Electronic Supplementary Material (ESI) for Chemical Communications

Ruthenium-catalyzed hydrophosphinylative cyclization of 1,6-diynes. Stereoselective synthesis of exocyclic 1,3-dienylphosphine oxides

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1. General Considerations

Column chromatography was performed on silica gel (Cica silica gel 60N) with solvents specified below. ^{1}H, ^{13}C, and ^{31}P NMR spectra were obtained for samples in $CDCl_3$ solutions at 25 ˚C. ^{1}H NMR chemical shifts are reported in terms of chemical shift (δ, ppm) relative to the singlet at 7.26 ppm for chloroform. Splitting patterns are designated as follows: s, singlet; d, doublet; t, triplet; q, quartet; quint, quintet; sext, sextet; sept, septet; m, multiplet. Coupling constants are reported in Hz. ^{13}C NMR spectra were fully decoupled and are reported in terms of chemical shift (δ, ppm) relative to the triplet at δ = 77.0 ppm for $CDCl_3$. Chemical shifts for ^{31}P NMR are reported relative to external H_3PO_4 standard. Mass mesurements and elemental analyses were performed in the Instrumental Analysis Facility of Nagoya University. Melting points were obtained in capillary tubes. Dry solvents were purchased and used directly as received. Cp*RuCl(cod) (**1a**),[1] $[Cp^*Ru(CH_3CN)_3]PF_6$ (**1b**),[2] and $[CpRu(CH_3CN)_3]PF_6$ (**1c**)[3] were prepared according to the reports. Diynes **2a**,[4] **2b**,[5] **2c**,[6] **2d**,[7] **2e**,[8] **2f**,[9] **2g**,[10] **2h**,[9] **2i**,[7] **2j**,[11] **2k**,[11] and **2l**[11] were known compounds.

2. Ruthenium-Catalyzed Reaction of Diynes with Diphenylphosphine Oxide.

General procedures – Cyclization of 2a: To a mixture of diyne **2a** (73.9 mg, 0.30 mmol), $Cp^*Ru(AN)_3PF_6$ (**1b**) (7.6 mg, 0.015 mmol), MS 4Å (10 mg) was added a 0.25 M $CHCl_3$ solution of $Ph_2P(O)H$ (1.2 mL, 0.3 mmol) at room temperature under an argon atmosphere. The resultant reaction mixture was stirred at 70 ˚C for 2 h. The reaction progress was traced by TLC analysis. After cooled to room temperature, the reaction mixture was concentrated *in vacuo*, and the crude material was purified with silica gel column chromatography (hexane:AcOEt = 1:1.5) to give **3a** (106.6 mg, 79% yield) as colorless solid (mp 147.0–148.0 ˚C): IR (KBr): 1173 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 4.28 (d, *J* = 3.6 Hz, 2 H), 4.69 (d, *J* = 2.1 Hz, 2 H), 6.93–6.97 (m, 4 H), 7.03–7.11 (m, 3 H), 7.21–7.38 (m, 9 H), 7.60–7.68 (m, 4 H), 8.07 (t, *J* = 2.1 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 72.1, 73.0 (*J* = 12.0 Hz), 126.7 (*J* = 1.7 Hz), 126.9 (*J* = 94.7 Hz), 127.5, 127.7, 127.8, 127.9 (d, *J* = 6.8 Hz), 128.1 (d, *J* = 1.1 Hz), 128.5 (d, *J* = 4.0 Hz), 128.9, 131.0

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(d, J = 2.3 Hz), 131.4 (d, J = 9.2 Hz), 132.8, 133.6 (d, J = 4.6 Hz), 133.8 (d, J = 1.7 Hz), 136.2, 138.8 (d, = 9.8 Hz), 152.4 (d, J = 5.7 Hz); ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 27.2; HRMS (FAB) *m/z* calcd for $C_{30}H_{25}O_2P$•H 449.1670, found 449.1670 $[M+H]^+$.

Analytical data for 3b; colorless solid (mp 178.0–178.5 ˚C); IR (KBr): 1166 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 2.46 (s, 3 H), 3.79 (d, J = 3.6 Hz, 2 H), 4.12 (d, J = 1.8 Hz, 2 H), 6.82–6.86 (m, 4 H), 7.08–7.11 (m, 3 H), 7.18–7.36 (m, 11 H), 7.45–7.54 (m, 6 H), 7.81 (t, J = 1.8 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 22.2, 52.2, 53.2 (d, J = 11.4 Hz), 127.5 (d, J = 2.3 Hz), 127.7, 128.2 (d, J = 4.6 Hz), 128.4, 128.6, 128.7 (d, J = 1.7 Hz), 128.9 (d, J = 4.0 Hz), 129.3, 130.0, 130.4, 130.8 (d, J = 5.1 Hz), 131.5 (d, J = 2.9 Hz), 131.6, 131.7 (d, J = 9.2 Hz), 133.1 (d, J = 18.2 Hz), 135.6 (d, J = 1.8 Hz), 135.7, 138.6 (d, J = 9.2 Hz), 144.0, 152.2 (d, J = 7.4 Hz); ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 27.2; HRMS (FAB) *m/z* calcd for $C_{37}H_{32}NO_3PS$•H 602.1919, found 602.1916 $[M+H]^+$.

Analytical data for 3c; colorless solid (mp 195.5–196.0 ˚C); IR (KBr): 1732 (C=O), 1173 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 2.88 (d, J = 3.3 Hz, 2 H), 3.11 (d, J = 2.4 Hz, 2 H), 3.68 (S, 6 H), 6.94–6.98 (m, 2 H), 7.02–7.12 (m, 5 H), 7.16–7.31 (m, 9 H), 7.56–7.64 (m, 4 H), 7.91 (t, J = 2.1 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 38.9, 41.5 (d, J = 11.4 Hz), 53.4, 57.0, 126.8 (d, J = 1.7 Hz), 127.8 (d, J = 12.0 Hz), 128.1 (d, J = 2.3 Hz), 128.4 (d, J = 1.7 Hz), 129.4, 129.5, 129.8, 131.0 (d, J = 2.3 Hz), 131.7 (d, J = 9.1 Hz), 132.5, 133.8, 134.9 (d, J = 1.7 Hz), 135.0 (d, J = 5.7 Hz), 136.7, 139.6 (d, J = 9.7 Hz), 156.9 (d, J = 7.4 Hz), 171.6; ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 26.9; HRMS (FAB) *m/z* calcd for $C_{35}H_{31}O_5P$•H 563.1987, found 563.1979 $[M+H]^+$.

Analytical data for 3d; colorless solid (mp 163.0–164.0 ˚C); IR (KBr): 1730 (C=O), 1189 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 1.17 (t, J = 7.2 Hz, 6 H), 2.87 (d, J = 3.3 Hz, 2 H), 3.09 (d, J = 2.1 Hz, 2 H), 4.14 (q, J = 7.2 Hz, 4 H), 6.94–6.98 (m, 2 H), 7.02–7.10 (m, 5 H), 7.16–7.31 (m, 9 H), 7.56–7.64 (m, 4 H), 7.88 (t, J = 2.1 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 14.1, 38.3, 40.9 (d, J = 10.9 Hz), 56.6, 61.8, 126.3 (d, J = 1.7 Hz), 127.3, 127.5, 127.6, 127.9 (d, J = 1.1 Hz), 129.0, 129.1 (d, J = 4.0 Hz), 129.8 (d, J = 95.3 Hz), 130.6 (d, J = 2.9 Hz), 131.2 (d, J = 9.2 Hz), 132.7 (d, J = 103.8 Hz), 134.2 (d, J = 1.7 Hz), 134.9 (d, J = 5.7 Hz), 136.2, 139.1 (d, J = 9.8 Hz), 156.8 (d, J = 7.4 Hz), 170.7; ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 26.9; HRMS (FAB) *m/z* calcd for $C_{37}H_{35}O_5P$•H 591.2300, found 591.2310 $[M+H]^+$.

Analytical data for 3e; colorless solid (mp 107.0–198.5 ˚C); IR (KBr): 1695 (C=O), 1172 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 2.00 (s, 6 H), 2.79 (d, J = 3.0 Hz, 2 H),

2.97 (d, J = 2.1 Hz, 2 H), 6.94–6.98 (m, 2 H), 7.01–7.15 (m, 5 H), 7.17–7.34 (m, 9 H), 7.52–7.60 (m, 4 H), 7.87 (t, J = 2.1 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 26.6, 35.4, 38.2 (d, J = 10.9 Hz), 70.8, 126.5 (d, J = 1.7 Hz), 127.5, 127.7 (d, J = 5.1 Hz), 128.1 (d, J = 1.1 Hz), 128.2 (d, J = 111.8 Hz), 129.0, 130.1, 130.7 (d, J = 2.9 Hz), 131.2 (d, J = 9.1 Hz), 131.9, 133.3, 134.4 (d, J = 1.7 Hz), 134.9 (d, J = 5.7 Hz), 136.1, 139.1 (d, J = 9.7 Hz), 156.3 (d, J = 7.4 Hz), 203.7; ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 26.9; HRMS (FAB) m/z calcd for $C_{35}H_{31}O_3P$•H 531.2089, found 531.2086 $[M+H]^+$.

Analytical data for 3f; colorless solid (mp 254.0–255.0 ˚C); IR (KBr): 2255 (C≡N), 1173 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 3.02 (d, J = 3.0 Hz, 2 H), 3.25 (d, J = 1.8 Hz, 2 H), 6.90–7.03 (m, 4 H), 7.09–7.20 (m, 3 H), 7.22–7.38 (m, 9 H), 7.59–7.68 (m, 4 H), 8.19 (t, J = 1.8 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 31.1, 42.3, 44.5 (d, J = 11.5 Hz), 115.4, 127.2 (d, J = 1.7 Hz), 127.9, 128.0, 128.2, 128.5 (d, J = 4.1 Hz), 128.9, 129.3 (d, J = 5.1 Hz), 131.0, 131.2, 131.4, 132.4, 135.2, 135.3, 137.9 (d, J = 1.7 Hz), 138.3 (d, J = 9.1 Hz), 150.2 (d, J = 8.0 Hz); ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 27.1; HRMS (FAB) m/z calcd for $C_{33}H_{25}N_2OP$•H 497.1783, found 497.1773 $[M+H]^+$.

Analytical data for 3g; colorless solid (mp 196.0–197.0 ˚C); IR (KBr): 1171 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 1.60–1.70 (m, 3 H), 2.32 (dt, J = 7.5, 3.9 Hz, 2 H), 2.38 (dt, J = 7.5, 1.8 Hz, 2 H), 6.97–7.08 (m, 6 H), 7.15–7.30 (m, 10 H), 7.56–7.64 (m, 4 H), 7.85 (t, J = 2.0 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 22.8, 31.9, 34.0 (d, J = 10.3 Hz), 126.0 (d, J = 1.7 Hz), 126.8, 127.4 (d, J = 2.9 Hz), 127.5, 127.8 (d, J = 1.1 Hz), 128.0 (d, J = 96.4 Hz), 129.0, 129.1 (d, J = 4.0 Hz), 130.3 (d, J = 2.9 Hz), 131.1 (d, J = 9.2 Hz), 132.6 (d, J = 11.9 Hz), 133.3 (d, J = 91.3 Hz), 136.9, 139.7 (d, J = 5.1 Hz), 140.0 (d, J = 10.3 Hz), 161.6 (d, J = 6.3 Hz); ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 43.6; HRMS (FAB) m/z calcd for $C_{31}H_{27}OP$•H 447.1878, found 447.1877 $[M+H]^+$.

Analytical data for 3h; colorless solid (mp 83.0–84.0 ˚C); IR (KBr): 1734 (C=O), 1174 (P=O) cm^{-1}; ^{1}H NMR (300 MHz, $CDCl_3$, 25 ˚C): δ 2.86 (d, J = 3.3 Hz, 2 H), 3.09 (d, J = 1.8 Hz, 2 H), 3.69 (s, 6 H), 3.71 (s, 3 H), 3.80 (s, 3 H), 6.63 (d, J = 8.7 Hz, 2 H), 6.75 (d, J = 8.7 Hz, 2 H), 6.91–6.96 (m, 4 H), 7.17–7.36 (m, 4 H), 7.55–7.63 (m, 4 H), 7.81 (t, J = 1.8 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 ˚C): δ 38.6, 41.2 (d, J = 11.4 Hz), 53.0, 55.2 (d, J = 1.7 Hz), 56.7, 113.2, 113 4, 127.6 (d, J = 12.0 Hz), 128.6 (d, J = 95.9 Hz), 129.2, 130.4 (d, J = 3.5 Hz), 130.6 (d, J = 2.9 Hz), 130.7, 131.3 (d, J = 9.2 Hz), 131.7 (d, J = 9.8 Hz), 132.4, 132.6 (d, J = 5.7 Hz), 133.7, 140.0 (d, J = 1.7 Hz), 157.3 (d, J = 8.6 Hz), 157.8 (d, J = 1.7 Hz), 158.8, 171.3; ^{31}P NMR (121 MHz, $CDCl_3$, 25 ˚C): δ 27.3; HRMS (FAB) m/z calcd for $C_{37}H_{35}O_7P$•H 623.2199, found 623.2211 $[M+H]^+$.

Analytical data for 3i; colorless solid (mp 166.0–167.0 °C); IR (KBr): 1731 (C=O), 1177 (P=O) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 2.84 (d, *J* = 3.3 Hz, 2 H), 3.06 (d, *J* = 2.4 Hz, 2 H), 3.70 (s, 6 H), 6.80 (t, *J* = 8.7 Hz, 2 H), 6.91 (d, *J* = 8.1 Hz, 2 H), 6.92 (d, *J* = 6.3 Hz, 2 H), 7.00 (ddd, *J* = 9.0, 5.1, 1.5 Hz, 2 H), 7.17–7.36 (m, 8 H), 7.54–7.62 (m, 4 H), 7.85 (t, *J* = 2.4 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 38.4, 41.0 (d, *J* = 11.4 Hz), 53.1, 56.5, 114.9 (d, *J* = 21.7 Hz), 115.0 (dd, *J* = 21.2, 1.2 Hz), 127.7 (d, *J* = 12.0 Hz), 129.2 (d, *J* = 95.9 Hz), 130.72, 130.74 (d, *J* = 11.4 Hz), 130.8, 131.2 (d, *J* = 9.1 Hz), 131.8, 132.2 (d, *J* = 3.5 Hz), 133.3 (d, *J* = 15.4 Hz), 134.2 (dd, *J* = 5.1, 1.5 Hz), 135.0 (dd, *J* = 8.1, 3.5 Hz), 157.0 (d, *J* = 7.4 Hz), 161.1 (dd, *J* = 244.7, 2.0 Hz), 161.8 (d, *J* = 245.8 Hz), 171.1; ^{31}P NMR (121 MHz, $CDCl_3$, 25 °C): δ 26.9 (J_{F-P} = 3.4 Hz); HRMS (FAB) *m/z* calcd for $C_{35}H_{29}F_2O_5P•H$ 599.1799, found 599.1814 $[M+H]^+$.

Analytical data for 3j; yellow solid (mp 167.0–168.0 °C); IR (KBr): 1727 (C=O), 1171 (P=O) cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, 25 °C): δ 3.07 (d, *J* = 3.0 Hz, 2 H), 3.18 (d, *J* = 2.4 Hz, 2 H), 3.75 (s, 6 H), 6.59 (ddd, *J* = 3.6, 2.1, 1.2 Hz, 1 H), 6.72 (dd, *J* = 5.4, 3.6 Hz, 1 H), 6.99 (dd, *J* = 5.1, 3.6 Hz, 1 H), 7.02 (d, *J* = 2.7 Hz, 1 H), 7.07 (dt, *J* = 5.4, 1.2 Hz, 1 H), 7.20–7.35 (m, 7 H), 7.60–7.68 (m, 4 H), 8.27 (t, *J* = 2.4 Hz, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, 25 °C): δ 39.4, 43.2 (d, *J* = 10.3 Hz), 53.5, 57.1, 121.6, 122.9, 126.5 (d, *J* = 2.3 Hz), 127.0 (d, *J* = 1.7 Hz), 127.5, 128.0 (d, *J* = 11.9 Hz), 128.2 (d, *J* = 6.3 Hz), 128.5 (d, *J* = 2.3 Hz), 130.7, 131.3 (d, *J* = 2.9 Hz), 131.7 (d, *J* = 9.2 Hz), 131.8 (d, *J* = 29.7 Hz), 133.4, 140.1, 140.6 (d, *J* = 10.8 Hz), 160.8 (d, *J* = 8.6 Hz), 171.7; ^{31}P NMR (121 MHz, $CDCl_3$, 25 °C): δ 27.4; HRMS (FAB) *m/z* calcd for $C_{31}H_{27}O_5PS_2•H$ 575.1116, found 575.1108 $[M+H]^+$.

3. Crystallographic Structural Determinations: A single crystal suitable for X-ray analysis was mounted on a glass fiber, and diffraction data were collected at 153 K on a Bruker SMART APEX CCD diffractometer with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å). The absorption correction was made using SADABS. The structure was solved by direct methods and refined by the full-matrix least-squares on F^2 by using SHELXTL.[12] All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions. CCDC 879594 (**3d**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033; or deposit@ccdc.cam.ac.uk).

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Table S1. Selected crystallographic data and collection parameters for **3d**.

	3d
Formula	$C_{37}H_{35}O_5P$
Fw	590.62
Crystal system	Triclinic
Space group	P-1 (#2)
a [Å]	11.0389(9)
b [Å]	11.7426(10)
c [Å]	13.2377(11)
α [°]	68.091(2)
β [°]	77.2830(10)
γ [°]	80.2790(10)
V [Å^3]	1545.8(2)
Z	2
D_{calc} [g cm^{-3}]	1.269
μ [mm^{-1}]	0.132
F(000)	624
Crystal size [mm^3]	0.70 × 0.20 × 0.10
Reflections collected	11532
Independent reflections	7520 (R_{int} = 0.0179)
GOF on F^2	1.029
R_1 [I>2σ(I)][a]	0.0443
wR_2 (all data)[b]	0.1309
Largest diff. peak / hole [e Å^{-3}]	0.583 / –0.333

[a] $R_1 = \Sigma|(F_o-F_c)|/\Sigma(F_o)$. [b] $wR_2 = \{\Sigma[(w(F_o^2-F_c^2)^2)]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

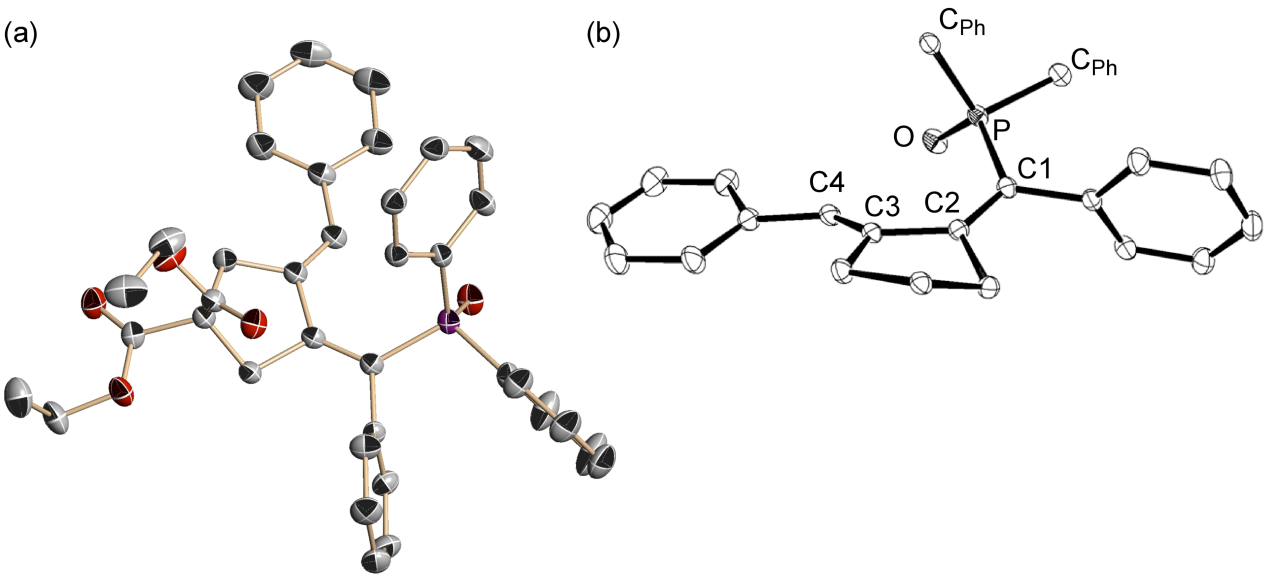

Figure S1. ORTEP diagrams for **3d**. Ellipsoids are shown at the 30% probability level. All hydrogen atoms are omitted for clarity. The phosphine phenyl rings and ester groups were also omitted in (b). C1–C2 = 1.3537(17) Å, C2–C3 = 1.4855(16) Å, C3–C4 = 1.3496(17) Å, ∠C1–C2–C3–C4 = 26.9 ° and ∠P–C1–C2–C3 = 6.1°.

4. Theoretical Calculations.

The Gaussian 09 program package was used for all geometry optimizations.[13] The geometries of stationary points and transition states were fully optimized by means of the Becke's three-parameter hybrid density functional method (B3LYP)[14] with the basis set, consisting of a

[13] Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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double-ζ basis set with the relativistic effective core potential of Hay and Wadt (LanL2DZ).[15] The vibrational frequencies, zero-point energy (ZPE) and thermal correction to Gibbs free energy (TCGFE) were calculated at the same level of theory. The obtained structures were characterized by the number of imaginary frequencies (one or zero for transition or ground states, respectively). The connectivity of each step was further confirmed by IRC calculation[16] from the transition states followed by optimization of the resulted geometries. Single-point energies for geometries obtained by the above method were calculated at the same level using the basis sets consisting of a [6*s*5*p*3*d*2*f*1*g*] contracted valence basis set with the Stuttgart-Dresden-Bonn energy-consistent pseudopotential (SDD)[17,18] for Ru and the 6-311++G(2d,p) basis sets[19] for other elements. The obtained results are summarized in Table S2.

Table S2. Summary of theoretical calculations.

Model	Energy/au	ZPE/au	TCGFE/au	IF/cm^{-1}
A	–1785.96615999	0.507307	0.437099	
TS-AB	–1785.94377874	0.507130	0.437735	208.3472i
B	–1786.02272489	0.511881	0.443419	
TS-BC	–1785.98501114	0.508454	0.441371	1050.8670i
C	–1785.99923137	0.513211	0.444642	
TS-CD	–1785.99149972	0.512885	0.447885	121.1288i
D	–1786.01165337	0.514077	0.449095	
TS-DE	–1785.99408022	0.513039	0.447880	357.2437i
E	–1786.06263541	0.515819	0.449208	

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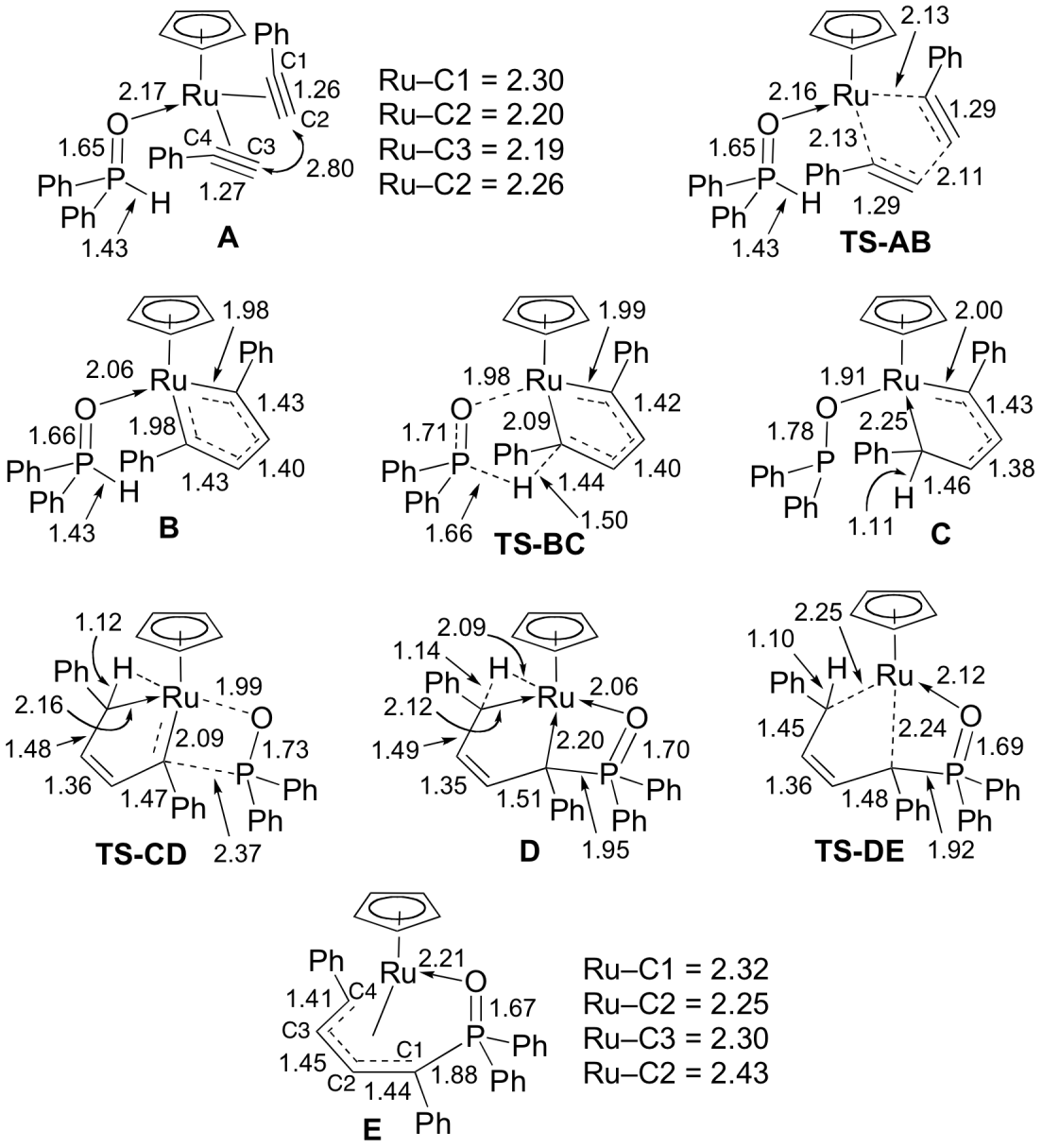


Figure S2. Interatomic distances (Å) of model complexes.

Standard orientations for **A**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	44	0	0.734106	-1.773044	0.186604
2	6	0	0.744917	-4.015234	-0.150620
3	6	0	2.098352	-3.576144	0.007447
4	6	0	2.418205	-2.704613	-1.113768
5	6	0	1.266351	-2.639330	-1.968262
6	6	0	0.220998	-3.419791	-1.372269
7	6	0	-1.531540	-1.842748	0.589233
8	6	0	-0.885823	-1.958182	1.669961
9	1	0	-0.817666	-2.039828	2.737424
10	6	0	1.744096	-1.056003	1.992892
11	1	0	1.519712	-1.223503	3.029525
12	6	0	2.424622	-0.542321	1.052205
13	6	0	-2.653025	-1.799550	-0.325031
14	6	0	-3.863359	-2.434250	0.063994
15	6	0	-2.581907	-1.152263	-1.582215
16	6	0	-4.976445	-2.414442	-0.791824
17	1	0	-3.920210	-2.938456	1.025221
18	6	0	-3.700270	-1.138241	-2.431539
19	1	0	-1.657676	-0.657406	-1.862279
20	6	0	-4.899701	-1.767978	-2.041985
21	1	0	-5.897894	-2.904496	-0.488702
22	1	0	-3.640173	-0.638156	-3.394681
23	1	0	-5.761870	-1.757642	-2.703420
24	6	0	3.482272	0.230418	0.430302
25	6	0	4.629424	0.557899	1.202427
26	6	0	3.404031	0.671720	-0.913411
27	6	0	5.670253	1.309758	0.635135
28	1	0	4.698856	0.215690	2.231733
29	6	0	4.448706	1.426106	-1.472117
30	1	0	2.523531	0.424356	-1.499496
31	6	0	5.584610v	1.746722	-0.702522

32	1	0	6.546803	1.551330	1.230408
33	1	0	4.380655	1.761698	-2.503515
34	1	0	6.393673	2.326415	-1.138431
35	1	0	0.208814	-4.682256	0.508924
36	1	0	2.770076	-3.850665	0.807998
37	1	0	3.374301	-2.236952	-1.297917
38	1	0	1.188833	-2.073609	-2.886467
39	1	0	-0.764754	-3.581422	-1.783696
40	1	0	1.214808	2.068866	0.858702
41	15	0	-0.036466	1.638847	0.325742
42	8	0	0.116903	0.199384	-0.467468
43	6	0	-1.166923	1.711476	1.784342
44	6	0	-2.560296	1.570076	1.612465
45	6	0	-0.619596	1.905970	3.069705
46	6	0	-3.405152	1.630470	2.733363
47	1	0	-2.985342	1.417992	0.623387
48	6	0	-1.471734	1.969135	4.187580
49	1	0	0.454764	2.015924	3.206844
50	6	0	-2.863106	1.830382	4.019612
51	1	0	-4.478790	1.526112	2.604959
52	1	0	-1.054316	2.129479	5.177703
53	1	0	-3.520901	1.882376	4.883127
54	6	0	-0.568095	2.883610	-0.937729
55	6	0	-0.992315	4.166840	-0.534961
56	6	0	-0.515780	2.536535	-2.301598
57	6	0	-1.361967	5.109602	-1.510837
58	1	0	-1.045582	4.434271	0.518021
59	6	0	-0.890497	3.484629	-3.271063
60	1	0	-0.192878	1.541085	-2.591671
61	6	0	-1.310275	4.769799	-2.877299
62	1	0	-1.689025	6.100042	-1.207221
63	1	0	-0.853560	3.223352	-4.325044
64	1	0	-1.597279	5.501207	-3.628060

Standard orientations for **TS-AB**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	44	0	0.523139	-1.754429	-0.132475
2	6	0	-0.158882	-3.692242	-1.204643
3	6	0	1.045272	-3.996034	-0.472673
4	6	0	2.105503	-3.186280	-1.019023
5	6	0	1.554137	-2.353740	-2.058815
6	6	0	0.140898	-2.669988	-2.173678
7	6	0	-1.435886	-1.683791	0.706998
8	6	0	-0.784447	-1.639972	1.817991
9	1	0	-0.897516	-1.620422	2.886719
10	6	0	1.278830	-1.229913	2.011031
11	1	0	1.221933	-1.337851	3.079910
12	6	0	2.071107	-0.892807	1.044359
13	6	0	-2.757704	-1.732411	0.093646
14	6	0	-3.822276	-2.383918	0.769111
15	6	0	-3.000179	-1.135316	-1.167102
16	6	0	-5.101286	-2.433523	0.189954
17	1	0	-3.641134	-2.852315	1.733355
18	6	0	-4.284142	-1.179466	-1.735177
19	1	0	-2.185709	-0.619706	-1.667122
20	6	0	-5.337269	-1.831393	-1.062320
21	1	0	-5.910004	-2.939788	0.710535
22	1	0	-4.465284	-0.711171	-2.699259
23	1	0	-6.327665	-1.872005	-1.507899
24	6	0	3.380826	-0.324293	0.742134
25	6	0	4.377168	-0.264372	1.753223
26	6	0	3.679405	0.183257	-0.545820
27	6	0	5.638463	0.284151	1.473260
28	1	0	4.162556	-0.658323	2.743504
29	6	0	4.939743	0.741176	-0.818114
30	1	0	2.915656	0.147205	-1.317310
31	6	0	5.924290	0.789711	0.187960

32	1	0	6.397710	0.316793	2.250196
33	1	0	5.156668	1.132164	-1.808644
34	1	0	6.902190	1.212923	-0.025081
35	1	0	-1.130930	-4.133859	-1.034540
36	1	0	1.142890	-4.723987	0.320502
37	1	0	3.134598	-3.185117	-0.687415
38	1	0	2.103366	-1.671085	-2.689731
39	1	0	-0.548805	-2.253924	-2.892970
40	1	0	1.452053	1.940198	0.609270
41	15	0	0.140542	1.718715	0.091457
42	8	0	0.028741	0.269037	-0.685891
43	6	0	-0.949718	2.002622	1.555886
44	6	0	-2.352396	1.999242	1.405099
45	6	0	-0.364591	2.225627	2.819387
46	6	0	-3.169012	2.225469	2.525962
47	1	0	-2.806267	1.824781	0.432680
48	6	0	-1.187982	2.458354	3.936426
49	1	0	0.717346	2.224418	2.940557
50	6	0	-2.588822	2.457261	3.789937
51	1	0	-4.249562	2.224571	2.414536
52	1	0	-0.740768	2.641981	4.909390
53	1	0	-3.223956	2.638897	4.652890
54	6	0	-0.191284	3.014498	-1.189072
55	6	0	-0.371639	4.360817	-0.810373
56	6	0	-0.239872	2.632843	-2.543836
57	6	0	-0.595234	5.332485	-1.802178
58	1	0	-0.349487	4.656600	0.236235
59	6	0	-0.469348	3.610770	-3.529034
60	1	0	-0.107845	1.588907	-2.812431
61	6	0	-0.643106	4.958589	-3.160010
62	1	0	-0.733631	6.371688	-1.517499
63	1	0	-0.510414	3.323413	-4.576046
64	1	0	-0.817557	5.712385	-3.923136

Standard orientations for **B**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	44	0	-0.119320	-1.373779	-0.568992
2	6	0	-0.553521	-3.519736	-1.151827
3	6	0	0.829726	-3.322910	-1.534887
4	6	0	0.860992	-2.433030	-2.657159
5	6	0	-0.488148	-2.075260	-2.983159
6	6	0	-1.363815	-2.745388	-2.068371
7	6	0	-1.678037	-1.179577	0.635893
8	6	0	-1.402209	-1.371841	2.021987
9	1	0	-2.154414	-1.238352	2.798425
10	6	0	-0.068993	-1.681183	2.308963
11	1	0	0.296532	-1.811478v	3.326600
12	6	0	0.776284	-1.751439	1.161425
13	6	0	-3.048590	-0.935313	0.157885
14	6	0	-4.174510	-1.507366	0.815687
15	6	0	-3.280139	-0.118427	-0.982179
16	6	0	-5.475314	-1.280708	0.341756
17	1	0	-4.024653	-2.151474	1.678712
18	6	0	-4.582923	0.115496	-1.449371
19	1	0	-2.433484	0.349747	-1.478358
20	6	0	-5.685097	-0.467878	-0.792111
21	1	0	-6.322884	-1.736816	0.846593
22	1	0	-4.742418	0.750288	-2.317096
23	1	0	-6.693914	-0.291670	-1.156254
24	6	0	2.189650	-2.149258	1.277951
25	6	0	2.633188	-3.025241	2.310176
26	6	0	3.155628	-1.659381	0.355527
27	6	0	3.981926	-3.397376	2.407776
28	1	0	1.915026	-3.434314	3.016056
29	6	0	4.507076	-2.023834	0.461043
30	1	0	2.839402	-0.979312	-0.431481
31	6	0	4.925259	-2.896267	1.485858

32	1	0	4.300395	-4.077185	3.193603
33	1	0	5.232290	-1.631505	-0.247088
34	1	0	5.970458	-3.183132	1.566137
35	1	0	-0.917550	-4.222114	-0.415385
36	1	0	1.684586	-3.796321	-1.074134
37	1	0	1.751578	-2.085077	-3.164206
38	1	0	-0.794170	-1.408601	-3.779052
39	1	0	-2.443344	-2.707610	-2.077675
40	1	0	1.274171	1.221611	1.537792
41	15	0	0.753389	1.790946	0.337238
42	8	0	0.485690	0.584394	-0.769383
43	6	0	-0.742201	2.721691	0.869572
44	6	0	-1.315320	3.680157	0.005544
45	6	0	-1.319082	2.451378	2.128441
46	6	0	-2.468194	4.372983	0.410926
47	1	0	-0.867300	3.894524	-0.961706
48	6	0	-2.468983	3.154033	2.528942
49	1	0	-0.882537	1.709184	2.793646
50	6	0	-3.044031	4.111210	1.670779
51	1	0	-2.911950	5.114400	-0.247303
52	1	0	-2.912770	2.955914	3.500319
53	1	0	-3.933268	4.652488	1.982315
54	6	0	1.997191	2.934178	-0.407334
55	6	0	2.384903	4.105523	0.276677
56	6	0	2.553553	2.606587	-1.659472
57	6	0	3.346368	4.952742	-0.301518
58	1	0	1.946932	4.367070	1.237677
59	6	0	3.510475	3.464694	-2.232120
60	1	0	2.232671	1.705436	-2.173945
61	6	0	3.908735	4.632562	-1.553838
62	1	0	3.652410	5.855701	0.218927
63	1	0	3.940817	3.223114	-3.199861
64	1	0	4.650006	5.291498	-1.997887

Standard orientations for **TS-BC**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.582788	-1.214903	-0.590274
2	6	0	-1.505789	-3.311143	-0.735516
3	6	0	-0.106665	-3.472428	-1.044772
4	6	0	0.157396	-2.848640	-2.320846
5	6	0	-1.052744	-2.252101	-2.773359
6	6	0	-2.087265	-2.525631	-1.794908
7	6	0	-2.005651	-0.644100	0.682624
8	6	0	-1.733812	-0.834470	2.064754
9	1	0	-2.451902	-0.587116	2.845048
10	6	0	-0.451781	-1.303543	2.353499
11	1	0	-0.125106	-1.499688	3.374484
12	6	0	0.432845	-1.413338	1.223684
13	6	0	-3.309866	-0.159199	0.207076
14	6	0	-4.513936	-0.458216	0.905323
15	6	0	-3.390717	0.625705	-0.975994
16	6	0	-5.750060	0.004459	0.430730
17	1	0	-4.481464	-1.072394	1.801791
18	6	0	-4.627499	1.097164	-1.442086
19	1	0	-2.476958	0.887839	-1.503853
20	6	0	-5.811322	0.785340	-0.742859
21	1	0	-6.662710	-0.240977	0.967153
22	1	0	-4.671491	1.708486	-2.339367
23	1	0	-6.769934	1.147120	-1.105373
24	6	0	1.699832	-2.186312	1.324474
25	6	0	1.914627	-3.145654	2.351763
26	6	0	2.734418	-1.987829	0.370864
27	6	0	3.115165	-3.870087	2.422513
28	1	0	1.136397	-3.341535	3.084575
29	6	0	3.936729	-2.707900	0.444739
30	1	0	2.594942	-1.268403	-0.432243
31	6	0	4.133412	-3.652677	1.471929

32	1	0	3.257438	-4.604192	3.211253
33	1	0	4.717923	-2.534782	-0.290683
34	1	0	5.062827	-4.212786	1.529699
35	1	0	-2.027796	-3.742958	0.105993
36	1	0	0.611080	-4.019142	-0.450833
37	1	0	1.117107	-2.812298	-2.818392
38	1	0	-1.183252	-1.684689	-3.685553
39	1	0	-3.126759	-2.243446	-1.879040
40	1	0	0.902267	0.006928	1.140626
41	15	0	1.089920	1.377389	0.216583
42	8	0	0.380723	0.458322	-1.042427
43	6	0	0.055174	2.836574	0.692934
44	6	0	0.099228	4.023877	-0.073477
45	6	0	-0.784975	2.751922	1.824915
46	6	0	-0.702772	5.117740	0.293225
47	1	0	0.749234	4.097747	-0.941078
48	6	0	-1.578774	3.853572	2.189691
49	1	0	-0.818083	1.844640	2.421570
50	6	0	-1.540280	5.034672	1.424194
51	1	0	-0.672526	6.029516	-0.296738
52	1	0	-2.220117	3.791495	3.064368
53	1	0	-2.154152	5.885428	1.707727
54	6	0	2.675459	2.011914	-0.499231
55	6	0	3.465164	2.927870	0.230650
56	6	0	3.108116	1.533795	-1.754243
57	6	0	4.689487	3.367546	-0.302863
58	1	0	3.137200	3.300405	1.198654
59	6	0	4.329889	1.986977	-2.284194
60	1	0	2.483614	0.841800	-2.312175
61	6	0	5.122532	2.898298	-1.559271
62	1	0	5.299528	4.071270	0.256483
63	1	0	4.659234	1.632937	-3.257290
64	1	0	6.068143	3.242182	-1.969866

Standard orientations for **C**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	-0.948785	-0.632819	0.658031
2	6	0	-2.268978	-2.243113	1.716969
3	6	0	-3.098381	-1.086535	1.607395
4	6	0	-2.542989	-0.025881	2.436692
5	6	0	-1.335476	-0.504624	2.998911
6	6	0	-1.127983	-1.874936	2.522849
7	6	0	-0.195956	-2.088974	-0.478760
8	6	0	-0.926040	-2.405581	-1.671503
9	1	0	-0.661031	-3.245934	-2.310090
10	6	0	-1.982219	-1.570075	-1.986058
11	1	0	-2.694630	-1.819334	-2.772101
12	6	0	-2.096540	-0.315030	-1.254500
13	6	0	0.912186	-2.934296	-0.018614
14	6	0	0.996539	-4.311403	-0.378948
15	6	0	1.926082	-2.393462	0.820943
16	6	0	2.046183	-5.112252	0.091711
17	1	0	0.229470	-4.760438	-1.003875
18	6	0	2.983570	-3.192846	1.275348
19	1	0	1.895502	-1.339526	1.081387
20	6	0	3.044714	-4.555865	0.918492
21	1	0	2.089955	-6.163105	-0.180681
22	1	0	3.759947	-2.758980	1.899132
23	1	0	3.860667	-5.177362	1.277881
24	6	0	-3.357812	0.457278	-1.238750
25	6	0	-4.617484	-0.164569	-1.448017
26	6	0	-3.322386	1.858685	-1.017412
27	6	0	-5.798642	0.593313	-1.447033
28	1	0	-4.675153	-1.238423	-1.615457
29	6	0	-4.504920	2.614757	-1.009673
30	1	0	-2.365017	2.353928	-0.868448
31	6	0	-5.747810	1.985690	-1.225927

32	1	0	-6.755226	0.106651	-1.617787
33	1	0	-4.460145	3.688315	-0.848287
34	1	0	-6.663209	2.571136	-1.226842
35	1	0	-2.449439	-3.208890	1.267945
36	1	0	-4.016266	-1.013238	1.042885
37	1	0	-2.968433	0.960706	2.559291
38	1	0	-0.663229	0.042746	3.645504
39	1	0	-0.323417	-2.532631	2.820750
40	1	0	-1.211579	0.322551	-1.436584
41	15	0	0.990290	1.729760	-0.867713
42	8	0	0.255455	0.838781	0.484204
43	6	0	2.574717	0.768864	-1.186760
44	6	0	3.698756	0.844509	-0.333702
45	6	0	2.625002	-0.047656	-2.338643
46	6	0	4.855941	0.101764	-0.628425
47	1	0	3.677028	1.489708	0.540649
48	6	0	3.785172	-0.788622	-2.632964
49	1	0	1.772072	-0.092086	-3.013460
50	6	0	4.900302	-0.715528	-1.776848
51	1	0	5.722083	0.169567	0.025020
52	1	0	3.822234	-1.407022	-3.525921
53	1	0	5.800331	-1.280012	-2.007331
54	6	0	1.601407	3.221927	0.096335
55	6	0	2.408851	4.170933	-0.569963
56	6	0	1.207795	3.451234	1.429983
57	6	0	2.829241	5.333880	0.100954
58	1	0	2.717106	4.011245	-1.601671
59	6	0	1.631738	4.616415	2.098235
60	1	0	0.585186	2.720550	1.937167
61	6	0	2.441457	5.559111	1.436694
62	1	0	3.452347	6.058714	-0.416269
63	1	0	1.330261	4.786650	3.128834
64	1	0	2.764909	6.459223	1.952990

Standard orientations for **TS-CD**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.855390	-0.808694	-0.701248
2	6	0	1.802483	-2.870488	-0.500619
3	6	0	2.834301	-2.098830	-1.117384
4	6	0	2.399855	-1.698648	-2.441245
5	6	0	1.078499	-2.180001	-2.631055
6	6	0	0.675656	-2.887450	-1.419689
7	6	0	-0.276389	-0.928105	1.055631
8	6	0	0.410442	-0.353704	2.221905
9	1	0	-0.037437	-0.385124	3.213795
10	6	0	1.632691	0.210709	2.008709
11	1	0	2.245557	0.579871	2.829748
12	6	0	2.097260	0.368242	0.613281
13	6	0	-1.215217	-2.070726	1.289567
14	6	0	-1.134723	-2.820771	2.493177
15	6	0	-2.164936	-2.482456	0.317293
16	6	0	-1.967437	-3.933390	2.712314
17	1	0	-0.408575	-2.554880	3.255393
18	6	0	-3.007307	-3.578440	0.543012
19	1	0	-2.253653	-1.933899	-0.616113
20	6	0	-2.912212	-4.314433	1.743687
21	1	0	-1.879716	-4.495388	3.638378
22	1	0	-3.738515	-3.860525	-0.209935
23	1	0	-3.563674	-5.166420	1.917526
24	6	0	3.534380	0.605149	0.346291
25	6	0	4.540907	0.079651	1.198952
26	6	0	3.931875	1.364500	-0.784881
27	6	0	5.898810	0.302712	0.922856
28	1	0	4.261996	-0.510378	2.068994
29	6	0	5.290447	1.587270	-1.059972
30	1	0	3.172499	1.794971	-1.435739
31	6	0	6.279672	1.056037	-0.207792

32	1	0	6.659765	-0.105396	1.582715
33	1	0	5.579089	2.179157	-1.924302
34	1	0	7.331522	1.231032	-0.416812
35	1	0	1.850143	-3.370266	0.455951
36	1	0	3.794884	-1.868375	-0.681414
37	1	0	2.976748	-1.109981	-3.141504
38	1	0	0.460723	-2.028537	-3.505935
39	1	0	-0.241299	-3.439385	-1.277415
40	1	0	1.471647	1.124637	0.071510
41	15	0	-1.589659	0.794180	0.087188
42	8	0	-0.696316	0.279681	-1.298743
43	6	0	-3.334306	1.000479	-0.539743
44	6	0	-3.701406	0.402218	-1.763901
45	6	0	-4.282687	1.721104	0.218577
46	6	0	-5.018902	0.542900	-2.236290
47	1	0	-2.959314	-0.129813	-2.353040
48	6	0	-5.599905	1.847581	-0.256372
49	1	0	-4.005260	2.193079	1.158508
50	6	0	-5.969474	1.258457	-1.482224
51	1	0	-5.300365	0.099917	-3.187808
52	1	0	-6.330789	2.405639	0.322306
53	1	0	-6.987799	1.360704	-1.847734
54	6	0	-0.971048	2.509232	0.484158
55	6	0	-0.965833	2.959933	1.820574
56	6	0	-0.539170	3.359472	-0.557955
57	6	0	-0.536329	4.268032	2.115439
58	1	0	-1.289683	2.306314	2.628137
59	6	0	-0.103583	4.662000	-0.254922
60	1	0	-0.550953	3.011668	-1.588027
61	6	0	-0.104627	5.117784	1.079197
62	1	0	-0.538609	4.619020	3.143753
63	1	0	0.222645	5.321098	-1.054999
64	1	0	0.225960	6.127529	1.307664

Standard orientations for **D**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.953080	-0.608845	-0.808894
2	6	0	1.657049	-2.704274	-0.422611
3	6	0	2.804206	-2.065162	-0.994867
4	6	0	2.519548	-1.734298	-2.377301
5	6	0	1.179710	-2.111314	-2.649649
6	6	0	0.613083	-2.689787	-1.435921
7	6	0	-0.441714	-0.448018	0.882407
8	6	0	0.243377	0.268677	2.015412
9	1	0	-0.283039	0.420979	2.957998
10	6	0	1.512827	0.698394	1.845193
11	1	0	2.064957	1.185271	2.647873
12	6	0	2.142472	0.563512	0.502389
13	6	0	-1.132729	-1.735354	1.288158
14	6	0	-0.760742	-2.370800	2.501285
15	6	0	-2.112348	-2.377569	0.487852
16	6	0	-1.344685	-3.587307	2.898645
17	1	0	-0.005642	-1.920386	3.139087
18	6	0	-2.701701	-3.587596	0.887891
19	1	0	-2.424844	-1.942620	-0.456729
20	6	0	-2.322836	-4.202617	2.097096
21	1	0	-1.038479	-4.048363	3.834304
22	1	0	-3.456280	-4.050010	0.256459
23	1	0	-2.780157	-5.138505	2.405885
24	6	0	3.619019	0.634091	0.408825
25	6	0	4.443363	0.159319	1.463190
26	6	0	4.240726	1.172854	-0.748113
27	6	0	5.841720	0.209831	1.354252
28	1	0	3.990069	-0.258918	2.358553
29	6	0	5.639243	1.228498	-0.853363
30	1	0	3.623652	1.567588	-1.553999
31	6	0	6.445863	0.744220	0.196708

32	1	0	6.461555	-0.160754	2.166297
33	1	0	6.100325	1.655488	-1.739783
34	1	0	7.528687	0.790045	0.118728
35	1	0	1.579511	-3.140927	0.562248
36	1	0	3.743754	-1.891123	-0.492316
37	1	0	3.201000	-1.246856	-3.061466
38	1	0	0.651001	-1.965298	-3.581937
39	1	0	-0.357701	-3.151364	-1.341216
40	1	0	1.682393	1.273745	-0.253953
41	15	0	-1.520708	0.776636	-0.179223
42	8	0	-0.622134	0.465007	-1.583435
43	6	0	-3.317621	0.514712	-0.563401
44	6	0	-3.677924	0.314946	-1.912031
45	6	0	-4.295047	0.555541	0.451277
46	6	0	-5.036458	0.161521	-2.244190
47	1	0	-2.911402	0.285014	-2.681960
48	6	0	-5.649126	0.395328	0.108637
49	1	0	-4.022084	0.691502	1.495336
50	6	0	-6.020311	0.201544	-1.237070
51	1	0	-5.323781	0.014949	-3.281601
52	1	0	-6.408264	0.420066	0.885233
53	1	0	-7.068436	0.081604	-1.497587
54	6	0	-1.249730	2.553935	0.278530
55	6	0	-1.728914	3.069331	1.500796
56	6	0	-0.584481	3.387165	-0.643189
57	6	0	-1.537471	4.429132	1.800565
58	1	0	-2.246103	2.434185	2.216962
59	6	0	-0.397305	4.747452	-0.334628
60	1	0	-0.235221	2.982041	-1.589779
61	6	0	-0.872030	5.268127	0.884165
62	1	0	-1.906479	4.831760	2.739666
63	1	0	0.108219	5.396481	-1.044255
64	1	0	-0.729259	6.319782	1.117478

Standard orientations for **TS-DE**

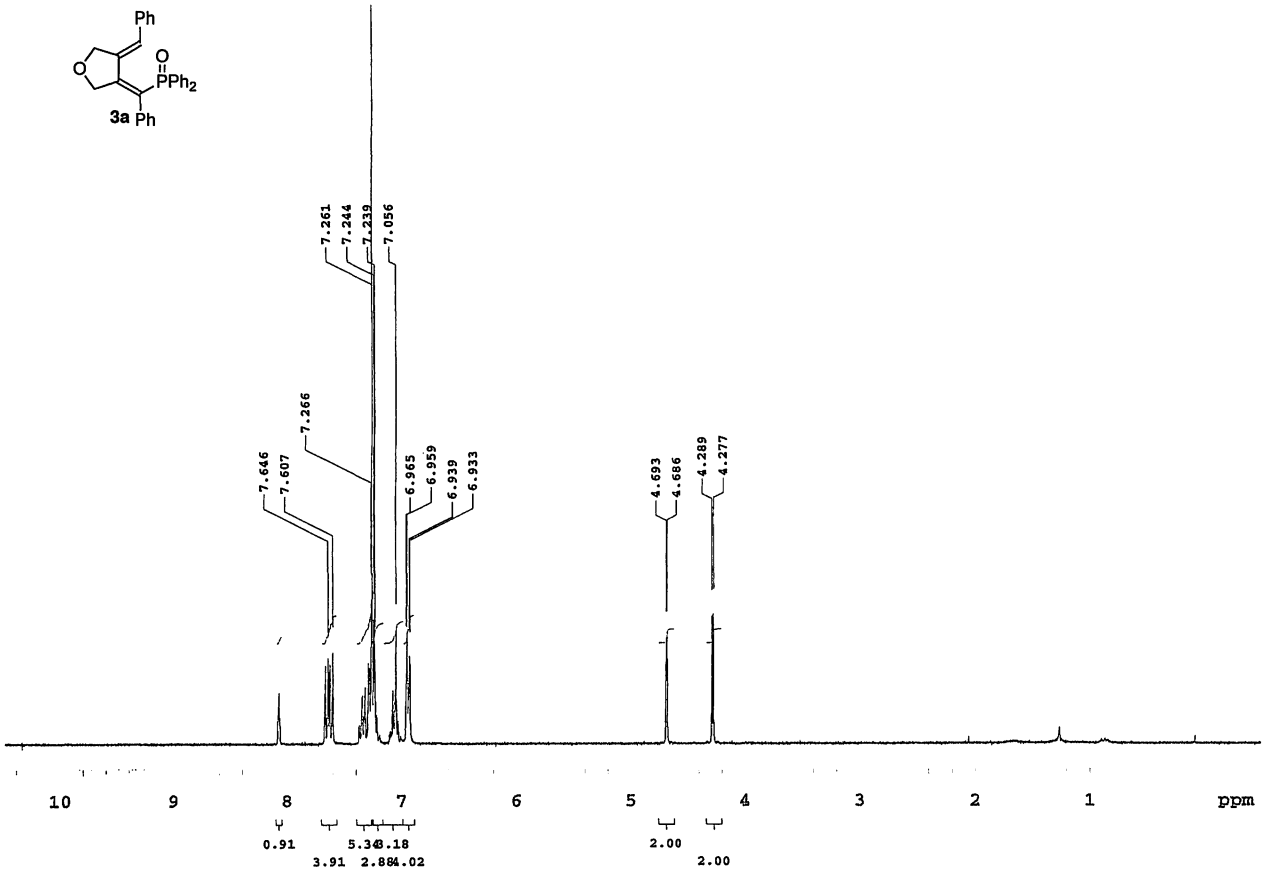
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.851940	-1.191499	-0.534814
2	6	0	1.574674	-3.311824	0.131683
3	6	0	2.711926	-2.637173	-0.417466
4	6	0	2.469729	-2.332982	-1.815178
5	6	0	1.140997	-2.764181	-2.114117
6	6	0	0.567722	-3.359829	-0.899826
7	6	0	-0.724633	-0.525790	0.917169
8	6	0	0.227062	-0.254458	2.019490
9	1	0	-0.088736	-0.514688	3.029812
10	6	0	1.552420	0.119417	1.875071
11	1	0	2.167982	0.183437	2.769057
12	6	0	2.172704	0.259157	0.572890
13	6	0	-1.936204	-1.365340	1.275908
14	6	0	-2.484190	-1.378016	2.582220
15	6	0	-2.584893	-2.139195	0.282969
16	6	0	-3.619554	-2.150608	2.887368
17	1	0	-2.045037	-0.779752	3.376726
18	6	0	-3.724106	-2.904043	0.582006
19	1	0	-2.192515	-2.142547	-0.730646
20	6	0	-4.245332	-2.920049	1.889768
21	1	0	-4.016348	-2.145668	3.899446
22	1	0	-4.201558	-3.487842	-0.200988
23	1	0	-5.122329	-3.516630	2.125527
24	6	0	3.622782	0.390094	0.391466
25	6	0	4.555892	0.004161	1.392596
26	6	0	4.119135	0.921393	-0.830280
27	6	0	5.933332	0.152028	1.177330
28	1	0	4.210137	-0.415887	2.333356
29	6	0	5.496908	1.069642	-1.043014
30	1	0	3.416670	1.222045	-1.605326
31	6	0	6.410000	0.685742	-0.039261

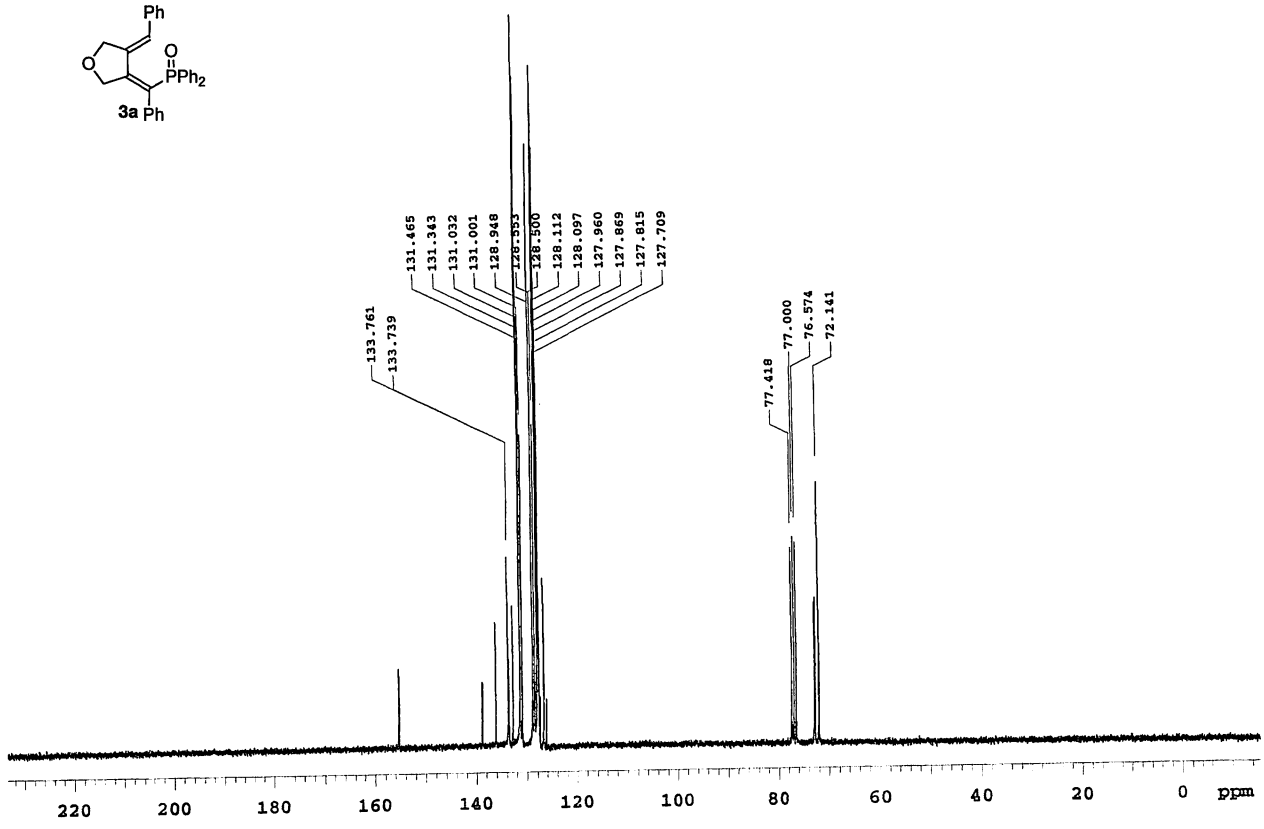
32	1	0	6.637130	-0.144966	1.949979
33	1	0	5.860975	1.484285	-1.978810
34	1	0	7.478347	0.800707	-0.201072
35	1	0	1.478816	-3.695388	1.137448
36	1	0	3.620777	-2.404325	0.118983
37	1	0	3.165015	-1.865303	-2.496359
38	1	0	0.644677	-2.683403	-3.071731
39	1	0	-0.396229	-3.841275	-0.820272
40	1	0	1.610990	0.827098	-0.189454
41	15	0	-1.174405	0.878412	-0.305939
42	8	0	-0.293377	0.240323	-1.592650
43	6	0	-2.940936	1.026520	-0.830740
44	6	0	-3.284217	0.575888	-2.121011
45	6	0	-3.908600	1.595951	0.021646
46	6	0	-4.613576	0.703674	-2.562205
47	1	0	-2.521490	0.149544	-2.766999
48	6	0	-5.236231	1.709495	-0.424976
49	1	0	-3.647066	1.948676	1.016595
50	6	0	-5.588475	1.265803	-1.715684
51	1	0	-4.885161	0.368816	-3.559424
52	1	0	-5.989488	2.143976	0.226138
53	1	0	-6.615260	1.360903	-2.058828
54	6	0	-0.520272	2.550503	0.159172
55	6	0	-0.714129	3.071773	1.454601
56	6	0	0.122901	3.315204	-0.836814
57	6	0	-0.262815	4.369713	1.753493
58	1	0	-1.200162	2.481553	2.228658
59	6	0	0.574054	4.611397	-0.528005
60	1	0	0.263860	2.906819	-1.834786
61	6	0	0.379695	5.139280	0.763397
62	1	0	-0.411770	4.777432	2.749400
63	1	0	1.067331	5.206878	-1.291167
64	1	0	0.725574	6.142621	0.996827

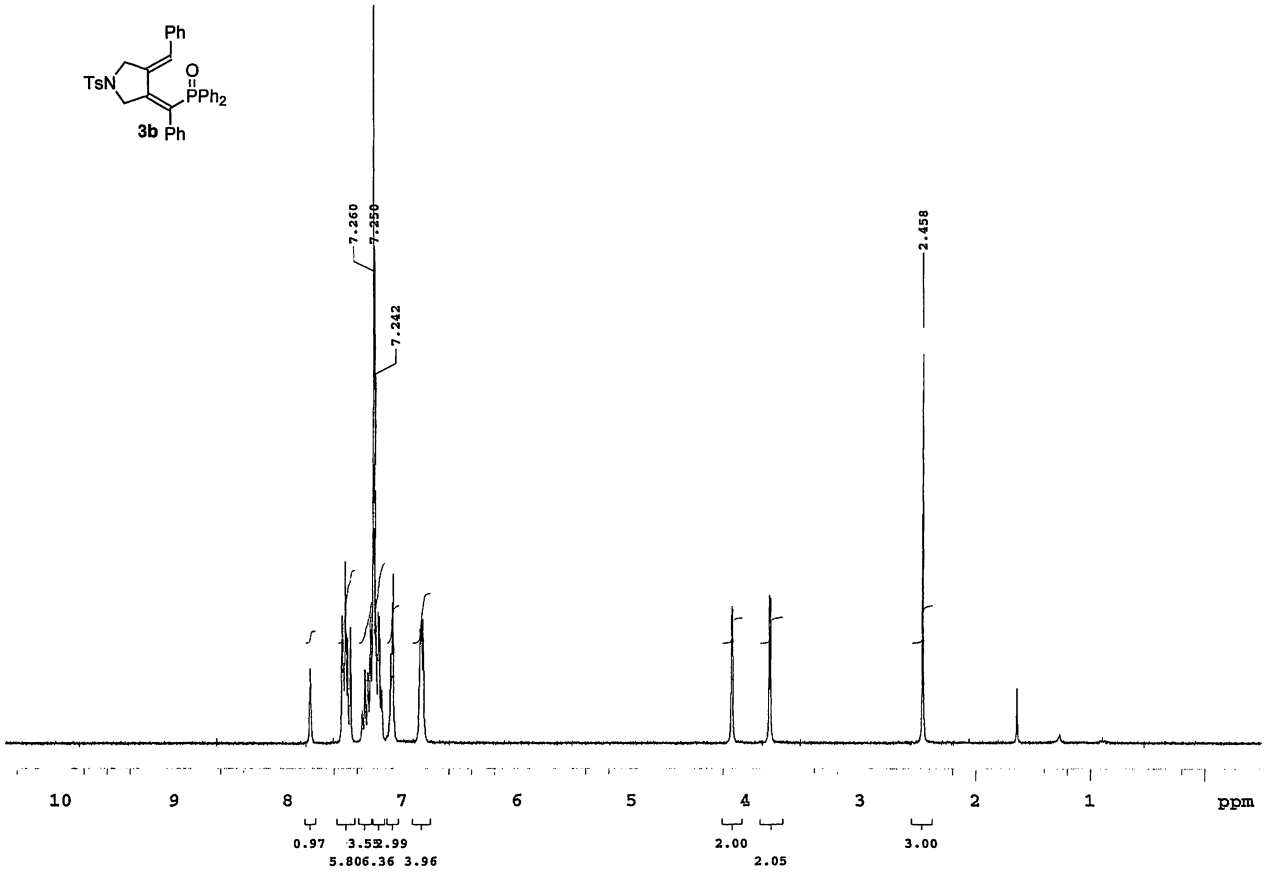
Standard orientations for **E**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	44	0	0.965408	-1.316382	-0.227030
2	6	0	0.670130	-3.547643	-0.099000
3	6	0	2.077531	-3.278430	0.062068
4	6	0	2.563911	-2.685916	-1.171821
5	6	0	1.459038	-2.580135	-2.076731
6	6	0	0.274037	-3.097439	-1.419869
7	6	0	-0.786948	-0.401394	0.977224
8	6	0	0.393851	-0.503952	1.785916
9	1	0	0.271737	-1.161025	2.645808
10	6	0	1.771541	-0.118390	1.561660
11	1	0	2.449477	-0.578064	2.276585
12	6	0	2.346905	0.553942	0.461851
13	6	0	-2.018438	-1.096190	1.485730
14	6	0	-2.418206	-0.916628	2.832688
15	6	0	-2.798709	-1.933524	0.655131
16	6	0	-3.563066	-1.560515	3.335320
17	1	0	-1.842180	-0.266315	3.487943
18	6	0	-3.942301	-2.576664	1.157183
19	1	0	-2.504949	-2.090320	-0.378437
20	6	0	-4.329404	-2.393898	2.499139
21	1	0	-3.855938	-1.409885	4.371030
22	1	0	-4.527182	-3.221123	0.506148
23	1	0	-5.213357	-2.893054	2.886613
24	6	0	3.799637	0.659991	0.233187
25	6	0	4.775335	-0.030268	0.999128
26	6	0	4.240818	1.509025	-0.813949
27	6	0	6.141953	0.133301	0.728993
28	1	0	4.479329	-0.693493	1.808447
29	6	0	5.608547	1.669943v	-1.086154
30	1	0	3.504405	2.041399	-1.412637
31	6	0	6.565711	0.983137	-0.314464

32	1	0	6.878853	-0.395839	1.327569
33	1	0	5.927635	2.326994	-1.890558
34	1	0	7.625533	1.107274	-0.519939
35	1	0	0.023765	-4.012393	0.632800
36	1	0	2.677828	-3.525000	0.926703
37	1	0	3.577315	-2.362515	-1.364633
38	1	0	1.495523	-2.146927	-3.067002
39	1	0	-0.702218	-3.209444	-1.867982
40	1	0	1.752914	1.216760	-0.156130
41	15	0	-1.007872	0.879724	-0.373833
42	8	0	0.226627	0.403443	-1.391596
43	6	0	-2.608634	0.735447	-1.280759
44	6	0	-2.593098	0.136713	-2.556533
45	6	0	-3.803591	1.242196	-0.730810
46	6	0	-3.792058	0.039569	-3.285809
47	1	0	-1.654445	-0.219277	-2.972578
48	6	0	-4.998153	1.133180	-1.463195
49	1	0	-3.810943	1.715331	0.248133
50	6	0	-4.992978	0.532015	-2.738393
51	1	0	-3.788200	-0.409156	-4.275245
52	1	0	-5.924380	1.517699	-1.045813
53	1	0	-5.917824	0.456152	-3.304166
54	6	0	-0.856888	2.614551	0.260366
55	6	0	-0.698551	2.886299	1.634578
56	6	0	-0.903592	3.670422	-0.678016
57	6	0	-0.592286	4.219413	2.071577
58	1	0	-0.659170	2.079362	2.360614
59	6	0	-0.786268	4.998118	-0.234506
60	1	0	-1.027999	3.464894	-1.738653
61	6	0	-0.633381	5.273500	1.139543
62	1	0	-0.476313	4.432604	3.130450
63	1	0	-0.818060	5.812179	-0.953043
64	1	0	-0.548406	6.301941	1.479915



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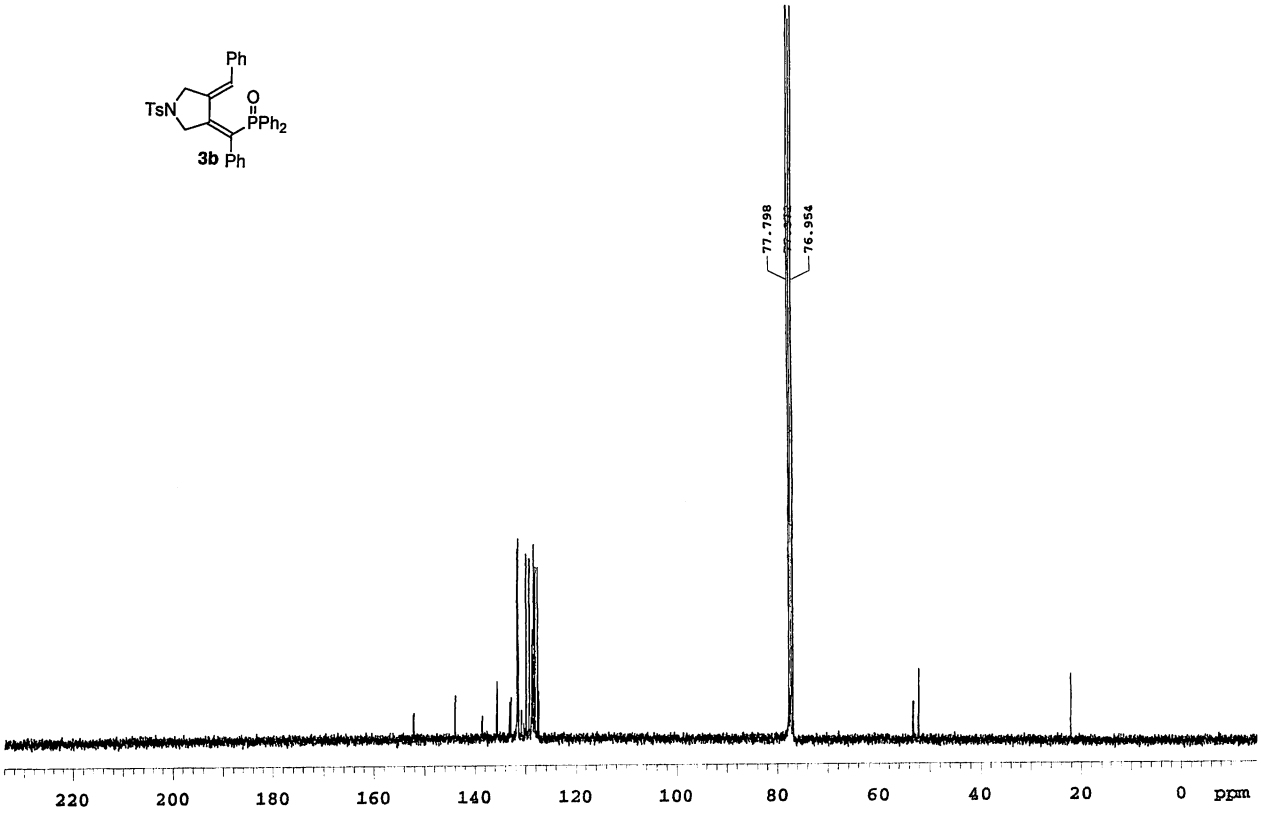
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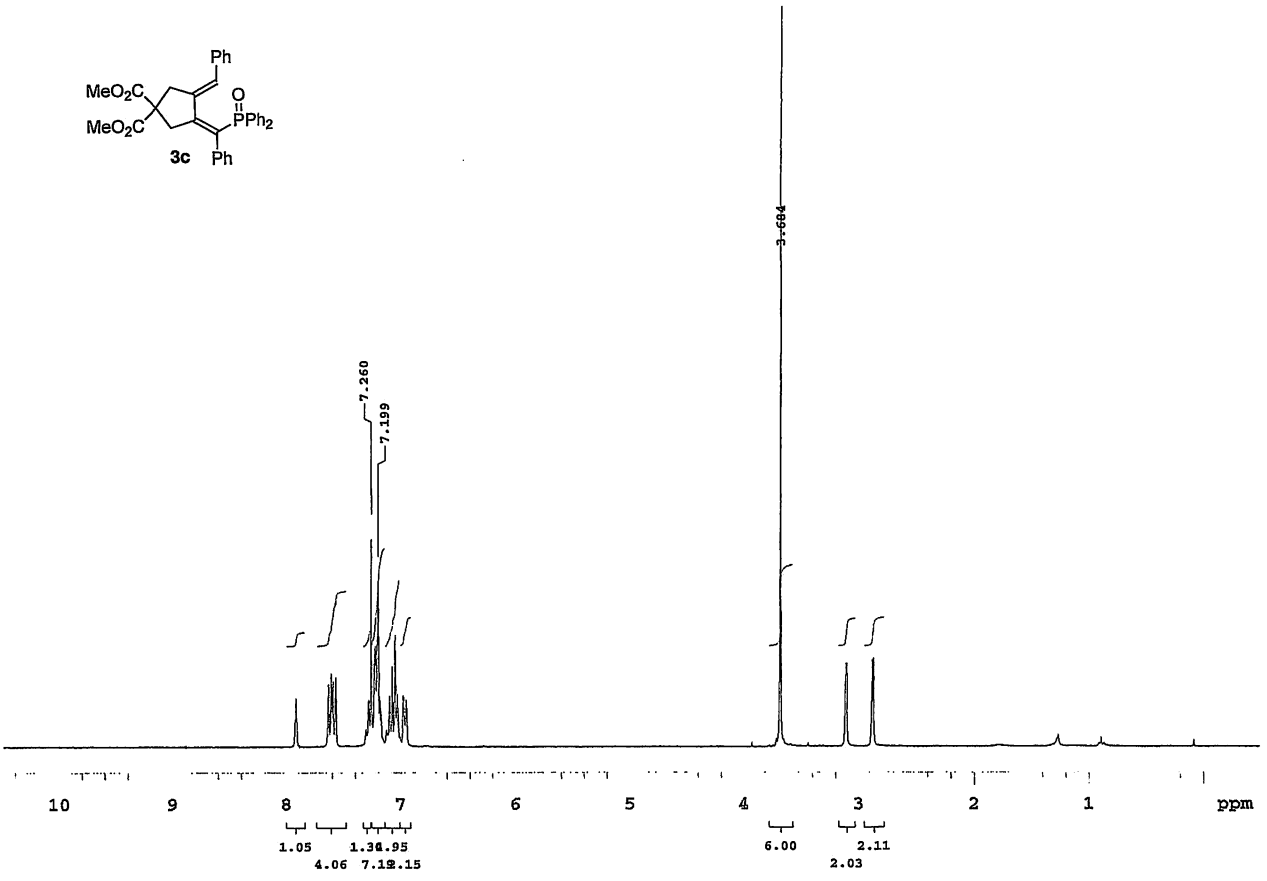
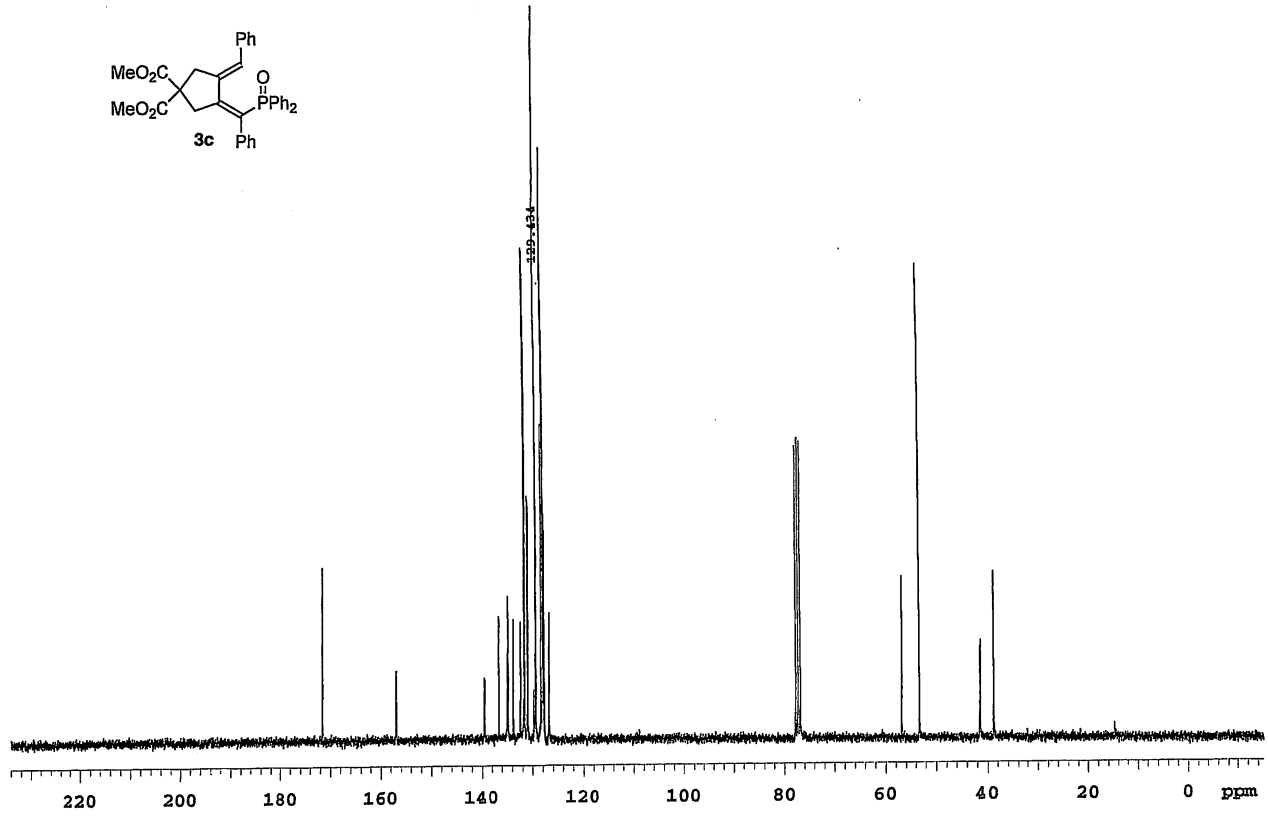
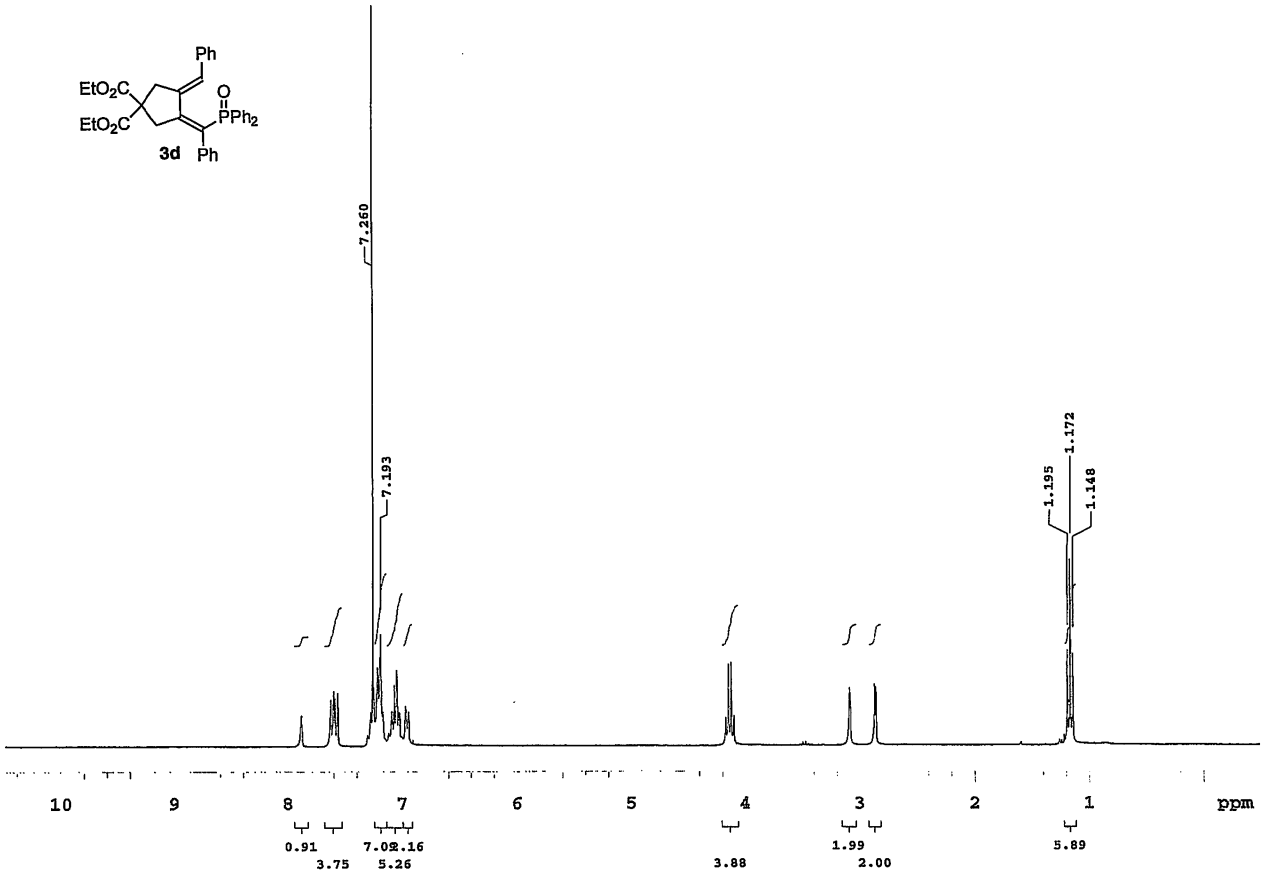
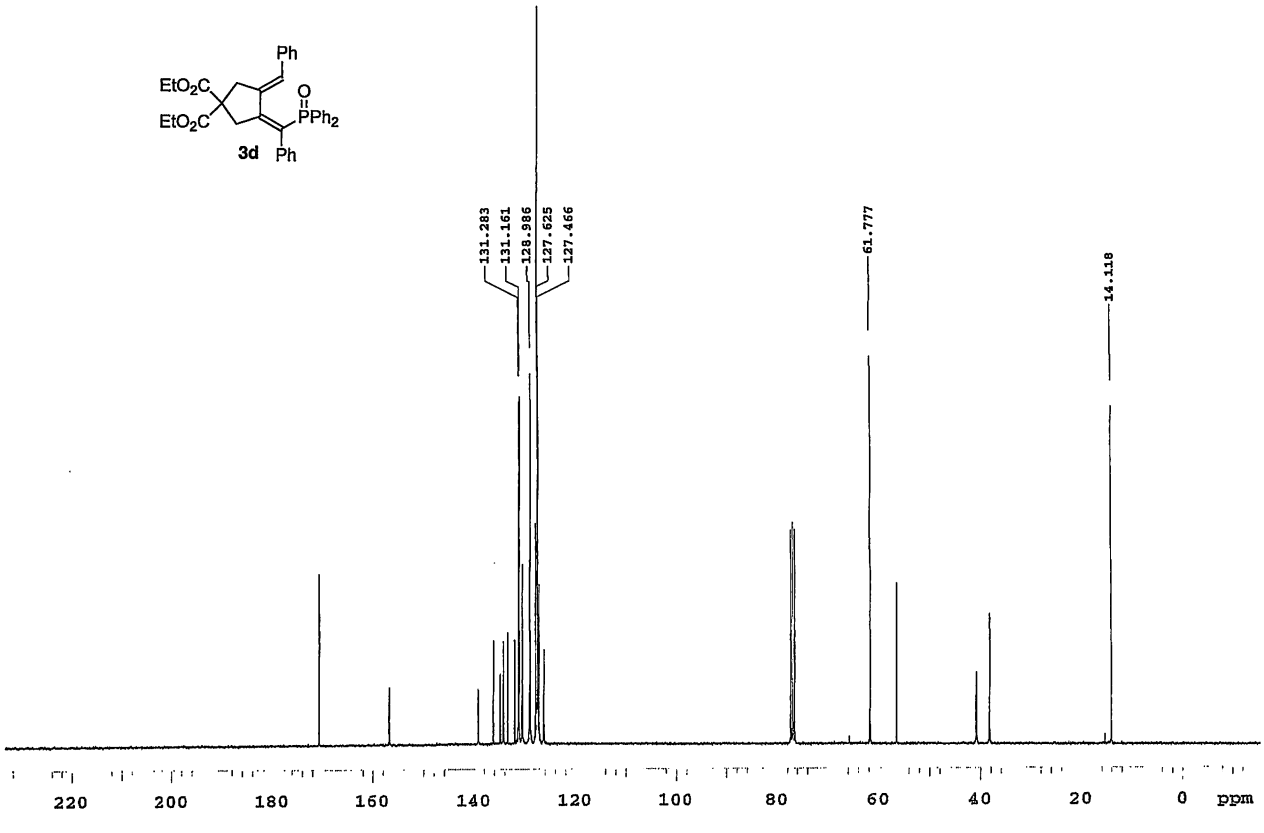
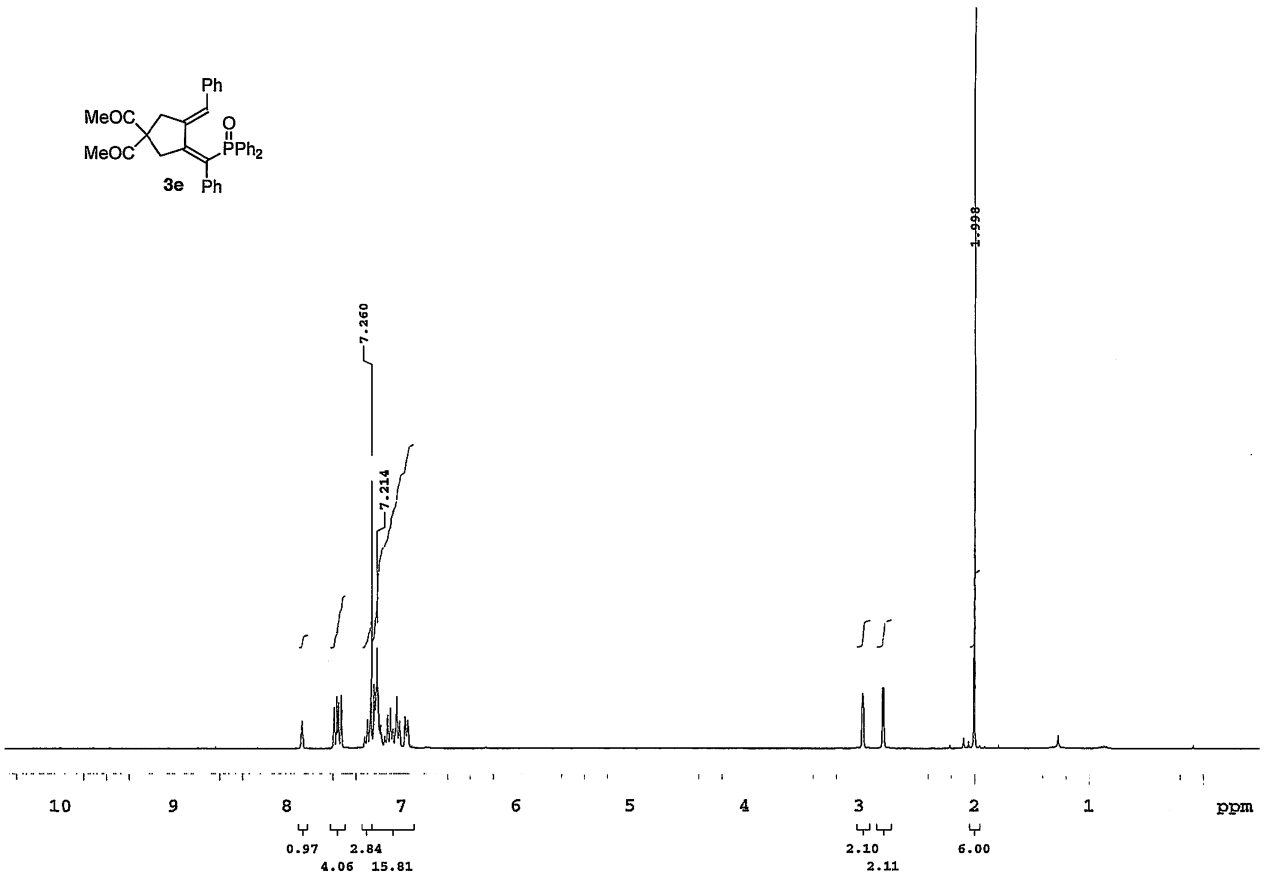
200
180
160
140
120
100
80
60
40
20
0
ppm

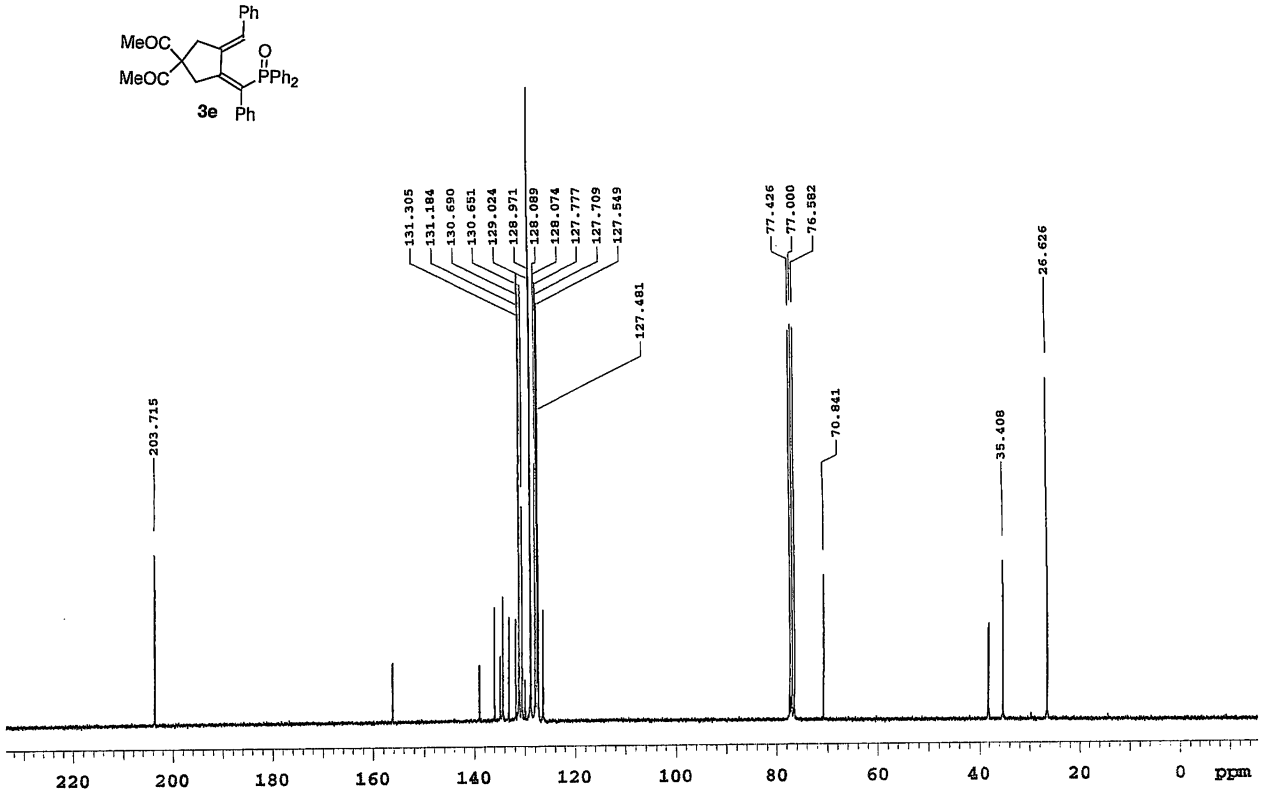

Ph
MeO2C
MeO2C
O
PPh2
3c
Ph
3.684
7.260
7.199
10
9
8
7
6
5
4
3
2
1
ppm
1.05
4.06
1.36
7.12
4.95
2.15
6.00
2.03
2.11

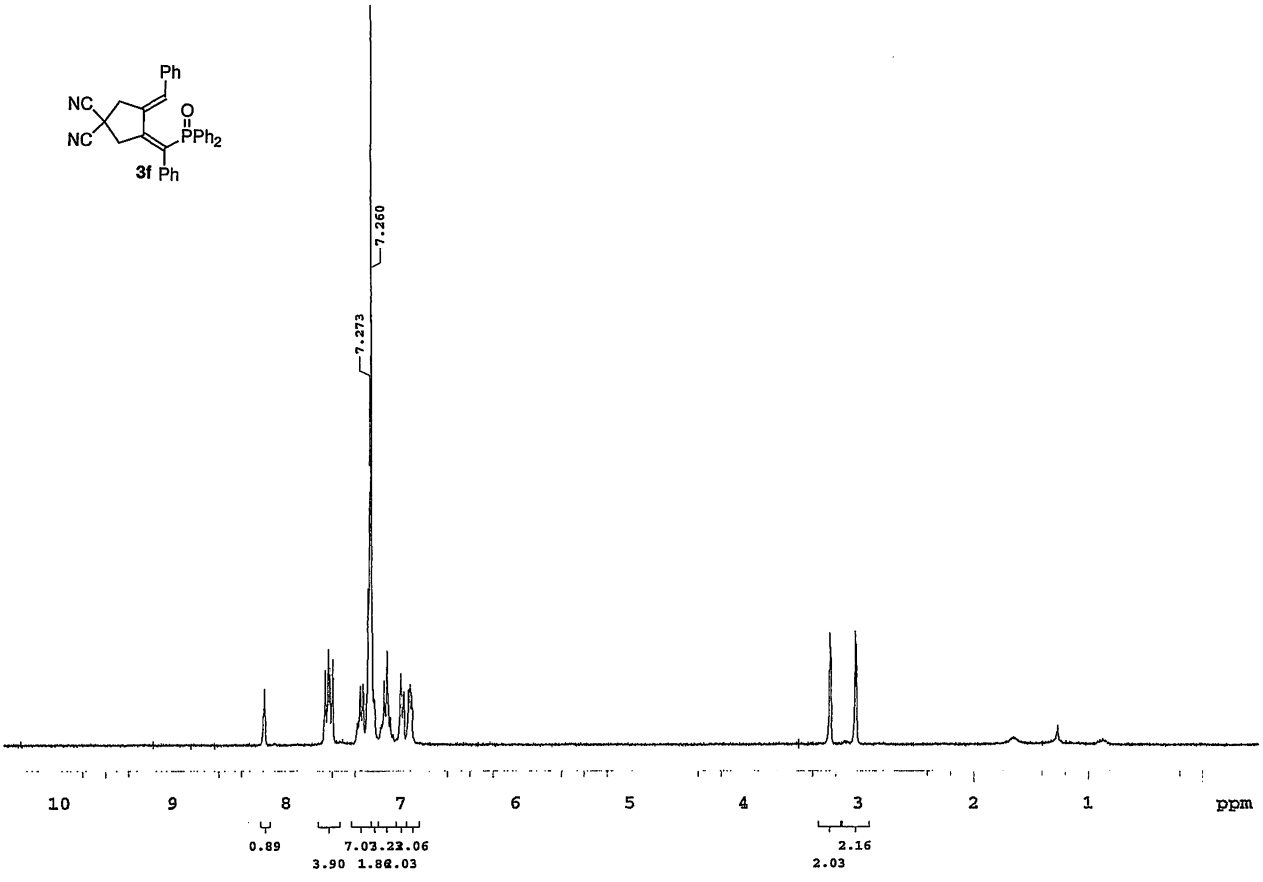

Ph
MeO2C
MeO2C
O
PPh2
3c
Ph
129.434
220
200
180
160
140
120
100
80
60
40
20
0
ppm

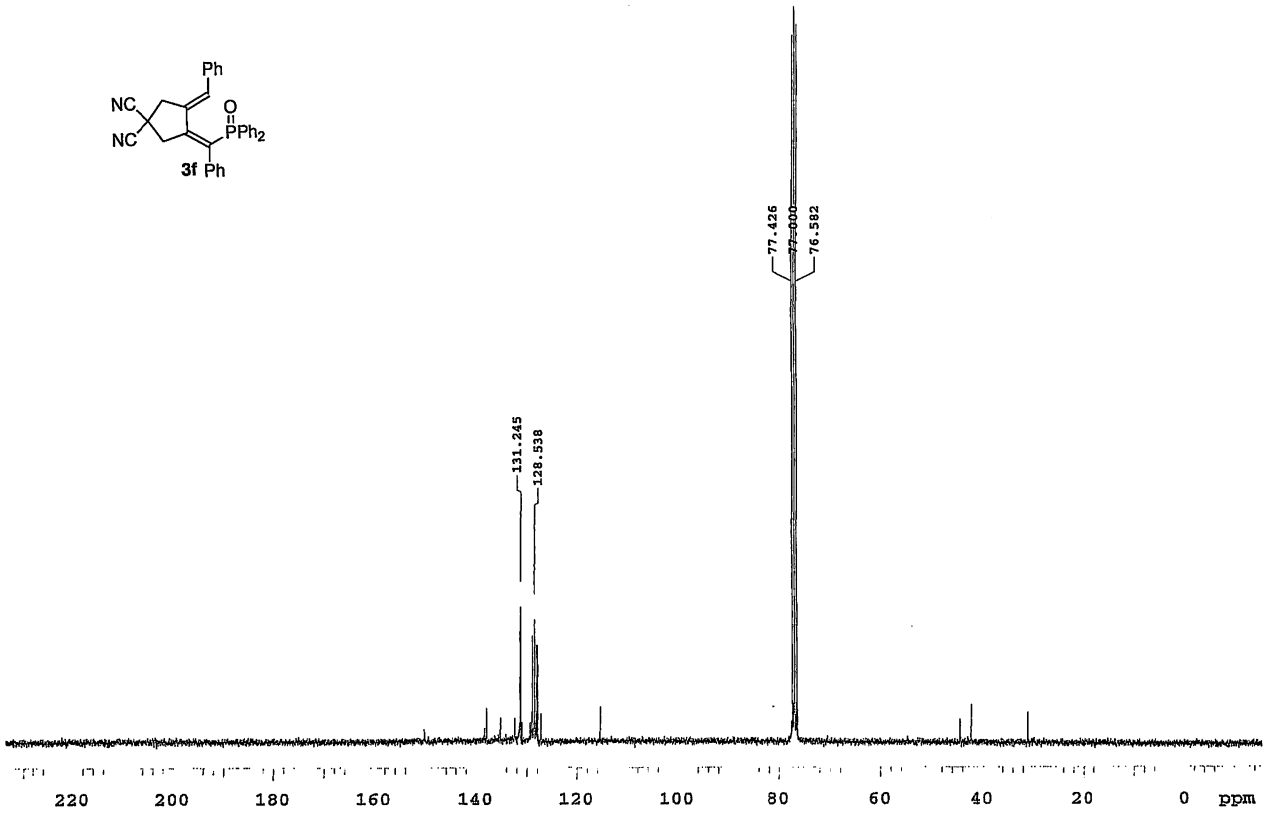

Ph
EtO2C
EtO2C
O
PPh2
3d
Ph
7.260
7.193
1.172
1.195
1.148
10
9
8
7
6
5
4
3
2
1
ppm
0.91
3.75
7.09
2.16
5.26
3.88
1.99
2.00
5.89

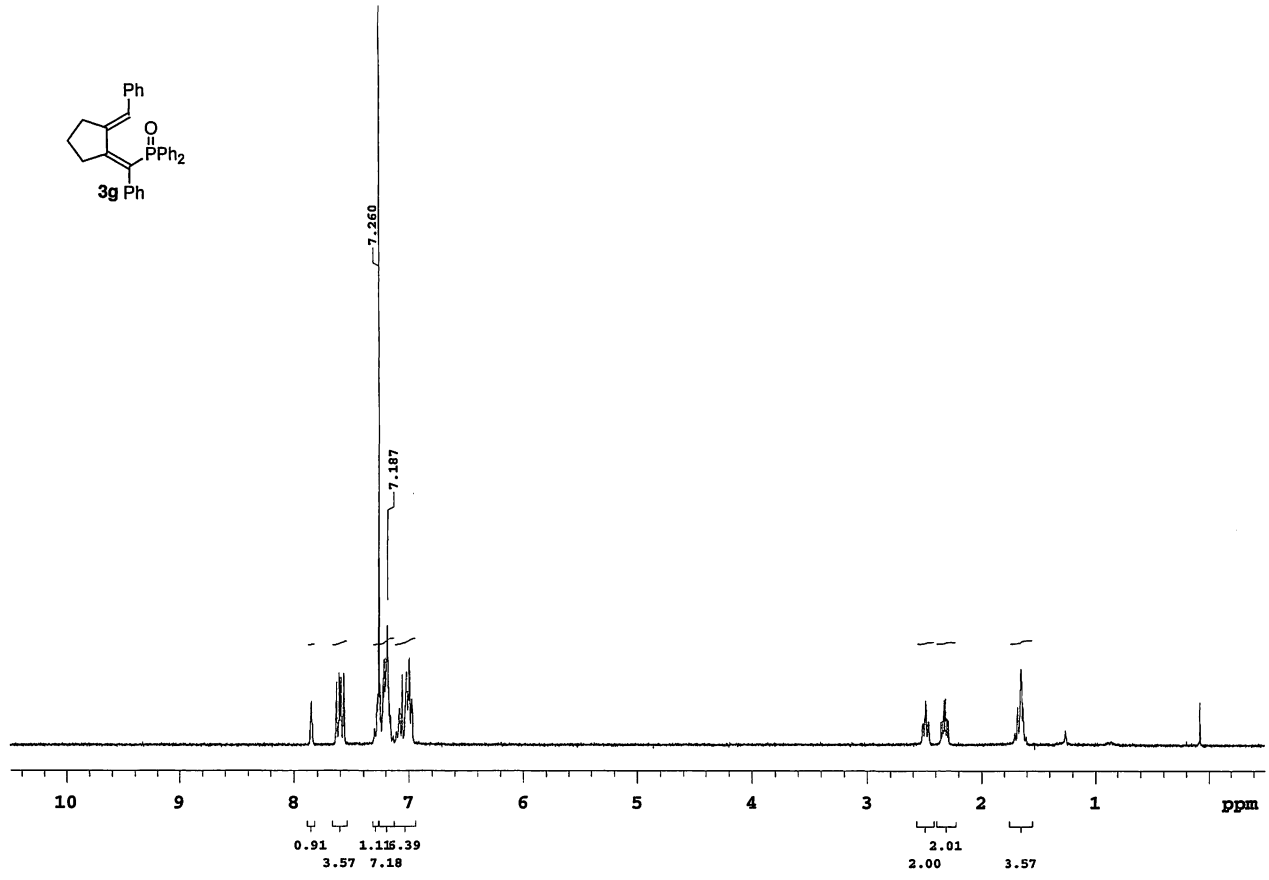

Ph
EtO2C
EtO2C
O
PPh2
3d
Ph
131.283
131.161
128.986
127.625
127.466
61.777
14.118
220
200
180
160
140
120
100
80
60
40
20
0
ppm

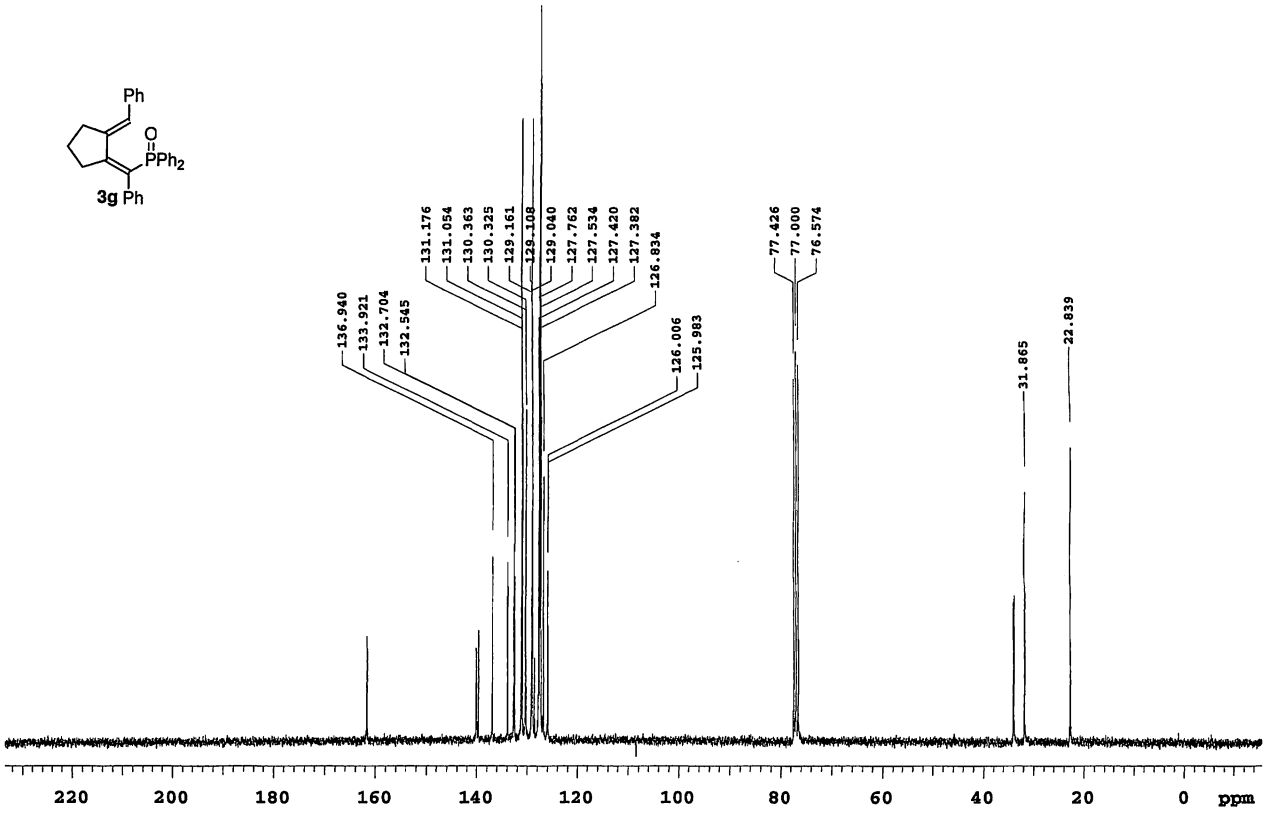


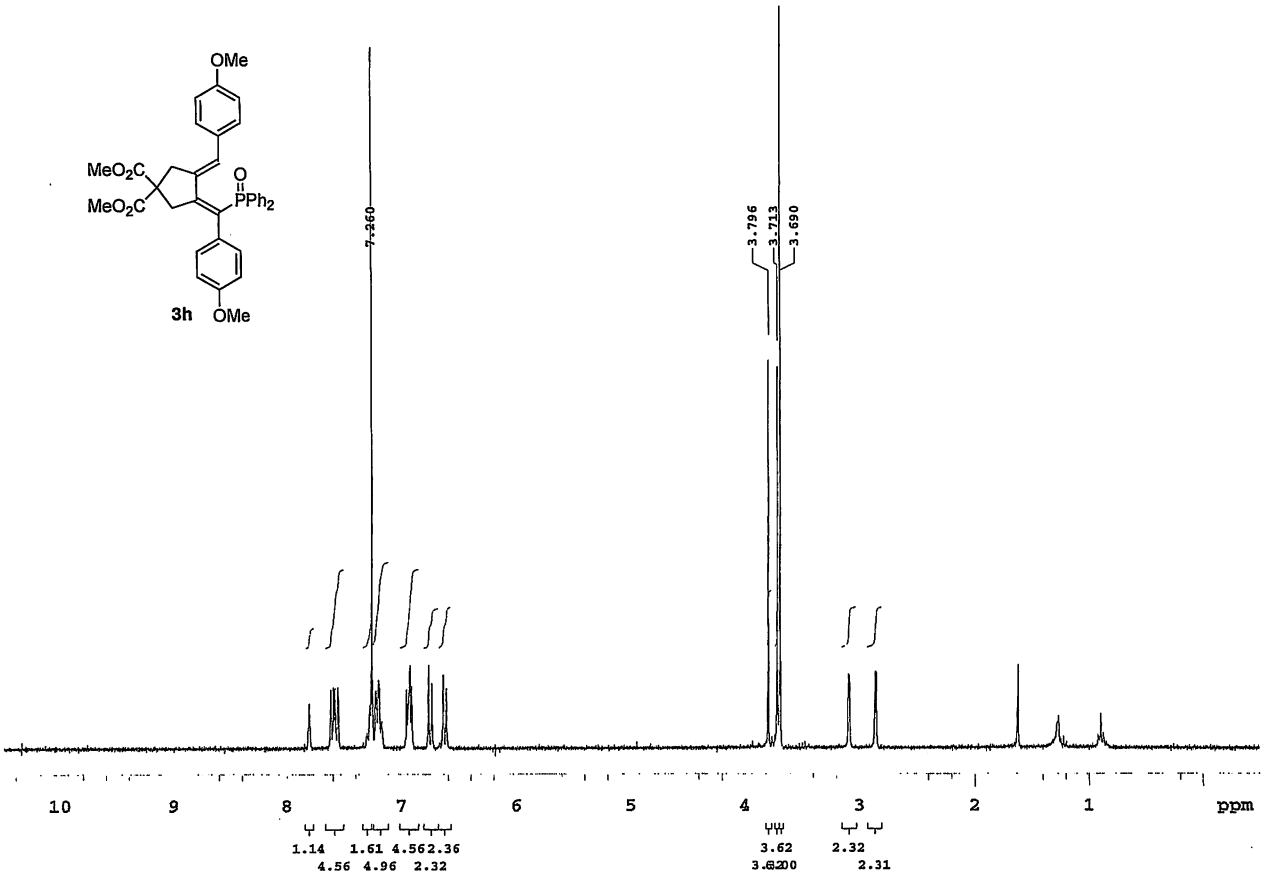


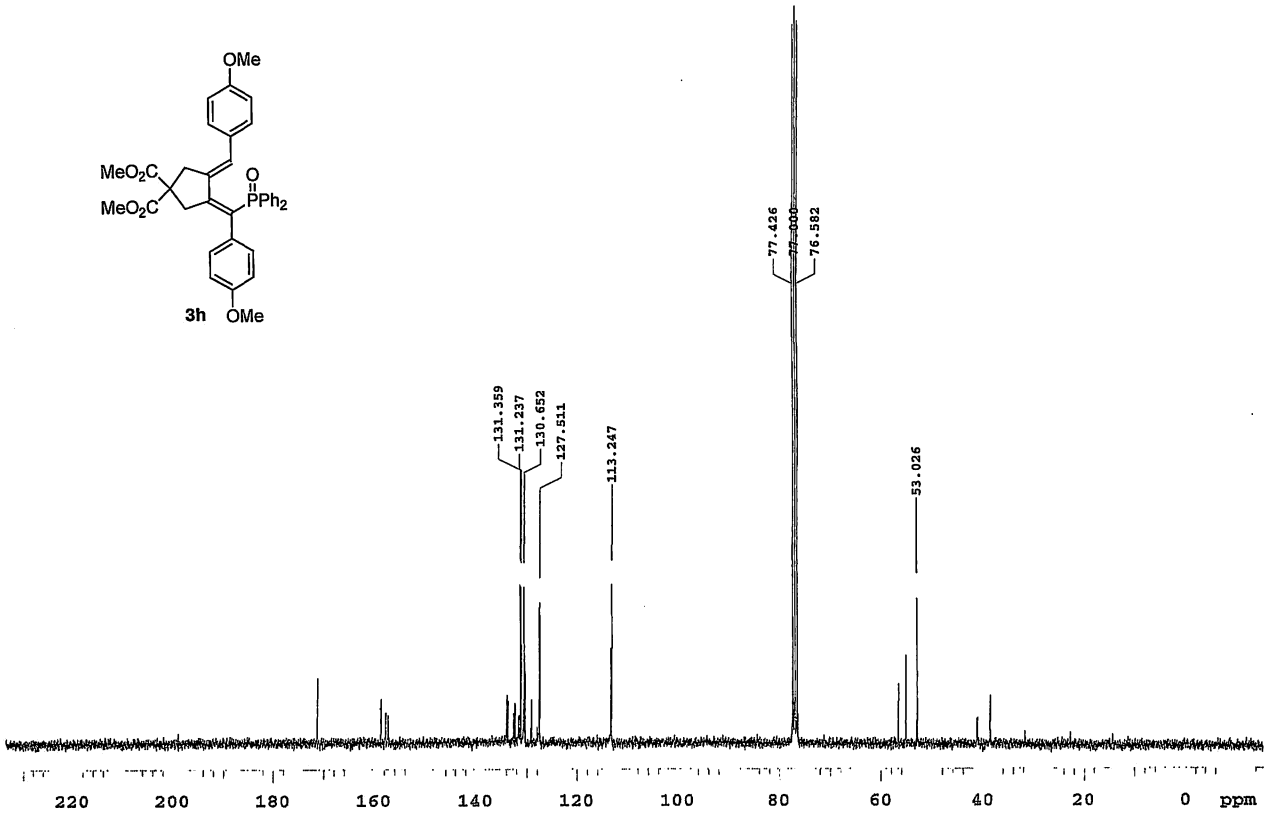


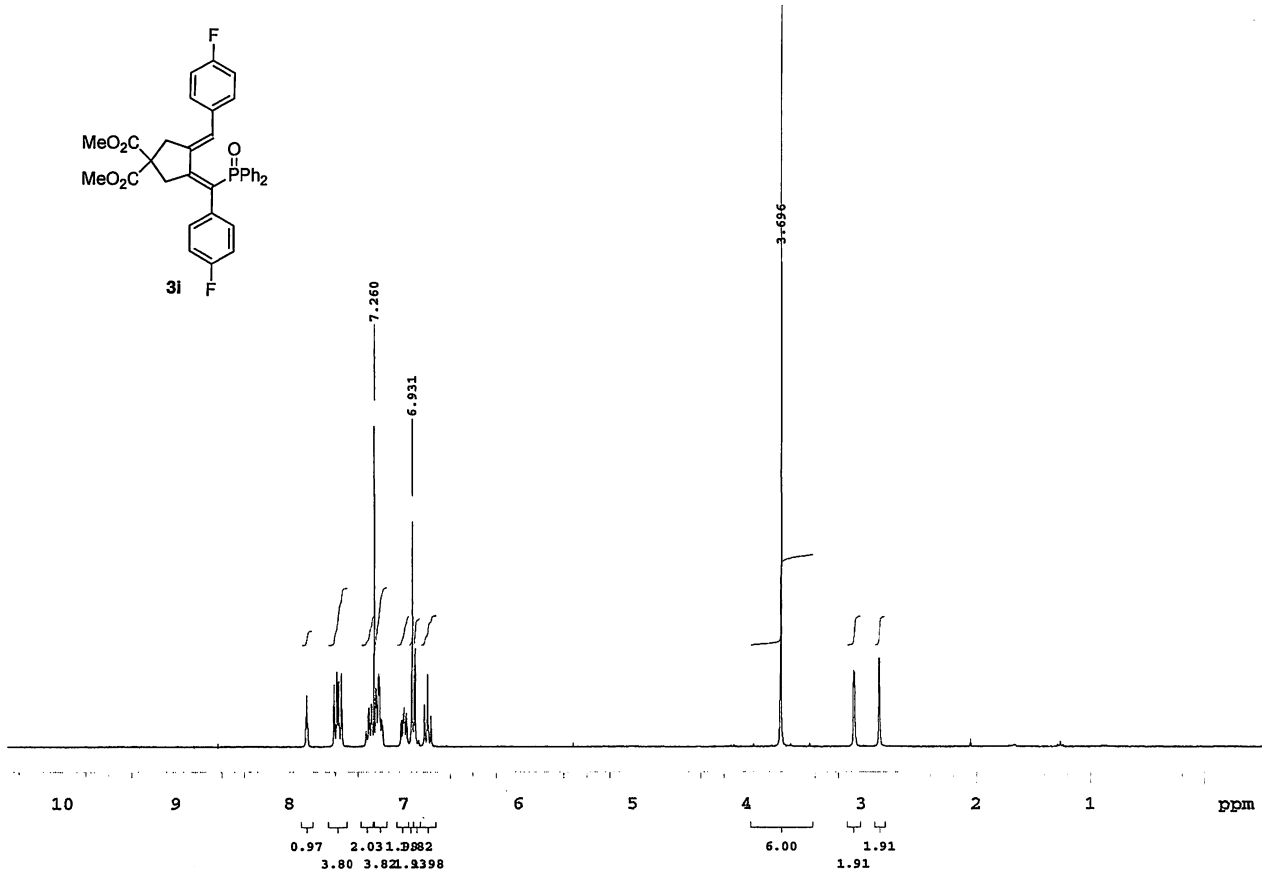


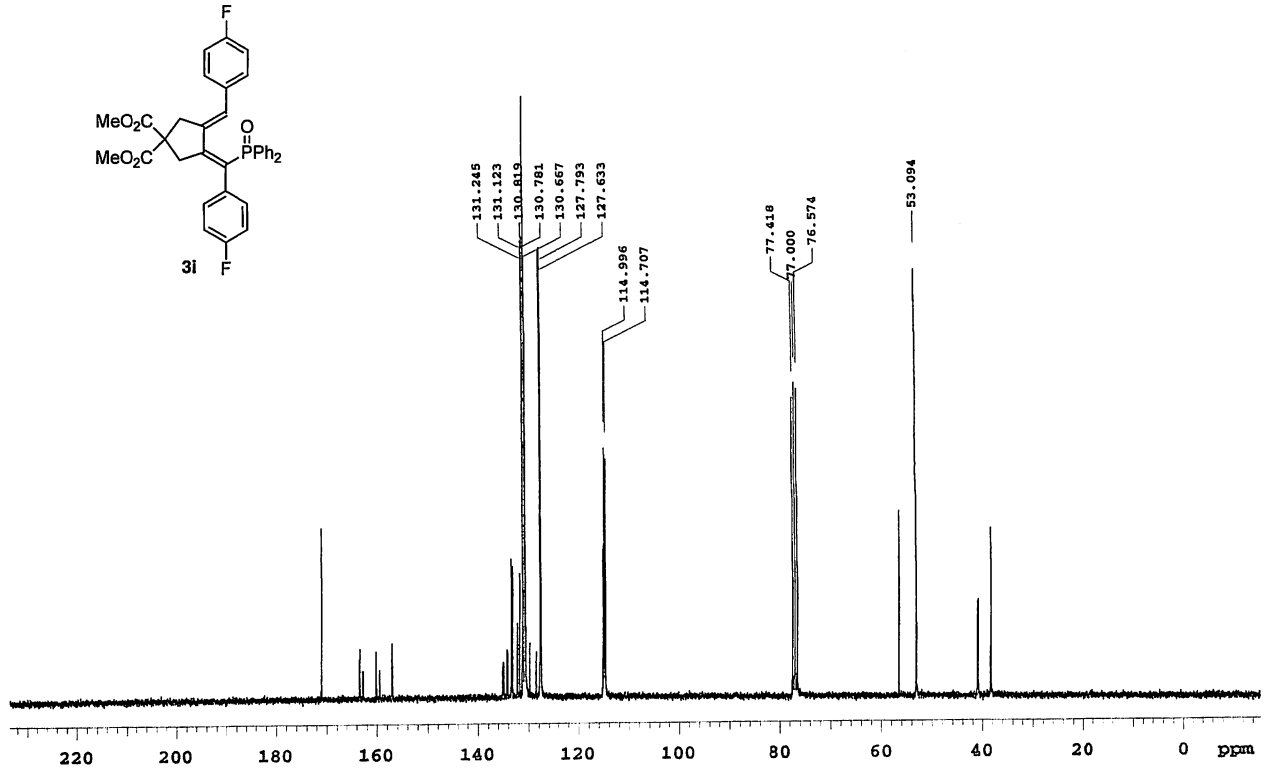

Ph
O
PPh2
3g Ph
7.260
7.187
10
9
8
7
6
5
4
3
2
1
ppm
0.91
1.11
5.39
3.57
7.18
2.01
2.00
3.57

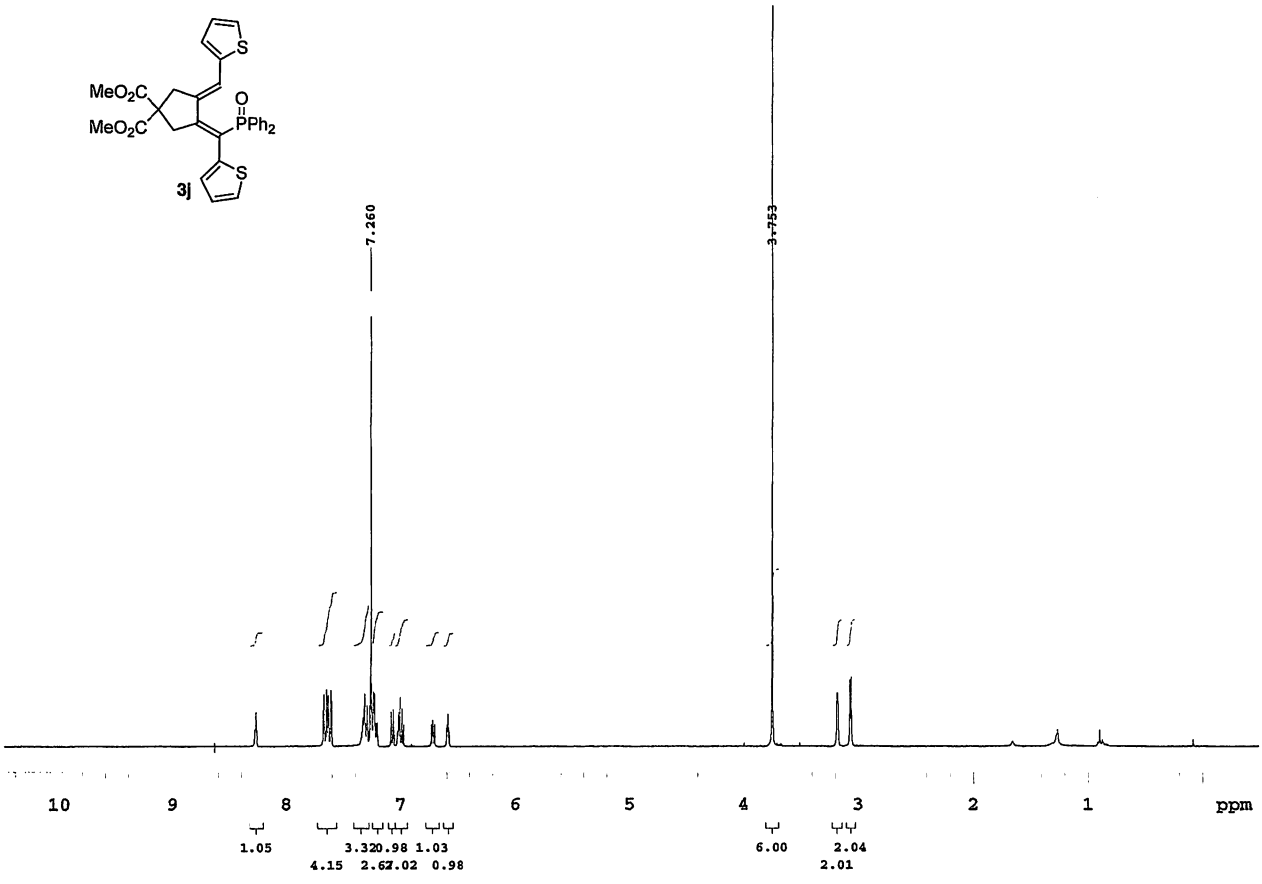

Ph
O
PPh2
3g Ph
131.176
131.054
130.363
130.325
129.161
129.108
129.040
127.762
127.534
127.420
127.382
126.834
126.006
125.983
136.940
133.921
132.704
132.545
77.426
77.000
76.574
31.865
22.839
220
200
180
160
140
120
100
80
60
40
20
0
ppm

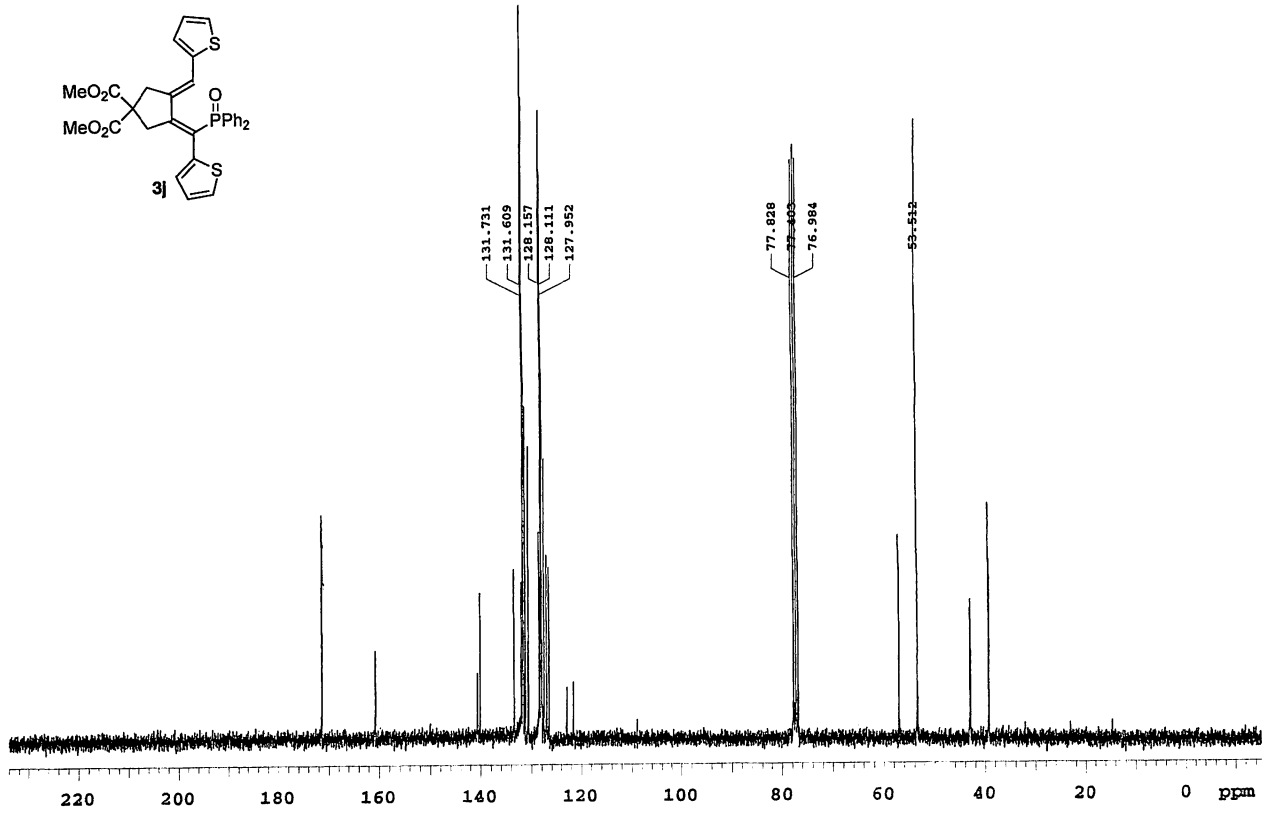









MeO2C
MeO2C
O
PPh2
S
S
3j
7.260
3.753
10
9
8
7
6
5
4
3
2
1
ppm
1.05
3.32
0.98
1.03
4.15
2.67
2.02
0.98
6.00
2.04
2.01


MeO2C
MeO2C
O
PPh2
S
S
3j
131.731
131.609
128.157
128.111
127.952
77.828
77.403
76.984
53.512
220
200
180
160
140
120
100
80
60
40
20
0
ppm