
C	1.78650200	3.46047100	-1.55103000
H	0.75177600	3.31848500	-1.23347400
H	1.93370600	2.92234400	-2.49392100
H	1.90121300	4.53036700	-1.75531700
C	4.13318900	3.73520800	-0.92593500
H	4.52452900	3.29018800	-1.84677300
H	4.91682300	3.69468300	-0.16667000
H	3.93534400	4.79482600	-1.11536500
C	0.81666300	-2.61740900	-0.29333000
H	0.40112500	-3.56884600	-0.64447700
H	-0.02034300	-1.93651300	-0.12773800
H	1.31297100	-2.79143300	0.66762400
C	1.08585400	-1.72769300	-2.63783700
H	0.25346500	-1.03247400	-2.50216000
H	0.65460400	-2.64141500	-3.06213500
H	1.77730500	-1.29724200	-3.37067700
C	2.76296800	-3.24069700	-1.68555000

H	3.17781500	-3.72869000	-0.79869200
H	3.59041600	-2.91416100	-2.32443500
H	2.19299800	-4.00191500	-2.22657100
C	6.04438800	-0.57186200	0.92790200
C	6.81647000	0.63314900	1.47393400
H	7.06671800	1.34609900	0.68071700
H	7.75509000	0.29371500	1.92406200
H	6.24544800	1.16072400	2.24557100
C	6.91435700	-1.26140700	-0.13650000
H	6.42836900	-2.15654500	-0.53735300
H	7.87417200	-1.56470000	0.29722300
H	7.11273900	-0.58224500	-0.97216500
C	5.78828600	-1.54805100	2.08816400
H	5.27461400	-2.45261200	1.74802900
H	5.16898300	-1.07956000	2.86001600
H	6.73773100	-1.85152000	2.54366700
H	-2.62671300	-0.47406800	-2.45058800
C	-1.43451500	3.65999300	1.38699900
H	-0.68294800	3.89536200	0.62446300
H	-0.89609700	3.24996500	2.24949200
H	-1.90796700	4.59598700	1.69413500

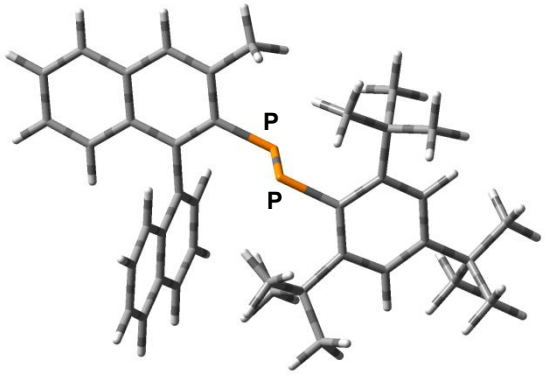
rac-**1** (X-ray)



P	-0.43235100	0.92288700	-0.84138800
P	0.38278100	1.03206900	1.01710100
C	2.10351700	1.52082100	0.53618200
C	-2.18926700	0.42909100	-0.50089200
C	3.10768900	0.56815500	0.60086700
C	4.76626100	2.26756200	-0.01933400
C	-3.21041300	1.42293100	-0.32420900
C	-4.82505700	-0.33629900	0.22145800
C	-6.25184300	-0.71618200	0.63794100
C	2.42125900	2.88338200	0.21850100
C	4.46964400	0.92322300	0.32488000
C	-2.54633700	-0.95041400	-0.43933600
C	2.79451000	-1.88291300	-0.00697100
C	2.66406400	-3.23882400	0.40652900
C	2.82557400	-0.84938400	0.98365300
C	-1.60738800	-2.15437000	-0.73651300
C	-3.01864500	2.95813300	-0.48108500
C	-0.75416500	-2.47436900	0.50208200
C	-2.42044600	3.54480800	0.80944100
C	1.36182900	3.95452300	0.16816600
C	-0.70608900	-1.92638800	-1.95840100
C	-6.68701000	0.12467300	1.84206000
C	-4.36452000	3.67880300	-0.70688500
C	-2.16352100	3.33053000	-1.70419000
C	-7.18116900	-0.44610500	-0.54530800
C	-6.37126600	-2.18428400	1.04037600
C	3.72095600	3.21787000	-0.04759600
C	6.10328900	2.63266800	-0.31729800
C	7.10566300	1.70335200	-0.25835700
C	6.82321900	0.37513900	0.11658200
C	5.53868900	-0.00907800	0.39948500
C	2.66138800	-1.18170500	2.30730300
C	2.49816200	-2.52121000	2.71417200
C	2.53149100	-3.52847400	1.78841900
C	2.62926100	-4.25753300	-0.57936500
C	2.68236100	-3.94802100	-1.90817700
C	2.79641000	-2.60390300	-2.32064700
C	2.86576700	-1.59727500	-1.39658200
C	-4.48441300	0.99822500	0.04334000
C	-3.85385000	-1.28144300	-0.05351100
C	-2.40898700	-3.42690000	-1.06773500
H	-4.11672600	-2.32389400	0.03904500
H	1.82043100	4.93715700	0.03284200
H	0.65917600	3.79178500	-0.65537900
H	0.77042500	3.97882800	1.09089000
H	3.96860700	4.24819000	-0.29572100
H	6.31423900	3.66351400	-0.58986500
H	8.12743900	1.98962700	-0.48956300
H	7.62912800	-0.34980800	0.17677300
H	5.32777800	-1.03527300	0.68290800
H	2.67974000	-0.39178900	3.05387700
H	2.37254400	-2.74811700	3.76814200

H	2.42826600	-4.56638800	2.09546200
H	2.53656900	-5.29079200	-0.25354900
H	2.63786700	-4.73653500	-2.65368800
H	2.83000800	-2.36871800	-3.38017000
H	2.95238800	-0.56168000	-1.71435000
H	-0.04241100	-1.68147500	0.73938700
H	-0.18060000	-3.39242700	0.32531900
H	-1.39503700	-2.63178600	1.37670600
H	-1.71189400	-4.19801500	-1.40875000
H	-2.92951200	-3.83797100	-0.19771800
H	-0.18732200	-2.86058000	-2.20147100
H	0.08087100	-1.18806100	-1.79947700
H	-1.29429800	-1.61788800	-2.83029400
H	-1.42965000	3.14071900	1.02105700
H	-3.06654700	3.31653200	1.66340900
H	-2.33576300	4.63503200	0.72135100
H	-1.11999300	3.02223800	-1.63298300
H	-2.57713800	2.88490800	-2.61565900
H	-2.16168000	4.41922500	-1.82663000
H	-4.16427400	4.72639700	-0.95116400
H	-4.92786900	3.23748600	-1.53596500
H	-4.99702100	3.67871100	0.18529600
H	-5.25802600	1.73818800	0.19461300
H	-3.14148700	-3.25319200	-1.86328000
H	-5.68158300	-2.43329700	1.85416200
H	-7.39044600	-2.38825100	1.38474100
H	-6.16968500	-2.85794700	0.20070200
H	-6.00985900	-0.02898400	2.68875600
H	-7.69710800	-0.16340500	2.15444500
H	-6.70828800	1.19500000	1.61713600
H	-8.21727100	-0.69615400	-0.28727700
H	-6.88880500	-1.04644300	-1.41317200
H	-7.15137300	0.60810700	-0.84085700

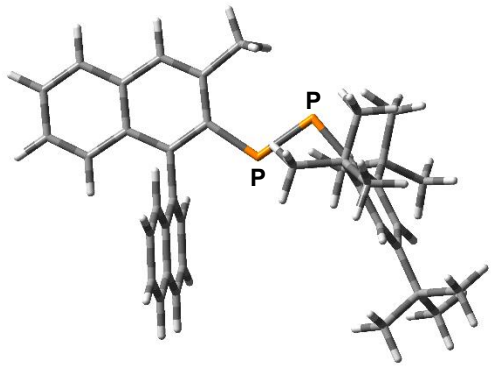
(*S*)-**1** (X-ray)



P	0.40528700	0.80743100	1.22081700
P	-0.22933800	1.16085500	-0.68022200
C	4.26618700	1.07273600	-0.21305100
C	-4.37209000	0.88025400	-0.58908800
C	-2.67123900	-1.83786200	0.07264500
C	3.11403600	1.42010200	0.51066100
C	-2.02191700	1.56481200	-0.44064900
C	2.56460700	-0.96559300	0.64715800
C	-3.77866800	3.21659500	-0.19835000
C	2.17866700	0.39510200	0.82010100
C	-2.60527100	-0.84251200	-0.96001900
C	-2.46458100	-3.20236900	-0.27394100
C	-6.70403300	0.22090600	-0.72065800
C	-2.43705300	2.92214800	-0.20800500
C	-2.93295500	-2.48533500	2.39380300
C	-2.91324800	-1.51178800	1.42939600
C	-2.31634600	-1.21461400	-2.24718600
C	6.80685900	-1.38993900	-0.55043600
C	-2.97370900	0.57380000	-0.64293700
C	-4.77750300	2.22530100	-0.37686700
C	5.36589000	-1.51523100	-2.59018100
C	-2.17437800	-3.53972500	-1.61946400
C	-2.52935500	-4.18814700	0.74059300
C	-1.42760000	4.00682400	0.06165100
C	-6.15927400	2.53399300	-0.36509700
C	4.57296500	-0.23258600	-0.56192300
C	-2.09172400	-2.57272200	-2.57985000
C	-2.74947900	-3.83948300	2.04518600
C	3.74097100	-1.22933800	-0.05188500
C	1.76146900	-2.19019600	1.15662400
C	1.96527000	3.22025300	2.00340000
C	2.72188900	3.76984400	-0.31793900
C	-5.37514900	-0.11037200	-0.76168500
C	3.01120900	2.91202200	0.92294300
C	6.49371500	0.62852500	-2.00712300
C	5.79716300	-0.60774400	-1.41485400
C	2.69136900	-3.37857600	1.45302100
C	-7.10734300	1.55962200	-0.52975400
C	4.36100100	3.34214800	1.54822600
C	0.78855000	-2.63214200	0.06107300

C	1.00010500	-1.92724400	2.44858200	H	4.58811300	2.73216500	2.42873400
H	-3.10244200	-2.21517800	3.43156800	H	5.20130300	3.26183300	0.85550500
H	-2.78429100	-4.60343400	2.81621000	H	1.63024500	-1.43332000	3.19728000
H	-2.37945800	-5.22895300	0.46329800	H	0.09899800	-1.32601100	2.30821000
H	-2.01227200	-4.58517900	-1.87035200	H	0.65648100	-2.87961800	2.86727300
H	-1.86190700	-2.83723800	-3.60728100	H	0.05976200	-1.85325700	-0.18016300
H	-2.27698600	-0.45482600	-3.02310700	H	0.23203500	-3.51897100	0.38823100
H	-3.06218600	-0.46995400	1.69931700	H	1.33011100	-2.88304100	-0.85798300
H	-5.08134800	-1.14164200	-0.92522300	H	2.10839300	-4.17627200	1.92282600
H	-7.45500500	-0.55258900	-0.84951800	H	3.13503600	-3.80672400	0.55035800
H	-8.16278600	1.81257200	-0.51240700	H	3.50088500	-3.09805300	2.13599200
H	-6.45430800	3.56983100	-0.21434500	H	4.01882900	-2.26105200	-0.23134400
H	-4.09759400	4.24400600	-0.03149200	H	4.93183100	1.86815600	-0.52623700
H	-1.89736200	4.99259700	0.01119600	H	5.80174400	1.22274400	-2.61341000
H	-0.60017100	3.98457800	-0.65663800	H	6.91038900	1.27289600	-1.22557400
H	-0.99288600	3.89314000	1.06073100	H	7.32106700	0.30991300	-2.64938400
H	1.77191300	3.47399700	-0.77519500	H	7.14218400	-0.78574000	0.29915500
H	3.50682400	3.65521900	-1.07227000	H	7.68393000	-1.66445900	-1.14736500
H	2.66270000	4.83020700	-0.04435800	H	6.36260100	-2.30955900	-0.15624100
H	0.94706300	3.24523200	1.61646700	H	6.24088500	-1.78357400	-3.19204100
H	2.16654300	4.21619600	2.41411700	H	4.90368600	-2.44206200	-2.23754000
H	2.01145200	2.50486800	2.83174200	H	4.64530600	-1.00178300	-3.23507900
H	4.29743100	4.38923600	1.86268300				

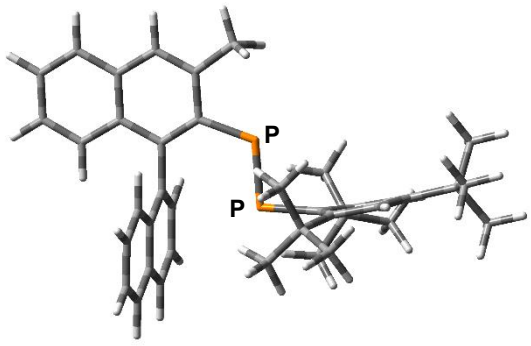
TS-A



C	4.36608035	0.73546368	0.26177807	C	4.02205179	-0.37737872	1.02200557
C	5.37063300	1.80084035	0.73764237	H	4.11538817	1.64381183	-1.64453648
C	6.59472951	1.82320203	-0.20875772	H	4.51431788	-0.51884246	1.97148626
H	7.10265691	0.85190992	-0.21460917	C	2.89510551	-2.57921108	1.53635638
H	7.31643962	2.58240534	0.11756688	C	2.39182191	0.11214295	-2.98480641
H	6.30957192	2.05699175	-1.23982232	C	1.00885558	0.79315395	-3.13375645
C	5.87749922	1.53509247	2.16808380	H	0.97055383	1.72986745	-2.56659302
H	6.56609842	2.33275137	2.46941750	H	0.18986578	0.16194193	-2.78855838
H	6.42212418	0.58675014	2.24044338	H	0.82631835	1.02816956	-4.19019512
H	5.05629661	1.51456011	2.89358914	C	2.39566127	-1.25031025	-3.71869104
C	4.68709268	3.18903447	0.72274279	H	1.66598130	-1.95614425	-3.31202038
H	3.82199099	3.20648160	1.39526270	H	3.38416148	-1.72090370	-3.66380711
H	4.33547098	3.45991919	-0.27820188	H	2.14692106	-1.10268895	-4.77666548
H	5.39041039	3.96449709	1.05093497	C	3.39283700	1.00046412	-3.76792107
C	3.79264051	0.83233777	-1.00750856	H	4.42448776	0.64514581	-3.67050794

H	3.35672883	2.05079439	-3.45957091
H	3.12927710	0.97363048	-4.83086039
C	1.68358298	-2.45092220	2.49168067
H	1.68173774	-3.28655637	3.20335253
H	0.73078700	-2.46161582	1.96106836
H	1.73800029	-1.51818500	3.06441762
C	2.78036525	-3.87825277	0.70472019
H	3.64903897	-4.00080067	0.04748167
H	1.88322706	-3.91140293	0.08000384
H	2.73562685	-4.74437167	1.37591506
C	4.14048222	-2.78665201	2.43860156
H	5.07082282	-2.79339921	1.86020157
H	4.05232423	-3.75481578	2.94359617
H	4.22728440	-2.02906376	3.22436361
C	2.36791508	-1.08790865	-0.60608707
C	2.82836987	-0.05823708	-1.49134945
C	3.06433081	-1.32259610	0.61853568
C	-6.83940787	0.02577606	0.95050956
C	-2.61482420	3.48610674	-1.46091098
C	-4.55733017	-0.62206085	0.38666246
C	-2.50550001	2.06627642	0.51666784
C	-2.64554489	0.79526613	1.16548923
C	-3.14047256	-0.41109842	0.41486019
C	-1.96817184	1.81094732	3.27770316
C	-1.81388883	3.03670118	2.67442774
C	-2.07834195	3.19784593	1.28835253
C	-1.93232967	4.45640859	0.64526126
C	-2.19364096	4.60114421	-0.69800945
H	-2.07709290	5.56990585	-1.17638587
H	-1.60702644	5.30797754	1.23853228
H	-1.48947308	3.90071710	3.24960389
C	-7.34143310	-1.11633016	0.28129826
C	-6.47296320	-1.99534158	-0.32407957
C	-5.07139646	-1.77144040	-0.28835572
H	-8.41272420	-1.29566533	0.24810461
H	-6.84700911	-2.87628241	-0.84041324
C	-4.15936337	-2.66048806	-0.90288606
H	-4.56214315	-3.53554575	-1.40888577
C	-2.76623603	2.25176125	-0.86882394
H	-3.08946033	1.40150768	-1.46080401
C	-5.48506120	0.26658442	1.00402377
H	-5.11278835	1.14315766	1.52156991
H	-2.81989119	3.60615759	-2.52129699
H	-7.52972346	0.71708323	1.42612697
C	-2.25425492	-1.30683889	-0.21731313
C	-2.38987428	0.69355766	2.52082018
C	-2.79518423	-2.46717472	-0.88834514
H	-1.76752747	1.69163997	4.33890906
H	-2.50919647	-0.26896838	3.01082347
C	-1.93867447	-3.49498156	-1.58055103
H	-1.21392350	-3.95422149	-0.89877110
H	-1.35846885	-3.06201104	-2.40336410
H	-2.56348160	-4.29288689	-1.99401245
P	-0.49169663	-0.75451189	-0.04872655
P	0.80277047	-2.04262105	-1.01363026

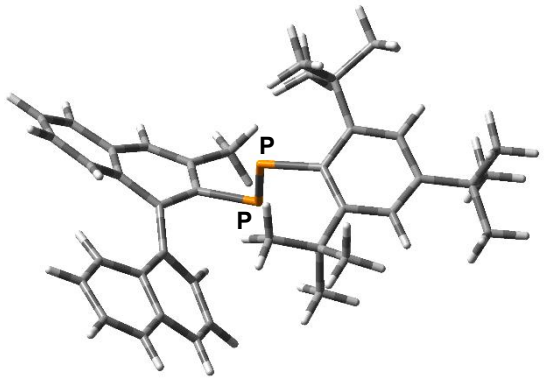
TS-B



C	-2.14755166	0.31685396	-0.27961459
C	-2.94622553	-0.31922295	-1.28766712
C	-2.76694277	0.75836112	0.92689836
C	-4.24826424	-0.69643934	-0.94483926
C	-4.07917164	0.32834165	1.18951574
C	-4.82329566	-0.44132617	0.30292482
H	-4.84871649	-1.21705520	-1.67756773
H	-4.53109951	0.60926226	2.12863414
C	-2.13707567	1.72536828	1.98325755
C	-2.49670886	-0.56798911	-2.76551890
C	-1.53027867	-1.77008836	-2.90453160
H	-1.95166874	-2.66475715	-2.43183441
H	-0.55574334	-1.58233027	-2.45300879
H	-1.36841635	-1.99250057	-3.96697814
C	-1.85163164	0.70604595	-3.36337161
H	-1.60602938	0.53629810	-4.41895248
H	-0.92486142	0.99405052	-2.85954281
H	-2.54315935	1.55477675	-3.30814156
C	-3.70644757	-0.88487313	-3.68117686
H	-4.48594917	-0.11793588	-3.61637385

H	-4.15818837	-1.85846253	-3.46240265
H	-3.36077424	-0.92180266	-4.72000689
C	-1.36823567	0.94851013	3.07866890
H	-0.49261038	0.43318680	2.67871947
H	-2.01384573	0.19781995	3.54868148
H	-1.02759924	1.64007830	3.86007759
C	-1.21123981	2.78469517	1.34421935
H	-1.72800094	3.33460481	0.54919968
H	-0.29399446	2.36710803	0.91946367
H	-0.89678248	3.50563254	2.10803179
C	-3.24487783	2.54301661	2.70318434
H	-3.84626637	1.93844316	3.38915549
H	-3.92048685	3.02886203	1.99053297
H	-2.77290666	3.32492638	3.30816185
C	-6.23902912	-0.95703535	0.61960336
C	-6.26408643	-2.49813310	0.48197530
H	-5.99060749	-2.82217176	-0.52755912
H	-7.26834845	-2.88451796	0.69594185
H	-5.56301427	-2.96504029	1.18312733
C	-7.25304891	-0.33867936	-0.37232510
H	-7.26125277	0.75447923	-0.29275643
H	-8.26608910	-0.70281088	-0.16038168
H	-7.01754016	-0.59598397	-1.41031982
C	-6.68958167	-0.59961340	2.04892963
H	-6.74756726	0.48414678	2.20136778
H	-6.01370996	-1.01591881	2.80461439
H	-7.68827364	-1.01110226	2.23470913
C	6.81513112	-0.91541662	-0.29670553
C	3.03739557	3.11394375	1.82208333
C	4.42712766	-1.23322904	0.09249630
C	2.83514662	1.72152421	-0.16721147
C	2.81981312	0.44206081	-0.81469725
C	3.05813721	-0.81823767	-0.04140862
C	2.48873617	1.54454325	-2.96535215
C	2.47746015	2.78089860	-2.36345081
C	2.65582315	2.90390194	-0.95992056
C	2.67109593	4.17293042	-0.32039187
C	2.85700464	4.27939087	1.03883396
H	2.86782978	5.25648842	1.51427012
H	2.53310469	5.06329893	-0.92953729
H	2.34154562	3.68338776	-2.95476480
C	7.10182113	-2.11350426	0.39921587
C	6.07527509	-2.85854022	0.93331743
C	4.72594739	-2.44055300	0.79601276
H	8.13183356	-2.44171734	0.51010271
H	6.28208391	-3.78124198	1.47044587
C	3.65661858	-3.19054265	1.33949127
H	3.89331157	-4.10931697	1.87218792
C	3.02675490	1.86850821	1.23438747
H	3.16673433	0.97921365	1.84058441
C	5.51504278	-0.48678061	-0.44710621
H	5.31148317	0.43219444	-0.98420786
H	3.18704498	3.20464049	2.89460388
H	7.62809607	-0.32880342	-0.71590488
C	2.01696145	-1.57856091	0.51077534
C	2.66603141	0.37712543	-2.18753718
C	2.34249811	-2.80251156	1.22004217
H	2.36406363	1.45621601	-4.04110968
H	2.67725584	-0.59382183	-2.67540453
C	1.28539409	-3.69116938	1.84626934
H	0.56764263	-4.06574756	1.10817533
H	0.70128588	-3.16644261	2.61033293
H	1.76106196	-4.55526756	2.32113182
P	0.18382148	-1.26841625	0.48514208
P	-0.28915565	0.46402885	-0.52721899

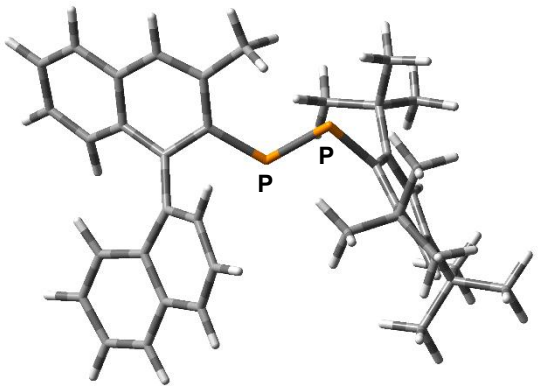
TS-C



C	1.99362082	2.63591068	-2.30685304
C	2.34243121	3.63180454	-1.43325786
C	3.17156338	3.32470186	-0.32461819
C	3.58563012	1.96422728	-0.06348703
C	2.95965693	0.88597365	-0.82673999
C	2.30977037	1.29829747	-2.00116436
H	3.29471590	5.39222079	0.27383926
H	1.45597469	2.85646794	-3.22449632
H	2.06423488	4.66711445	-1.61318856
C	3.66760651	4.39050297	0.47432240

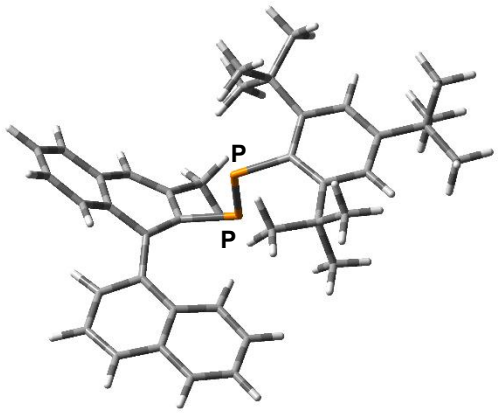
C	4.65958792	1.82709209	0.85813390
H	2.03997944	0.55027584	-2.73433916
C	5.16323170	2.88803790	1.58231269
C	4.62877042	4.18351195	1.43418208
H	5.16452500	0.88170506	0.94080662
H	5.99892742	2.72005312	2.25664653
H	5.00939901	5.01012756	2.02752729
C	2.91368138	-0.61211645	-0.62499857
C	3.92182635	-1.48321366	-0.03047101
C	1.83827161	-1.29031801	-1.25544841
C	4.60968231	-1.24230853	1.18960195
C	4.12714621	-2.77609576	-0.62087133
C	2.01338070	-2.60737732	-1.79598534
C	5.57641597	-2.10374186	1.67024690
H	4.29301861	-0.42210973	1.81681286
C	5.17934862	-3.60860342	-0.15498294
C	3.20403521	-3.26208866	-1.57906550
C	5.91779081	-3.27084380	0.95597808
H	6.05219240	-1.89318214	2.62439955
H	5.34639384	-4.55609911	-0.66198318
H	3.38837462	-4.22945597	-2.04129796
H	6.70293967	-3.92796564	1.31930202
P	0.09163651	-0.61450994	-1.34456799
P	-0.30792318	-0.64441013	0.67517145
C	-2.12376407	-0.18274628	0.65211370
C	-2.57027620	1.13904839	0.38428863
C	-3.09439077	-1.23682776	0.78167717
C	-3.90626920	1.31795882	-0.02276231
C	-4.40655073	-0.96439720	0.39083016
C	-4.83066490	0.28464372	-0.07976913
H	-4.22164632	2.31309304	-0.30524924
H	-5.14027320	-1.75647771	0.44307651
C	-2.80072046	-2.64472681	1.39400293
C	-1.75824106	2.46137955	0.54941664
C	0.93453595	-3.27708876	-2.62104920
H	0.56234603	-2.62947982	-3.42323609
H	0.06757952	-3.55580903	-2.00969083
H	1.32324961	-4.19192190	-3.08000472
C	-1.48671191	3.09195319	-0.83574137
H	-2.41832454	3.28921842	-1.37750105
H	-0.86970336	2.43216285	-1.45304684
H	-0.95393230	4.04452608	-0.72324924
C	-0.42222289	2.33528512	1.31094754
H	-0.54383225	1.80331472	2.26151632
H	-0.04973146	3.34032935	1.54363494
H	0.36316023	1.84376879	0.73567198
C	-2.60568897	3.45395571	1.39640093
H	-2.83705110	3.02960655	2.38008937
H	-3.55000072	3.73263399	0.92220495
H	-2.03708387	4.37816988	1.55214663
C	-1.98705791	-3.55895932	0.44461203
H	-0.96001427	-3.21598109	0.30853406
H	-2.45991197	-3.61262046	-0.54321021
H	-1.94435587	-4.57499032	0.85655858
C	-4.10704611	-3.41493684	1.70897409
H	-4.78224667	-2.83904773	2.35103838
H	-3.85128448	-4.33828200	2.23998968
H	-4.65214624	-3.70696147	0.80462773
C	-2.06714872	-2.49581891	2.74984804
H	-2.66212213	-1.89594271	3.44803729
H	-1.08501953	-2.02605317	2.65220371
H	-1.91081690	-3.48416512	3.19903158
C	-6.27655289	0.47153796	-0.57352185
C	-6.54545030	-0.50127065	-1.74653674
H	-7.57548176	-0.38922674	-2.10711222
H	-6.40829323	-1.54621941	-1.44949709
H	-5.86779804	-0.30106232	-2.58428859
C	-6.54720340	1.90417648	-1.07111859
H	-5.88146954	2.18083680	-1.89659978
H	-6.42799191	2.64471358	-0.27195831
H	-7.57756620	1.97935140	-1.43691355
C	-7.26390047	0.16849264	0.57881282
H	-7.15781876	-0.85659488	0.94894246
H	-8.29906104	0.29383735	0.23770384
H	-7.09975407	0.84739803	1.42347641

TS-C’



C	2.81352300	1.42049900	0.46986900
C	3.17319600	-0.01506500	0.21129500
C	4.39505000	-0.57220800	-0.35169700
C	3.09558000	2.66426000	-0.24919400
C	6.28167900	-0.65279200	-1.91729800
C	6.84240400	-1.75146500	-1.23453700
C	6.12590300	-2.33301300	-0.21346600
C	4.87038800	-1.81108300	0.19400800
C	2.27979500	3.82075200	0.03735900
C	2.43078100	5.01069000	-0.72285200
C	3.41836900	5.13892600	-1.67087100
C	4.32591400	4.07641800	-1.84265000
H	6.76385000	-0.26603500	-2.81110000
H	7.79078900	-2.17299900	-1.55546500
H	6.48205500	-3.24336500	0.26284700
C	4.16594900	2.89008000	-1.15423200
C	5.09874900	-0.08505000	-1.48624900
H	4.64164800	0.67233800	-2.10336100
C	4.03685100	-2.55628300	1.06216100
H	4.43285900	-3.46690600	1.50591000
C	2.70995900	-2.23484100	1.23254100
C	1.34698700	2.75023600	1.98356100
C	1.38603600	3.82693200	1.14070800
H	0.75949300	2.77020400	2.89602900
H	0.80575700	4.72409000	1.34092100
H	1.76483700	5.84202900	-0.50428200
H	3.53062100	6.05975600	-2.23611400
H	5.17812200	4.19246100	-2.50710700
H	4.93826400	2.14955400	-1.25185700
C	2.23516700	-0.97099500	0.72983000
C	2.04445700	1.57470700	1.63998000
H	1.99731100	0.75043300	2.33837600
C	1.83842600	-3.20476000	1.99017200
H	1.30143200	-2.72583100	2.81517400
H	1.07782800	-3.66303300	1.34756200
H	2.45125100	-4.01055200	2.40667600
P	0.48239500	-0.48405800	0.35733600
P	-0.88491100	-1.71651600	1.30506600
C	-2.40873000	-1.01608600	0.45498800
C	-2.77172200	-1.42542200	-0.86440200
C	-3.17946800	0.00293800	1.10704000
C	-3.69130900	-0.63017000	-1.56990800
C	-4.08768300	0.73194700	0.33304000
C	-4.31913200	0.48297000	-1.02205100
H	-3.92307200	-0.89728300	-2.58937400
H	-4.64134800	1.53533100	0.79844600
C	-3.13579800	0.31215200	2.63926100
C	-2.29630800	-2.73449200	-1.58130400
C	-3.26795400	-0.99622400	3.45661200
H	-4.19837900	-1.51804600	3.20465500
H	-2.43725300	-1.68597700	3.28775900
H	-3.28832700	-0.76482300	4.52878500
C	-1.85896700	1.07854400	3.06012300
H	-0.95846600	0.47010700	2.96784700
H	-1.72408200	1.97413400	2.44303900
H	-1.94523100	1.39447600	4.10790000
C	-4.32823900	1.19790700	3.07943700
H	-4.26832300	2.21586500	2.67883400
H	-5.29276400	0.76714500	2.78971500
H	-4.31759500	1.28378000	4.17155700
C	-0.94201200	-2.55785400	-2.30976800
H	-0.97145000	-1.69263500	-2.98160500
H	-0.11169800	-2.41440300	-1.61723500
H	-0.72638100	-3.44863000	-2.91391900
C	-2.21841900	-3.92647700	-0.59924700
H	-1.46631500	-3.79060400	0.18263000
H	-3.18380400	-4.09284400	-0.10720700
H	-1.95362500	-4.83889700	-1.14709200
C	-3.31854000	-3.17420900	-2.66458600
H	-4.33949400	-3.22236700	-2.27034000
H	-3.31765000	-2.51937000	-3.54203400
H	-3.04752000	-4.17453300	-3.01973200
C	-5.27854700	1.38526600	-1.81939000
C	-4.76425500	2.84399300	-1.77232500
H	-5.44009700	3.50561800	-2.32842600
H	-4.69905900	3.22029500	-0.74606600
H	-3.76682000	2.92163100	-2.21972200
C	-6.69364300	1.32176100	-1.19652600
H	-7.38616100	1.96480500	-1.75394700
H	-7.08604700	0.29860800	-1.22046800
H	-6.69615000	1.65577300	-0.15366800
C	-5.38790500	0.96681000	-3.29810100
H	-4.41523200	0.99623000	-3.80221900
H	-5.80042400	-0.04249600	-3.40874500
H	-6.05696000	1.65468100	-3.82771900

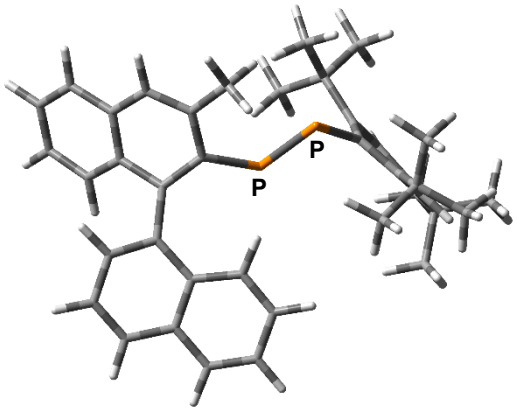
TS-D



C	2.68944484	1.05061720	-0.55805790	H	5.72512181	-0.29955556	2.71215751
C	2.05354549	2.41637744	-0.95668211	C	6.70000064	1.55627921	0.91804746
C	1.92089683	3.31739271	0.29254953	H	6.69104737	2.17610595	0.01414511
H	1.46626297	4.27919267	0.02528544	H	6.05451879	2.03119883	1.66569036
H	1.29041489	2.83995525	1.04872706	H	7.72314871	1.56413853	1.31059585
H	2.89444989	3.52232762	0.75044000	C	7.23434058	-0.48090565	-0.42875332
C	0.68512586	2.34057835	-1.66315975	H	8.26958123	-0.42701753	-0.06975101
H	-0.13595530	2.07877008	-0.99439243	H	7.01265422	-1.53084145	-0.64678021
H	0.44431234	3.32795869	-2.07555263	H	7.17166887	0.07652538	-1.37036932
H	0.69761520	1.63366013	-2.50070064	C	-1.96562273	-2.22702390	1.80708003
C	2.99746523	3.10760898	-1.98160367	C	-2.86558691	-3.17272717	1.37683147
H	3.99707173	3.30137714	-1.58464284	C	-3.67240927	-2.92447415	0.24125724
H	3.10881205	2.49395614	-2.88286676	C	-3.75532320	-1.58698107	-0.25605493
H	2.57124653	4.07269503	-2.28003165	C	-3.07460818	-0.49604389	0.44571777
C	2.08932417	-0.23291412	-0.64080364	C	-1.96256890	-0.90447980	1.22848808
C	2.92968379	-1.40164054	-0.58612894	H	-4.30175689	-4.97563368	-0.00266666
C	4.03106950	1.13233375	-0.13797428	H	-2.88543904	-4.15705905	1.83939946
C	4.25587002	-1.22851199	-0.18682364	C	-4.35484899	-3.97555174	-0.42656723
C	4.82011671	0.01870862	0.11047756	C	-4.41992969	-1.40397896	-1.50447968
H	4.46165206	2.11554621	-0.00363328	C	-5.02138408	-2.45253838	-2.16744565
H	4.88951863	-2.09947438	-0.09650230	C	-5.02331742	-3.74958891	-1.60736930
C	2.48936653	-2.83698123	-1.02412356	H	-4.42130378	-0.41996478	-1.95911884
C	1.53339435	-3.51964180	-0.01511091	H	-5.49028805	-2.27796010	-3.13207901
H	0.54406592	-3.05929265	0.01243731	H	-5.52148507	-4.56599549	-2.12322900
H	1.39590559	-4.57229829	-0.29203388	C	-3.74423004	0.85777487	0.37423712
H	1.95216449	-3.48880022	0.99783457	C	-3.22731891	2.19825139	0.62869820
C	3.70389510	-3.78795341	-1.16504681	C	-5.12637063	0.79439971	0.14774076
H	4.46707138	-3.38801327	-1.84123051	C	-1.97548955	2.49875450	1.22123046
H	4.17577160	-4.01388828	-0.20237240	C	-4.06930466	3.34188077	0.35683991
H	3.35743853	-4.73958049	-1.58231214	C	-5.95331299	1.91182377	-0.06816558
C	1.83522716	-2.78574696	-2.42752348	H	-5.60852519	-0.17174184	0.12601362
H	0.91376104	-2.19829219	-2.44540710	C	-1.54390076	3.78673220	1.46219947
H	2.52673377	-2.35606111	-3.16133424	H	-1.33783093	1.69394907	1.55564728
H	1.57919754	-3.80049752	-2.75559539	C	-3.57887466	4.66015054	0.55714418
C	6.26733481	0.10670923	0.62678504	C	-5.42053472	3.17283808	-0.03319662
C	6.39020811	-0.70268607	1.93998201	H	-7.00887204	1.75457689	-0.27184651
H	6.13219746	-1.75692409	1.79513940	C	-2.33649765	4.89202289	1.09575978
H	7.41847574	-0.65989949	2.31978461	H	-0.58646538	3.94332119	1.94916684

H	-4.23626339	5.49005297	0.30871678
H	-6.02792253	4.05230227	-0.23147487
H	-1.98376831	5.90520883	1.26705903
C	-0.99039288	-2.60166138	2.90952508
H	0.01427278	-2.81756646	2.52754830
H	-0.88877150	-1.80852971	3.65793542
H	-1.34531181	-3.50219861	3.42168910
P	-0.23773756	-0.17209390	1.31822297
P	0.23563172	-0.50643381	-0.66154653

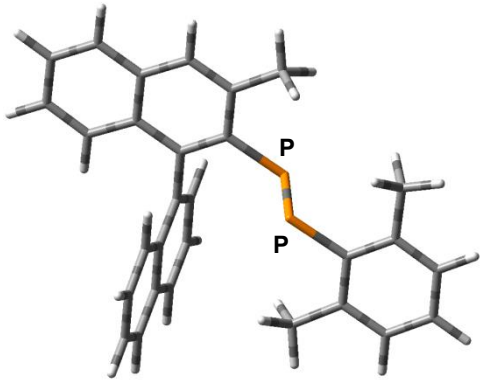
TS-D’



C	2.31726406	-1.84065233	2.27721757
C	3.40046054	-2.66541385	2.07984342
C	4.19033133	-2.55448938	0.91329284
C	4.05361228	-1.37502447	0.11533799
C	3.14042109	-0.31507728	0.52668087
C	2.05433459	-0.74520262	1.36530882
H	5.19989284	-4.44621117	1.16690776
H	3.60303120	-3.46956871	2.78353425
C	5.09025156	-3.57911222	0.52002757
C	4.75057146	-1.35313814	-1.13088345
C	5.56923080	-2.39059872	-1.52060879
C	5.77256359	-3.50284047	-0.67212120
H	4.59886874	-0.51648923	-1.80264393
H	6.05506919	-2.35421117	-2.49179688
H	6.44029185	-4.30453451	-0.97572156
C	3.53181313	1.08249324	0.11779605
C	2.74352070	2.29999622	-0.05988970
C	4.91746435	1.24933732	-0.03604286
C	1.41987477	2.50860968	0.40439008
C	3.36204289	3.44573299	-0.68728226
C	5.52665469	2.40140385	-0.56405379
H	5.57491748	0.44141170	0.25145429
C	0.71107941	3.66591594	0.16191887
H	0.95185458	1.75596332	1.01821775
C	2.59720651	4.61022953	-0.96863231
C	4.75175974	3.45911253	-0.96254343
H	6.60726366	2.42485146	-0.67328695
C	1.28615560	4.72135277	-0.57342564
H	-0.29610992	3.76268840	0.55684965
H	3.09278271	5.43359808	-1.47755143
H	5.18917188	4.33862272	-1.42833041
H	0.71611899	5.62182794	-0.78449856
C	1.45334104	-2.09597169	3.48865379
H	1.14388177	-1.16752627	3.97758264
H	0.53600839	-2.64820409	3.24933250
H	2.01371934	-2.69337828	4.21530184
P	0.34631934	-0.38041768	0.76593256
P	-1.11779803	-0.92720048	2.13035376
C	-2.55639176	-0.66382531	0.96216115
C	-2.76974170	-1.50164394	-0.16752312
C	-3.38427261	0.49869004	1.13858394
C	-3.57047287	-1.00417053	-1.21410256
C	-4.18571566	0.89658876	0.06779868
C	-4.24594818	0.20623899	-1.14985573
H	-3.66077139	-1.60156112	-2.11118938
H	-4.78479057	1.79083953	0.16894699
C	-2.29261668	-2.97822559	-0.36851272
C	-3.49044561	1.31265839	2.46725726
C	-3.73966136	0.35874394	3.66172091
H	-4.65094271	-0.22913007	3.50267119
H	-2.91345282	-0.33668179	3.82886039
H	-3.86775001	0.94066090	4.58265732
C	-2.24151384	2.18778390	2.73146842
H	-2.40458098	2.81236853	3.61869544
H	-1.34038034	1.59602945	2.90477026
H	-2.05138773	2.85277840	1.88066042
C	-4.69605209	2.28421088	2.45041082
H	-4.57152412	3.09784088	1.72741498
H	-5.63835328	1.76923565	2.23421576
H	-4.78957447	2.74677191	3.43903737
C	-1.26942558	-3.06690346	-1.52500483
H	-1.67894974	-2.67290010	-2.46134351
H	-0.36373931	-2.49777618	-1.29161023
H	-0.98261721	-4.11180657	-1.69879886
C	-1.68943339	-3.67917859	0.86865348
H	-0.67183380	-3.35781767	1.09246109

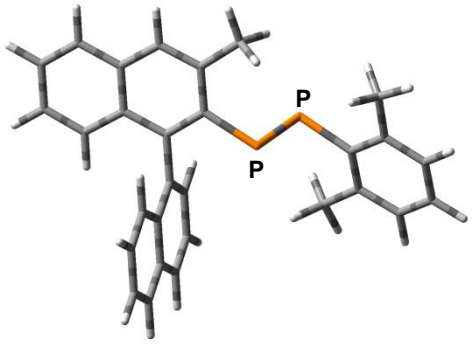
H	-2.30469362	-3.53543210	1.76403961
H	-1.64424631	-4.75749846	0.67247028
C	-3.54117903	-3.83385567	-0.73409832
H	-4.28842927	-3.79450211	0.06683983
H	-4.02765198	-3.51664270	-1.65942157
H	-3.24202606	-4.88007438	-0.86695181
C	-5.07901548	0.77076453	-2.31452942
C	-4.55164226	2.17798048	-2.68391788
H	-5.13793948	2.60074299	-3.50918313
H	-4.61629471	2.87230427	-1.83966341
H	-3.50304030	2.13266230	-2.99908445
C	-6.56347373	0.87565539	-1.89041734
H	-7.16731591	1.28209700	-2.71126605
H	-6.96602146	-0.10938229	-1.62773774
H	-6.69569875	1.53218381	-1.02402331
C	-5.00215827	-0.11214489	-3.57459372
H	-3.97189963	-0.22302584	-3.93141522
H	-5.41384364	-1.11274816	-3.39962219
H	-5.58516245	0.34553865	-4.38189183

syn-(*S*)-**1**$_{\mathbf{Dmp}}$



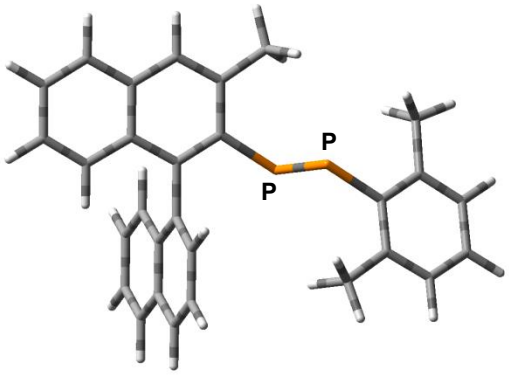
C	-5.52475700	0.05183300	-0.14687900
C	-0.90495800	2.67652200	-2.43223400
C	-3.22349100	-0.69384800	0.14454400
C	-1.12851400	1.93854500	-0.12058100
C	-1.41628200	0.93141900	0.85905800
C	-1.84547700	-0.45030200	0.45848600
C	-0.92356200	2.53507500	2.63421000
C	-0.64461700	3.51592500	1.71216100
C	-0.73744200	3.24740800	0.31997400
C	-0.44531300	4.24380500	-0.64968400
C	-0.52659500	3.96816300	-1.99603000
H	-0.29890100	4.73971800	-2.72656600
H	-0.15203500	5.23321600	-0.30626400
H	-0.34769700	4.51122200	2.03447700
C	-5.92022300	-1.26437100	-0.48450000
C	-4.99003100	-2.27848700	-0.50359700
C	-3.62793600	-2.02417700	-0.19167000
H	-6.95946200	-1.47113600	-0.72564300
H	-5.28495300	-3.29402700	-0.75764800
C	-2.65845300	-3.05801400	-0.19142000
H	-2.98210400	-4.06781900	-0.43662600
C	-1.19910500	1.68779700	-1.51829100
H	-1.48883000	0.70010600	-1.86086700
C	-4.21139100	0.33011200	0.16108200
H	-3.91836600	1.34163800	0.42099400
H	-0.96324100	2.46323300	-3.49604300
H	-6.26401100	0.84812500	-0.13002100
C	-0.91937900	-1.48939700	0.42798600
C	-1.31268400	1.24496400	2.20376500
P	0.83617700	-1.14835700	0.95806500
P	1.74851500	-0.86933700	-0.85721400
C	3.50110200	-0.55107200	-0.31926700
C	4.41724400	-1.62565700	-0.23831000
C	3.94093800	0.77674900	-0.10955400
C	5.75552200	-1.35552900	0.06947900
C	5.28844500	1.00331000	0.19559900
C	6.19185100	-0.05167100	0.28900600
H	6.46024500	-2.18135700	0.13362400
H	5.62800300	2.02351900	0.35871700
C	-1.33438200	-2.82736200	0.11032500
H	-0.85068100	2.74351300	3.69796400
H	-1.53928500	0.48161700	2.94290000
C	-0.35293200	-3.97669400	0.10264300
H	0.38126900	-3.87810700	-0.70546700
H	0.21515900	-4.03172200	1.04013200
H	-0.87515900	-4.92928500	-0.03042200
C	2.99506700	1.95364100	-0.19392100
H	2.38630000	1.92959300	-1.10623900
H	2.29251600	1.97013800	0.64771700
H	3.54918600	2.89771200	-0.18479000
C	3.98836100	-3.05804900	-0.46871500
H	3.33030800	-3.41683800	0.33189300
H	3.43285600	-3.17129300	-1.40866400
H	4.85710300	-3.72254600	-0.51124100
H	7.23535400	0.14235800	0.52331300

anti-(*S*)-**1**$_{\mathbf{Dmp}}$



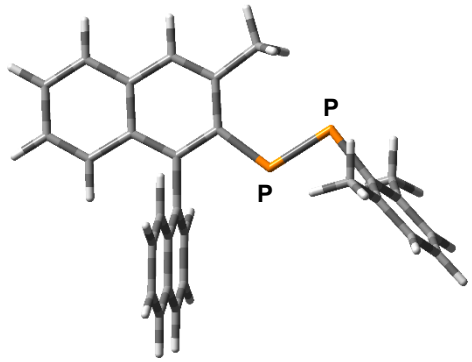
C	5.29862200	-0.87409200	-1.19123900	C	0.93522500	1.31339000	-1.72932700
C	2.58603200	2.60471700	2.66615500	P	-0.96957500	-0.48948500	0.63867200
C	2.98512100	-1.07493000	-0.45449700	P	-2.22576300	-1.32266800	-0.75259500
C	1.76452400	1.93223200	0.47345500	C	-3.81907500	-0.46154300	-0.32464500
C	1.44099900	0.92778400	-0.49993000	C	-4.72219700	-1.05525100	0.58737200
C	1.68218800	-0.52652300	-0.21446200	C	-4.17409100	0.72632500	-1.00558300
C	0.72218600	2.67524500	-2.04589700	C	-5.95759800	-0.43894200	0.81808500
C	1.01859000	3.65341500	-1.12536600	C	-5.41910700	1.31085000	-0.74589300
C	1.54306400	3.31250000	0.14945900	C	-6.30609400	0.73822300	0.16158800
C	1.85797300	4.30804200	1.11335600	H	-6.65220000	-0.89417000	1.52022400
C	2.36825700	3.96557200	2.34433400	H	-5.69225400	2.22537400	-1.26710100
H	2.60394200	4.73702400	3.07240500	C	0.89316500	-2.71251100	0.58336900
H	1.68565200	5.35116500	0.85829500	H	0.32578500	2.94116400	-3.02199800
H	0.85720400	4.70266600	-1.36133500	H	0.69938200	0.55051300	-2.46602300
C	5.52245400	-2.24011100	-0.89703900	C	-0.18047300	-3.60252700	1.16766100
C	4.50029300	-3.01164800	-0.39261100	H	-0.96998100	-3.82196700	0.44041400
C	3.21437100	-2.45547100	-0.16097800	H	-0.66855700	-3.13672200	2.03246300
H	6.50206100	-2.67679300	-1.07194600	H	0.24933000	-4.55412600	1.49547400
H	4.66184100	-4.06268000	-0.16450300	C	-3.24234600	1.38190000	-2.00032800
C	2.15092500	-3.23047600	0.36552900	H	-2.87093700	0.66315300	-2.74227700
H	2.34634000	-4.27348200	0.60736000	H	-2.36061700	1.81158000	-1.51018400
C	2.29141700	1.61462400	1.75534700	H	-3.75268300	2.18656400	-2.53939400
H	2.45938500	0.57341700	2.01042900	C	-4.38803700	-2.33382300	1.32345300
C	4.06245800	-0.30574100	-0.97637100	H	-3.59468200	-2.17825500	2.06444000
H	3.89911800	0.74084500	-1.20982100	H	-4.03447500	-3.11695900	0.64061600
H	2.98768300	2.34044200	3.64065100	H	-5.26618700	-2.72010400	1.85041000
H	6.10854300	-0.27034100	-1.59170500	H	-7.27060300	1.20276900	0.34936000
C	0.65065300	-1.33102600	0.26710100				

anti-(*R*)-**1**$_{\mathbf{Dmp}}$



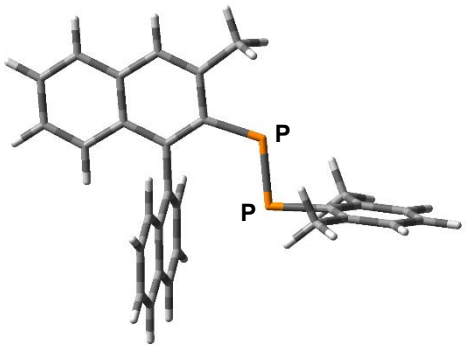
C	-5.29822900	-0.87482000	-1.19115900	C	-0.93506800	1.31332400	-1.72897200
C	-2.58748100	2.60450000	2.66595500	P	0.96992300	-0.48935400	0.63879300
C	-2.98472600	-1.07532100	-0.45434100	P	2.22600600	-1.32257200	-0.75255800
C	-1.76509800	1.93208100	0.47356000	C	3.81929000	-0.46124300	-0.32497900
C	-1.44098800	0.92764800	-0.49965900	C	4.72256000	-1.05474100	0.58702600
C	-1.68191000	-0.52669600	-0.21419400	C	4.17399000	0.72674000	-1.00587200
C	-0.72233900	2.67522000	-2.04558500	C	5.95781500	-0.43812700	0.81775100
C	-1.01923500	3.65336600	-1.12519000	C	5.41885900	1.31157300	-0.74616900
C	-1.54395500	3.31238700	0.14952100	C	6.30602200	0.73913000	0.16126300
C	-1.85942400	4.30791000	1.11325300	H	6.65248900	-0.89317300	1.51993100
C	-2.36996400	3.96538800	2.34411200	H	5.69175200	2.22622100	-1.26728900
H	-2.60608900	4.73682600	3.07205400	C	-0.89254600	-2.71260300	0.58353500
H	-1.68733300	5.35106200	0.85815600	H	-0.32578000	2.94117800	-3.02161000
H	-0.85812700	4.70264800	-1.36120400	H	-0.69885000	0.55046400	-2.46556800
C	-5.52184900	-2.24089700	-0.89706100	C	0.18126300	-3.60253000	1.16765900
C	-4.49957900	-3.01229800	-0.39264100	H	0.97066800	-3.82188300	0.44026600
C	-3.21376000	-2.45591800	-0.16090800	H	0.66945100	-3.13670900	2.03238700
H	-6.50137600	-2.67772700	-1.07204000	H	-0.24840600	-4.55417400	1.49551900
H	-4.66096100	-4.06337200	-0.16460900	C	3.24192800	1.38227700	-2.00034700
C	-2.15020900	-3.23077700	0.36559900	H	2.87055900	0.66358300	-2.74234800
H	-2.34544200	-4.27384600	0.60730300	H	2.36015900	1.81162300	-1.50996200
C	-2.29234700	1.61442500	1.75529300	H	3.75195600	2.18718800	-2.53932000
H	-2.46013200	0.57319400	2.01039300	C	4.38865000	-2.33330800	1.32322300
C	-4.06217000	-0.30627700	-0.97620000	H	3.59518000	-2.17785500	2.06411600
H	-3.89899900	0.74035400	-1.20957100	H	4.03535900	-3.11660500	0.64043600
H	-2.98934200	2.34017800	3.64035100	H	5.26683800	-2.71929700	1.85032300
H	-6.10823100	-0.27117200	-1.59162100	H	7.27037400	1.20397700	0.34907900
C	-0.65027600	-1.33104600	0.26740800				

TS-A_{Dmp}



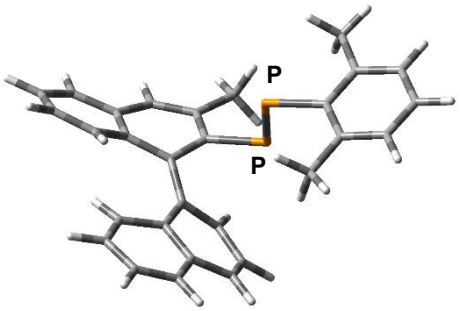
C	5.56991900	-0.35407400	-0.47033800	C	1.36205000	1.14181000	-2.15311100
C	1.49068500	2.95159400	2.36502100	P	-0.88809800	-0.61645100	-0.12066400
C	3.19414100	-0.84514400	-0.22756700	P	-2.38863000	-1.93495800	0.39819400
C	1.42630100	2.02050700	0.11399200	C	-3.80882400	-0.76567700	0.10395800
C	1.50490400	0.91541100	-0.79633900	C	-4.28936700	0.04398400	1.15969000
C	1.81315600	-0.47337400	-0.30739600	C	-4.48267500	-0.78369200	-1.13976100
C	1.11451200	2.43752300	-2.66221700	C	-5.42633200	0.83265600	0.94727600
C	1.02061600	3.51021900	-1.80746400	C	-5.61548200	0.02044400	-1.31112200
C	1.17491200	3.33355100	-0.40670200	C	-6.08563000	0.82730400	-0.27870300
C	1.08813700	4.42861300	0.49446700	H	-5.79553800	1.45602800	1.75834500
C	1.24211400	4.24588800	1.84963900	H	-6.13243900	0.00812700	-2.26788800
H	1.17253300	5.09277000	2.52698700	C	1.15266100	-2.71159700	0.47115100
H	0.89521200	5.41966300	0.09018500	H	0.99852100	2.57686400	-3.73352000
H	0.82867300	4.50938400	-2.19130000	H	1.43503200	0.30302800	-2.84010500
C	5.89581300	-1.66315200	-0.04082500	C	0.13941700	-3.76034500	0.84869900
C	4.89502400	-2.54774500	0.28978600	H	-0.55028700	-3.98231500	0.02628200
C	3.53058500	-2.16401500	0.20686100	H	-0.48050000	-3.45001600	1.69774200
H	6.93732200	-1.96595000	0.02604700	H	0.64298600	-4.69212600	1.12443600
H	5.13377000	-3.55592900	0.61999800	C	-4.00748400	-1.64092900	-2.29191800
C	2.48493500	-3.05613500	0.54006200	H	-3.84124400	-2.68133700	-1.98501700
H	2.75370100	-4.05957500	0.86383600	H	-3.05615800	-1.27826300	-2.69999900
C	1.57956400	1.86801900	1.51946900	H	-4.74166400	-1.64237700	-3.10388000
H	1.77027900	0.87884800	1.92340300	C	-3.60617500	0.08809400	2.50868400
C	4.25572600	0.04482500	-0.56305400	H	-2.63497000	0.59461500	2.45274900
H	4.01822500	1.04895300	-0.89490100	H	-3.41422100	-0.91815000	2.90182900
H	1.61158700	2.81312500	3.43608500	H	-4.22213100	0.62345900	3.23826200
H	6.36449300	0.34038000	-0.72911100	H	-6.96907000	1.44316100	-0.42613700
C	0.79126500	-1.37976600	0.04154800				

TS-B_{Dmp}



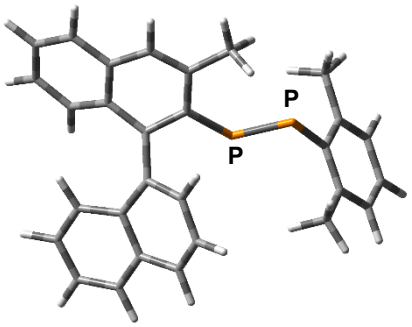
C	5.46505500	0.09147700	-0.61085900
C	1.24477100	2.87989000	2.38811400
C	3.19546100	-0.72090400	-0.23385600
C	1.12917800	1.89487200	0.16286800
C	1.27228900	0.78539500	-0.73449600
C	1.77051300	-0.54074800	-0.24754900
C	0.60300900	2.21427100	-2.59466400
C	0.44115400	3.28750200	-1.75040600
C	0.70314300	3.16091600	-0.36052900
C	0.56028700	4.26199600	0.52631800
C	0.82337400	4.12811800	1.87011700
H	0.70967100	4.97864500	2.53686300
H	0.23616700	5.21741300	0.12016400
H	0.11709100	4.25125000	-2.13608200
C	5.99398900	-1.14814700	-0.18008300
C	5.14495400	-2.15573300	0.21766600
C	3.73819300	-1.96915100	0.20197200
H	7.06977000	-1.30101800	-0.16429900
H	5.53949200	-3.11268300	0.55109300
C	2.84839100	-2.99121000	0.60913300
H	3.27126900	-3.93675000	0.94233200
C	1.39439800	1.79275200	1.55640100
H	1.71798900	0.83880800	1.96038400
C	4.10419800	0.30027600	-0.63773300
H	3.71315100	1.25440000	-0.97113700
H	1.45284500	2.78112800	3.45013800
H	6.13875800	0.88488900	-0.92273400
C	0.91151700	-1.57274000	0.15818000
C	1.02543300	0.96558100	-2.08341700
P	-0.94392300	-1.60207200	0.19446100
P	-1.75959700	0.22694900	-0.28094700
C	-3.54195400	-0.29400700	-0.09245800
C	-4.26319600	-0.76251500	-1.21516200
C	-4.20485000	-0.08528000	1.13949200
C	-5.63017800	-1.03261000	-1.08142900
C	-5.57315100	-0.36654100	1.23156200
C	-6.28410000	-0.84106600	0.13267000
H	-6.18425000	-1.39471400	-1.94442800
H	-6.08278000	-0.20694700	2.17907000
C	1.48240300	-2.83184800	0.59888400
H	0.41089900	2.31859400	-3.65903100
H	1.15525800	0.12629200	-2.76143900
C	0.63019600	-3.99811000	1.05938500
H	-0.04625200	-4.35339600	0.27421500
H	0.00174400	-3.73848600	1.91848800
H	1.27247200	-4.83428900	1.35351700
C	-3.47333200	0.42521100	2.36126700
H	-2.86628700	1.31074600	2.13467700
H	-2.78702900	-0.32926300	2.76502600
H	-4.17973000	0.69364600	3.15337400
C	-3.59589500	-0.98429100	-2.55457200
H	-2.90936500	-1.83918700	-2.52740900
H	-3.00178700	-0.11442300	-2.86238000
H	-4.34075400	-1.17673300	-3.33341900
H	-7.34705000	-1.05118100	0.21941300

TS-C_{Dmp}



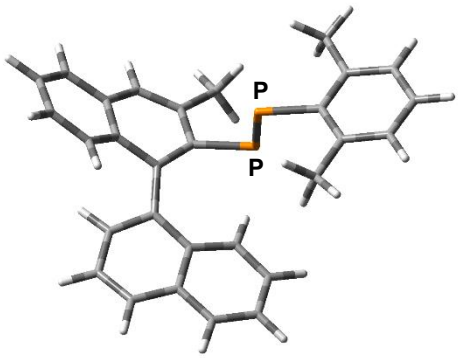
C	0.16163900	2.19706800	-2.49508300	H	4.96534800	-0.89530400	2.83819200
C	0.34726700	3.33611700	-1.75686800	H	4.42497400	-4.22334600	0.18818800
C	1.26607200	3.32004800	-0.67487000	H	2.40262100	-4.37068400	-1.11555300
C	1.92590400	2.09532300	-0.28437600	H	5.77457700	-3.08380800	1.93180100
C	1.45482100	0.83956400	-0.86225900	P	-1.19194100	-0.97129700	-1.10003700
C	0.72053600	0.98160300	-2.05050400	P	-1.68255100	-0.67869500	0.87358900
H	1.05507400	5.43821000	-0.33181700	C	-3.47773200	-0.21239500	0.69760600
H	-0.43513100	2.20507400	-3.40252400	C	-3.84381600	1.15330800	0.64770900
H	-0.12277100	4.27579600	-2.03561500	C	-4.47698900	-1.21319900	0.74183000
C	1.60864000	4.54702700	-0.04562900	C	-5.20164500	1.49274100	0.62076500
C	3.06300800	2.25840200	0.55320000	C	-5.82349300	-0.83125600	0.71376600
H	0.57447900	0.11237300	-2.67818900	C	-6.18804200	0.51079600	0.64930200
C	3.41297700	3.47399200	1.10475800	H	-5.48300300	2.54256700	0.58092900
C	2.64577700	4.62905100	0.85272900	H	-6.59172200	-1.60033500	0.74646700
H	3.73336800	1.42889100	0.69695300	H	-7.23815100	0.79099100	0.63171300
H	4.30647000	3.54017700	1.71998200	C	-4.13348600	-2.68490400	0.81575100
H	2.90753000	5.57732900	1.31361700	H	-3.41191500	-2.89620300	1.61475400
C	1.60395800	-0.59860100	-0.42552000	H	-3.68291000	-3.04259100	-0.11799800
C	2.71276400	-1.23386800	0.27618000	H	-5.03016500	-3.28356100	1.00525800
C	0.59670600	-1.48505500	-0.88589800	C	-2.80789100	2.25480000	0.61817600
C	3.41486900	-0.68702500	1.38431500	H	-2.25207600	2.26717900	-0.32691300
C	3.03177300	-2.59369300	-0.05874800	H	-2.06378800	2.13539800	1.41565800
C	0.88461700	-2.86266600	-1.15442200	H	-3.27968700	3.23492900	0.74277100
C	4.48016600	-1.33923600	1.97296100	C	-0.14557200	-3.78290000	-1.77343900
H	3.04140000	0.21194000	1.85069300	H	-0.60023100	-3.35453500	-2.67430500
C	4.17828500	-3.21326900	0.50677400	H	-0.96389800	-3.99984700	-1.07558600
C	2.13647600	-3.34864200	-0.85473400	H	0.31446500	-4.73704200	-2.04992400
C	4.91449700	-2.59041600	1.48789100				

TS-C'$_{Dmp}$



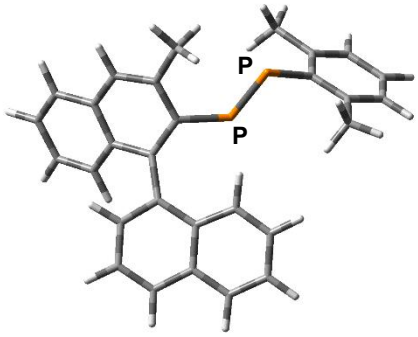
C	-1.57200700	0.90569500	-0.58770600	H	-4.06896800	1.43674600	0.63525000
C	-1.75651400	-0.54432700	-0.23653900	C	-0.60555100	-1.36203200	-0.48532800
C	-2.95930000	-1.24856600	0.18401400	C	-0.63325800	1.08757700	-1.62267500
C	-2.14964500	2.14335800	-0.05989200	H	-0.35599400	0.23230900	-2.22303300
C	-5.07413000	-1.49925000	1.40192400	P	0.97423800	-0.54626900	0.05465500
C	-5.31577800	-2.74647200	0.79041800	P	2.63890200	-1.38463700	-0.83515900
C	-4.33543100	-3.29531200	-0.00389700	C	0.37600700	-3.62321300	-1.30522800
C	-3.12260700	-2.60301800	-0.26007500	H	0.92263900	-3.19939600	-2.15362400
C	-1.45565500	3.38410700	-0.31292300	H	1.11011200	-3.77988200	-0.50694100
C	-1.90418500	4.59071600	0.28624100	H	-0.00455600	-4.60425500	-1.60635500
C	-3.06380900	4.64028000	1.02384200	C	3.91710600	-0.42619300	0.12817400
C	-3.84039900	3.47129000	1.13297600	C	4.44947200	-0.96507000	1.32380900
H	-5.77261300	-1.11204400	2.13892200	C	4.44889800	0.77260800	-0.40306200
H	-6.23034900	-3.29409500	0.99961500	C	5.48915200	-0.28815300	1.97275900
H	-4.44694900	-4.30005700	-0.40452400	C	5.48887500	1.41834300	0.27596300
C	-3.39564400	2.27391300	0.60781500	C	6.00654300	0.89730200	1.45838300
C	-3.93394000	-0.77878100	1.10552700	H	5.89604900	-0.70261100	2.89225200
H	-3.72753400	0.10820900	1.68271600	H	5.89527100	2.34028400	-0.13370400
C	-2.03294600	-3.27936600	-0.85858500	H	6.81657700	1.40841200	1.97238300
H	-2.18911400	-4.29447000	-1.21647800	C	3.91911200	1.38286900	-1.68143700
C	-0.76613300	-2.74235400	-0.86105300	H	3.86138000	0.64531500	-2.49147500
C	-0.05025300	2.32709600	-1.95925300	H	2.90711900	1.78317700	-1.54481900
C	-0.38307700	3.44341900	-1.24242900	H	4.56241400	2.20328600	-2.01613800
H	0.68130000	2.36850300	-2.76067200	C	3.92655300	-2.25037900	1.92620000
H	0.09915400	4.39998200	-1.42684200	H	3.87894200	-3.05736900	1.18457300
H	-1.32496200	5.49354500	0.10817100	H	4.56911100	-2.58316100	2.74775400
H	-3.40279800	5.57330000	1.46483500	H	2.91128600	-2.12772500	2.32216200
H	-4.81336200	3.50907200	1.61574300				

TS-D_{Dmp}



C	-0.95542500	-2.35177900	1.58324200	H	1.56246800	3.44798600	1.84481300
C	-2.03727400	-3.09677000	1.17797700	H	-1.52343800	5.66882700	-0.14801500
C	-2.84964800	-2.65376700	0.10956500	H	-3.63010500	4.66207800	-0.59508000
C	-2.70082400	-1.30877700	-0.35334900	H	0.74276200	5.60723300	0.86256500
C	-1.79738600	-0.38759100	0.34123600	P	1.03816700	-0.51475800	1.21027500
C	-0.75581400	-1.01996200	1.06949800	P	1.58379900	-0.84257700	-0.74087300
H	-3.87367900	-4.53905200	-0.13585800	C	0.01125800	-2.96688800	2.57906400
H	-2.20629300	-4.08554700	1.59865500	H	0.92491100	-3.33787300	2.09756700
C	-3.75546400	-3.53585100	-0.53849600	H	0.31950600	-2.25779600	3.35512600
C	-3.36883200	-0.97432100	-1.56913000	H	-0.46264300	-3.81998600	3.07578000
C	-4.19114200	-1.87000700	-2.21832300	C	3.41213200	-0.49888100	-0.64142700
C	-4.42328500	-3.15480000	-1.67820400	C	3.90101000	0.75090600	-1.09059500
H	-3.19499900	-0.00188500	-2.01423600	C	4.31538800	-1.51437300	-0.24813800
H	-4.65532000	-1.58543000	-3.15870500	C	5.28234800	0.97511700	-1.10536400
H	-5.09436500	-3.84570700	-2.18117900	C	5.68992100	-1.24949600	-0.28006200
C	-2.16861900	1.07690300	0.27876200	C	6.17428700	-0.01319700	-0.69775900
C	-1.36485300	2.27678900	0.48989100	H	5.65773000	1.93695000	-1.44698100
C	-3.52926300	1.32273400	0.05210800	H	6.38488000	-2.02877100	0.02405300
C	-0.11732400	2.32602200	1.15880400	H	7.24459900	0.17508000	-0.71800600
C	-1.89818600	3.55961400	0.09530600	C	3.84550700	-2.88037700	0.20313700
C	-4.07067700	2.58873300	-0.24224500	H	3.37830600	-2.84246200	1.19478900
H	-4.22144500	0.49340400	0.07471700	H	3.09999500	-3.30245500	-0.48181700
C	0.62218400	3.48209100	1.30102800	H	4.68620200	-3.57923300	0.25834700
H	0.25690200	1.44029200	1.65016100	C	2.96954300	1.84734800	-1.55752100
C	-1.09887200	4.73028800	0.20045700	H	2.27888500	1.48978900	-2.33212800
C	-3.25047200	3.68431300	-0.30965200	H	2.35051900	2.23688400	-0.74115800
H	-5.13506300	2.67284000	-0.44308200	H	3.53556400	2.68508700	-1.97730200
C	0.15055300	4.70093800	0.77284600				

TS-D'$_{Dmp}$



C	0.83772800	-2.20693000	1.47663200	H	-1.50878700	3.70006500	0.59212000
C	1.93220600	-3.01017500	1.24818100	H	2.12037300	5.64736100	-0.60903400
C	2.87568300	-2.68372900	0.24985900	H	4.19439900	4.50994600	-0.49531400
C	2.85494000	-1.36053300	-0.29477600	H	-0.32818900	5.75598900	-0.21407500
C	1.90014700	-0.38028600	0.20449200	P	-0.91179800	-0.41794400	0.09071300
C	0.71342900	-0.93228200	0.79855000	P	-2.53132500	-0.98892400	1.24669000
H	3.83540700	-4.61846900	0.23658000	C	-0.18760000	-2.69227700	2.47203900
H	2.03012600	-3.95295500	1.78126300	H	-0.53089100	-1.89275200	3.13508800
C	3.81911800	-3.63348300	-0.22362900	H	-1.08105300	-3.11135300	1.99184300
C	3.71830400	-1.10431600	-1.40387100	H	0.25188600	-3.48126200	3.09069800
C	4.57953800	-2.06439900	-1.88697900	C	-3.85208900	-0.53900200	0.01061300
C	4.66019500	-3.33414500	-1.26950200	C	-4.23394600	-1.44754500	-1.00499000
H	3.66319000	-0.14331900	-1.90140500	C	-4.56632600	0.67101900	0.18255500
H	5.19510000	-1.84447400	-2.75485300	C	-5.30507100	-1.11656100	-1.84414000
H	5.36142600	-4.07644100	-1.64093900	C	-5.63011400	0.96382000	-0.67806500
C	2.34550600	1.05917700	0.14148300	C	-5.99727900	0.08096400	-1.68989700
C	1.58778800	2.30725400	0.10346700	H	-5.59774400	-1.81394300	-2.62553800
C	3.73860000	1.21595300	0.21107900	H	-6.17548000	1.89558600	-0.54741500
C	0.21341500	2.45399400	0.42003600	H	-6.82776600	0.32038400	-2.34896300
C	2.28395700	3.53723200	-0.19712800	C	-3.52727800	-2.76930900	-1.21223600
C	4.41275600	2.43329500	0.00791800	H	-2.51870500	-2.63258800	-1.61996000
H	4.35106700	0.34987300	0.41763500	H	-3.41377900	-3.32127100	-0.27098800
C	-0.45797500	3.65378200	0.31976100	H	-4.08708900	-3.40096800	-1.90929900
H	-0.32912000	1.60953600	0.81392200	C	-4.20698800	1.65871500	1.26986000
C	1.56210100	4.75294900	-0.34294600	H	-4.15041800	1.17933600	2.25508800
C	3.69833500	3.56805400	-0.27504100	H	-3.22816600	2.11941900	1.08918600
H	5.49808500	2.45002700	0.05155600	H	-4.94866900	2.46173100	1.32846400
C	0.20952600	4.81769100	-0.11111100				

7. References

S1. T. Hartman and R. Cibulka, *Org. Lett.*, 2016, **18**, 3710-3713.

S2. (a) S. S. Moleele, J. P. Michael and C. B. de Koning, *Tetrahedron*, 2006, **62**, 2831-2844. (b) F. Liu, L.-H. Xie, C. Tang, J. Liang, Q.-Q. Chen, B. Peng, W. Wei, Y. Cao and W. Huang, *Org. Lett.*, 2009, **11**, 3850-3853. (c) C. Wang, S. Rakshit and F. Glorius, *J. Am. Chem. Soc.*, 2010, **132**, 14006-14008.

S3. D. R. Coulson, L. C. Satek and S. O. Grim, *Inorg. Synth.*, 1972, **13**, 121-124.

S4. (a) M. Yoshifuji, I. Shima, N. Inamoto, K. Hirotsu and T. Higuchi, *J. Am. Chem. Soc.*, 1981, **103**, 4587-4589. (b) E. Öberg, B. Schäfer, X.-L. Geng, J. Pettersson, Q. Hu, M. Kritikos, T. Rasmussen and S. Ott, *J. Org. Chem.*, 2009, **74**, 9265-9273.

S5. V. H. G. Rohde, M. F. Müller and M. Oestreich, *Organometallics*, 2015, **34**, 3358-3373.

S6. M. C. Burla, R. Caliandro, B. Carrozzini, G. L. Cascarano, C. Cuocci, C. Giacovazzo, M. Mallamo, A. Mazzone and G. Polidori, *J. Appl. Cryst.*, 2015, **48**, 306-309.

S7. C. Kabuto, S. Akine, T. Nemoto and E. Kwon, *J. Cryst. Soc. Jpn.*, 2009, **51**, 218-224.

S8. G. M. Sheldrick, *Acta Crystallogr., Sect. A*, 2008, **64**, 112-122.

S9. R. C. Smith, E. Urnezius, K.-C. Lam, A. L. Rheingold and J. D. Protasiewicz, *Inorg. Chem.*, 2002, **41**, 5296.

S10. K. Toyota, A. Nakamura and M. Yoshifuji, *Chem. Commun.*, 2002, 3012-3013.

S11. 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. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision D.01*,, Gaussian, Inc., Wallingford CT, 2013.

S12. (a) K. Ohno and S. Maeda, *Chem. Phys. Lett.*, 2004, **384**, 277-282. (b) S. Maeda and K. Ohno, *J. Phys. Chem. A*, 2005, **109**, 5742-5753. (c) K. Ohno and S. Maeda, *J. Phys. Chem. A*, 2006, **110**, 8933-8941.

S13. (a) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789. (b) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100. (c) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.

S14. C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158-6170.

S15. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.

S16. T. Yanai, D. P. Tew and N. C. Handy, *Chem. Phys. Lett.*, 2004, **393**, 51-57.

S17. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615-6620.

S18. M. Cossi, V. Barone, R. Cammi and J. Tomasi, *Chem. Phys. Lett.*, 1996, **255**, 327-335.