Supporting Information:

Chain-Length-Dependent Reactivity of Alkenyl Phosphates in Ruthenium-Catalyzed Cross-Metathesis

Apicha Pontavatchai,[a,b] Kevin Schwedtmann,[a] Philipp Royla,[a] Kai Schwedtmann,[a] Tossapol Khamnaen,[c] Uwe Schwarzenbolz,[a] Thomas Henle,[a] Ekasith Somsook,[*,b] Jan J. Weigand[*,a]

Electronic Supplementary Information (ESI) for Chemical Communications.

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S1. Chemicals and instruments

All manipulations were performed in a Glovebox or using Schlenk techniques under an atmosphere of purified argon or nitrogen. Dry, oxygen-free solvents were distilled either from CaH_2 or from potassium. Deuterated solvents were purchased from Merck, Deutero, or Eurisotop. Dry solvents were stored over molecular sieves (4 Å: CH_2Cl_2, *n*-hexane, cyclohexane, $CDCl_3$). All glassware was oven-dried at 160 °C prior to use. Flash column chromatography: Merk silica gel 60 (200-400 mesh). Anhydrous deuterated chloroform ($CDCl_3$) methanol (CD_3OD) were purchased from Sigma-Aldrich. 2nd generation Grubbs catalyst was purchased from BLD pharm and used as received. Phosphorus substrates **1a**[1] and **3a**[2], were prepared according to procedures given by literature. Diethyl chlorophosphate and **2a** were purchased from Sigma Aldrich. Alkene substrates styrene (**a**) was purchased from Acros Organics. Allyl bromide (**b**) was purchased from Honeywell Fluka. 2-Methyl-3-buten-2-ol (**c**), 2-methylpent-1-ene (**f**), hex-5-en-1-yl acetate (**h**), and β-Methallyl Alcohol from TCI chemicals. 5-Hexen-2-one (**d**) allyl acetate (**e**) were purchased from Sigma Aldrich. 6-bromohex-1-ene (**g**) and 3-Buten-1-ol were purchased from BLD pharm. *n*-butyl lithium (2.5 M in hexane) was purchased from Sigma Aldrich and used as received. Trimethylamine was purchased from Sigma Aldrich, distilled in an inert atmosphere, and stored over 4 Å molecular sieve. **NMR spectra** were measured on a Bruker AVANCE III HD Nanobay 400 MHz UltraShield (^{1}H: 400.13 MHz, ^{13}C: 100.61 MHz, ^{31}P: 161.98 MHz), or on a Bruker AVANCE III HDX, 500 MHz Ascend (^{1}H: 500.13 MHz, ^{13}C: 125.75 MHz, ^{31}P: 202.45 MHz). Reported numbers assigning atoms in the ^{13}C spectra were indirectly deduced from the cross-peaks in 2D correlation experiments (HMBC, HSQC). Chemical shifts are referenced to δ(Me_4Si) = 0.00 ppm (^{1}H, ^{13}C, externally), δ($CFCl_3$) = 0.00 ppm (externally) and δ(H_3PO_4, 85%) = 0.00 ppm (externally). Unless stated otherwise, all NMR spectra were measured at 300 K. Chemical shifts (δ) are reported in ppm. Coupling constants (J) are reported in Hz. **Melting points** were recorded on an electrothermal melting point apparatus (Büchi Switzerland, Melting point

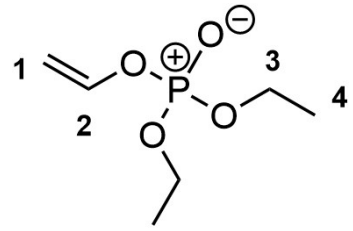
M-560) in sealed capillaries under a Nitrogen atmosphere and are uncorrected. **Infrared (IR)** spectra were recorded at ambient temperature using a Bruker Vertex 70 instrument equipped with a RAM II module (Nd: YAG laser, 1064 nm). An ATR unit (diamond) was used to record IR spectra. The intensities are reported relative to the most intense peak and are given in parenthesis using the following abbreviations: vw = very weak, w = weak, m = medium, s = strong, vs = very strong. **High-resolution mass spectrometry** (**HRMS**) HR-MS data were recorded on a Bruker Impact II Q-TOF mass spectrometer using electrospray ionization (ESI) in positive mode. The samples were directly injected using an eluent mixture of water/acetonitrile (50/50) and 0.1% formic acid with a flow of 0.3 ml/min.

S2. Synthetic procedures

S2.1 General synthesis of diethyl alkenyl phosphates 1-3a.

Alkenyl alcohol (136 mmol) and triethylamine (136 mmol) were added to a 250 mL Schlenk flask and suspended in cyclohexane (60 mL) at 0 °C. Then, diethyl chlorophosphate (120 mmol) was added dropwise, resulting in the formation of a white precipitate. The reaction mixture was stirred overnight and then quenched with 1 M HCl solution (30 mL). The organic layer was washed with brine, and the aqueous layer was separated and removed. The aqueous layer was further extracted with CH_2Cl_2 (3 × 10 mL). The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure using a rotary evaporator. The crude product was purified by reduced-pressure distillation.

S2.2 Preparation of Diethyl vinyl phosphate (1a)



To a solution of vinyl alcohol (1.32 g, 30 mmol) in THF (70 mL), *n*-butyl lithium (2.5 M in hexane, 12 mL, 30 mmol) was added dropwise under N_2 atmosphere at 0 °C. The mixture was stirred at room temperature overnight (16 h). Then, diethyl chlorophosphate (4.35 mL, 30 mmol) was slowly added dropwise at −76 °C and stirred for 1 h at 0 °C. The reaction mixture was stirred again overnight at room temperature. Subsequently, the colorless precipitate was filtered off, and the solvent was removed under reduced pressure. The pale-yellow crude product was purified by distillation to afford **1a** as a colorless liquid (3 g, 60% yield, Bp: 214-218 °C); **IR** (ATR, 298 K, in cm^{-1}): 3501 (vw), 3079 (vw), 2986 (vw), 2936 (vw), 2912 (vw), 2874 (vw), 2360 (vw), 2341 (vw), 1844 (vw), 1772 (vw), 1644 (m), 1480 (vw), 1445 (vw), 1394 (vw), 1371 (vw), 1314 (vw), 1269 (s), 1165 (w), 1136 (m), 1099 (w), 1011 (vs), 979 (vs), 873 (w), 819 (s), 753 (w), 705 (w), 526 (m), 470 (m); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.36 (6H, m, H4), 4.17 (4H, m, H3), 6.57 (1H, m, H2), 4.56, 4.89 (2H, ddd, m, $^3J_{HH}$ = 13.6 Hz, $^3J_{HH}$ = 1.9 Hz, H1); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.2 (2C, d, $^3J_{CP}$ = 6 Hz, C4), 64.5 (2C, d, $^2J_{CP}$ = 6 Hz, C3), 99.9 (1C, d, $^3J_{CP}$ = 10 Hz, C1), 142.3 (1C, d, $^2J_{CP}$ = 6 Hz, C2); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -4.9 (1P,

s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_6H_{14}O_4P$ 181.0624 found 181.0625, $[M + Na]^+$ calcd for $C_6H_{13}O_4PNa$ 203.0444 found 203.0444.

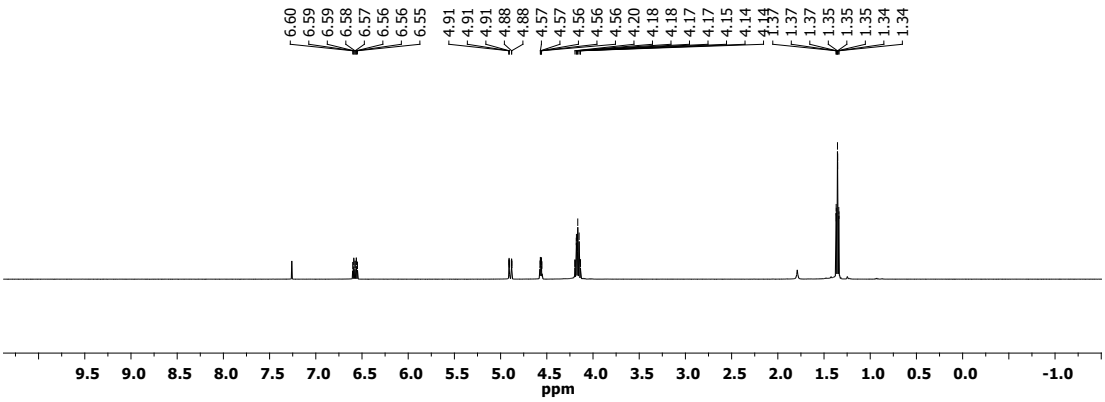


Figure S1 ^1H NMR spectrum of **1a** ($CDCl_3$, 300 K).

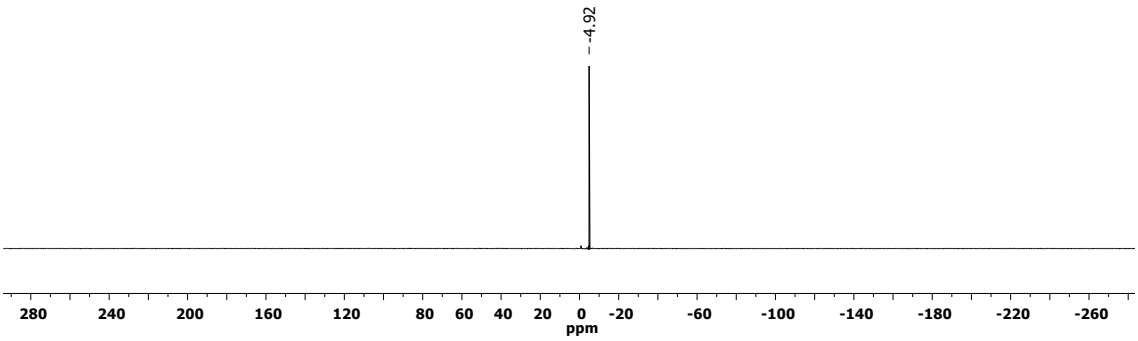


Figure S2 $^{31}P\{^1H\}$ NMR spectrum of **1a** ($CDCl_3$, 300 K).

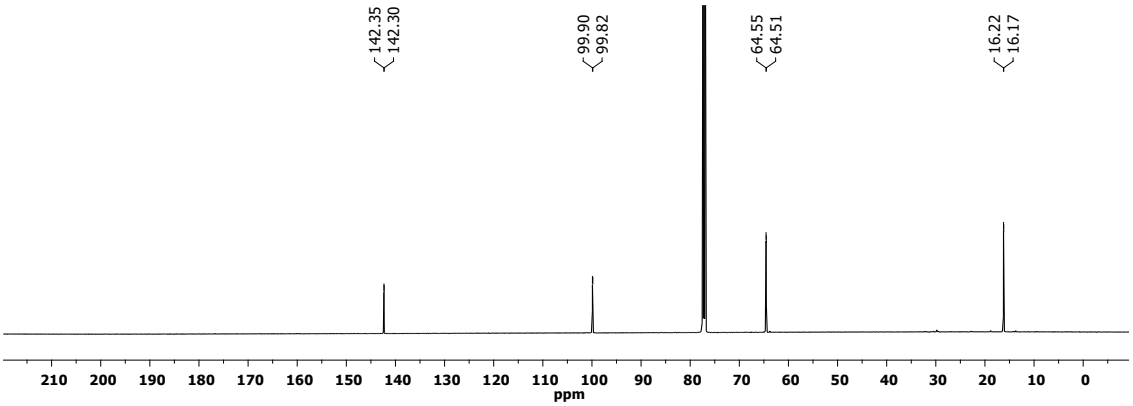
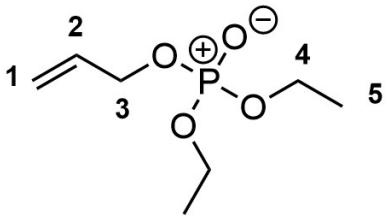


Figure S3 $^{13}C\{^1H\}$ NMR spectrum of **1a** ($CDCl_3$, 300 K).

S2.3 Preparation of Diethyl allyl phosphate (2a)



Compound **2a** was synthesized from diethyl chlorophosphate (17 mL, 117 mmol), allyl alcohol (8.75 mL, 129 mmol), and triethylamine (18 mL, 129 mmol) following the procedure outlined in S2.1. After distillation, **2a** was obtained as a colorless liquid (19 g, 70% yield, 39–42 °C (38 mbar)); **IR** (ATR, 298 K, in cm^{-1}): 3545 (vw), 3486 (vw), 2984 (vw), 2935 (vw), 2911 (vw), 2361 (w), 2341 (vw), 1650 (vw), 1479 (vw), 1457 (vw), 1445 (vw), 1426 (vw), 1410 (vw), 1394 (vw), 1370 (vw), 1262 (s), 1165 (w), 1100 (w), 1015 (vs), 977 (vs), 863 (m), 842 (m), 816 (m), 801 (m), 751 (w), 669 (w), 632 (w), 592 (w); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.34 (6H, ddd, H5), 4.53 (2H, ddt, H3), 5.95 (1H, dtd, $^{3}J_{HH}$ = 16.0 Hz, $^{3}J_{HH}$ = 10.6 Hz, $^{4}J_{HP}$ = 5.6 Hz, H2), 4.11 (4H, ddd, m, H4), 5.24, 5.36 (2H, dd, ddd, $^{3}J_{HH}$ = 10.4 Hz, $^{2}J_{HH}$ = 1.3 Hz, $^{3}J_{HH}$ = 17.1 Hz, $^{2}J_{HH}$ = 1.3 Hz, H1); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C5), 63.9 (2C, d, $^{2}J_{CP}$ = 6 Hz, C4), 68.0 (1C, d, $^{2}J_{CP}$ = 5 Hz, C3), 118.2 (1C, s, C1), 132.8 (1C, d, $^{3}J_{CP}$ = 7 Hz, C2); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_7H_{16}O_4P$ 195.0781 found 195.0784, $[M + Na]^+$ calcd for $C_7H_{15}O_4PNa$ 217.0600 found 217.0603.

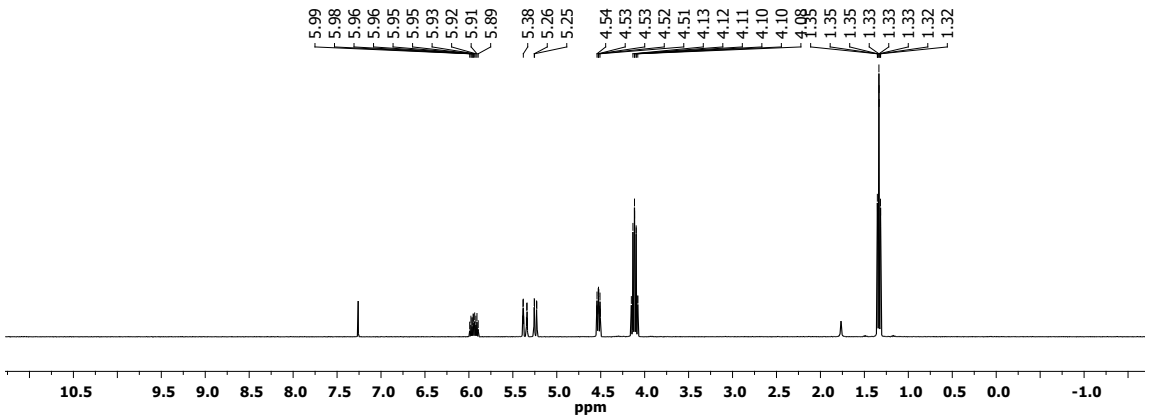


Figure S4 ^{1}H NMR spectrum of **2a** ($CDCl_3$, 300 K).

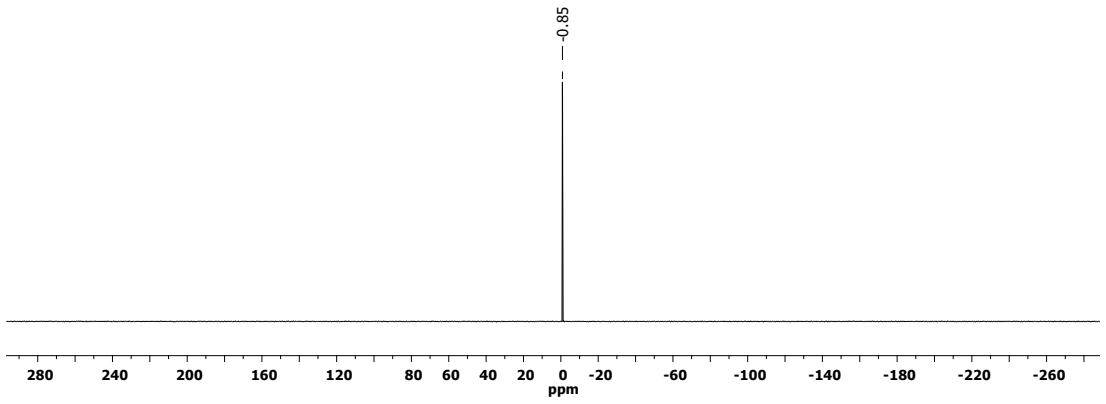


Figure S5 $^{31}P\{^{1}H\}$ NMR spectrum of **2a** ($CDCl_3$, 300 K).

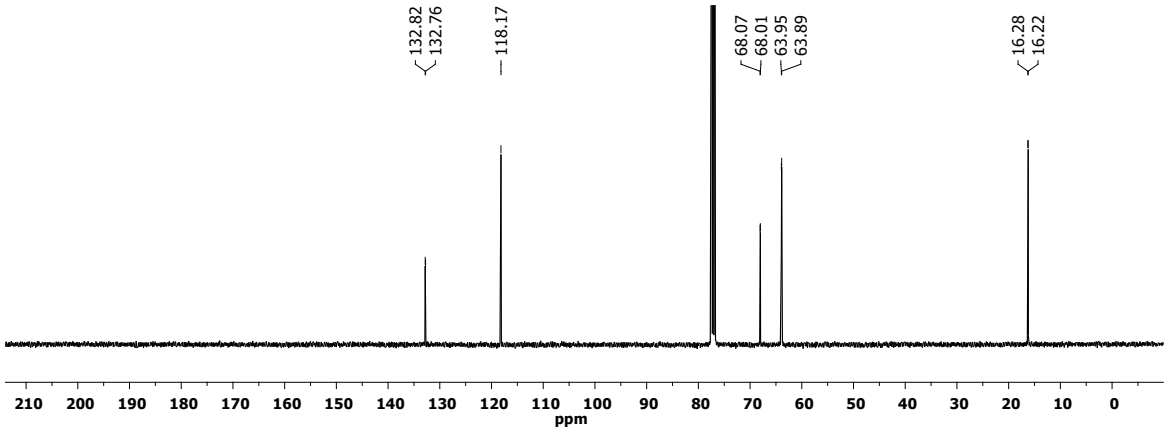
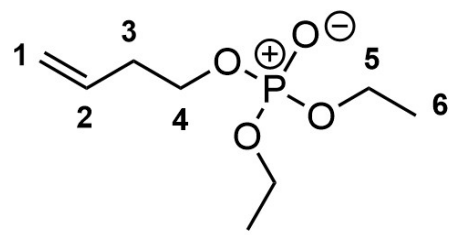


Figure S6 $^{13}C\{^{1}H\}$ NMR spectrum of **2a** ($CDCl_3$, 300 K).

S2.4 Preparation of Butenyl phosphate (3a)



Compound **3a** was synthesized from diethyl chlorophosphate (17.4 mL, 120 mmol), 3-buten-1-ol (11.36 mL, 132 mmol), and triethylamine (18.4 mL, 132 mmol) following the procedure outlined in S2.1. After distillation, **3a** was obtained as a colorless liquid (17 g, 66% yield, Bp: 50–53 °C (38 mbar)); **IR** (ATR, 298 K, in cm^{-1}): 2983 (vw), 2935 (vw), 2909 (vw), 2360 (w), 2341 (vw), 1643 (vw), 1477 (vw), 1445 (vw), 1393 (vw), 1370 (vw), 1261 (m), 1166 (vw), 1100 (vw), 1018 (vs), 975 (vs), 918 (m), 861 (w), 799 (m), 745 (w), 669 (vw), 636 (vw), 521 (m); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.33 (6H, t, $^{3}J_{HH}$ = 7.1 Hz, H6), 2.43 (2H, q, $^{3}J_{HH}$ = 6.7 Hz, H3), 4.09 (6H, tt, H4,5), 5.11 (2H, dd, $^{3}J_{HH}$ = 13.7 Hz, H1), 5.79 (1H, ddt, $^{3}J_{HH}$ = 17.0 Hz, $^{3}J_{HH}$ = 10.3 Hz, $^{3}J_{HH}$ = 6.7 Hz, H2);

$^{13}C\{^1H\}$ NMR (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C6), 34.8 (1C, d, $^3J_{CP}$ = 7 Hz, C3), 63.9 (2C, d, $^2J_{CP}$ = 6 Hz, C5), 66.7 (1C, d, $^2J_{CP}$ = 6 Hz, C4), 117.8 (1C, s, C1), 133.6 (1C, s, C2); **$^{31}P\{^1H\}$ NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_8H_{18}O_4P$ 209.0937 found 209.0942, $[M + Na]^+$ calcd for $C_8H_{17}O_4PNa$ 231.0757 found 231.0761.

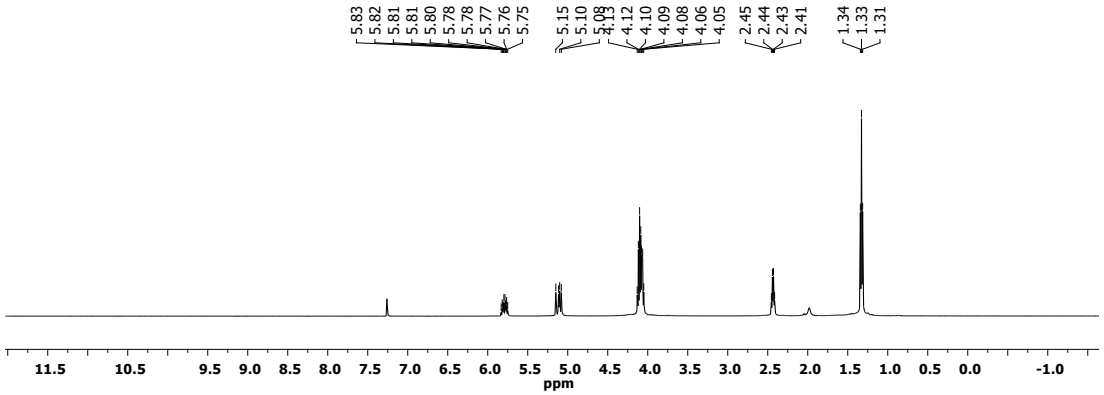


Figure S7 ^1H NMR spectrum of **3a** ($CDCl_3$, 300 K).

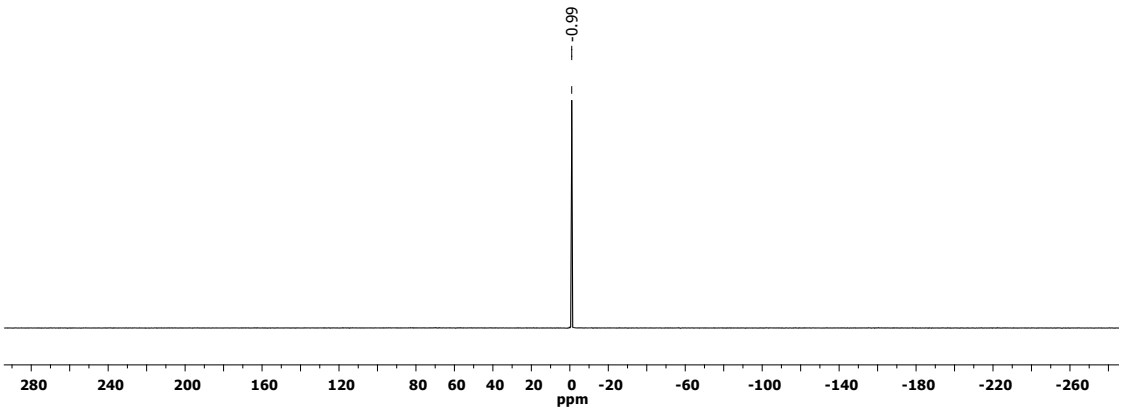


Figure S8 $^{31}P\{^1H\}$ NMR spectrum of **3a** ($CDCl_3$, 300 K).

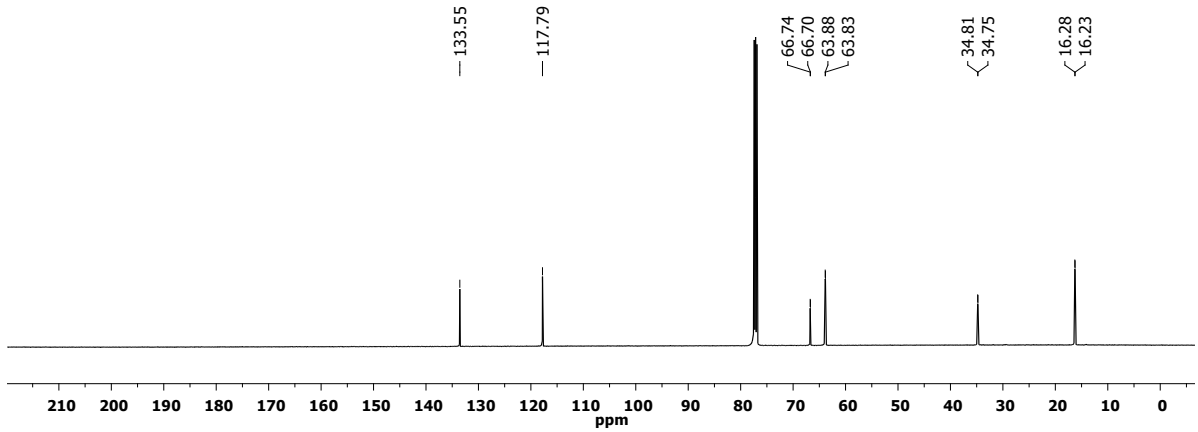
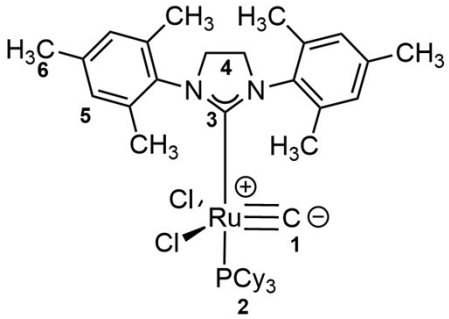


Figure S9 $^{13}C\{^{1}H\}$ NMR spectrum of **3a** ($CDCl_3$, 300 K).

S2.5 Preparation of Ru-carbide (4)



Method A: To a solution of **1a** (0.5 mmol, 0.096 mL) in CH_2Cl_2 (3 mL) was added a solution of 2nd generation Grubbs catalyst (0.5 mmol, 0.424 g) in CH_2Cl_2 (1 mL). The resulting mixture was stirred at 45 °C for 24 h, during which the solution changed color to brown and yellow. The solvent was evaporated under reduced pressure, and the yellow-brown residue was washed with methanol, filtered, and dried in vacuo to afford **4** (0.27 g, 70%) as a pale yellow powder.

Method B: To a solution of **1a** (0.08 mmol, 0.016 mL) in CH_2Cl_2 (1 mL) was added a solution of 2nd generation Grubbs catalyst (0.08 mmol, 0.069 g) in CH_2Cl_2 (1 mL). After 1 hour, the $^{31}P\{^{1}H\}$ NMR spectrum showed four peaks at 34.2, 29, 0, and −4.9 ppm, corresponding to **1** (39%), 2nd generation Grubbs catalyst (61%), phosphoric acid diethyl ester, and **1a**, respectively. After overnight stirring (16 h), the $^{31}P\{^{1}H\}$ NMR spectrum indicated complete conversion to **4** and phosphoric acid diethyl ester. Complex **4** was precipitated by the addition of *n*-hexane and dried in vacuo. Yield: 70%; pale yellow powder; **m.p**.: 246-248 °C; **IR** (ATR, 298 K, in cm^{-1}): 2915 (m), 2848 (m), 2735 (vw), 1943 (vw), 1748 (vw), 1606 (vw), 1481 (m), 1441 (s), 1377 (vw), 1349 (vw), 1329 (vw), 1289 (w), 1265 (vs), 1231 (vw), 1202 (vw), 1176 (vw), 1129 (vw), 1114 (vw), 1079 (vw), 1033 (w), 1005 (w), 950 (vw), 918 (vw), 899 (vw), 889 (w), 861 (w), 848 (m), 818 (vw), 451 (vw), 421 (vw), 411 (vw); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.11-2.30 (33H, m,

H2), 2.24-2.54 (18H, s, H4), 4.02, 4.11 (4H, m, H5), 6.89, 6.95 (4H, s, H6); **$^{13}C\{^{1}H\}$ NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 479.5 (1C, s, C1), 129.5-138.5 (12C, s, C5), 18.9-21.4 (18C, s, C2), 18.9-21.4 (6C, s, C6), 212.2, 212.9 (1C, s, C3), 51.0, 52.1 (2C, d, $^{4}J_{CP}$ = 2.0, 3.4 Hz, C4); **$^{31}P\{^{1}H\}$ NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = 34.2 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{40}H_{60}Cl_2N_2PRu$ 771.2904 found 771.2905.

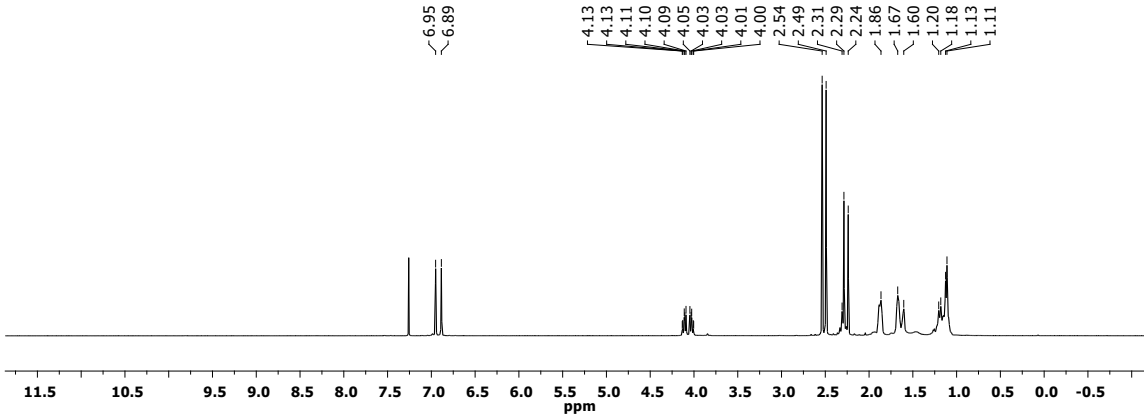


Figure S13 ^{1}H NMR spectrum of **4** ($CDCl_3$, 300 K).

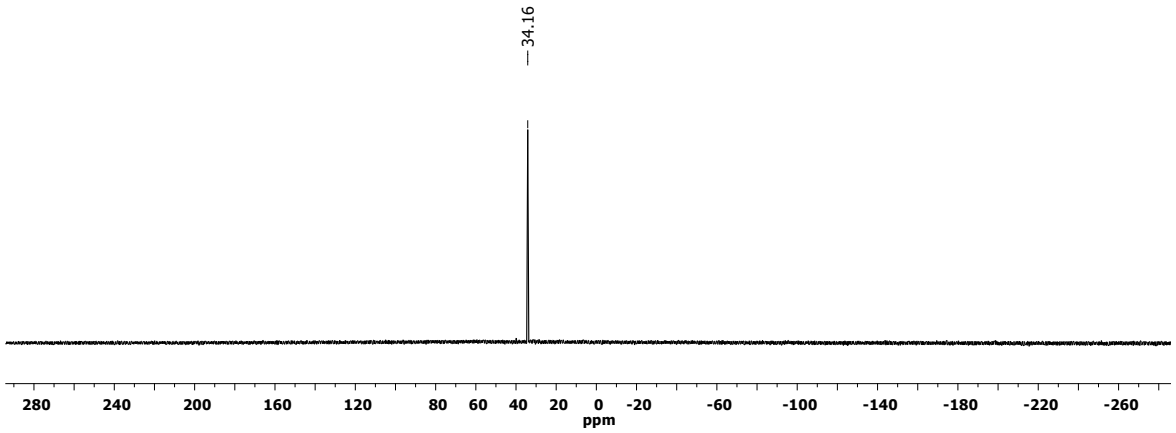


Figure S14 $^{31}P\{^{1}H\}$ NMR spectrum of **4** ($CDCl_3$, 300 K).

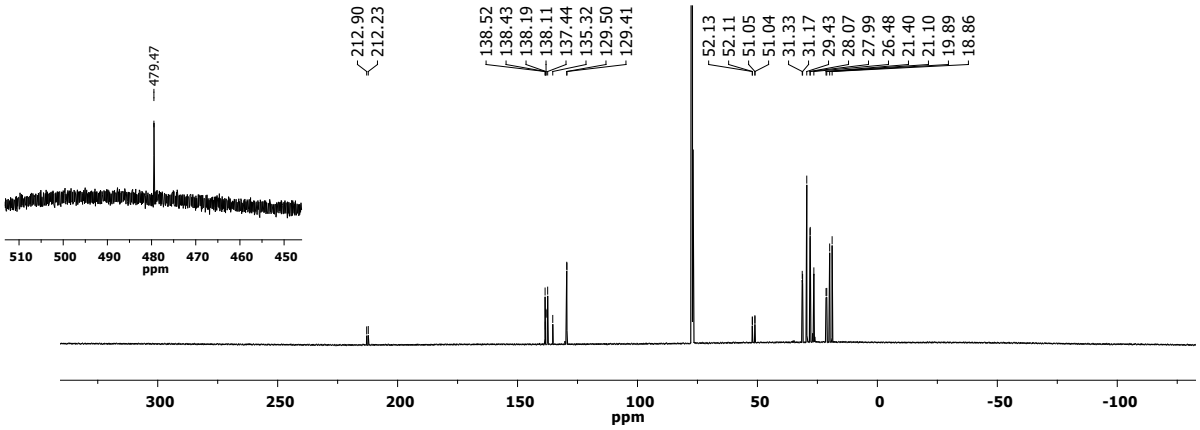


Figure S15 $^{13}C\{^{1}H\}$ NMR spectrum of **4** ($CDCl_3$, 300 K).

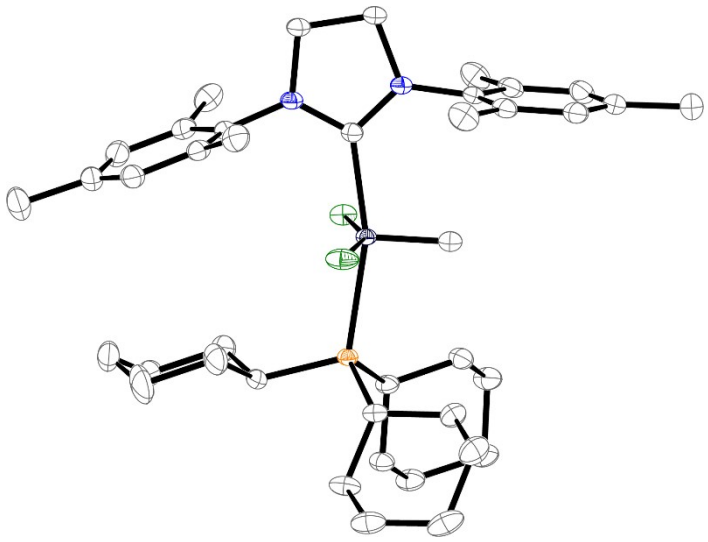
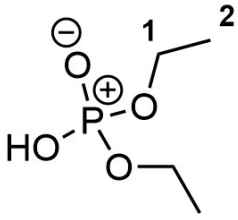


Figure S16 Molecular structure of **4**; hydrogen atoms are omitted for clarity, and thermal ellipsoids are displayed at 50% probability.[3]

S2.6 Preparation of Phosphoric acid diethyl ester (5)



Compound **5** was synthesized from the reaction procedures outlined in S2.5 and separated by column chromatography using ethyl acetate/methanol (6:4). **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.33 (6H, t, $^{3}J_{HH}$ = 7.0 Hz, H1), 4.09 (4H, t, $^{3}J_{HH}$ = 7.2 Hz, H2); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 63.8 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = 0.6 (1P, s, P).

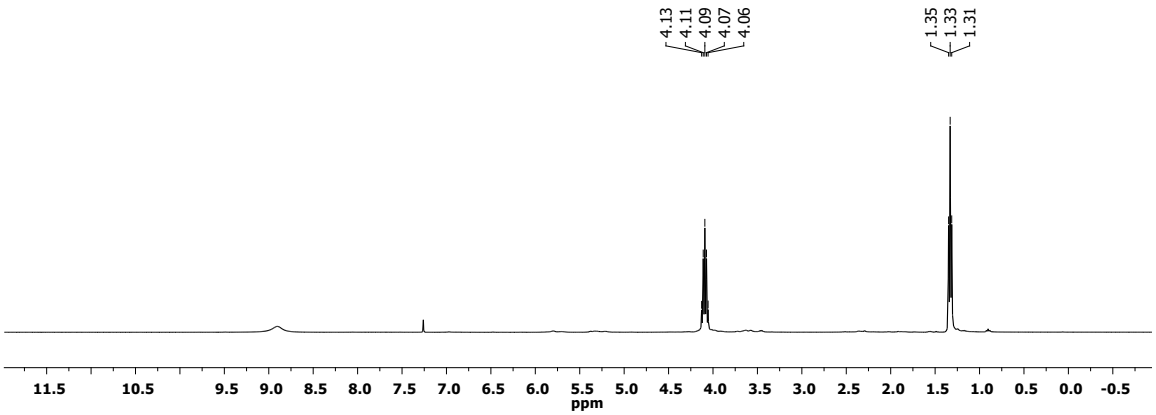


Figure S17 ^{1}H NMR spectrum of **5** ($CDCl_3$, 300 K).

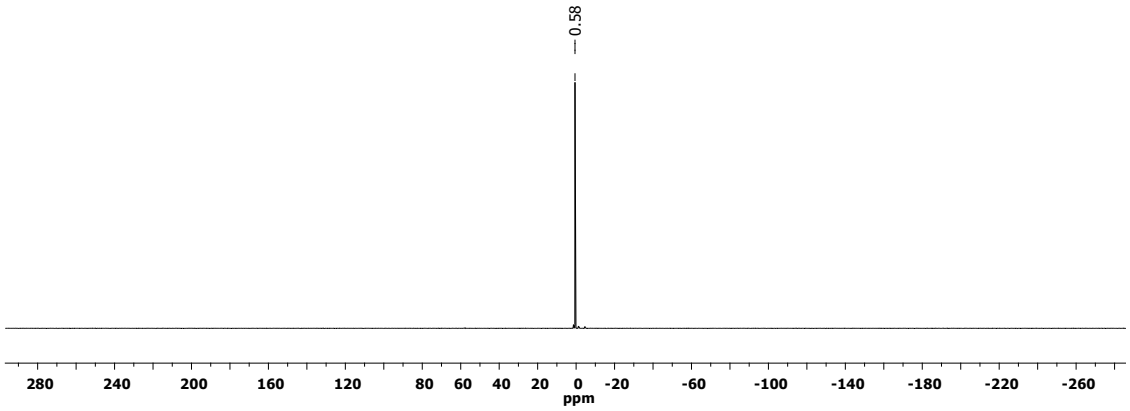


Figure S18 $^{31}P\{^{1}H\}$ NMR spectrum of **5** ($CDCl_3$, 300 K).

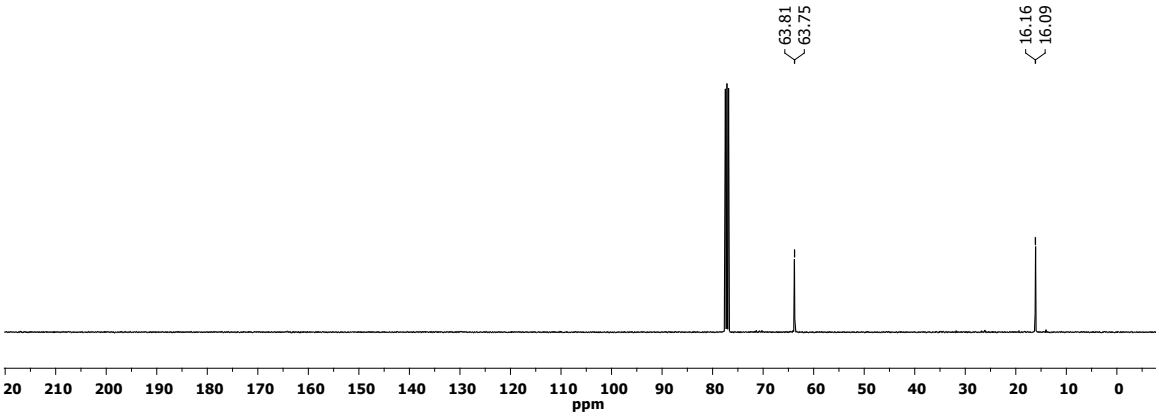
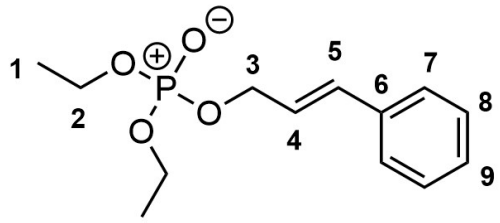


Figure S19 $^{13}C\{^{1}H\}$ NMR spectrum of **5** ($CDCl_3$, 300 K).

S2.7 General procedure for the cross-metathesis of diethyl alkenyl phosphates 1-3a with alkene substrates.

In a Schlenk flask, diethyl alkenyl phosphates (1.0 mmol) and alkene substrates (3.0 mmol) were mixed in CH_2Cl_2 (3 mL) and added to a solution of 2nd Generation Grubbs catalyst (**GII**) in CH_2Cl_2 (1 mL). The resulting mixture was stirred at 45 °C for 24 hours. Afterward, the solvent was removed under reduced pressure to yield a dark brown liquid. The crude product was purified by column chromatography using ethyl acetate/cyclohexane (6:4).

S2.8 Cross metathesis of diethyl allyl phosphate (2a) with styrene (a)



Compound **2aa** was synthesized from **2a** (0.089 mL, 0.5 mmol) and styrene (0.19 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2aa** (47 mg, 35% yield; *E/Z*, 100:0); **IR** (ATR, 298 K, in cm^{-1}): 3061 (vw), 3028 (vw), 2984 (vw), 2911 (w), 2848 (vw), 2737 (vw), 2360 (vw), 2331 (vw), 1717 (vw), 1701 (vw), 1679 (vw), 1627 (vw), 1601 (vw), 1480 (vw), 1446 (w), 1394 (vw), 1370 (vw), 1289 (vw), 1228 (m), 1166 (m), 1100 (w), 1023 (vs), 971 (vs), 862 (w), 848 (w), 817 (m), 803 (m), 746 (m); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.34 (6H, t, $^3J_{HH}$ = 7.1 Hz, H1), 4.13 (4H, p, $^3J_{HH}$ = 7.3 Hz, H2), 4.69 (2H, m, H3), 6.30 (1H, dt, $^3J_{HH}$ = 15.8 Hz, $^3J_{HH}$ = 6.2 Hz, H4), 6.68 (1H, d, $^3J_{HH}$ = 15.9 Hz, H5), 7.26 (1H, t, $^3J_{HH}$ = 7.7 Hz, H9), 7.32 (2H, t, $^3J_{HH}$ = 7.5 Hz, H8), 7.39 (2H, d, $^3J_{HH}$ = 7.2 Hz, H7); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 64.0 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 68.1 (1C, d, $^2J_{CP}$ = 5 Hz, C3), 123.7 (1C, d, C4), 126.8 (2C, s, C7), 128.3 (1C, s, C9), 128.8 (2C, s, C8), 134.0 (1C, s, C6), 136.2 (1C, s, C5); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.8 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{13}H_{20}O_4P$ 271.1094 found 271.1098, $[M + Na]^+$ calcd for $C_{13}H_{19}O_4PNa$ 293.0913 found 293.0917.

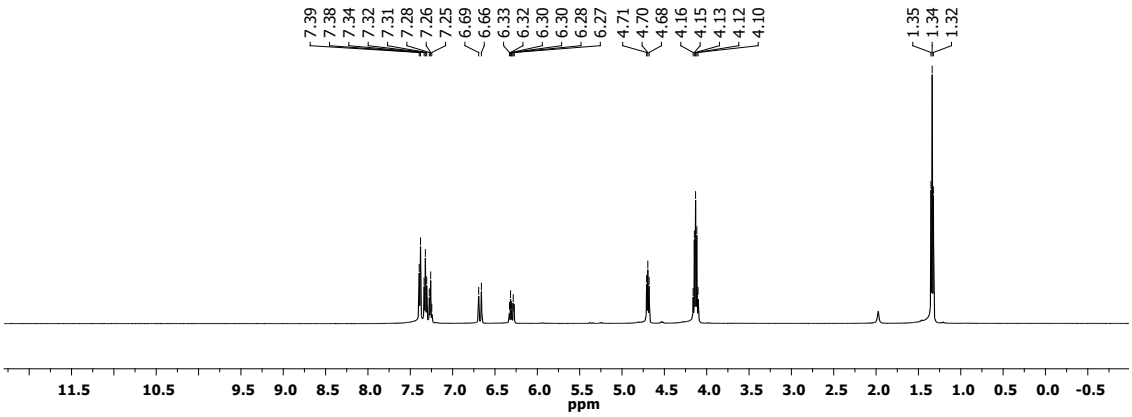


Figure S20 ^{1}H NMR spectrum of **2aa** ($CDCl_3$, 300 K).

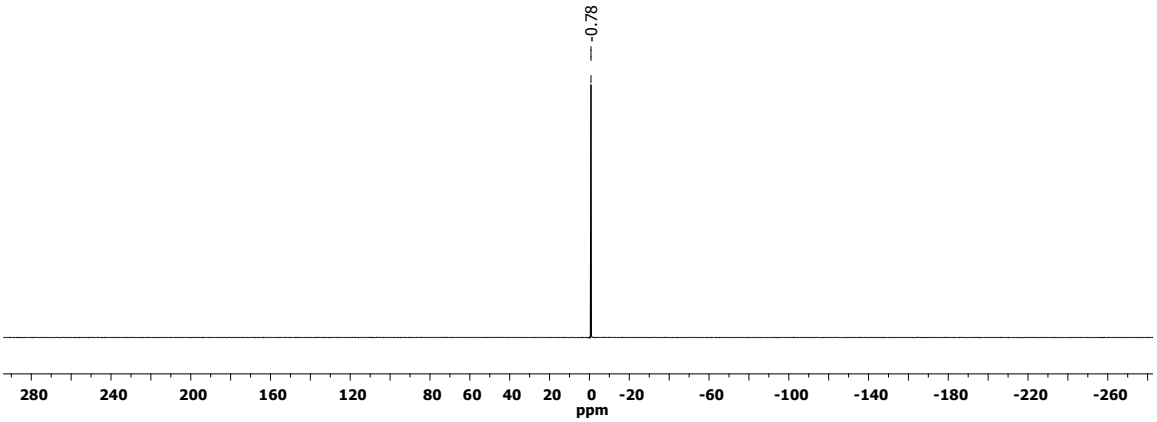


Figure S21 $^{31}P\{^{1}H\}$ NMR spectrum of **2aa** ($CDCl_3$, 300 K).

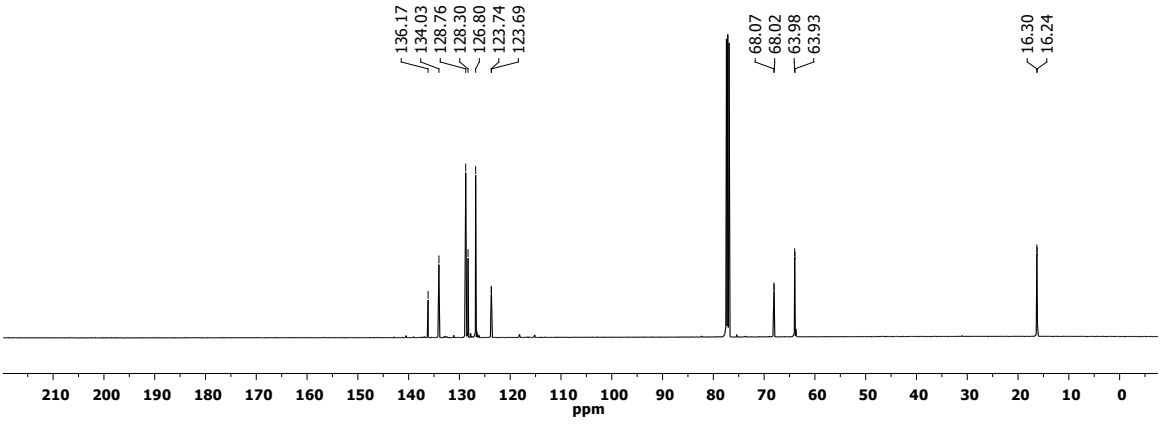
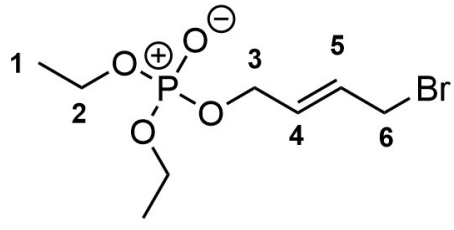


Figure S22 $^{13}C\{^{1}H\}$ NMR spectrum of **2aa** ($CDCl_3$, 300 K).

S2.9 Cross metathesis of diethyl allyl phosphate (2a) with allyl bromide (b)



Compound **2ab** was synthesized from **2a** (0.089 mL, 0.5 mmol) and allyl bromide (0.13 mL, 1.5 mmol) in CH_2Cl_2

(3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2ab** (60 mg, 42% yield; *E/Z*, 91:9); **IR** (ATR, 298 K, in cm^{-1}): 3404 (vw), 2984 (vw), 2934 (vw), 2910 (vw), 2360 (vw), 2341 (vw), 1733 (vw), 1717 (vw), 1698 (vw), 1671 (vw), 1652 (vw), 1636 (vw), 1478 (vw), 1456 (vw), 1444 (vw), 1393 (vw), 1370 (vw), 1258 (m), 1211 (w), 1165 (w), 1095 (w), 1019 (vs), 972 (vs), 846 (w), 816 (m), 802 (m), 748 (w), 669 (vw); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.34 (6H, t, $^3J_{HH}$ = 7.1 Hz, H1), 3.95 (2H, dt, $^3J_{HH}$ = 7.4 Hz, H6), 4.12 (4H, m, H2), 4.55 (2H, m, H3), 5.88 (1H, dt, $^3J_{HH}$ = 15.2 Hz, $^3J_{HH}$ = 5.6 Hz, H4), 6.68 (1H, dt, $^3J_{HH}$ = 15.0 Hz, $^3J_{HH}$ = 7.4 Hz, H5); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 31.2 (1C, s, C6), 64.1 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 66.4 (1C, d, $^2J_{CP}$ = 5 Hz, C3), 123.5 (1C, d, $^3J_{CP}$ = 7 Hz, C4), 129.9 (1C, s, C5); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_8H_{17}O_4BrP$ 287.0042 found 287.0043, 289.0024, $[M + Na]^+$ calcd for $C_8H_{16}O_4BrPNa$ 308.9862 found 308.9863.

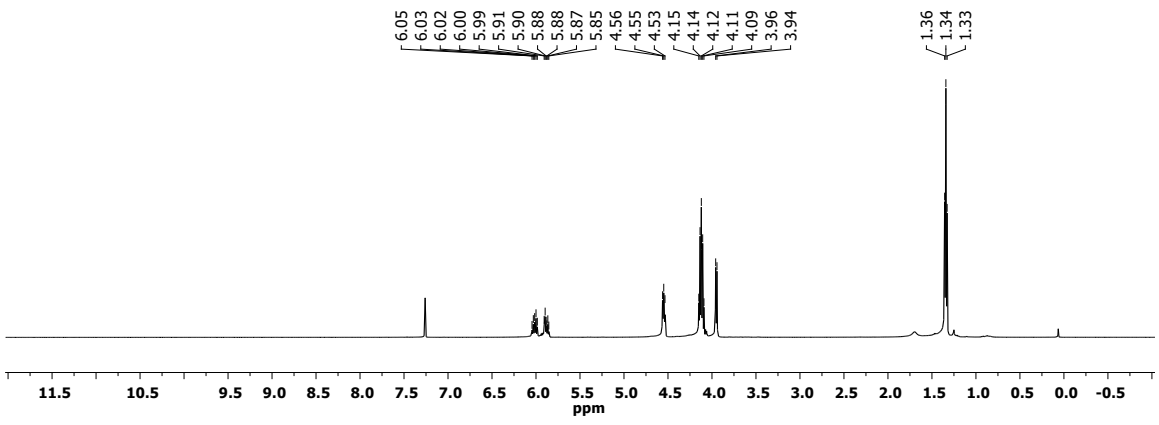


Figure S23 ^{1}H NMR spectrum of **2ab** ($CDCl_3$, 300 K).

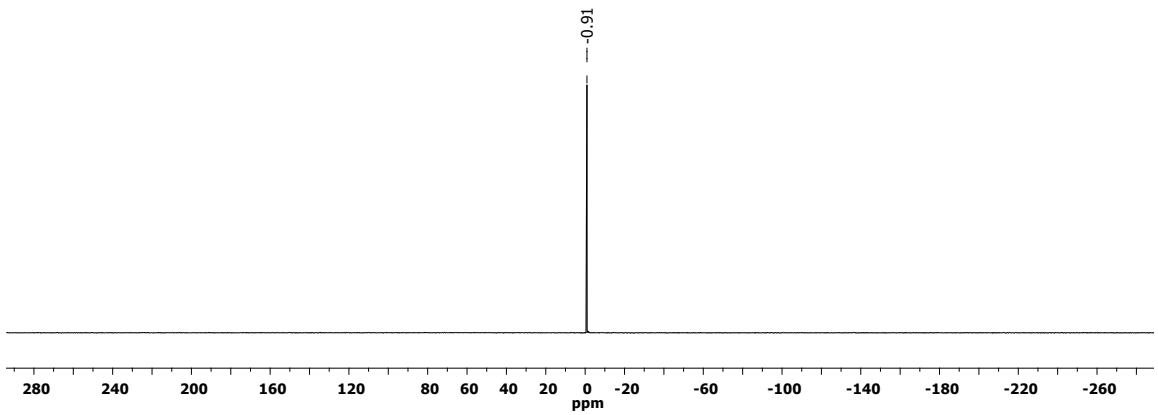


Figure S24 $^{31}P\{^{1}H\}$ NMR spectrum of **2ab** ($CDCl_3$, 300 K).

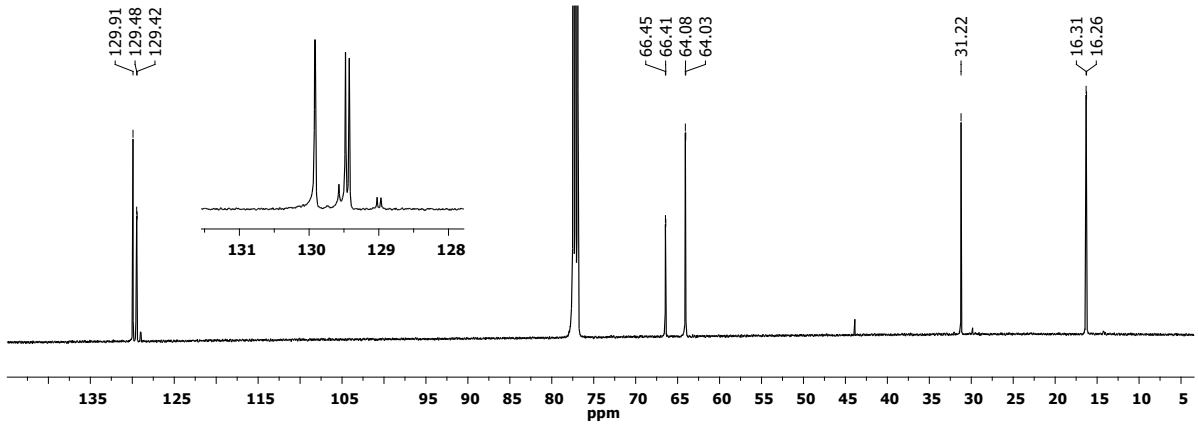
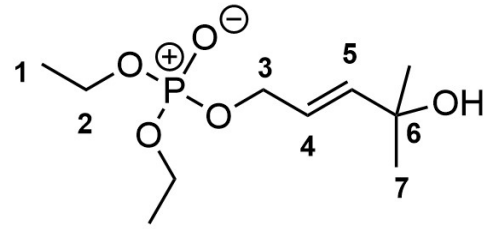


Figure S25 $^{13}C\{^{1}H\}$ NMR spectrum of **2ab** ($CDCl_3$, 300 K).

S2.10 Cross metathesis of diethyl allyl phosphate (2a) with 2-Methyl-3-buten-2-ol (c)



Compound **2ac** was synthesized from **2a** (0.089 mL, 0.5 mmol) and 2-methyl-3-buten-2-ol (0.16 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7 The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2ac** (70 mg, 56% yield; *E/Z*, 100:0); **IR** (ATR, 298 K, in cm^{-1}): 3401 (w), 2975 (w), 2934 (vw), 2911 (vw), 2361 (vw), 2341 (vw), 1868 (vw), 1845 (vw), 1772 (vw), 1733 (vw), 1717 (vw), 1698 (vw), 1670 (vw), 1653 (vw), 1636 (vw), 1558 (vw), 1541 (vw), 1521 (vw), 1507 (vw), 1459 (w), 1445 (vw), 1394 (w), 1372

(w), 1245 (s), 1164 (m), 1099 (w), 1018 (vs), 969 (vs); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.27 (12H, m, H1, H7), 4.05 (4H, p, $^{3}J_{HH}$ = 7.2 Hz, H2), 4.46 (2H, m, H3), 5.73 (1H, dt, $^{3}J_{HH}$ = 15.6 Hz, $^{3}J_{HH}$ = 6.0 Hz, H4), 5.88 (1H, d, $^{3}J_{HH}$ = 15.6 Hz, H5); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.1 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 29.5 (2C, s, C7), 63.8 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 67.6 (2C, d, $^{2}J_{CP}$ = 6 Hz, C3), 70.2 (1C, s, C6), 121.1 (1C, d, $^{3}J_{CP}$ = 5 Hz, C4), 142.7 (1C, s, C5); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.1 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{10}H_{22}O_5P$ 253.1199 found 253.1198, $[M + Na]^+$ calcd for $C_{10}H_{21}O_5PNa$ 275.1019 found 275.1018, $[M - OH^-]^+$ calcd for $C_{10}H_{20}O_4P$ 235.1094 found 235.1093.

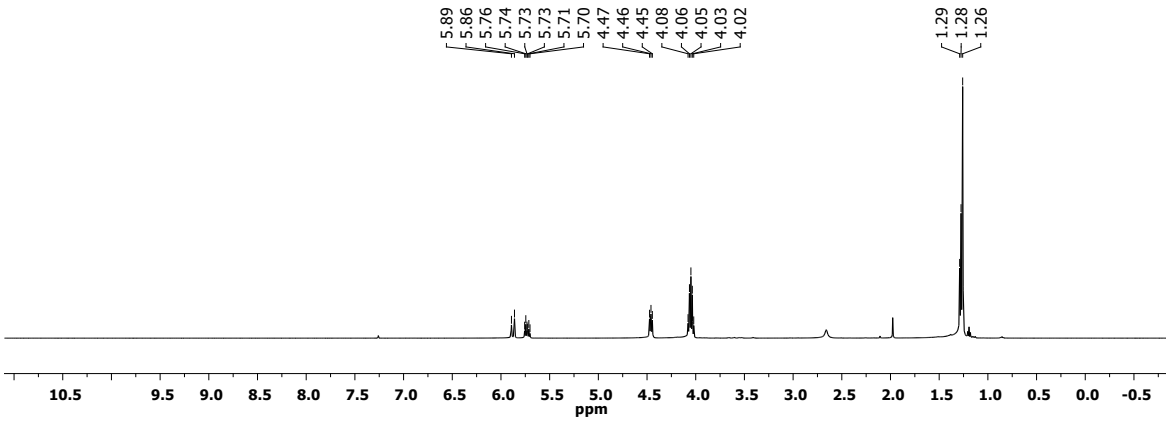


Figure S26 ^{1}H NMR spectrum of **2ac** ($CDCl_3$, 300 K).

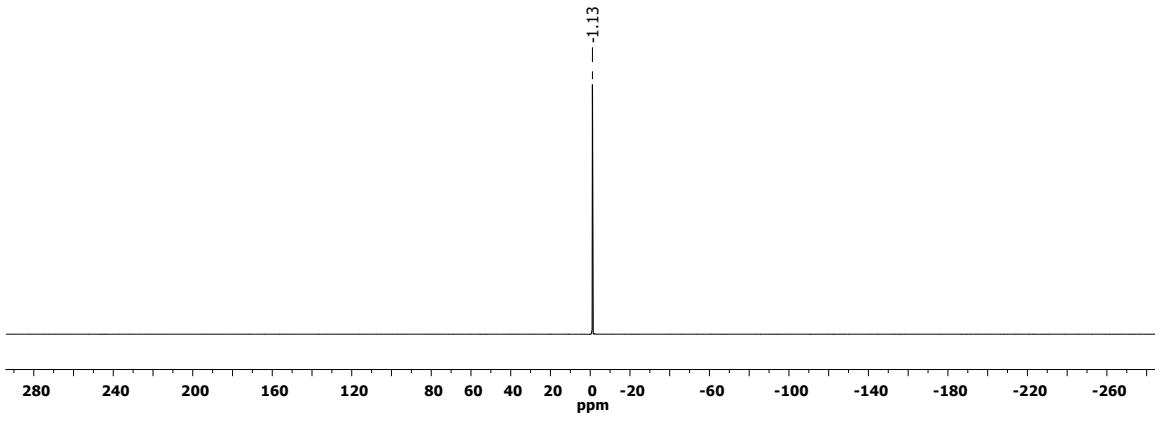


Figure S27 ^{31}P{^{1}H} NMR spectrum of **2ac** ($CDCl_3$, 300 K).

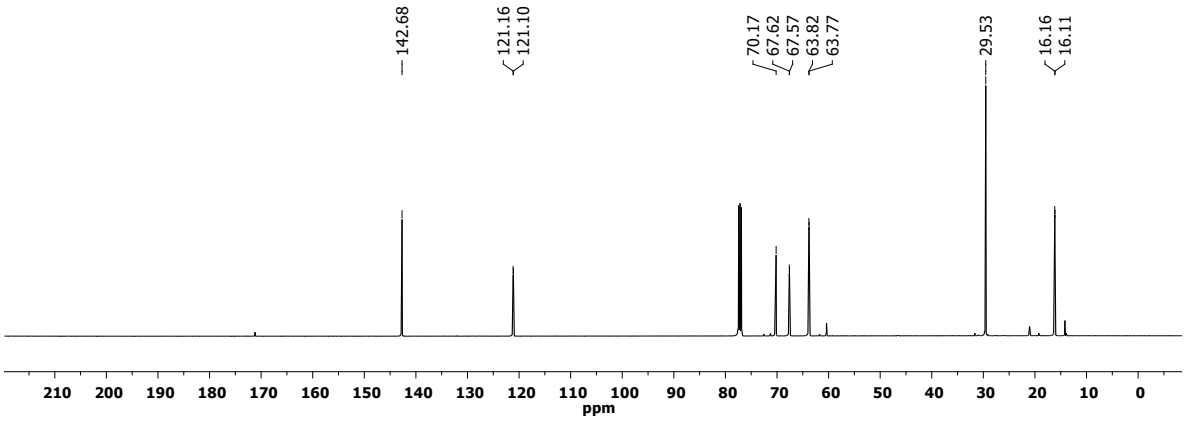
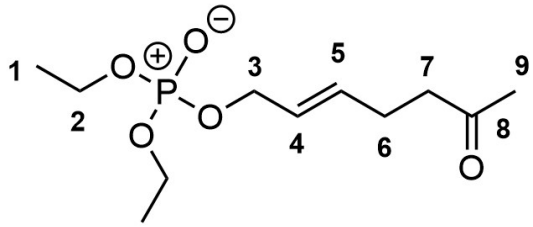


Figure S28 $^{13}C\{^{1}H\}$ NMR spectrum of **2ac** ($CDCl_3$, 300 K).

S2.11 Cross metathesis of diethyl allyl phosphate (2a) with 5-Hexen-2-one (d)



Compound **2ad** was synthesized from **2a** (0.089 mL, 0.5 mmol) and 5-hexen-2-one (0.18 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2ad** (30 mg, 23% yield; *E/Z*, 91:9); **IR** (ATR, 298 K, in cm^{-1}): 2984 (vw), 2934 (vw), 2911 (vw), 2361 (vw), 2341 (vw), 1714 (m), 1653 (vw), 1479 (vw), 1444 (vw), 1420 (vw), 1395 (vw), 1369 (w), 1231 (m), 1164 (m), 1099 (w), 1025 (vs), 972 (vs), 817 (m), 802 (m), 749 (w), 670 (vw), 505 (m), 473 (m), 419 (w); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.33 (6H, t, $^{3}J_{HH}$ = 7.1 Hz, H1), 2.14 (3H, s, H9), 2.33 (2H, q, $^{3}J_{HH}$ = 6.9 Hz, H6), 2.52 (2H, m, H7), 4.10 (4H, m, H2), 4.46 (2H, m, H3 *E*), 4.61 (2H, dd, $^{3}J_{HH}$ = 8.5 Hz, $^{3}J_{HH}$ = 5.6 Hz, H3 *Z*), 5.62 (1H, ddd, $^{3}J_{HH}$ = 15.6 Hz, $^{3}J_{HH}$ = 6.0 Hz, H4), 5.78 (1H, m, H5); **^{13}C{^{1}H} NMR** (100,61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 26.2 (1C, s, C6), 30.1 (1C, s, C9), 42.7 (1C, s, C7), 63.9 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 207.8 (1C, s, C8), 125.6, 125.4 (1C, d, $^{3}J_{CP}$ = 7, 7 Hz, C4 (*E/Z*)), 134.3, 133.3 (1C, s, C5 (*E/Z*)), 68.0, 63.0 (1C, d, $^{2}J_{CP}$ = 6, 6 Hz, C3 (*E/Z*)); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P(*E*)), -0.7 (1P, s, P(*Z*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{11}H_{22}O_5P$ 265.1199 found 265.1200, $[M + Na]^+$ calcd for $C_{11}H_{21}O_5PNa$ 287.1019 found 287.1019.

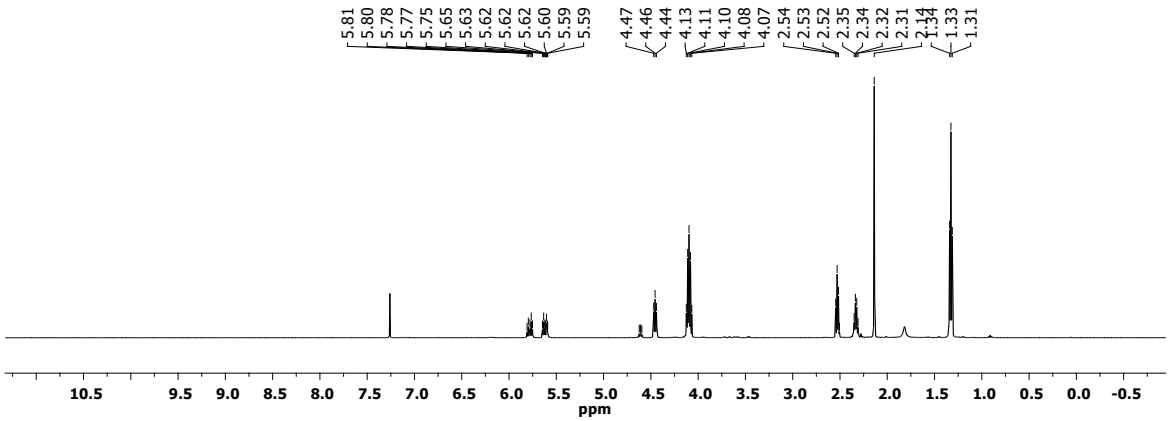


Figure S29 ^{1}H NMR spectrum of **2ad** ($CDCl_3$, 300 K).

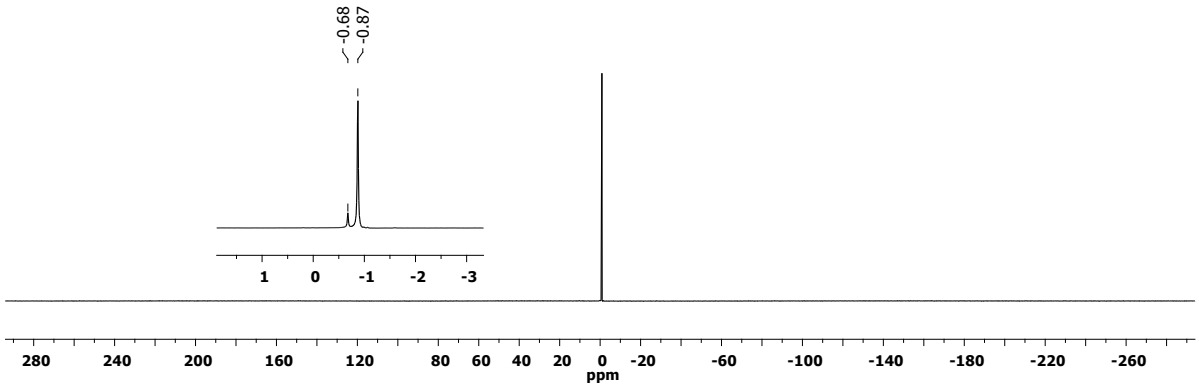


Figure S30 $^{31}P\{^{1}H\}$ NMR spectrum of **2ad** ($CDCl_3$, 300 K).

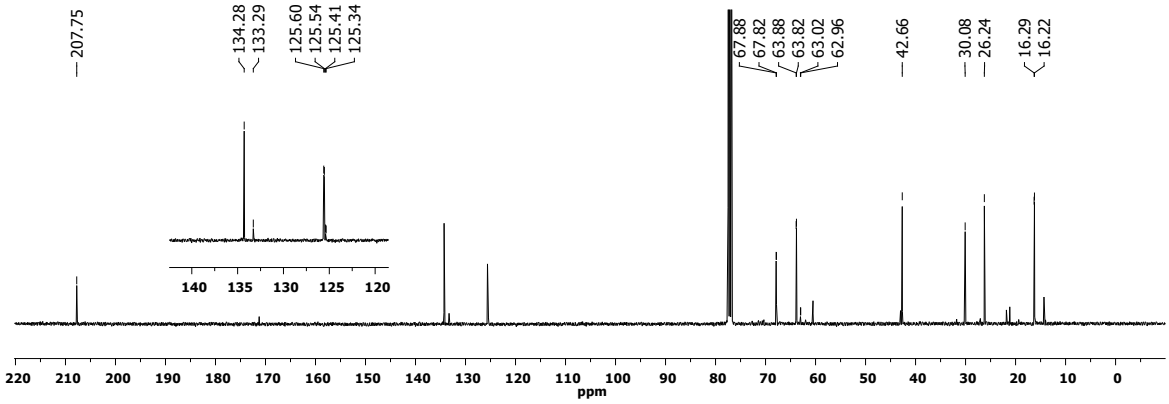
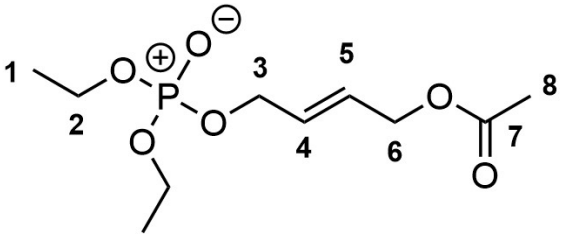


Figure S31 $^{13}C\{^{1}H\}$ NMR spectrum of **2ad** ($CDCl_3$, 300 K).

S2.12 Cross metathesis of diethyl allyl phosphate (2a) with allyl acetate (e)



Compound **2ae** was synthesized from **2a** (0.089 mL, 0.5 mmol) and allyl acetate (0.16 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2ae** (56 mg, 40% yield; *E/Z*, 91:9); **IR** (ATR, 298 K, in cm^{-1}): 2985 (w), 2915 (w), 2852 (vw), 2361 (w), 2341 (vw), 1740 (m), 1653 (vw), 1637 (vw), 1558 (vw), 1541 (vw), 1507 (vw), 1456 (w), 1445 (w), 1374 (w), 1226 (s), 1166 (m), 1094 (m), 1018 (vs), 971 (vs), 847 (m), 817 (m), 802 (m), 748 (m), 669 (w), 608 (m), 518 (m), 474 (m), 419 (w); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.31 (6H, t, $^3J_{HH}$ = 7.1 Hz, H1), 2.04 (3H, s, H8), 4.08 (4H, m, H2), 4.51 (2H, dd, $^3J_{HH}$ = 7.9 Hz, $^3J_{HP}$ = 3.5 Hz, H3), 4.55 (2H, d, H6), 5.86 (2H, q, H4, H5); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.2 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 20.9 (1C, s, C8), 63.8 (1C, s, C6), 63.8 (1C, d, $^2J_{CP}$ = 5 Hz, C3), 63.9 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 128.0 (1C, s, C5), 128.5 (1C, d, $^3J_{CP}$ = 7 Hz, C4), 170.7, 171.2 (1C, s, C7 (*E/Z*)); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P(*E*)), -0.9 (1P, s, P(*Z*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{10}H_{20}O_6P$ 267.0992 found 267.0994, $[M + Na]^+$ calcd for $C_{10}H_{19}O_6PNa$ 289.0811 found 289.0813.

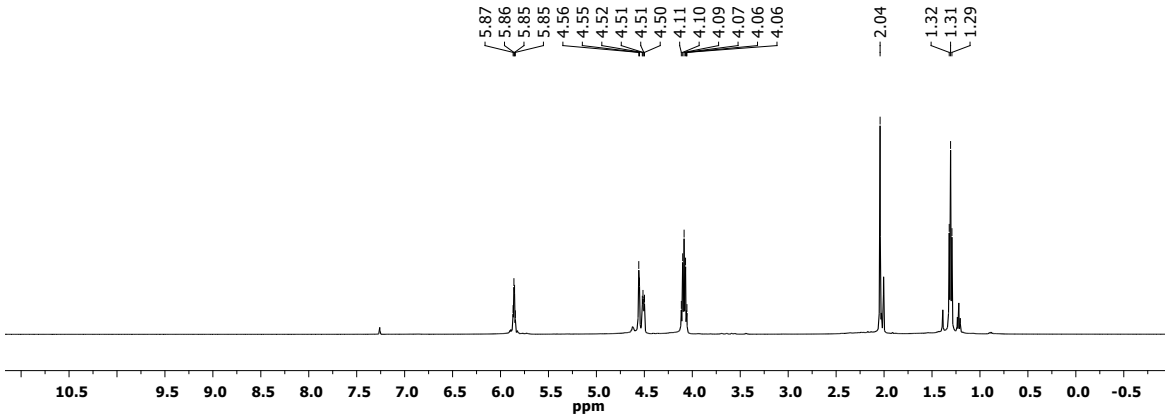


Figure S32 ^{1}H NMR spectrum of **2ae** ($CDCl_3$, 300 K).

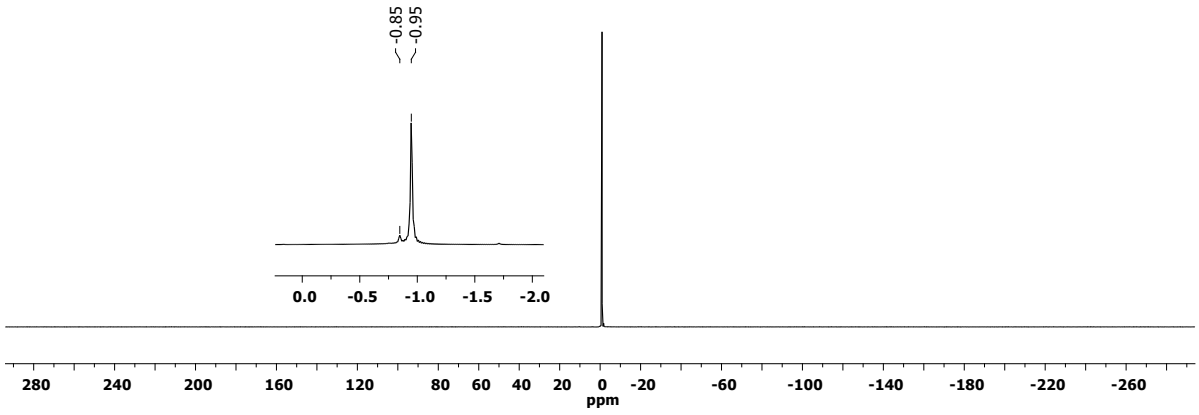


Figure S33 $^{31}P\{^{1}H\}$ NMR spectrum of **2ae** ($CDCl_3$, 300 K).

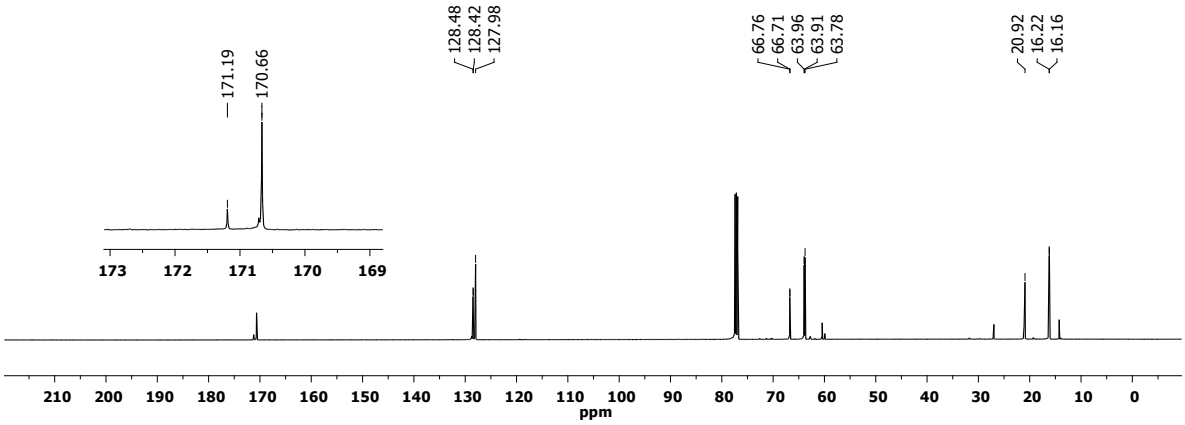
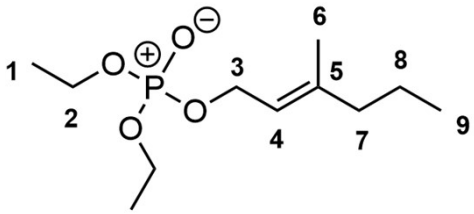


Figure S34 $^{13}C\{^{1}H\}$ NMR spectrum of **2ae** ($CDCl_3$, 300 K).

S2.13 Cross metathesis of diethyl allyl phosphate (2a) with 2-methylpent-1-ene (f)



Compound **2af** was synthesized from **2a** (0.089 mL, 0.5 mmol) and 2-methylpent-1-ene (0.19 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2af** (9 mg, 7% yield; *E/Z*, 63:37); **IR** (ATR, 298 K, in cm^{-1}): 2983 (w), 2933 (w), 2910 (w), 2872 (w), 2360 (w), 2341 (w), 1733 (w), 1716 (w), 1698 (w), 1672 (w), 1653 (w), 1637 (w), 1577 (w), 1559 (w), 1541 (w), 1522 (w), 1508 (w), 1480 (w), 1445 (w), 1394 (w), 1370 (w), 1231 (m), 1165 (m), 1099 (m), 1024 (vs), 973 (vs), 817 (s), 802 (s); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 0.88 (3H, t,

$^3J_{HH}$ = 7.3 Hz, H9), 1.33 (6H, t, $^3J_{HH}$ = 7.1 Hz, H1), 1.43 (2H, m, H8), 4.18 (4H, q, $^3J_{HH}$ = 7.2 Hz, H2), 4.55 (2H, q, $^3J_{HH}$ = 7.8 Hz, H3), 5.40 (1H, q, $^3J_{HH}$ = 7.3 Hz, H4), 1.68, 1.75 (3H, s, H6 (*E/Z*)), 2.00, 2.06 (2H, t, $^3J_{HH}$ = 7.5 Hz, H7 (*E/Z*)); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 16.4 (1C, s, C6), 20.8 (1C, s, C8), 63.7 (2C, d, $^3J_{CP}$ = 6 Hz, C2), 119.1, 120.0 (1C, d, $^3J_{CP}$ = 7 Hz, C4 (*E/Z*)), 13.8, 14.0 (1C, s, C9 (*E/Z*)), 142.8, 143.1 (1C, s, C5 (*E/Z*)), 41.7, 34.1 (1C, s, C7 (*E/Z*)), 64.2, 63.9 (1C, d, $^3J_{CP}$ = 6 Hz, C3 (*E/Z*)); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.6 (1P, s, P(*Z*)), -0.5 (1P, s, P(*E*)). **HR-MS** (ESI+) *m/z*: $[M + 2H]^+$ calcd for $C_{11}H_{25}O_4P$ 252.1407 found 252.0312.

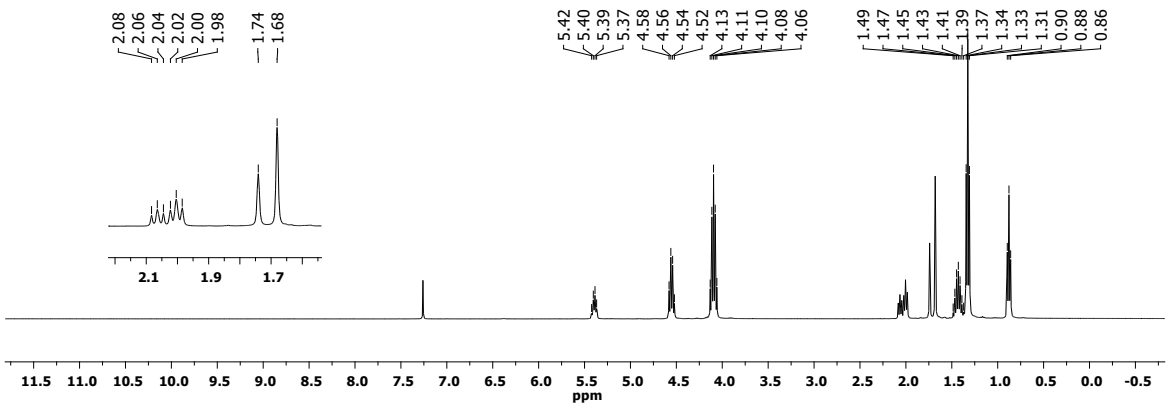


Figure S35 ^{1}H NMR spectrum of **2af** ($CDCl_3$, 300 K).

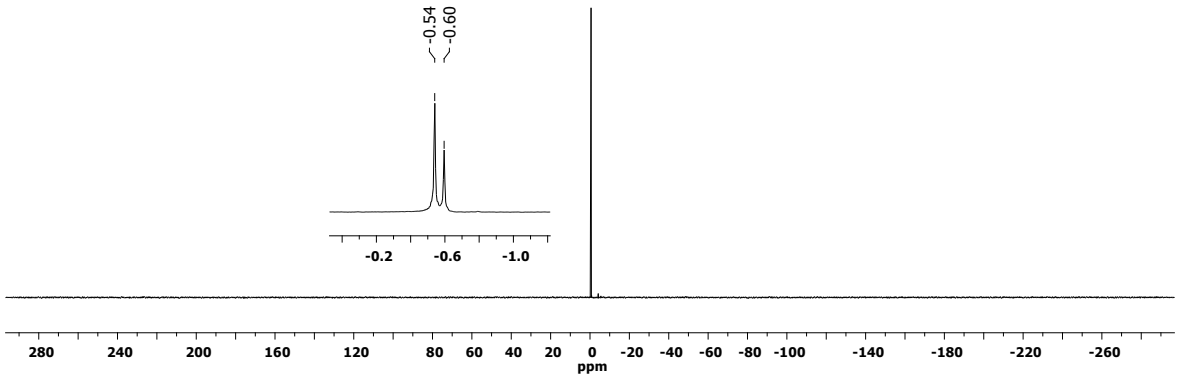


Figure S36 ^{31}P{^{1}H} NMR spectrum of **2af** ($CDCl_3$, 300 K).

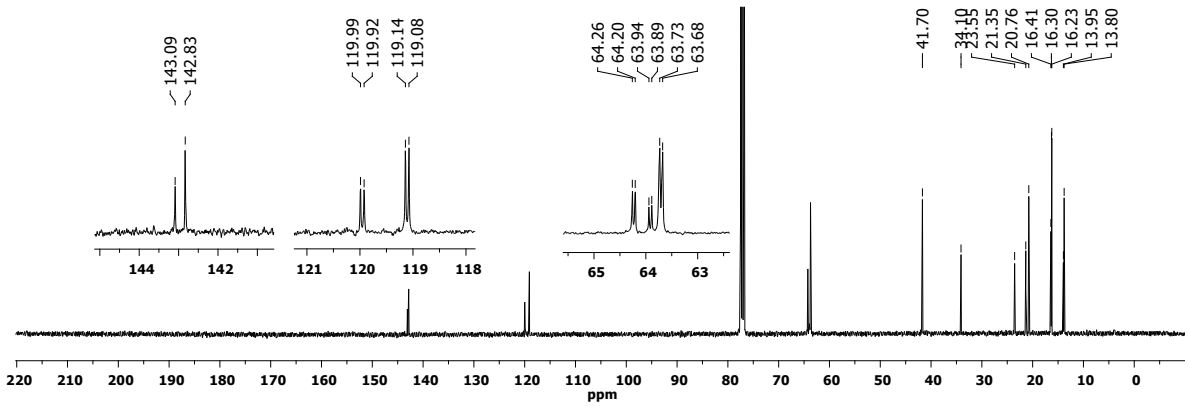
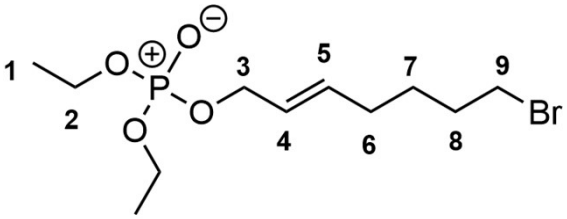


Figure S37 $^{13}C\{^{1}H\}$ NMR spectrum of **2af** ($CDCl_3$, 300 K).

S2.14 Cross metathesis of diethyl allyl phosphate (2a) with 6-bromohex-1-ene (g)



Compound **2ag** was synthesized from **2a** (0.089 mL, 0.5 mmol) and 6-bromohex-1-ene (0.20 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2ag** (100 mg, 62% yield; *E/Z*, 86:14); **IR** (ATR, 298 K, in cm^{-1}): 2981 (w), 2924 (w), 2852 (w), 2361 (w), 2341 (w), 1732 (w), 1717 (w), 1671 (vw), 1457 (w), 1443 (w), 1394 (w), 1370 (w), 1340 (vw), 1248 (m), 1165 (m), 1099 (m), 1026 (vs), 970 (vs), 851 (m), 817 (m), 802 (m), 743 (m), 669 (w), 645 (w), 518 (m), 474 (m), 420 (m); **^{1}H NMR** (400,13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.34 (6H, t, $^{3}J_{HH}$ = 7.0 Hz, H1), 1.55 (2H, m, H7), 1.87 (2H, m, H8), 2.10 (2H, dd, $^{3}J_{HH}$ = 14.3 Hz, $^{3}J_{HH}$ = 7.1 Hz, H6), 3.40 (2H, t, $^{3}J_{HH}$ = 6.8 Hz, H9), 4.11 (4H, p, $^{3}J_{HH}$ = 7.2 Hz, H2), 4.48 (2H, m, H3), 5.63 (1H, m, H4), 5.78 (1H, m, H5); **$^{13}C\{^{1}H\}$ NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 27.4 (1C, s, C7), 31.4 (1C, s, C6), 32.3 (1C, s, C8), 33.6 (1C, s, C9), 68.1 (1C, d, $^{2}J_{CP}$ = 6 Hz, C3), 68.9 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 125.3 (1C, d, $^{3}J_{CP}$ = 7 Hz, C4), 135.5 (1C, s, C5); **$^{31}P\{^{1}H\}$ NMR** (161,98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P(*Z*)), -0.8 (1P, s, P(*E*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{11}H_{23}O_4BrP$ 329.0512 found 329.0512, 331.0492, $[M + Na]^+$ calcd for $C_{11}H_{22}O_4BrPNa$ 351.0331 found 351.0329, 353.0310.

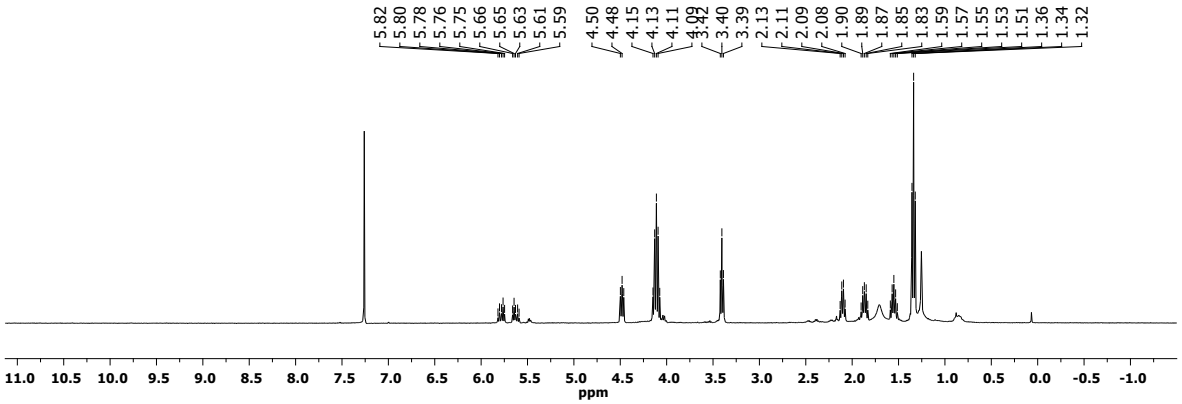


Figure S38 ^{1}H NMR spectrum of **2ag** ($CDCl_3$, 300 K).

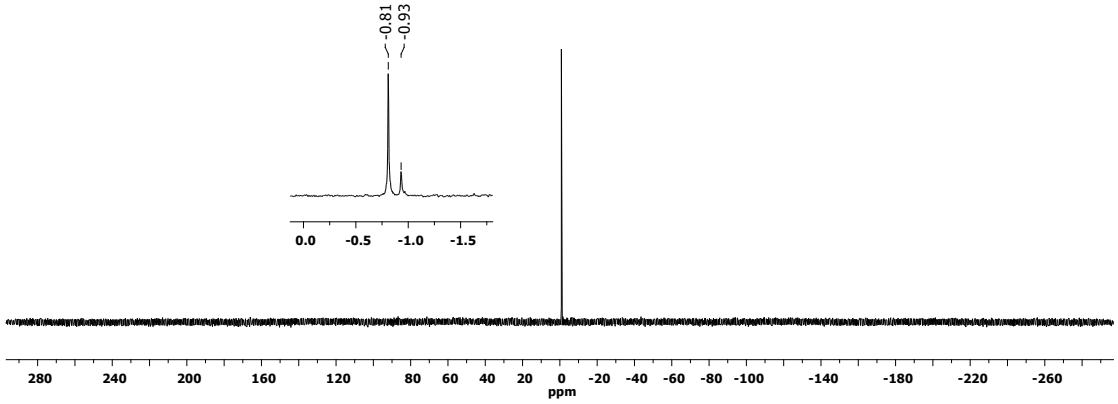


Figure S39 $^{31}P\{^{1}H\}$ NMR spectrum of **2ag** ($CDCl_3$, 300 K).

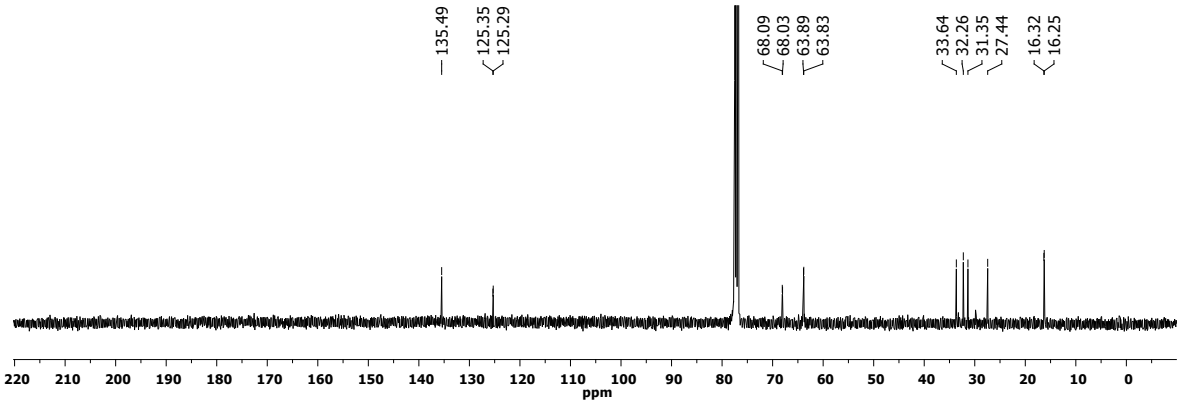
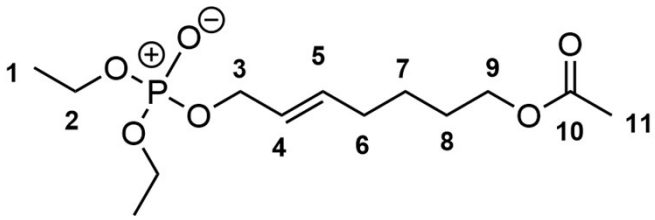


Figure S40 $^{13}C\{^{1}H\}$ NMR spectrum of **2ag** ($CDCl_3$, 300 K).

S2.15 Cross metathesis of diethyl allyl phosphate (2a) with hex-5-en-1-yl acetate (h)



Compound **2ah** was synthesized from **2a** (0.089 mL, 0.5 mmol) and hex-5-en-1-yl acetate (0.24 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **2ah** (100 mg, 66% yield; *E/Z*, 93:7); **IR** (ATR, 298 K, in cm^{-1}): 3421 (w), 2983 (w), 2933 (w), 2862 (w), 2361 (w), 2341 (w), 1734 (vw), 1671 (vw), 1475 (w), 1457 (w), 1444 (w), 1394 (w), 1370 (w), 1340 (w), 1254 (s), 1166 (w), 1096 (m), 1024 (vs), 1003 (vs), 970 (vs), 849 (m), 817 (m), 801 (m), 745 (m), 669 (w), 519 (m), 420 (m); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.32 (6H, t, $^3J_{HH}$ = 7.0 Hz, H1), 1.45 (2H, dq, $^3J_{HH}$ = 14.8 Hz, $^3J_{HH}$ = 7.5 Hz, H7), 1.63 (2H, m, H8), 2.03 (3H, s, H11), 2.09 (2H, dd, $^3J_{HH}$ = 14.4 Hz, $^3J_{HH}$ = 7.1 Hz, H6), 4.10 (4H, m, H2), 4.47 (2H, m, H3), 5.61 (1H, m, H4), 5.77 (1H, m, H5), 6.53 (2H, t, $^3J_{HH}$ = 6.5 Hz, H9); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.2 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 21.1 (1C, s, C11), 25.3 (1C, s, C7), 28.2 (1C, s, C8), 31.8 (1C, s, C6), 63.8 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 64.4 (1C, s, C9), 68.1 (1C, d, $^2J_{CP}$ = 6 Hz, C3), 171.3 (1C, s, C10), 125.1, 124.8 (1C, d, $^3J_{CP}$ = 7, 7 Hz, C4 (*E/Z*)), 135.7, 134.7 (1C, s, C5 (*E/Z*)); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.8 (1P, s, P(*E*)), -0.6 (1P, s, P(*Z*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{13}H_{26}O_6P$ 309.1462 found 309.1459, $[M + Na]^+$ calcd for $C_{13}H_{25}O_6PNa$ 331.1281 found 331.1278.

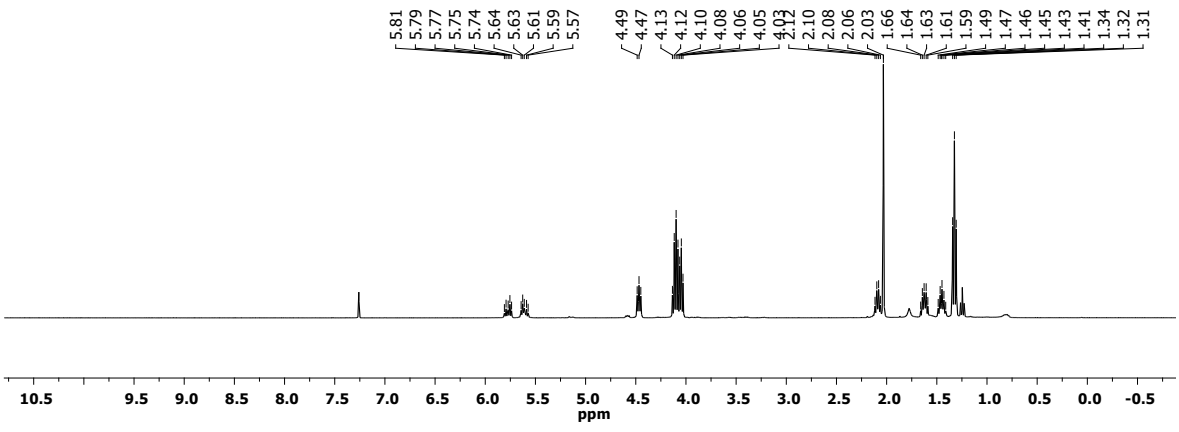


Figure S41 ^{1}H NMR spectrum of **2ah** ($CDCl_3$, 300 K).

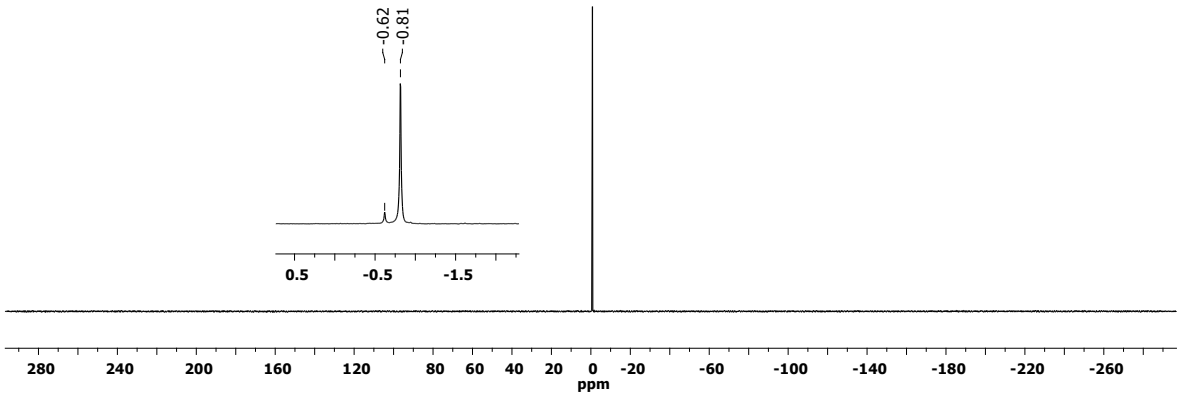


Figure S42 $^{31}P\{^{1}H\}$ NMR spectrum of **2ah** ($CDCl_3$, 300 K).

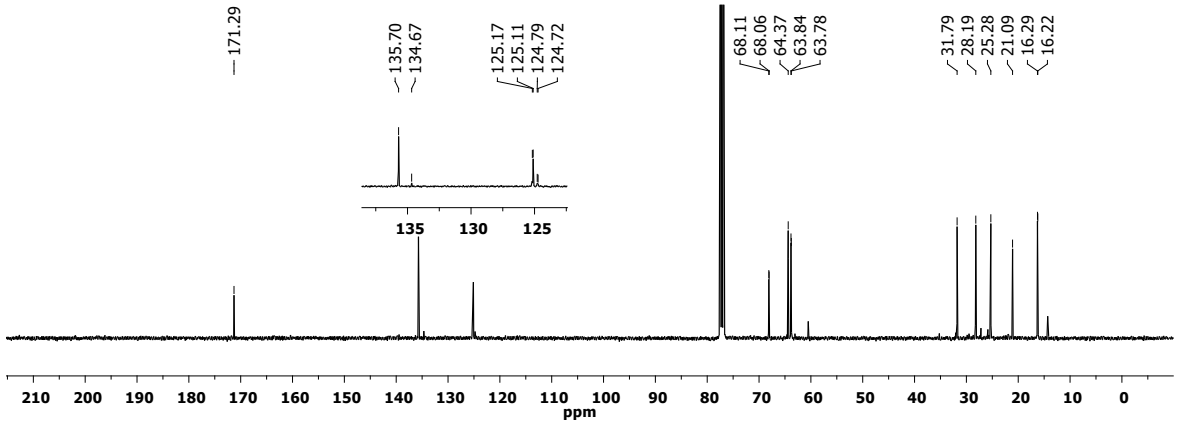
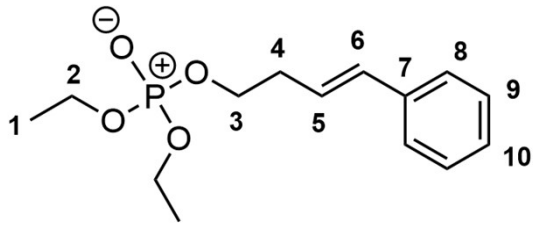


Figure S43 $^{13}C\{^{1}H\}$ NMR spectrum of **2ah** ($CDCl_3$, 300 K).

S2.16 Cross metathesis of diethyl butenyl phosphate (3a) with styrene (a)



Compound **3aa** was synthesized from **3a** (0.195 mL, 1 mmol) and styrene (0.39 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3aa** (142 mg, 50% yield; *E/Z*, 100:0); **IR** (ATR, 298 K, in cm^{-1}): 3027 (vw), 2982 (w), 2932 (vw), 2906 (vw), 2361 (vw), 2341 (vw), 1653 (vw), 1598 (vw), 1494 (vw), 1475 (vw), 1447 (w), 1393 (w), 1369 (vw), 1261 (s), 1165 (w), 1100 (w), 1015 (vs), 965 (vs), 872 (w), 818 (m), 800 (m), 745 (s), 694 (m), 669 (w), 619

(w), 607 (w), 512 (m); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.32 (6H, t, $^{3}J_{HH}$ = 7.0 Hz, H1), 2.60 (2H, q, $^{3}J_{HH}$ = 6.7 Hz, H4), 4.13 (6H, m, H2, H3), 6.18 (1H, dtd, $^{3}J_{HH}$ = 8.8 Hz, $^{3}J_{HH}$ = 7.0 Hz, $^{2}J_{HH}$ = 1.8 Hz, H5), 6.49 (1H, d, $^{3}J_{HH}$ = 15.9 Hz, H6), 7.21 (1H, t, $^{3}J_{HH}$ = 7.2 Hz, H10), 7.30 (2H, m, H9), 7.34 (2H, d, $^{3}J_{HH}$ = 7.3 Hz, H8); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 34.1 (1C, d, $^{3}J_{CP}$ = 7 Hz, C4), 63.9 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 66.9 (1C, d, $^{2}J_{CP}$ = 6 Hz, C3), 125.1 (1C, s, C5), 126.2 (1C, s, C8), 127.5 (1C, s, C10), 128.7 (1C, s, C9), 133.0 (1C, s, C6), 137.3 (2C, s, C7); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{14}H_{22}O_4P$ 285.1250 found 285.1247, $[M + Na]^+$ calcd for $C_{13}H_{25}O_6PNa$ 307.1070 found 307.1066.

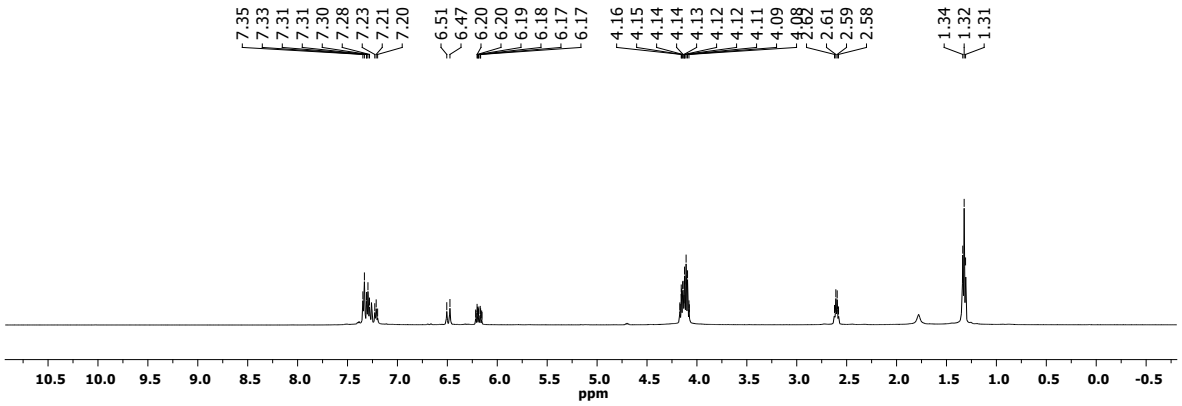


Figure S44 ^{1}H NMR spectrum of **3aa** ($CDCl_3$, 300 K).

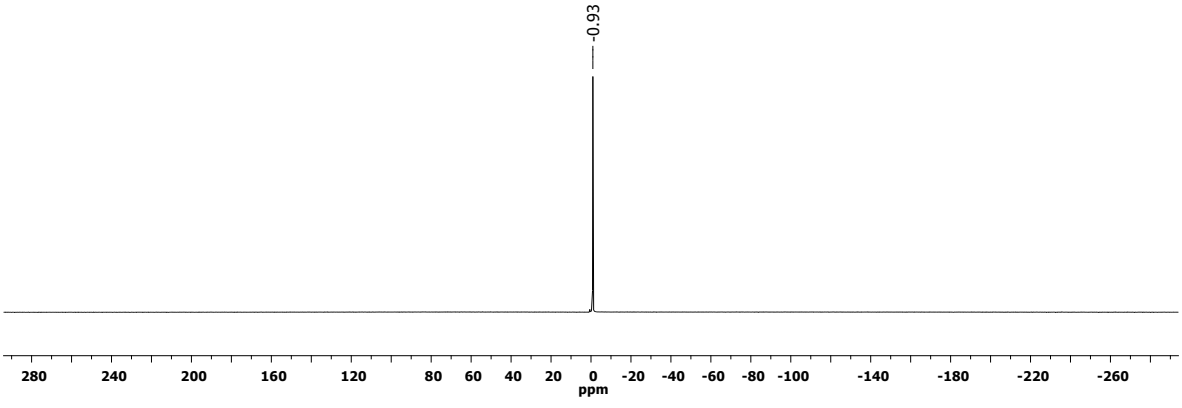


Figure S45 ^{31}P{^{1}H} NMR spectrum of **3aa** ($CDCl_3$, 300 K).

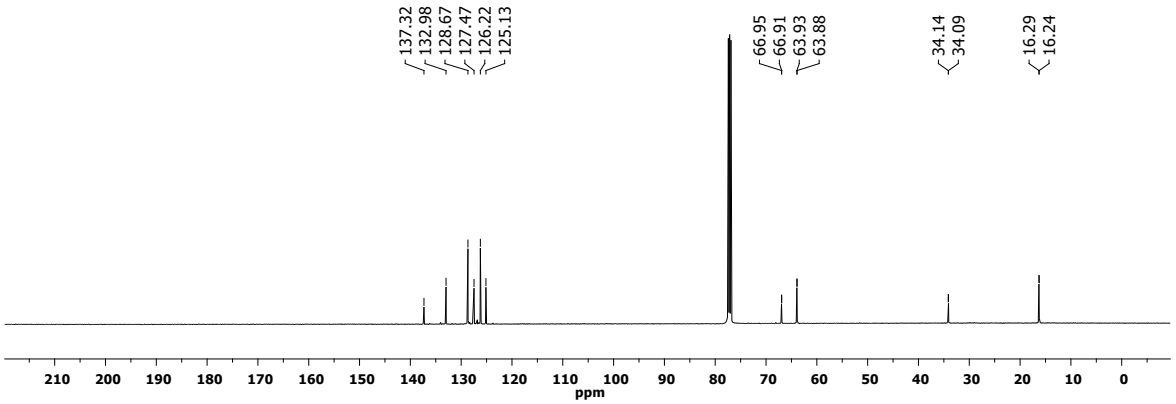
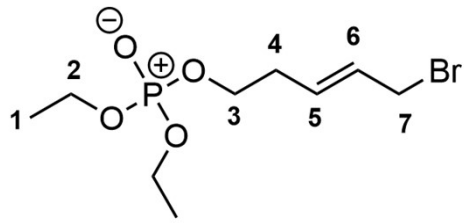


Figure S46 $^{13}C\{^{1}H\}$ NMR spectrum of **3aa** ($CDCl_3$, 300 K).



S2.17 Cross metathesis of diethyl butenyl phosphate (3a) with allyl bromide (b)

Compound **3ab** was synthesized from **3a** (0.195 mL, 1 mmol) and allyl bromide (0.26 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3ab** (251 mg, 83% yield; *E/Z*, 91:9); **IR** (ATR, 298 K, in cm^{-1}): 2982 (w), 2933 (vw), 2907 (vw), 2360 (w), 2341 (vw), 1662 (vw), 1653 (vw), 1474 (vw), 1456 (vw), 1443 (w), 1393 (w), 1369 (w), 1261 (s), 1206 (w), 1165 (w), 1097 (w), 1017 (vs), 967 (vs), 854 (w), 817 (m), 800 (m), 743 (m), 669 (w), 592 (w), 526 (m), 473 (m), 420 (w); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.34 (6H, t, $^{3}J_{HH}$ = 7.0 Hz, H1), 4.10 (6H, m, H2, H3), 5.78 (2H, m, H5, H6), 2.46, 2.54 (2H, q, dd, 3 J_{HH} = 6.3 Hz, $^{3}J_{HH}$ = 13.8 Hz, H7 (*E/Z*)), 3.93, 3.98 (2H, d, d, $^{3}J_{HH}$ = 6.5 Hz, $^{3}J_{HH}$ = 8.4 Hz, H4 (*E/Z*)); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 32.6 (1C, s, C7), 33.2 (1C, d, $^{3}J_{CP}$ = 7 Hz, C4), 64.0 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 66.3 (1C, d, $^{2}J_{CP}$ = 6 Hz, C3), 128.5, 128.5 (1C, s, C5 (*E/Z*)), 130.9, 130.0 (1C, s, C6 (*E/Z*)); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_9H_{19}O_4BrP$ 301.0199 found 301.0196, $[M + Na]^+$ calcd for $C_9H_{18}O_4BrPNa$ 323.0018 found 323.0014.

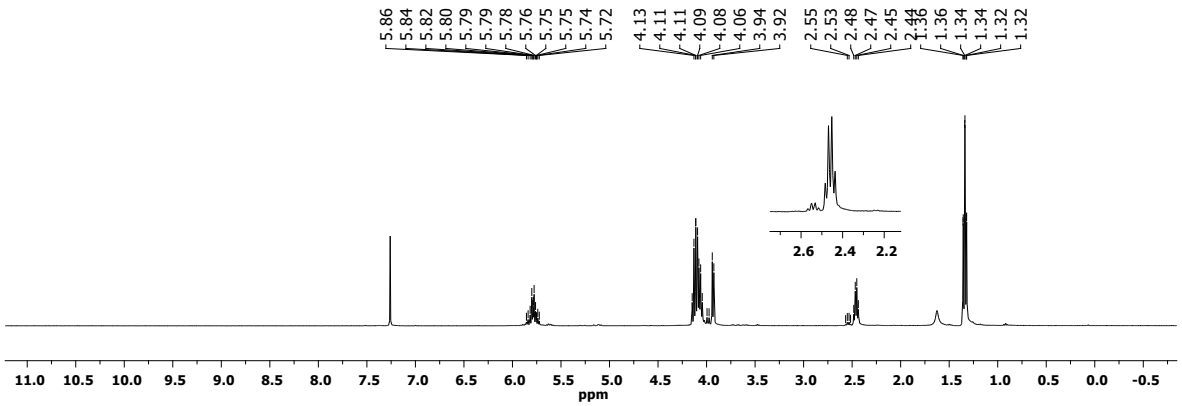


Figure S47 ^{1}H NMR spectrum of **3ab** ($CDCl_3$, 300 K).

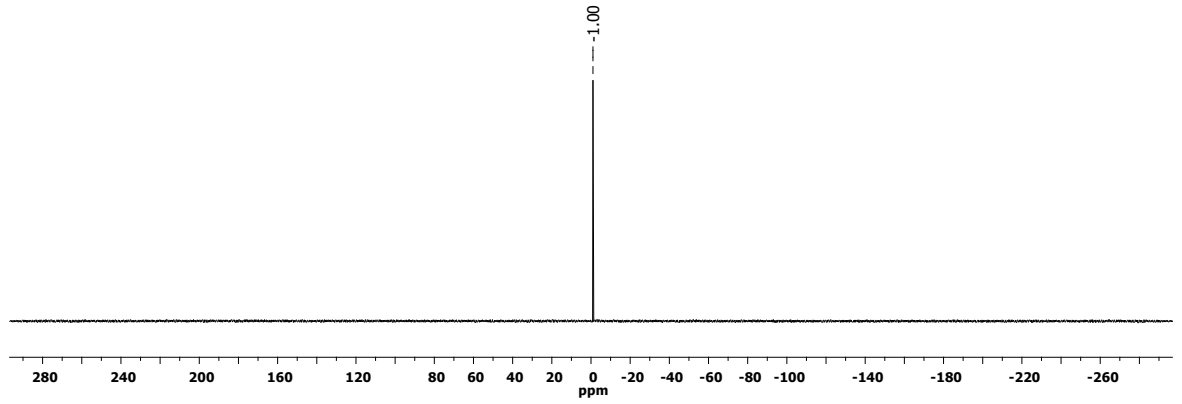


Figure S48 $^{31}P\{^{1}H\}$ NMR spectrum of **3ab** ($CDCl_3$, 300 K).

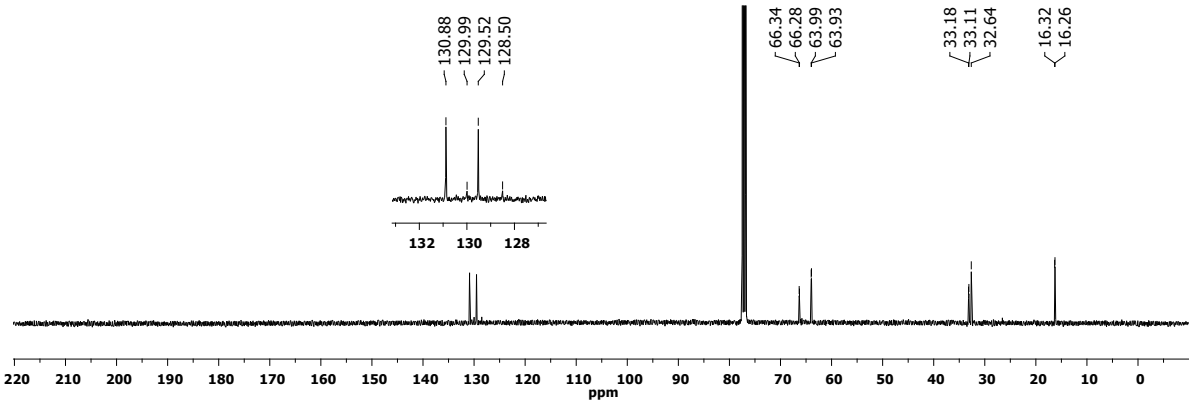
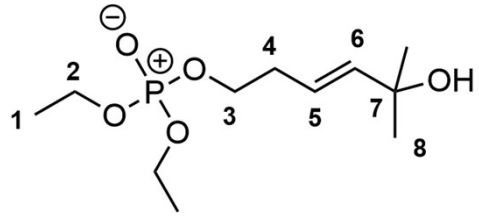


Figure S49 $^{13}C\{^{1}H\}$ NMR spectrum of **3ab** ($CDCl_3$, 300 K).

S2.18 Cross metathesis of diethyl butenyl phosphate (3a) with 2-Methyl-3-buten-2-ol (c)



Compound **3ac** was synthesized from **3a** (0.195 mL, 1 mmol) and 2-methyl-3-buten-2-ol (0.32 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the reaction mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3ac** (223 mg, 84% yield; *E/Z*, 100:0); **IR** (ATR, 298 K, in cm^{-1}): 3419 (w), 2972 (w), 2931 (w), 2909 (w), 2872 (vw), 2361 (w), 2341 (vw), 1473 (w), 1458 (w), 1445 (w), 1394 (w), 1371 (w), 1258 (m), 1163 (m), 1099 (w), 1015 (vs), 970 (vs), 913 (m), 872 (w), 819 (m), 801 (m), 741 (w), 669 (w), 511 (m), 473 (m), 419 (w); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.30 (6H, s, H8), 1.34 (6H, t, $^3J_{HH}$ = 7.0 Hz, H1), 2.41 (2H, q, $^3J_{HH}$ = 6.7 Hz, H4), 4.08 (6H, m, H2, H3), 5.61 (1H, dt, 3 J_{HH} = 15.6 Hz, $^3J_{HH}$ = 5.6 Hz, H5), 5.73 (1H, d, $^3J_{HH}$ = 15.7 Hz, H6); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 29.9 (1C, s, C8), 33.2 (1C, d, $^3J_{CP}$ = 7 Hz, C4), 63.9 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 67.0 (1C, d, $^2J_{CP}$ = 6 Hz, C3), 70.7 (1C, s, C7), 121.8 (1C, s, C5), 141.4 (1C, s, C6); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M - OH^-]^+$ calcd for $C_{11}H_{22}O_4P$ 249.1245 found 249.1247, $[M + Na]^+$ calcd for $C_{11}H_{23}O_5PNa$ 289.1175 found 289.1172.

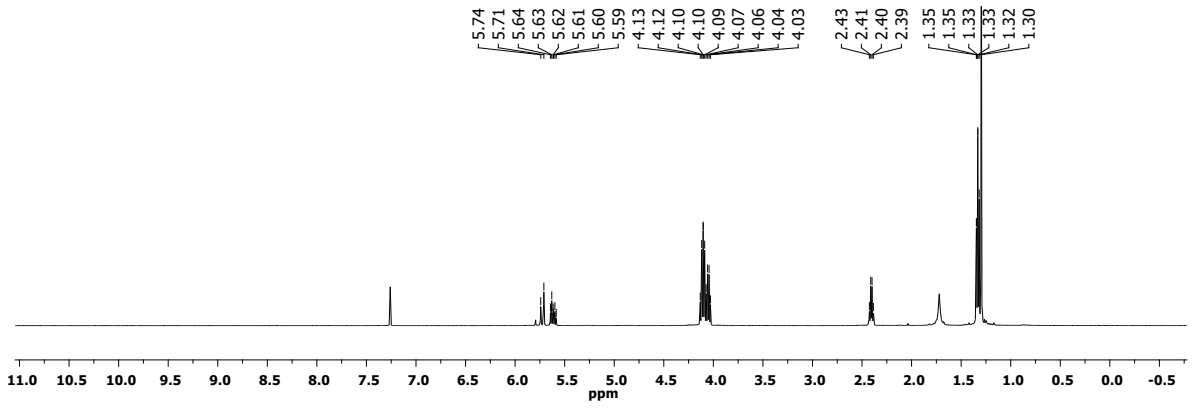


Figure S50 ^{1}H NMR spectrum of **3ac** ($CDCl_3$, 300 K).

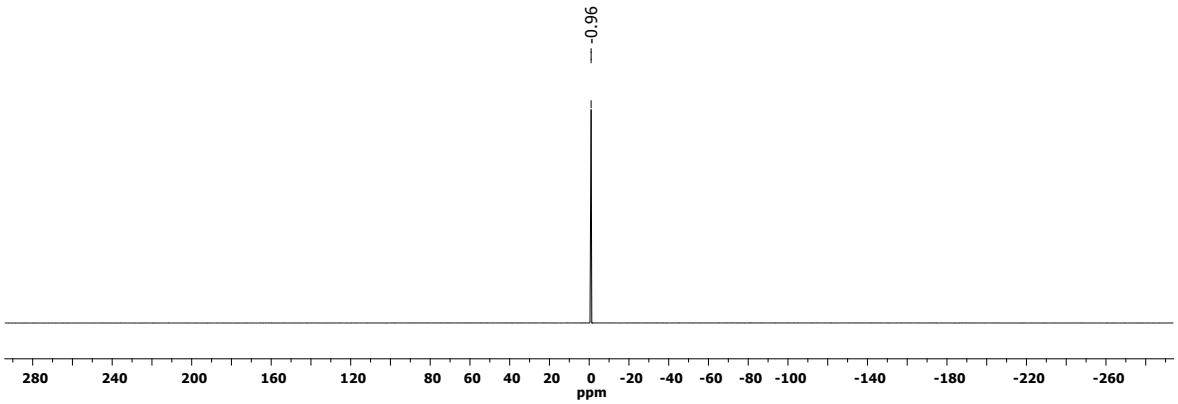


Figure S51 $^{31}P\{^{1}H\}$ NMR spectrum of **3ac** ($CDCl_3$, 300 K).

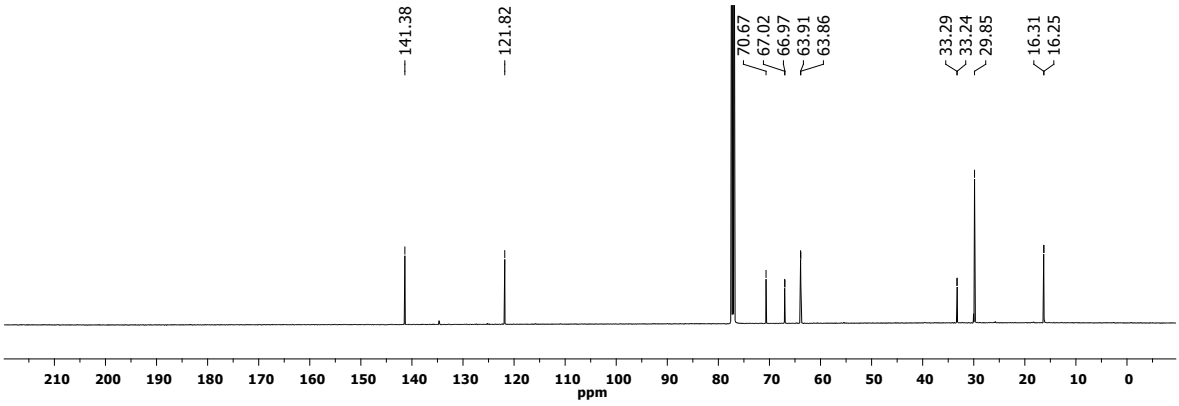
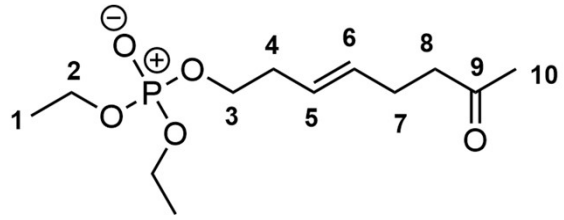


Figure S52 $^{13}C\{^{1}H\}$ NMR spectrum of **3ac** ($CDCl_3$, 300 K).

S2.19 Cross metathesis of diethyl butenyl phosphate (3a) with 5-Hexen-2-one (d)



Compound **3ad** was synthesized from **3a** (0.195 mL, 1 mmol) and 5-hexen-2-one (0.36 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3ad** (180 mg, 65% yield; *E/Z*, 85:15); **IR** (ATR, 298 K, in cm^{-1}): 2983 (w), 2909 (w), 2361 (w), 2341 (vw), 1714 (m), 1676 (w), 1653 (vw), 1636 (vw), 1474 (vw), 1443 (w), 1394 (w), 1364 (w), 1260 (s), 1163 (m), 1100 (w), 1016 (vs), 969 (vs), 866 (w), 818 (m), 801 (m), 743 (w), 669 (w), 651 (w), 600 (w), 520 (m), 472 (m), 419 (w); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.33 (6H,

t, $^3J_{HH}$ = 7.1 Hz, H1), 2.13 (3H, s, H10), 2.27 (2H, dd, $^3J_{HH}$ = 14.0 Hz, $^3J_{HH}$ = 6.9 Hz, H7), 2.36 (2H, dd, $^3J_{HH}$ = 13.1 Hz, $^3J_{HH}$ = 6.4 Hz, H4), 2.49 (2H, t, $^3J_{HH}$ = 7.3 Hz, H8), 4.02 (2H, m, H3), 4.10 (4H, m, H2), 5.42 (1H, m, H5), 5.52 (1H, m, H6); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 26.8 (1C, s, C7), 29.9 (1C, s, C8), 30.1 (1C, s, C10), 33.6 (1C, d, $^3J_{CP}$ = 7 Hz, C4), 63.9 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 125.9, 125.3 (1C, s, C5 (*E/Z*)), 132.0, 131.2 (1C, s, C6 (*E/Z*)), 208.3, 208.2 (1C, s, C9 (*E/Z*)), 67.1, 66.9 (1C, d, $^2J_{CP}$ = 6 Hz, $^2J_{CP}$ = 6 Hz, C3 (*E/Z*)); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{12}H_{24}O_5P$ 279.1356 found 279.1353, $[M + Na]^+$ calcd for $C_{12}H_{23}O_5PNa$ 301.1175 found 301.1172.

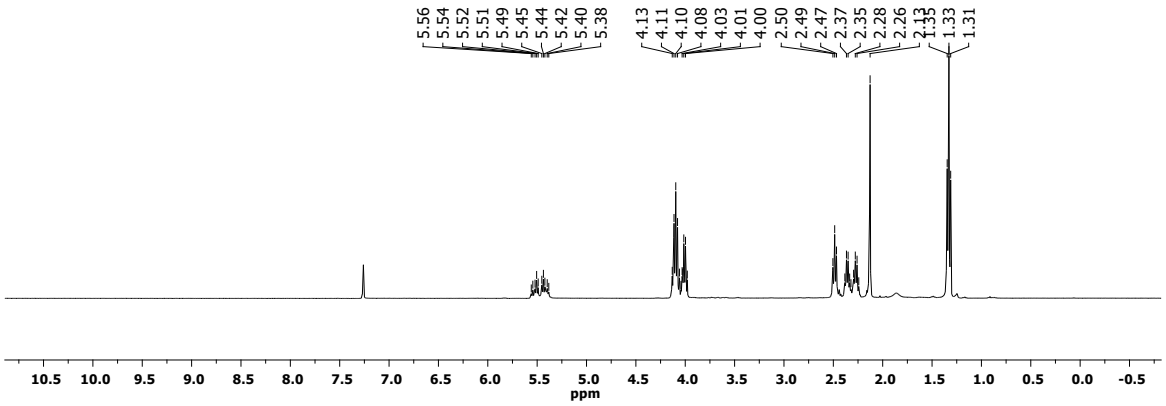


Figure S53 ^{1}H NMR spectrum of **3ad** ($CDCl_3$, 300 K).

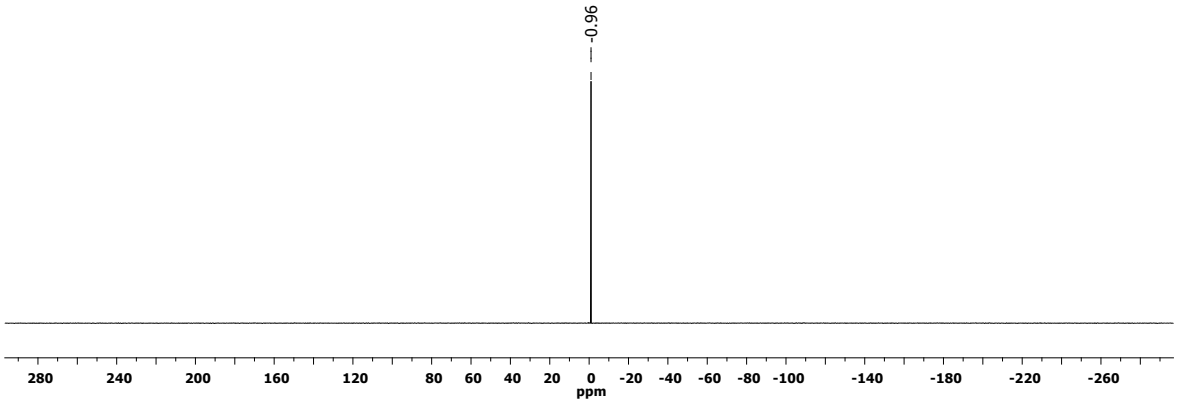


Figure S54 ^{31}P{^{1}H} NMR spectrum of **3ad** ($CDCl_3$, 300 K).

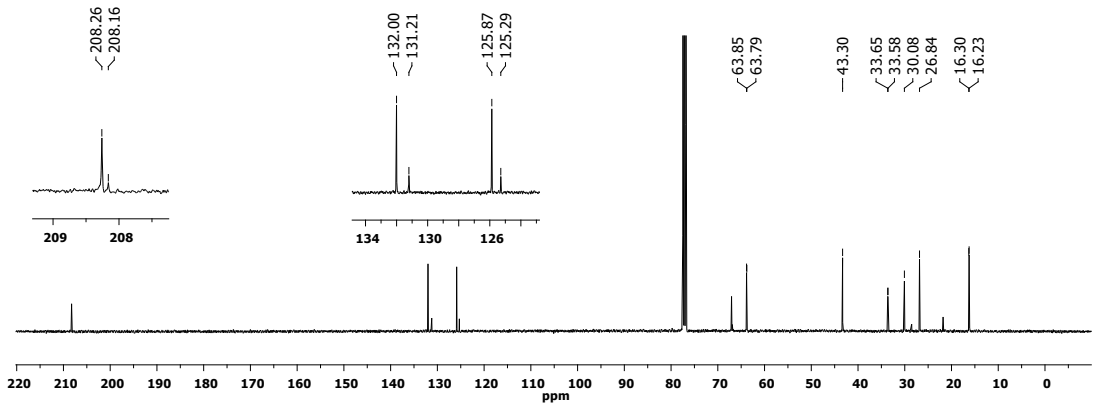
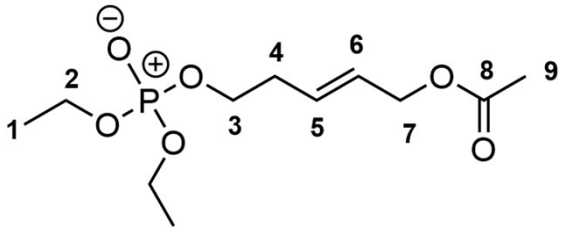


Figure S55 $^{13}C\{^{1}H\}$ NMR spectrum of **3ad** ($CDCl_3$, 300 K).

S2.20 Cross metathesis of diethyl butenyl phosphate (3a) with allyl acetate (e)



Compound **3ae** was synthesized from **3a** (0.096 mL, 0.5 mmol) and allyl acetate (0.16 mL, 1.5 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (21 mg, 0.025 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3ae** (69 mg, 49% yield; *E/Z*, 87:13); **IR** (ATR, 298 K, in cm^{-1}): 2983 (vw), 2935 (vw), 2910 (vw), 1737 (m), 1477 (vw), 1444 (w), 1383 (w), 1367 (w), 1229 (s), 1166 (w), 1015 (vs), 969 (vs), 868 (w), 818 (m), 801 (m), 744 (w), 642 (w), 608 (w), 521 (m), 472 (m); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.30 (6H, t, $^{3}J_{HH}$ = 7.1 Hz, H1), 2.02 (3H, s, H9), 4.05 (6H, m, H2, H3), 5.69 (2H, m, H5, H6), 2.42, 2.48 (2H, q, dd, $^{3}J_{HH}$ = 6.5 Hz, $^{3}J_{HH}$ = 6.36, 12.66 Hz, 4H (*E/Z*)), 4.49, 4.59 (2H, d, $^{3}J_{HH}$ = 5.7 Hz, $^{3}J_{HH}$ = 5.5 Hz, H7 (*E/Z*)); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.2 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 21.0 (1C, s, C9), 63.8 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 66.4 (1C, d, $^{2}J_{CP}$ = 6 Hz, C3), 127.2, 126.7 (1C, s, C5 (*E/Z*)), 130.4, 129.4 (1C, s, C6 (*E/Z*)), 170.8, 170.9 (1C, s, C8 (*E/Z*)), 33.2, 28.8 (1C, d, $^{3}J_{CP}$ = 7, 7 Hz, C4), 64.8, 60.2 (1C, s, C7); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.1 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{11}H_{22}O_6P$ 281.1149 found 281.1147, $[M + Na]^+$ calcd for $C_{11}H_{21}O_6PNa$ 303.0968 found 303.0964.

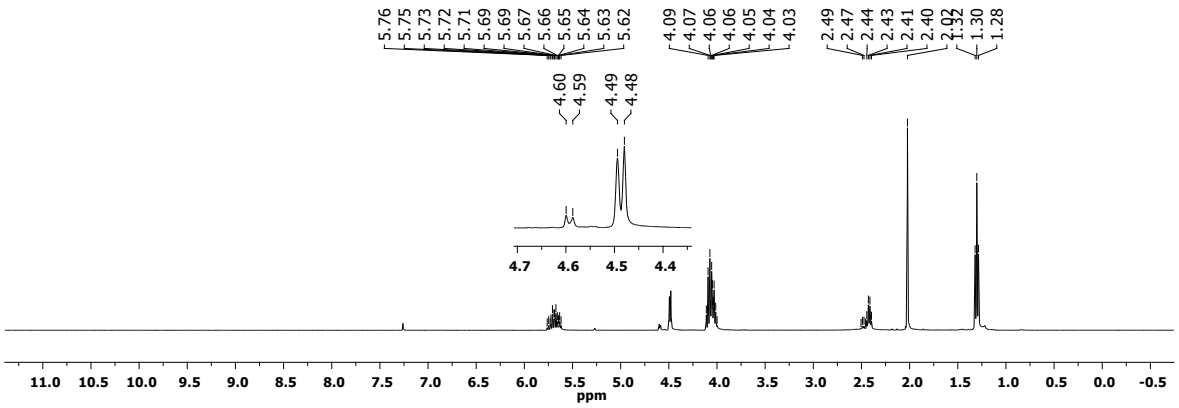


Figure S56 ^{1}H NMR spectrum of **3ae** ($CDCl_3$, 300 K).

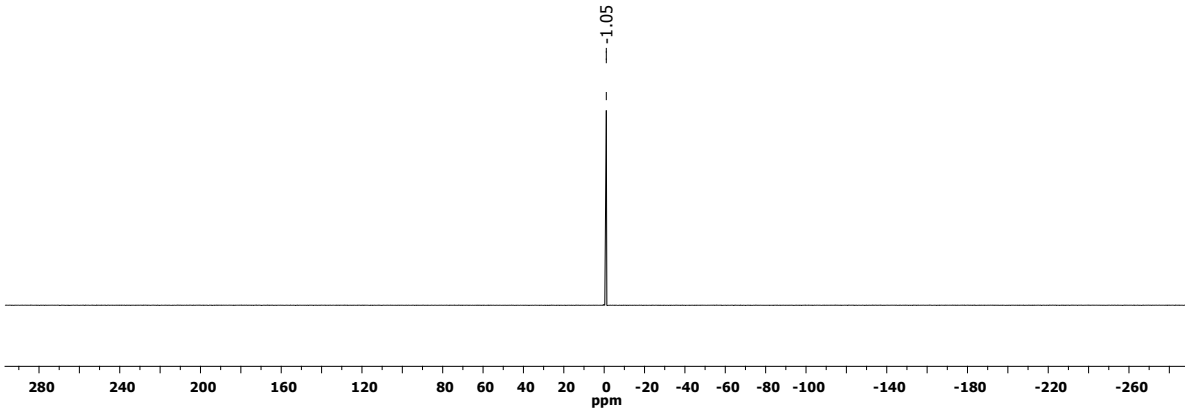


Figure S57 $^{31}P\{^{1}H\}$ NMR spectrum of **3ae** ($CDCl_3$, 300 K).

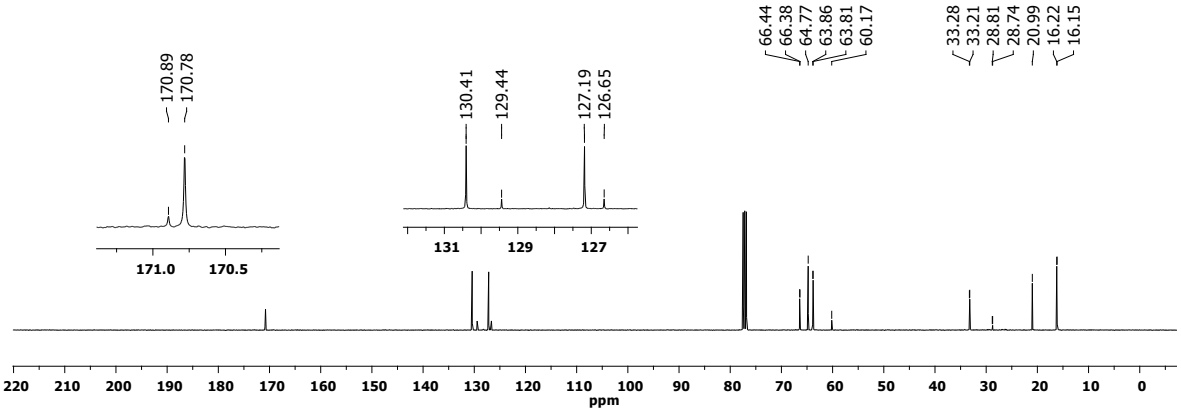
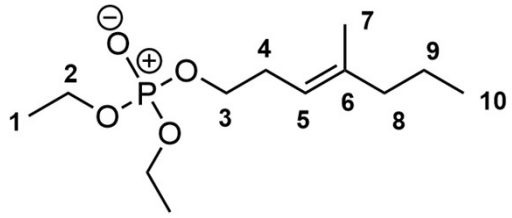


Figure S58 $^{13}C\{^{1}H\}$ NMR spectrum of **3ae** ($CDCl_3$, 300 K).

S2.21 Cross metathesis of diethyl butenyl phosphate (3a) with 2-methylpent-1-ene (f)



Compound **3af** was synthesized from **3a** (0.195 mL, 1 mmol) and 2-methylpent-1-ene (0.38 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3af** (132 mg, 50% yield; *E/Z*, 68:32); **IR** (ATR, 298 K, in cm^{-1}): 2960 (w), 2932 (w), 2910 (w), 2872 (vw), 1445 (w), 1392 (w), 1370 (vw), 1263 (m), 1166 (w), 1012 (vs), 967 (vs), 866 (w), 817 (m), 803 (m), 743 (w), 526 (m), 475 (m); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 0.87 (3H, m, 10H), 1.33 (6H, t, $^3J_{HH}$ = 7.1 Hz, H1), 1.41 (2H, m, H9), 1.95 (2H, m, H8), 2.39 (2H, q, $^3J_{HH}$ = 7.1 Hz, H4), 3.98 (2H, m, H3), 4.10 (4H, m, H2), 5.10 (1H, t, $^3J_{HH}$ = 6.4 Hz, H5), 1.6, 1.7 (3H, s, H7 (*E/Z*)); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^3J_{CP}$ = 7 Hz, C1), 63.8 (2C, d, $^2J_{CP}$ = 6 Hz, C2), 118.5, 119.3 (1C, s, C5 (*E/Z*)), 13.8, 14.1 (1C, s, C10 (*E/Z*)), 138.9, 139.1 (1C, s, C6 (*E/Z*)), 16.1, 23.5 (1C, s, C7 (*E/Z*)), 20.0, 21.2 (1C, s, C9 (*E/Z*)), 29.6, 29.2 (1C, d, $^3J_{CP}$ = 7, 7 Hz, C4 (*E/Z*)), 41.9, 34.0 (1C, s, C8 (*E/Z*)), 67.3, 67.4 (1C, d, $^2J_{CP}$ = 6, 6 Hz, C3 (*E/Z*)); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P (*Z*)), -0.9 (1P, s, P (*E*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{12}H_{26}O_4P$ 265.1563 found 265.1558, $[M + Na]^+$ calcd for $C_{12}H_{25}O_4PNa$ 287.1383 found 287.1376.

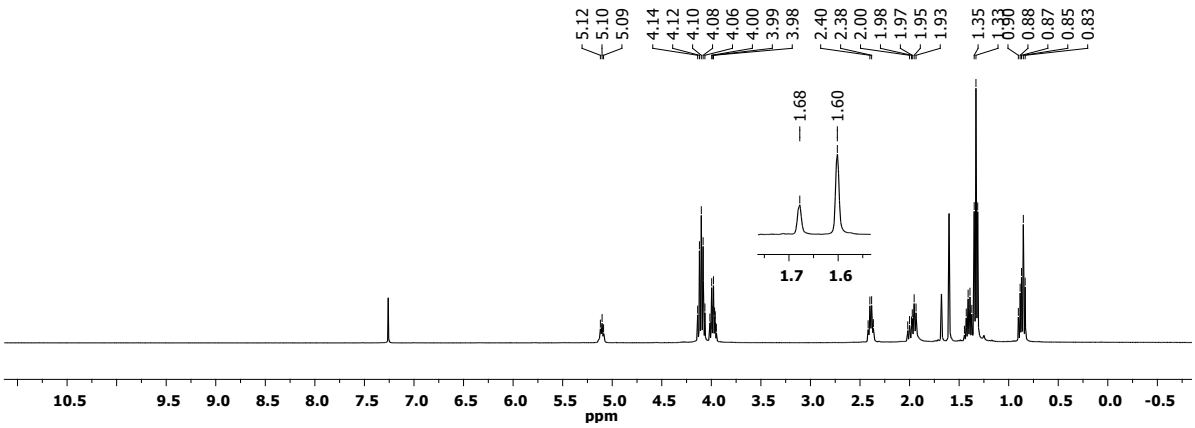


Figure S59 ^{1}H NMR spectrum of **3af** ($CDCl_3$, 300 K).

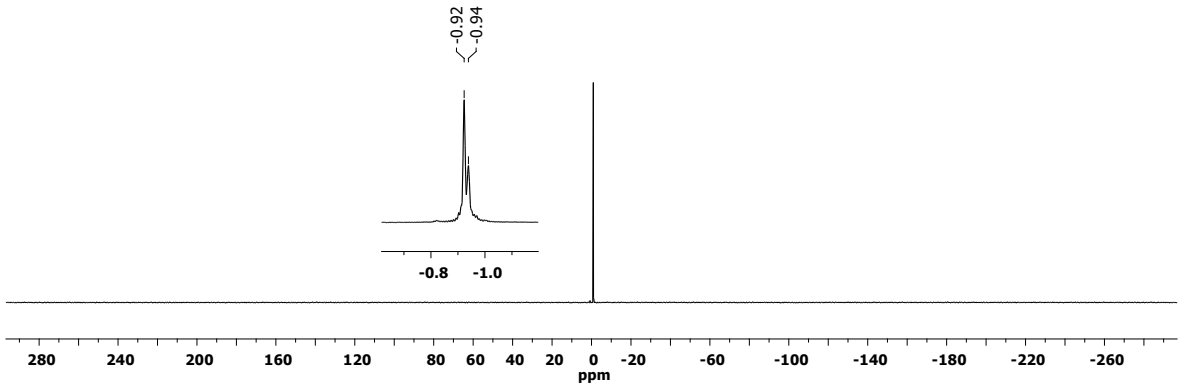


Figure S60 $^{31}P\{^{1}H\}$ NMR spectrum of **3af** ($CDCl_3$, 300 K).

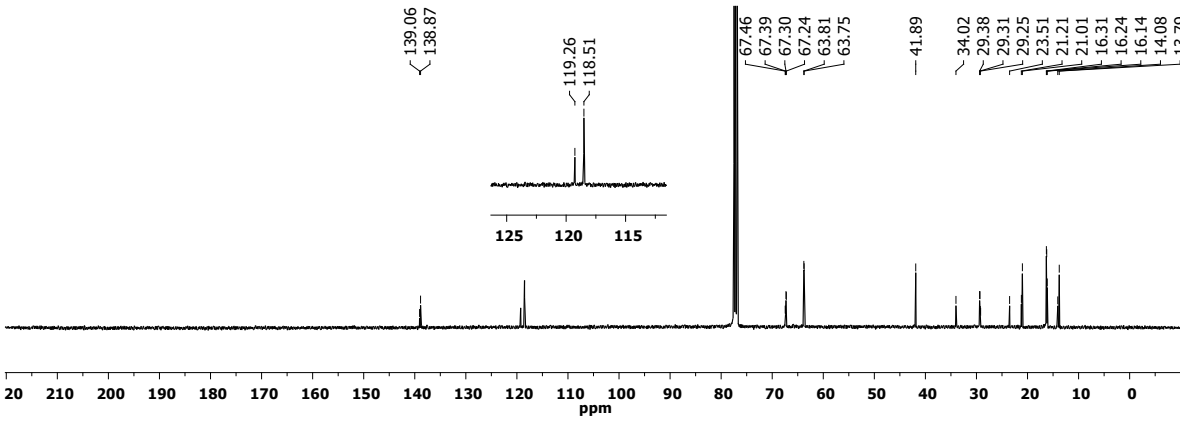
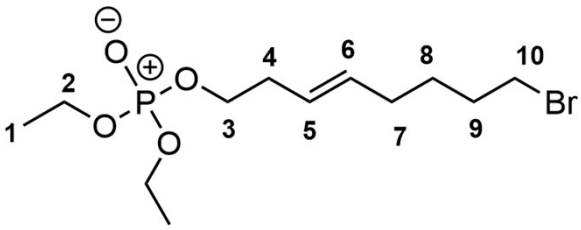


Figure S61 $^{13}C\{^{1}H\}$ NMR spectrum of **3af** ($CDCl_3$, 300 K).

S2.22 Cross metathesis of diethyl butenyl phosphate (3a) with 6-bromo hex-1-ene (g)



Compound **3ag** was synthesized from **3a** (0.195 mL, 1 mmol) and 6-bromo hex-1-ene (0.41 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3ag** (250 mg, 73% yield; *E/Z*, 87:13); **IR** (ATR, 298 K, in cm^{-1}): 2981 (w), 2933 (w), 2908 (w), 2859 (vw), 1476 (w), 1442 (w), 1392 (w), 1369 (w), 1262 (s), 1165 (w), 1099 (w), 1016 (vs), 967 (vs), 860 (m), 817 (m), 800 (m), 742 (m), 643 (w), 520 (m), 472 (m); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K,

[ppm]): δ = 1.33 (6H, t, $^{3}J_{HH}$ = 7.1 Hz, H1), 1.50 (2H, m, H8), 1.84 (2H, m, H9), 2.03 (2H, m, H7), 2.37 (2H, m, H4), 3.39 (2H, t, $^{3}J_{HH}$ = 6.8 Hz, 10H), 4.02 (2H, q, $^{3}J_{HHP}$ = 7.0 Hz, H3), 4.10 (4H, p, $^{3}J_{HHP}$ = 7.2 Hz, H2), 5.40 (1H, m, H5), 5.51 (1H, m, H6); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 27.9 (1C, s, C8), 31.8 (1C, s, C7), 32.3 (1C, s, C9), 33.7 (1C, d, $^{3}J_{CP}$ = 7 Hz, C4), 33.8 (1C, s, C10), 63.8 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 67.2 (1C, d, $^{2}J_{CP}$ = 6 Hz, C3), 125.5 (1C, s, C5), 133.1 (1C, s, C6); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -0.9 (1P, s, P (*E*)), -0.8 (1P, s, P (*Z*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{12}H_{25}O_4BrP$ 343.0668 found 343.0663.

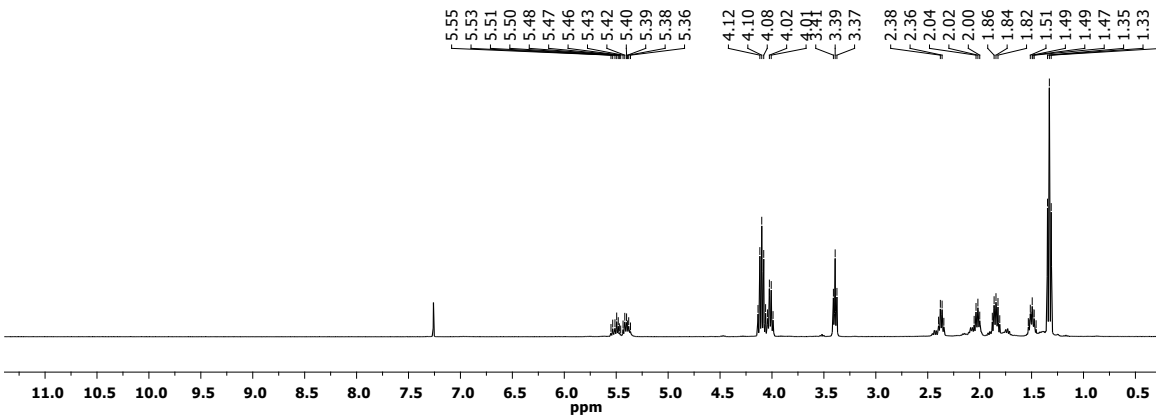


Figure S62 ^{1}H NMR spectrum of **3ag** ($CDCl_3$, 300 K).

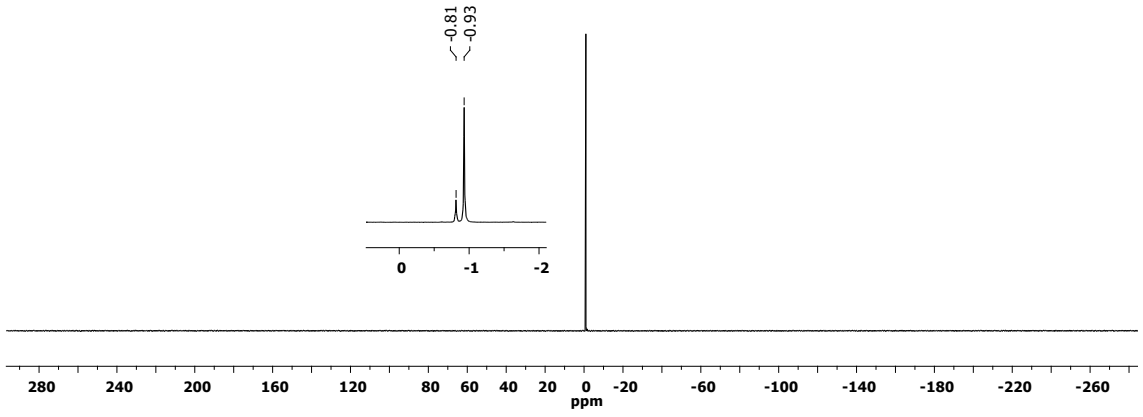


Figure S63 ^{31}P{^{1}H} NMR spectrum of **3ag** ($CDCl_3$, 300 K).

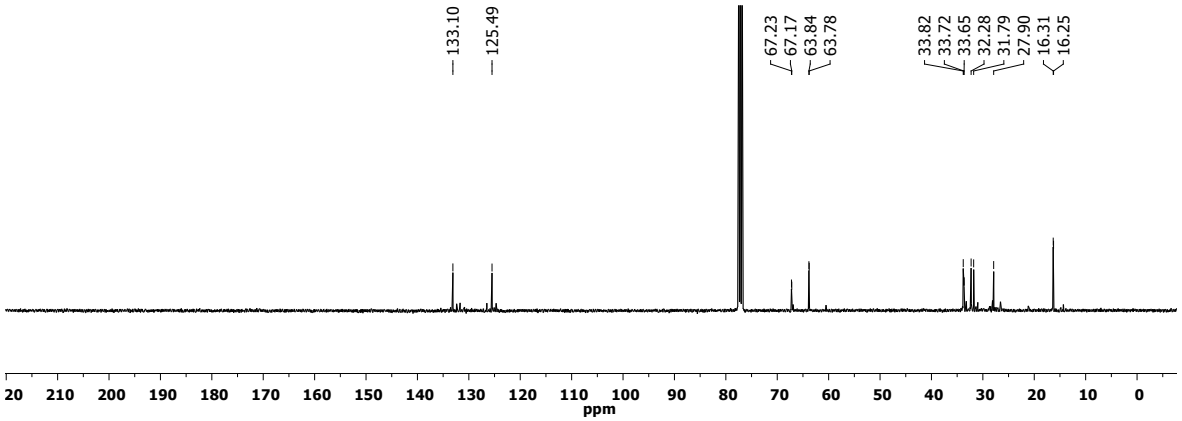
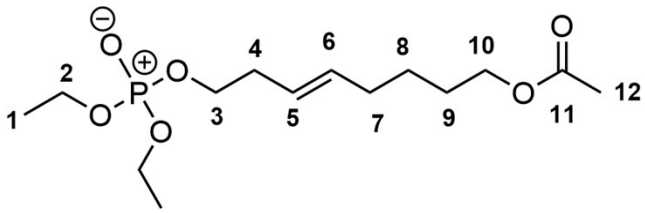


Figure S64 $^{13}C\{^{1}H\}$ NMR spectrum of **3ag** ($CDCl_3$, 300 K).

S2.23 Cross metathesis of diethyl butenyl phosphate (3a) with hex-5-en-1-yl acetate (h)



Compound **3ah** was synthesized from **3a** (0.195 mL, 1 mmol) and hex-5-en-1-yl acetate (0.49 mL, 3 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 6:4) to afford **3ah** (225 mg, 70% yield; *E/Z*, 85:15); **IR** (ATR, 298 K, in cm^{-1}): 2982 (vw), 2935 (vw), 2910 (vw), 2862 (vw), 1736 (m), 1473 (vw), 1444 (vw), 1390 (vw), 1367 (w), 1239 (s), 1166 (w), 1017 (vs), 968 (vs), 864 (w), 817 (m), 800 (m), 744 (w), 634 (vw), 607 (w), 523 (w), 473 (w); **^{1}H NMR** (500.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.33 (6H, t, $^{3}J_{HH}$ = 7.0 Hz, H1), 1.41 (2H, m, H8), 1.61 (2H, m, H9), 2.04 (4H, m, H7, H12), 2.37 (2H, d, $^{3}J_{HH}$ = 6.7 Hz, H4), 4.03 (4H, m, H3, H10), 4.11 (4H, m, H2), 5.41 (1H, m, H5), 5.51 (1H, m, H6); **^{13}C{^{1}H} NMR** (125.76 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (2C, d, $^{3}J_{CP}$ = 7 Hz, C1), 21.0 (1C, s, C12), 25.7 (1C, s, C8), 28.2 (1C, s, C7), 32.3 (1C, s, C9), 33.7 (1C, d, $^{3}J_{CP}$ = 7 Hz, C4), 63.8 (2C, d, $^{2}J_{CP}$ = 6 Hz, C2), 64.5 (1C, s, C10), 67.3 (1C, d, $^{2}J_{CP}$ = 6 Hz, C3), 125.3 (1C, s, C5), 133.3 (1C, s, C6), 171.4, 171.3 (1C, s, C11 (*E,Z*)); **^{31}P{^{1}H} NMR** (202.46 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P (*E*)), -0.9 (1P, s, P (*Z*)); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{14}H_{28}O_6P$ 323.1618 found 323.1620, $[M + Na]^+$ calcd for $C_{14}H_{27}O_6PNa$ 345.1437 found 345.1439.

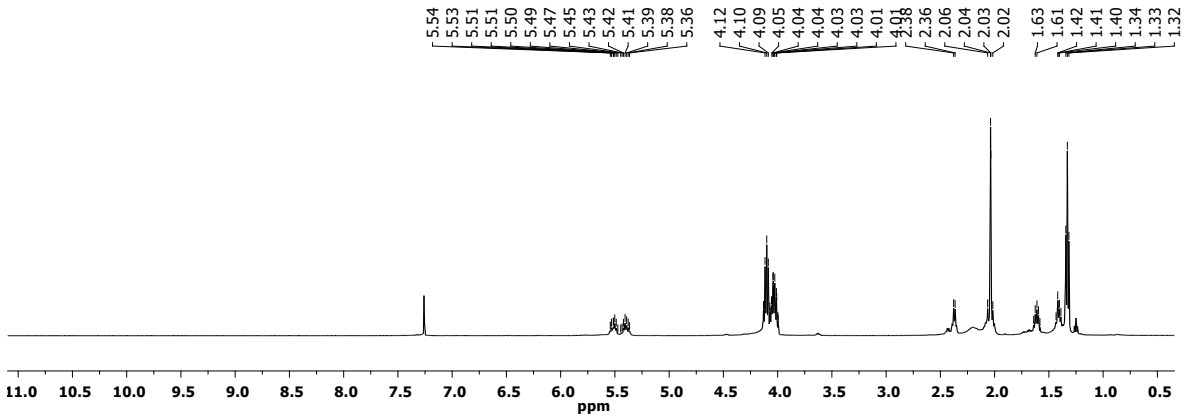


Figure S65 ^{1}H NMR spectrum of **3ah** ($CDCl_3$, 300 K).

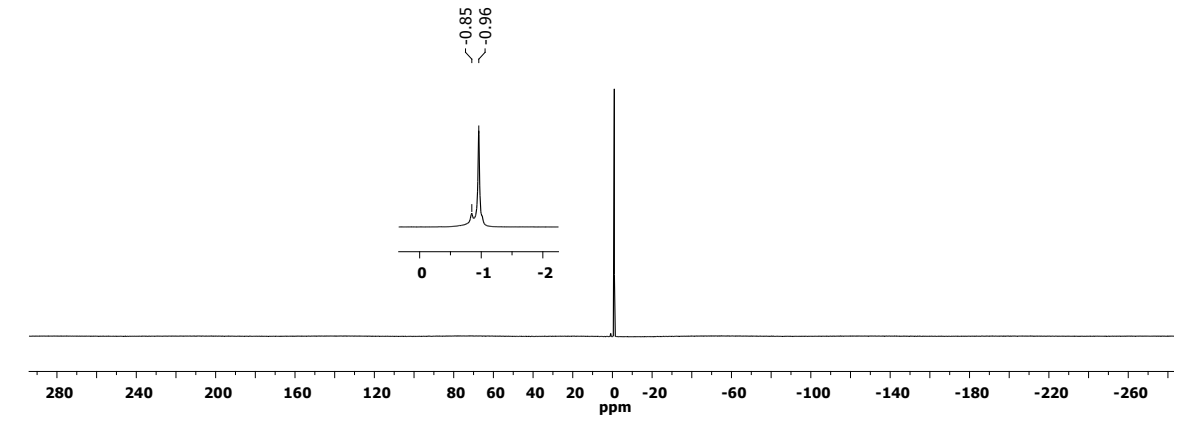


Figure S66 $^{31}P\{^{1}H\}$ NMR spectrum of **3ah** ($CDCl_3$, 300 K).

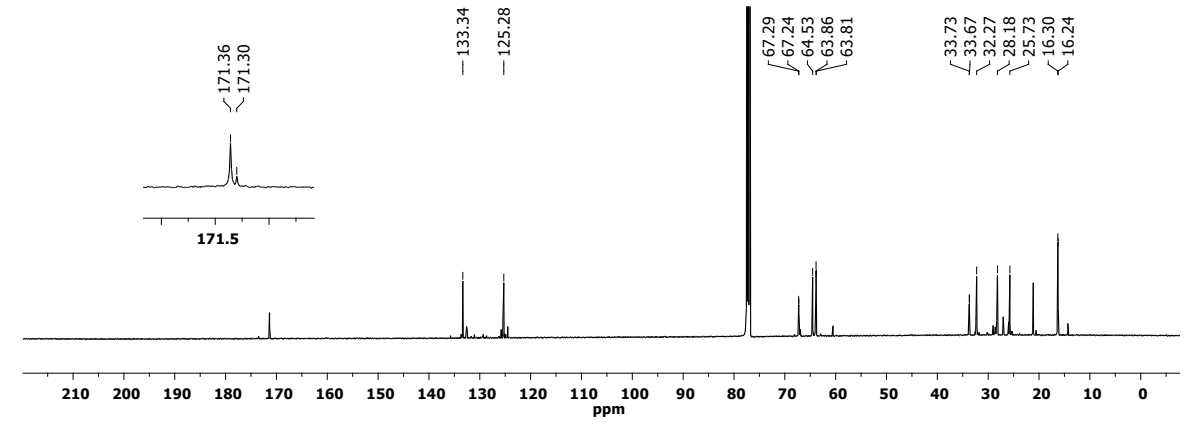
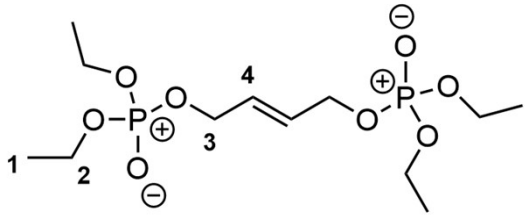


Figure S67 $^{13}C\{^{1}H\}$ NMR spectrum of **3ah** ($CDCl_3$, 300 K).

S2.24 Dimerization of diethyl allyl phosphate (dimer 2a)



Compound **dimer 2a** was synthesized from **2a** (0.36 mL, 2 mmol) in CH_2Cl_2 (3 mL). A solution of

2nd generation Grubbs catalyst (85 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (10% methanol:ethyl acetate) to afford **dimer 2a** (270 mg, 75% yield; *E/Z*, 100:0); **^{1}H NMR** (500.13 MHz, CD_3OD, 300 K, [ppm]): δ = 1.34 (12H, t, $^3J_{HH}$ = 7.0 Hz, H1), 4.12 (8H, m, H2), 4.57 (4H, d, $^3J_{HH}$ = 7.7 Hz, H3), 5.98 (4H, m, H4); **^{13}C{^{1}H} NMR** (125.76 MHz, CD_3OD, 300 K, [ppm]): δ = 15.0 (4C, d, $^3J_{CP}$ = 6 Hz, C1), 64.1 (4C, d, $^2J_{CP}$ = 6 Hz, C2), 66.6 (2C, d, $^2J_{CP}$ = 5 Hz, C3), 128.0 (2C, d, $^3J_{CP}$ = 7 Hz, C4); **^{31}P{^{1}H} NMR** (202.46 MHz, CD_3OD, 300 K, [ppm]): δ = -1.3 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{12}H_{27}O_8P_2$ 361.1176 found 361.1173.

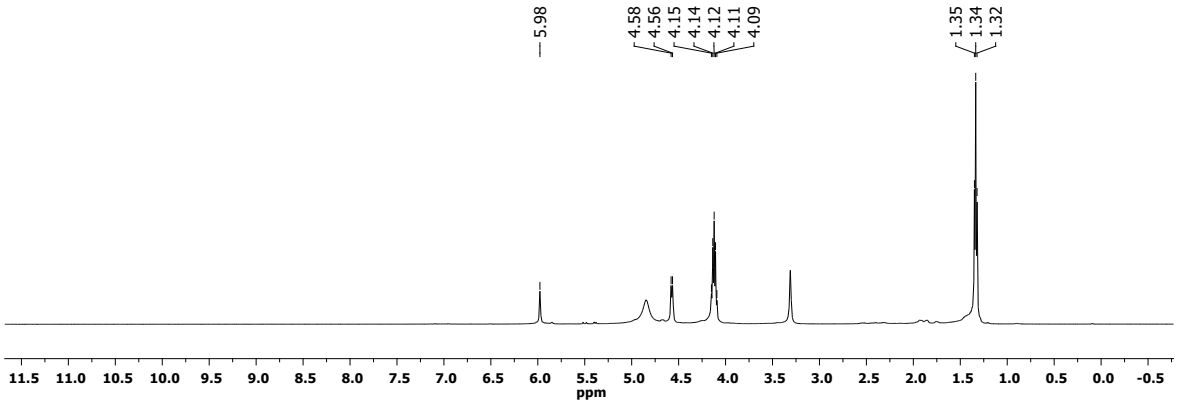


Figure S68 ^{1}H NMR spectrum of **dimer 2a** (CD_3OD, 300 K).

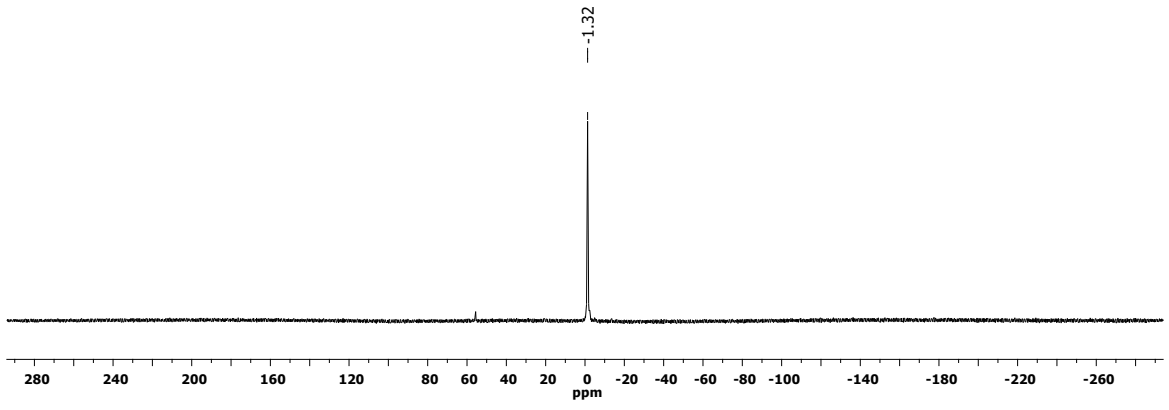


Figure S69 ^{31}P{^{1}H} NMR spectrum of **dimer 2a** (CD_3OD, 300 K).

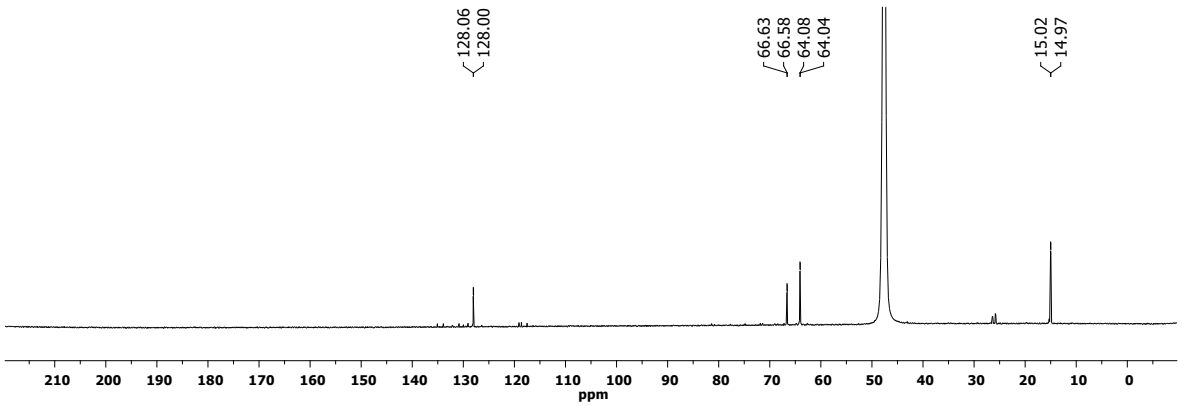
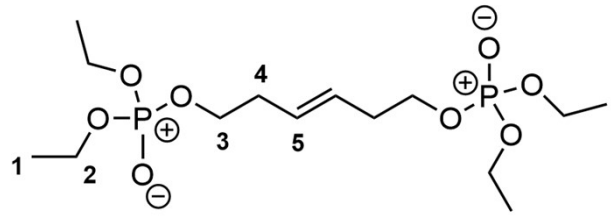


Figure S70 $^{13}C\{^{1}H\}$ NMR spectrum of **dimer 2a** (CD_3OD, 300 K).

S2.25 Dimerization of diethyl butenyl phosphate (dimer 3a)



Compound **dimer 3a** was synthesized from **3a** (0.195 mL, 1 mmol) in CH_2Cl_2 (3 mL). A solution of 2nd generation Grubbs catalyst (43 mg, 0.05 mmol) in CH_2Cl_2 (1 mL) was added to the mixture. The reaction was carried out following the procedure outlined in S2.7. The crude product was purified by column chromatography (ethyl acetate:cyclohexane = 8:2) to afford **dimer 3a** (131 mg, 66% yield; *E/Z*, 89:11); **IR** (ATR, 298 K, in cm^{-1}): 2982 (w), 2934 (vw), 2908 (w), 1477 (vw), 1445 (vw), 1393 (w), 1369 (vw), 1260 (s), 1165 (w), 1098 (w), 1010 (vs), 968 (vs), 867 (w), 817 (m), 799 (m), 743 (m), 524 (m), 471 (m); **^{1}H NMR** (400.13 MHz, $CDCl_3$, 300 K, [ppm]): δ = 1.30 (12H, t, $^{3}J_{HH}$ = 7.1 Hz, H1), 3.99 (4H, q, $^{3}J_{HHP}$ = 6.9 Hz, H3), 4.06 (8H, p, $^{3}J_{HHP}$ = 7.2 Hz, H2), 5.50 (2H, m, H5), 2.36, 2.42 (4H, dd, $^{3}J_{HH}$ = 11.2,6.0 Hz, H4); **^{13}C{^{1}H} NMR** (100.61 MHz, $CDCl_3$, 300 K, [ppm]): δ = 16.3 (4C, d, $^{3}J_{CP}$ = 7 Hz, C1), 63.8 (4C, d, $^{2}J_{CP}$ = 6 Hz, C2), 128.2, 137.3 (2C, s, C5 (*E/Z*)), 33.6, 28.7 (2C, d, $^{3}J_{CP}$ = 7 Hz, C4 (*E/Z*)), 66.9, 66.6 (2C, d, $^{2}J_{CP}$ = 6 Hz, C3 (*E/Z*)); **^{31}P{^{1}H} NMR** (161.98 MHz, $CDCl_3$, 300 K, [ppm]): δ = -1.0 (1P, s, P); **HR-MS** (ESI+) *m/z*: $[M + H]^+$ calcd for $C_{14}H_{30}O_8P_2$ 389.1489 found 389.1482.

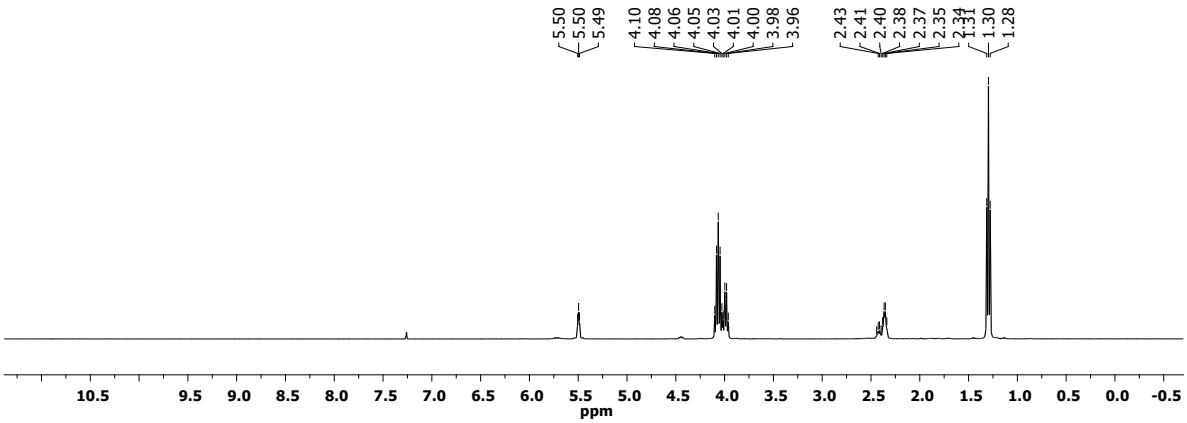


Figure S71 ^{1}H NMR spectrum of **dimer 3a** ($CDCl_3$, 300 K).

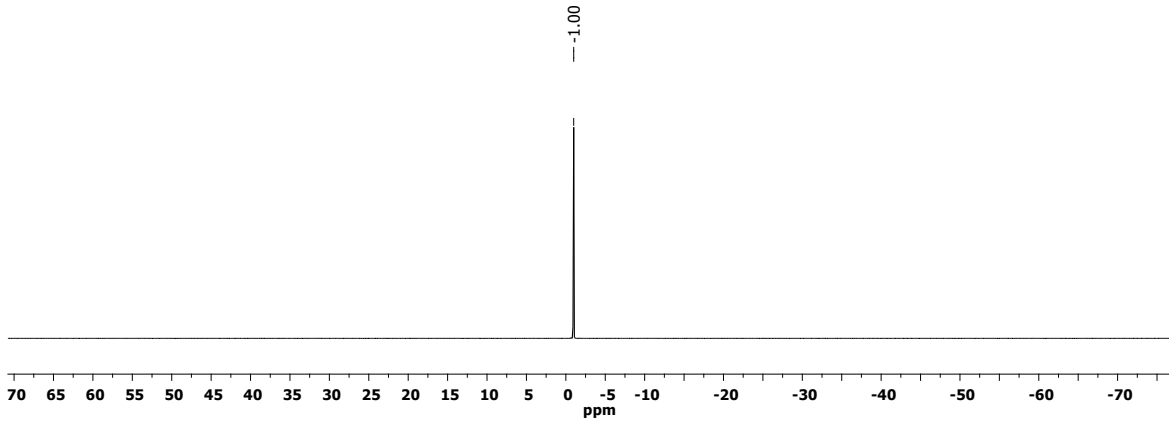


Figure S72 $^{31}P\{^{1}H\}$ NMR spectrum of **dimer 3a** ($CDCl_3$, 300 K).

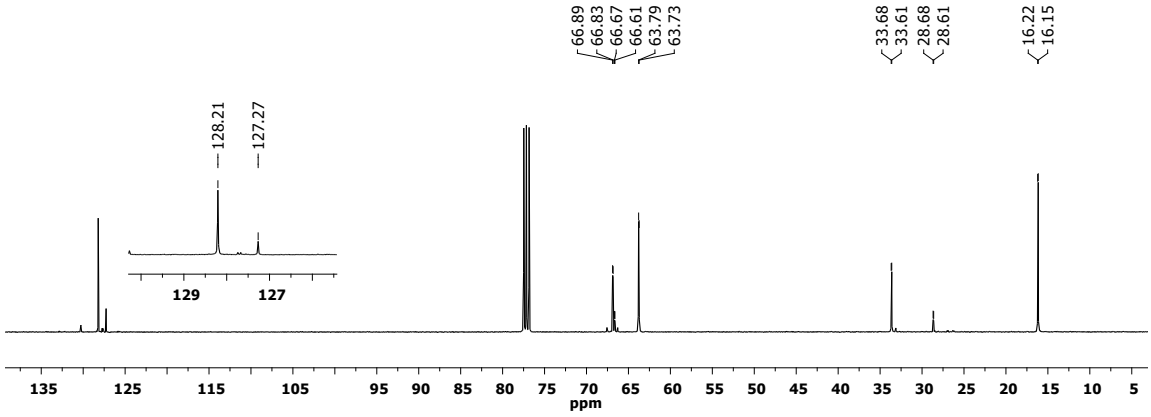


Figure S73 $^{13}C\{^{1}H\}$ NMR spectrum of **dimer 3a** ($CDCl_3$, 300 K).

S3. Single Crystal X-ray Diffraction Data.

S3.1General remarks

Suitable single crystals were coated with Paratone-N oil, mounted using a nylon loop, and frozen in a cold nitrogen stream. Crystals were measured at 100 K on a Rigaku Oxford Diffraction SuperNova system using Cu K_α radiation (λ = 1.54184 Å) generated by a Nova micro-focus X-ray source. Reflections were collected with an Atlas S2 detector. Data reduction and absorption correction were performed with CrysaAlisPro[4] software. Using Olex2[5], the structures were solved with SHELXS/T[6] by direct methods and refined with SHELXL[7] by least-square minimization against F^2 using first isotropic and later anisotropic thermal parameters for all non-hydrogen atoms. Hydrogen atoms bonded to carbon atoms were added to the structure models on calculated positions using the riding model. All other hydrogen atoms were localized in the different Fourier maps. Images of the structures were produced with Olex2[5] software.

S3.2Refinement details

Table S1 Crystallographic data of Ru carbide (**4**)

	Ru carbide (**4**)
Empirical formula	$C_{40}H_{59}Cl_2N_2PRu$
Formula weight	770.83
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.21890(10)
b/Å	18.29290(10)
c/Å	17.88730(10)
α/°	90
β/°	103.8900(10)
γ/°	90
Volume/Å^3	3881.24(5)
Z	4
ρ_{calc}g/cm^3	1.319
μ/mm^{-1}	5.137
F(000)	1624.0
Crystal size/mm^3	0.25 × 0.15 × 0.08

Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.018 to 153.372
Index ranges	-15 ≤ h ≤ 14, -15 ≤ k ≤ 23, -22 ≤ l ≤ 22
Reflections collected	46671
Independent reflections	8128 [R_{int} = 0.0531, R_{sigma} = 0.0276]
Data/restraints/parameters	8128/0/421
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0255, wR_2 = 0.0663
Final R indexes [all data]	R_1 = 0.0267, wR_2 = 0.0675
Largest diff. peak/hole/e $Å^{-3}$	0.51/-0.61

S4. Computational Details

The geometry optimization and frequency calculations were performed using Gaussian 16 software[8] at the meta-GGA functional M06-L[9] method as the recommended model for Grubbs II catalyst[10]. The def2-SVP[11] basis set was applied for all stationary points, followed by the triple-zeta valence def2-TZVPP[11] basis set with single point calculations and dichloromethane as SMD polarizable solvation model[12]. The transition state was confirmed by the presence of a single imaginary frequency representing the vibrational mode corresponding to the reaction, while the intermediate structure showed no imaginary frequencies, consistent with the reaction coordinate involving the phosphate motif and Ru catalyst. Intrinsic reaction coordinate (IRC)[13, 14] calculations were also conducted to verify the reaction pathway leading to the corresponding reactant and the product. Natural Population Analysis (NPA)[15, 16] charges have visualized by Cylview20[17] software.

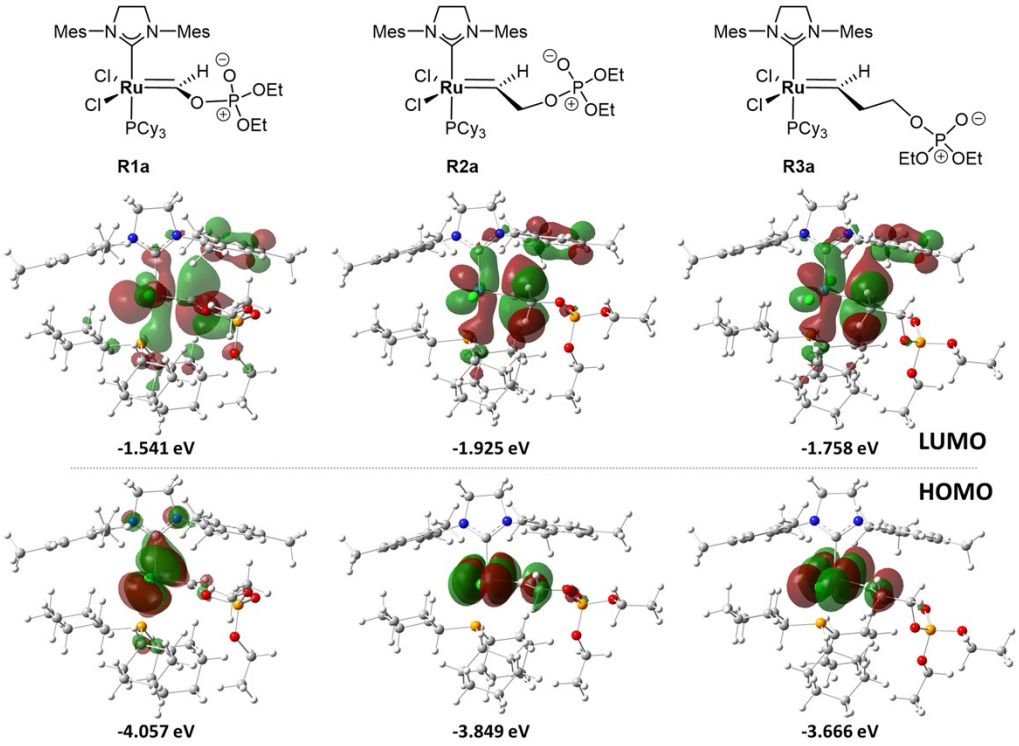


Figure S74 Optimized structures and frontier molecular orbitals (LUMO and HOMO) of Ru–carbene intermediate derived from chain-length-varied alkenyl phosphates (**1a**-**3a**) substrates.

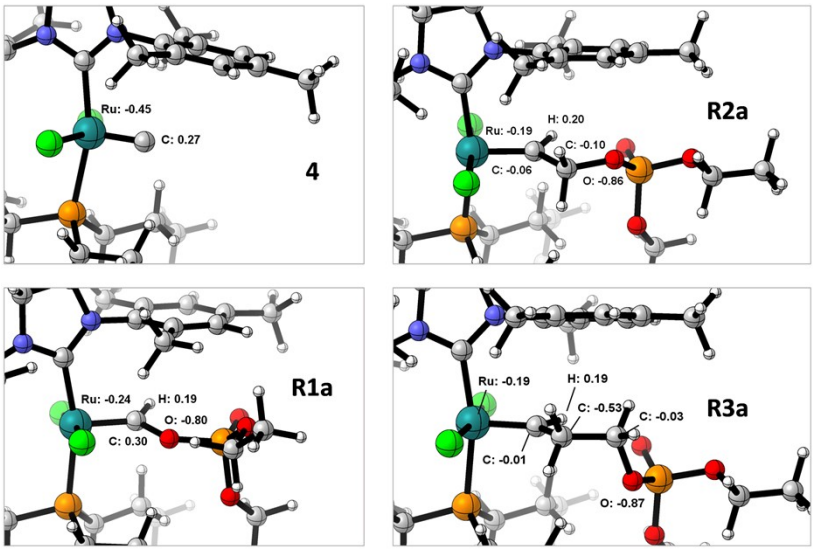


Figure S75. Natural Population Analysis charges of **R1a**, **R2a**, and **R3a**.

Table S2 Molecular orbital of correlated Ru catalyst in diethyl alkenyl phosphate metathesis reaction mechanism.

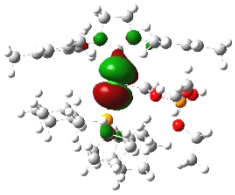
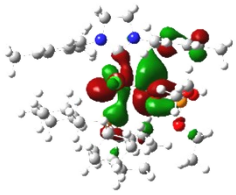
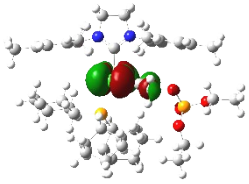
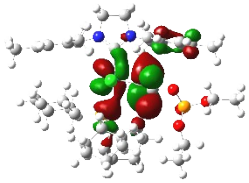
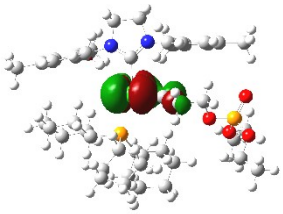
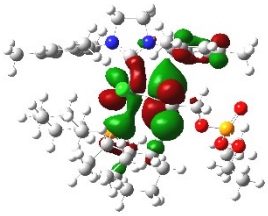
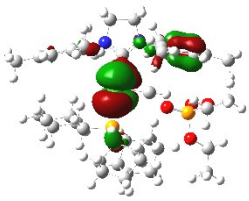
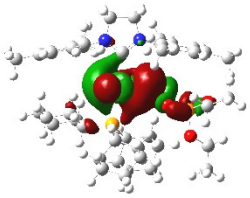
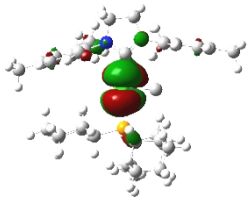
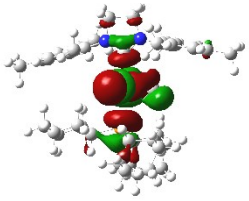
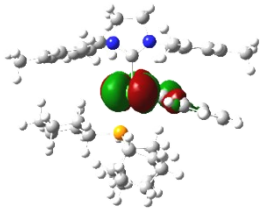
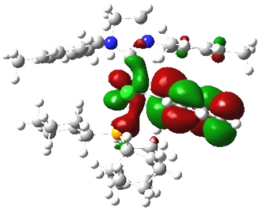
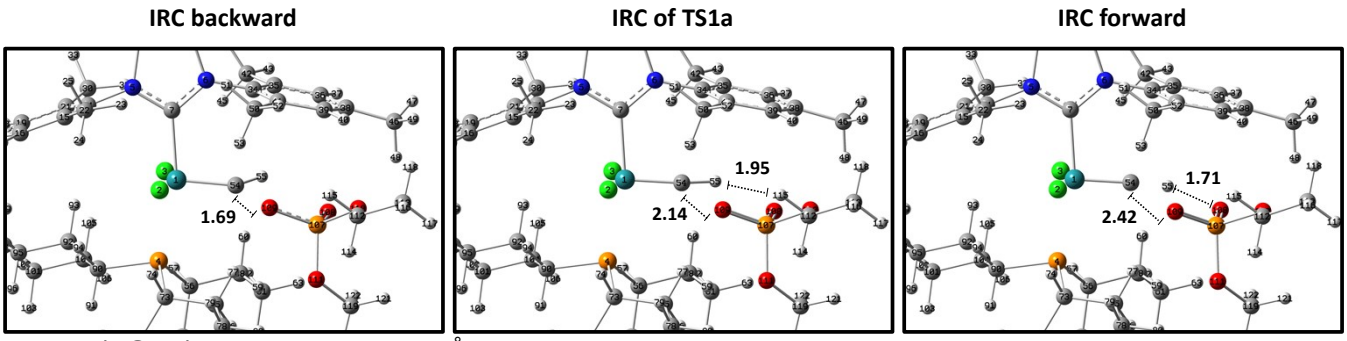
	HOMO	LUMO
R1a (**Ru** coordinate **1a**)		
R2a (**Ru** coordinate **2a**)		
R3a (**Ru** coordinate **3a**)		
TS1a		
P1a (ruthenium carbide **4**)		
GII		

Table S3 Frontier orbital energy levels of Ru catalyst and correlated intermediate at the M06L/def2-SVP level of theory.

	HOMO (eV)	LUMO (eV)	GAP(LUMO-HOMO)
R1a (**Ru** coordinate **1a**)	-4.057	-1.541	2.52
R2a (**Ru** coordinate **2a**)	-3.849	-1.925	1.92
R3a (**Ru** coordinate **3a**)	-3.666	-1.758	1.91
TS1a	-4.909	-2.434	2.47
4 (ruthenium carbide)	-4.577	-1.444	3.13
GII	-3.833	-2.406	1.43

Figure S76 The intrinsic reaction coordinate (IRC) profile for the molecular transformation of **TS1a** at the M06L/def2-SVP level of theory; Optimized geometries of the transition states (**TS1a**) with distances in Å.



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S6. Cartesian coordinate

Table S3 Cartesian coordinates of optimized geometries calculated at the M06L/def2-TZVPP level of theory.

Atom	**R1a** Total atom =125		
	X	Y	Z
Ru1	0.488332	-0.527438	-0.197225
Cl2	0.481874	-0.390754	2.243215
Cl3	0.717645	-0.494758	-2.648330
P4	0.754608	1.916453	-0.306804
N5	2.007748	-3.065505	0.379931
N6	-0.030357	-3.599276	-0.161653
C7	0.816521	-2.557644	-0.018768
C8	2.005444	-4.522256	0.521315
H9	2.293494	-4.808799	1.546332
H10	2.747152	-4.975975	-0.157977
C11	0.571354	-4.891717	0.175573

Atom	**R2a** Total atom =128		
	X	Y	Z
Ru1	-0.739488	-0.505098	-0.053175
Cl2	-0.849748	-0.442511	-2.500100
Cl3	-0.852174	-0.416100	2.394325
P4	-0.931207	1.946787	0.008243
N5	-2.327095	-3.020555	0.434751
N6	-0.194577	-3.467915	0.558688
C7	-1.090087	-2.509547	0.226986
C8	-2.305060	-4.356517	1.032207
H9	-2.948882	-5.045953	0.463276
H10	-2.692775	-4.323831	2.064499
C11	-0.829501	-4.720852	0.976116

H12	0.493190	-5.587699	-0.675806	H12	-0.426406	-5.050719	1.946167
H13	0.030358	-5.357611	1.015960	H13	-0.607605	-5.520949	0.247071
C14	3.234397	-2.354637	0.535846	C14	-3.557808	-2.408100	0.055495
C15	3.705689	-2.046400	1.824597	C15	-3.931336	-2.448905	-1.303246
C16	4.958509	-1.428961	1.934502	C16	-5.156619	-1.882094	-1.668032
H17	5.327464	-1.170598	2.932577	H17	-5.447143	-1.895147	-2.723150
C18	5.761022	-1.169846	0.822712	C18	-6.032904	-1.341795	-0.723360
C19	5.276097	-1.531392	-0.440696	C19	-5.653912	-1.376653	0.622623
H20	5.904197	-1.368254	-1.322691	H20	-6.339488	-0.984913	1.381495
C21	4.024327	-2.124672	-0.612299	C21	-4.426361	-1.898281	1.040828
C22	2.957607	-2.427493	3.061551	C22	-3.069089	-3.124803	-2.317986
H23	1.914454	-2.692484	2.858491	H23	-2.169370	-2.531064	-2.541696
H24	2.936979	-1.599878	3.782460	H24	-3.610362	-3.272638	-3.260579
H25	3.450566	-3.277908	3.560878	H25	-2.727949	-4.109927	-1.964543
C26	7.125540	-0.572579	0.971810	C26	-7.360958	-0.781672	-1.127325
H27	7.274680	-0.129341	1.965060	H27	-7.418317	-0.598633	-2.208102
H28	7.317241	0.206807	0.219986	H28	-7.578946	0.165155	-0.611878
H29	7.910480	-1.332915	0.835884	H29	-8.181607	-1.469690	-0.871013
C30	3.553808	-2.545637	-1.966467	C30	-4.081993	-1.951891	2.494367
H31	4.352310	-2.445809	-2.712152	H31	-4.650736	-1.204861	3.063696
H32	2.694415	-1.947611	-2.311980	H32	-3.012463	-1.771102	2.672781
H33	3.218733	-3.594484	-1.974629	H33	-4.335487	-2.933428	2.928204
C34	-1.402151	-3.553839	-0.542995	C34	1.213818	-3.475923	0.324360
C35	-1.739187	-3.731910	-1.894223	C35	2.113585	-3.280678	1.387254
C36	-3.095961	-3.726156	-2.234302	C36	3.481949	-3.405919	1.119278
H37	-3.374835	-3.847104	-3.285697	H37	4.188985	-3.219707	1.933860
C38	-4.099268	-3.560391	-1.276376	C38	3.966259	-3.734584	-0.146950
C39	-3.721437	-3.406854	0.062564	C39	3.041998	-3.910930	-1.183660
H40	-4.494903	-3.258880	0.822553	H40	3.402024	-4.146172	-2.190671
C41	-2.382109	-3.398154	0.454121	C41	1.667988	-3.785517	-0.973905
C42	-0.676227	-3.877710	-2.934346	C42	1.663212	-2.904712	2.761152
H43	-1.104904	-4.132091	-3.911493	H43	2.057616	-1.910759	3.024360
H44	0.055586	-4.658798	-2.677382	H44	2.051781	-3.606935	3.513692
H45	-0.107301	-2.939916	-3.048103	H45	0.573214	-2.844169	2.853763
C46	-5.538293	-3.482581	-1.668060	C46	5.436184	-3.892254	-0.379473
H47	-5.720687	-3.903912	-2.665059	H47	5.802771	-4.855154	0.009773
H48	-5.856866	-2.429130	-1.685560	H48	6.006743	-3.106421	0.134991
H49	-6.188746	-4.002676	-0.951218	H49	5.691466	-3.861559	-1.447488
C50	-1.983584	-3.194526	1.880317	C50	0.695542	-3.922705	-2.101119
H51	-1.399074	-4.041851	2.273080	H51	-0.107647	-4.641401	-1.876120
H52	-2.863807	-3.080237	2.525430	H52	1.190811	-4.254950	-3.022042
H53	-1.343851	-2.303789	2.003723	H53	0.192980	-2.962522	-2.315577
C54	-1.308503	-0.555685	-0.395531	C54	1.073894	-0.573408	-0.045579
H55	-1.809497	-0.905374	-1.324151	H55	1.576050	-0.702702	0.934805
C56	-0.107076	2.748724	-1.728603	C56	-0.183935	2.741326	1.507169
H57	0.456174	2.342494	-2.588987	H57	-0.781259	2.264274	2.305762

C58	-1.554358	2.306046	-1.944524	C58	1.260800	2.339192	1.805715
H59	-2.175715	2.608607	-1.082874	H59	1.946110	2.771472	1.056730
H60	-1.598154	1.208549	-2.001873	H60	1.374436	1.247890	1.746831
C61	-2.118247	2.895235	-3.230472	C61	1.665645	2.822458	3.189733
H62	-1.568196	2.460444	-4.084222	H62	1.040044	2.306328	3.939677
H63	-3.166419	2.583203	-3.364471	H63	2.701403	2.517644	3.408251
C64	-1.993980	4.410470	-3.269952	C64	1.491175	4.328205	3.321746
H65	-2.380660	4.808709	-4.221127	H65	1.769897	4.671034	4.330727
H66	-2.628668	4.851767	-2.478688	H66	2.187940	4.836850	2.627909
C67	-0.553393	4.845781	-3.051329	C67	0.065625	4.750035	2.993310
H68	-0.471614	5.944192	-3.048742	H68	-0.043678	5.844445	3.056414
H69	0.066400	4.496978	-3.897097	H69	-0.619069	4.332937	3.754101
C70	0.005554	4.273477	-1.754994	C70	-0.370788	4.255831	1.618253
H71	-0.562825	4.696288	-0.906071	H71	0.227978	4.767701	0.842749
H72	1.050137	4.597128	-1.613990	H72	-1.418404	4.544686	1.428032
C73	0.393537	2.819897	1.282359	C73	-0.341895	2.829508	-1.526402
H74	0.796689	2.106310	2.024432	H74	-0.484122	2.052986	-2.301249
C75	-1.109439	2.886612	1.542880	C75	1.154653	3.138591	-1.465745
H76	-1.584659	3.567035	0.811810	H76	1.324533	3.953918	-0.738890
H77	-1.559638	1.899134	1.383431	H77	1.731768	2.284317	-1.083634
C78	-1.411203	3.382884	2.947787	C78	1.679322	3.580559	-2.822705
H79	-1.040851	2.634994	3.672672	H79	1.558473	2.751738	-3.543760
H80	-2.501294	3.444419	3.100459	H80	2.761466	3.779731	-2.765401
C81	-0.751065	4.726286	3.214204	C81	0.925120	4.805833	-3.315908
H82	-1.201669	5.489617	2.552547	H82	1.146781	5.657517	-2.646517
H83	-0.949214	5.065794	4.243199	H83	1.276837	5.109094	-4.314477
C84	0.746016	4.659461	2.953401	C84	-0.575733	4.557840	-3.332776
H85	1.208266	3.968666	3.681480	H85	-0.806262	3.791799	-4.094420
H86	1.216659	5.640200	3.127048	H86	-1.115755	5.465402	-3.645651
C87	1.062640	4.171740	1.542796	C87	-1.104498	4.074620	-1.985406
H88	2.155443	4.105263	1.425375	H88	-2.181926	3.871346	-2.079534
H89	0.722373	4.927142	0.813588	H89	-1.007225	4.880686	-1.234176
C90	2.539907	2.351200	-0.584662	C90	-2.721552	2.421985	0.120082
H91	2.593652	3.448747	-0.452538	H91	-2.756622	3.503352	-0.111986
C92	3.419027	1.705316	0.490074	C92	-3.543386	1.683049	-0.939756
H93	3.410348	0.606615	0.345365	H93	-3.566551	0.603863	-0.685484
H94	3.011011	1.865798	1.501495	H94	-3.063932	1.728769	-1.931337
C95	4.847022	2.224591	0.398985	C95	-4.962424	2.231044	-0.991934
H96	4.851395	3.301855	0.650606	H96	-4.927570	3.276099	-1.353080
H97	5.477776	1.736850	1.159701	H97	-5.557339	1.676252	-1.735481
C98	5.431558	2.026827	-0.992076	C98	-5.636619	2.184617	0.372206
H99	5.556465	0.945150	-1.172289	H99	-5.813531	1.129972	0.639855
H100	6.439845	2.467423	-1.055582	H100	-6.629614	2.660866	0.330182
C101	4.527623	2.592812	-2.076615	C101	-4.785348	2.817641	1.462540
H102	4.942859	2.378347	-3.073759	H102	-5.266806	2.692595	2.445366
H103	4.497367	3.695240	-1.994045	H103	-4.721960	3.909348	1.297117

C104	3.109383	2.046550	-1.968792
H105	3.101565	0.956058	-2.141781
H106	2.482373	2.475424	-2.765531
P107	-3.822420	0.046448	0.344315
O108	-4.437808	-0.458945	-0.896249
O109	-2.198885	-0.134992	0.537755
O110	-4.336242	-0.602443	1.710802
O111	-3.958988	1.637987	0.585865
C112	-3.778628	-0.175719	2.974890
C113	-4.522082	-0.875803	4.072602
H114	-3.879974	0.919552	3.051542
H115	-2.700101	-0.408052	2.984737
H116	-4.124018	-0.574185	5.049761
H117	-5.592194	-0.631626	4.048031
H118	-4.423044	-1.966205	3.989702
C119	-4.834670	2.414272	-0.251001
C120	-4.649277	3.863060	0.091684
H121	-5.875790	2.090539	-0.086074
H122	-4.601965	2.207949	-1.308188
H123	-5.312900	4.486290	-0.521935
H124	-4.881175	4.056119	1.147645
H125	-3.615165	4.187482	-0.091350

C104	-3.372920	2.245755	1.491062
H105	-3.387478	1.173539	1.758952
H106	-2.790627	2.742703	2.281903
P107	4.181135	0.059184	0.319395
O108	3.792551	-0.099746	1.737077
O109	3.390354	-0.686768	-0.853592
O110	5.678193	-0.461677	0.040143
O111	4.149106	1.592488	-0.228692
C112	6.227237	-0.422887	-1.283875
C113	7.714398	-0.602573	-1.189275
H114	5.965743	0.538112	-1.759838
H115	5.755500	-1.217293	-1.885910
H116	8.167278	-0.581501	-2.188951
H117	8.173331	0.194853	-0.589707
H118	7.969786	-1.562667	-0.721557
C119	4.740727	2.602210	0.602102
C120	4.540692	3.942071	-0.042926
H121	5.815207	2.376759	0.729293
H122	4.284278	2.559600	1.605326
H123	5.002526	4.731026	0.564920
H124	4.991651	3.975101	-1.043959
H125	3.472130	4.177046	-0.145996
C126	2.011328	-0.492592	-1.204089
H127	1.902189	0.457980	-1.752649
H128	1.785945	-1.273447	-1.945215

Atom	**R3a** Total atom =131		
	X	Y	Z
Ru1	0.964340	0.497474	-0.068201
Cl2	1.423343	0.447730	-2.478711
Cl3	0.831233	0.380381	2.384834
P4	0.622099	-1.927732	-0.091727
N5	3.028659	2.558313	0.644967
N6	1.043577	3.464891	0.723798
C7	1.723249	2.356305	0.345532
C8	3.251761	3.795495	1.394838
H9	4.109143	4.350863	0.984919
H10	3.476810	3.569527	2.451835
C11	1.925408	4.519511	1.231659
H12	1.536115	4.931489	2.174784
H13	1.975898	5.355997	0.509741
C14	4.114883	1.727288	0.236060
C15	4.563161	1.833108	-1.095861

Atom	**Diethyl vinyl phosphate (1a)** Total atom =24		
	X	Y	Z
C1	-3.327353	-1.759387	-0.291225
C2	-2.210162	-1.281567	0.249431
H3	-4.043668	-2.287762	0.335709
H4	-3.547080	-1.635286	-1.352410
H5	-1.950640	-1.380162	1.309318
O6	-1.292348	-0.589339	-0.501080
P7	0.136665	-0.141539	0.138728
O8	0.178504	-0.060157	1.617215
C9	-1.455842	2.608816	0.022293
H10	-1.719548	3.626826	0.337782
H11	-1.959217	2.402781	-0.931664
H12	-1.855568	1.917335	0.777542
C13	2.422734	-1.425663	-0.027786
C14	3.319453	-0.220618	-0.112452
H15	2.313235	-1.769509	1.013428

C16	5.645770	1.043842	-1.493657
H17	5.988480	1.108104	-2.530959
C18	6.320888	0.208512	-0.599905
C19	5.883522	0.174965	0.728319
H20	6.416113	-0.451576	1.451885
C21	4.787211	0.919904	1.174161
C22	3.928108	2.794690	-2.045110
H23	2.932941	2.441611	-2.355583
H24	4.534307	2.915266	-2.951398
H25	3.798365	3.787826	-1.587668
C26	7.508780	-0.591338	-1.036051
H27	7.568763	-0.673427	-2.128993
H28	7.492811	-1.609802	-0.621874
H29	8.449263	-0.131862	-0.693992
C30	4.384964	0.888701	2.613501
H31	4.769457	-0.010690	3.112515
H32	3.292563	0.909977	2.741131
H33	4.799327	1.751127	3.161536
C34	-0.311705	3.792318	0.420986
C35	-1.296474	3.754369	1.425278
C36	-2.590590	4.170943	1.090363
H37	-3.369192	4.116066	1.857863
C38	-2.921998	4.623155	-0.188821
C39	-1.916257	4.649579	-1.161792
H40	-2.155907	4.991343	-2.174389
C41	-0.610562	4.239369	-0.881043
C42	-1.020290	3.241320	2.799633
H43	-1.381599	2.205188	2.896806
H44	-1.541539	3.839465	3.559424
H45	0.048488	3.201329	3.037878
C46	-4.333233	4.994964	-0.521117
H47	-4.777797	5.647325	0.243392
H48	-4.975741	4.099559	-0.570148
H49	-4.409961	5.506795	-1.489136
C50	0.437504	4.212779	-1.946222
H51	1.347958	4.756597	-1.651744
H52	0.073721	4.654405	-2.882402
H53	0.760139	3.177753	-2.161440
C54	-0.796162	0.884616	-0.317056
H55	-1.428423	0.985837	0.595523
C56	-0.236073	-2.602842	1.408870
H57	0.474416	-2.276054	2.189924
C58	-1.560149	-1.940223	1.793631
H59	-2.368917	-2.267652	1.119135
H60	-1.493711	-0.848533	1.701701
C61	-1.923356	-2.321256	3.220961
H16	2.816944	-2.265608	-0.614885
H17	4.337066	-0.481712	0.206660
H18	3.368461	0.166810	-1.138674
H19	2.966314	0.588830	0.542144
O20	1.115412	-1.185137	-0.577089
O21	0.438480	1.212833	-0.667382
C22	0.037328	2.475628	-0.108486
H23	0.451433	3.224905	-0.796382
H24	0.534973	2.606789	0.866546

Atom	**Diethyl allyl phosphate (2a)** Total atom =27		
	X	Y	Z
O1	-1.20418	0.295323	-0.253102
P2	0.246788	-0.183164	0.261010
O3	0.39418	-0.387260	1.721793
C4	2.467987	2.934529	-0.394211
H5	2.554419	3.944620	0.026251
H6	3.394662	2.390355	-0.168935
H7	2.385605	3.024569	-1.485201
C8	1.490987	-2.445554	-0.229102
C9	2.897962	-1.913246	-0.262263
H10	1.222259	-2.794549	0.781168
H11	1.361204	-3.289958	-0.919658
H12	3.616189	-2.712785	-0.037233
H13	3.140882	-1.498017	-1.249524
H14	3.038906	-1.120182	0.485517
O15	0.527929	-1.470518	-0.659048
O16	1.190585	0.925164	-0.419006
C17	1.275273	2.226949	0.178721
H18	1.352399	2.118866	1.273622
H19	0.340994	2.774297	-0.033052
C20	-4.692204	0.079798	-0.520383
H21	-4.805337	-0.921191	-0.947877
C22	-2.361814	-0.399016	0.230172
H23	-2.2088	-0.643126	1.297556
H24	-2.474176	-1.350957	-0.315843
C25	-3.556088	0.467327	0.058266
H26	-5.558703	0.740729	-0.585859
H27	-3.463045	1.478389	0.471622

Atom	**Diethyl butenyl phosphate (3a)** Total atom =30		
	X	Y	Z
O1	-0.663575	0.320266	-0.380835
P2	0.805968	-0.061547	0.156649

H62	-1.148502	-1.923116	3.900036
H63	-2.861265	-1.825140	3.518906
C64	-2.027790	-3.831995	3.377806
H65	-2.255956	-4.106646	4.420103
H66	-2.881768	-4.199489	2.777876
C67	-0.759192	-4.535189	2.912939
H68	-0.875006	-5.629107	2.975906
H69	0.068308	-4.279056	3.599562
C70	-0.358369	-4.125307	1.498804
H71	-1.120733	-4.483069	0.781335
H72	0.581045	-4.628947	1.215300
C73	-0.232759	-2.549332	-1.623991
H74	0.064943	-1.797368	-2.380832
C75	-1.749848	-2.475407	-1.457458
H76	-2.069867	-3.243449	-0.731532
H77	-2.058346	-1.512845	-1.026231
C78	-2.470894	-2.732130	-2.769691
H79	-2.215266	-1.934883	-3.491622
H80	-3.559576	-2.664755	-2.614693
C81	-2.075753	-4.087147	-3.337873
H82	-2.448035	-4.880439	-2.663049
H83	-2.563819	-4.265984	-4.308986
C84	-0.564705	-4.213437	-3.471593
H85	-0.208221	-3.499253	-4.235261
H86	-0.290308	-5.213289	-3.843635
C87	0.163525	-3.925400	-2.161943
H88	1.249792	-3.992241	-2.328885
H89	-0.083171	-4.706959	-1.418938
C90	2.246026	-2.829160	-0.067922
H91	2.004015	-3.879502	-0.320790
C92	3.200460	-2.293428	-1.137472
H93	3.490705	-1.257734	-0.872314
H94	2.701870	-2.199116	-2.115033
C95	4.441088	-3.169458	-1.235111
H96	4.147158	-4.171151	-1.601402
H97	5.133103	-2.763983	-1.990899
C98	5.141818	-3.301792	0.109287
H99	5.564348	-2.320603	0.380400
H100	5.995405	-3.995345	0.038481
C101	4.191612	-3.733010	1.215545
H102	4.711001	-3.740069	2.187253
H103	3.868155	-4.776266	1.041668
C104	2.953880	-2.846718	1.287358
H105	3.229766	-1.813398	1.569813
H106	2.291759	-3.209498	2.087776
P107	-4.477362	0.026143	0.242646
O3	1.028237	0.003734	1.621314
C4	1.056481	3.1344	0.025773
H5	1.452633	4.106665	0.347468
H6	0.481932	3.283733	-0.898181
H7	0.365677	2.782419	0.804717
C8	2.021702	-2.387968	0.001679
C9	3.420237	-1.866737	-0.192084
H10	1.810509	-2.568715	1.068272
H11	1.866279	-3.334591	-0.533597
H12	4.155926	-2.621553	0.115749
H13	3.60625	-1.612081	-1.244017
H14	3.597179	-0.967067	0.414352
O15	1.025103	-1.500952	-0.527899
O16	1.719287	0.910664	-0.740606
C17	2.177432	2.153191	-0.185944
H18	2.912566	2.528341	-0.910999
H19	2.711251	1.9513	0.757564
C20	-4.277852	-0.188297	0.366742
H21	-4.309534	-0.225669	1.464196
C22	-1.794582	-0.350191	0.178858
H23	-1.69713	-0.390255	1.278195
H24	-1.821139	-1.390687	-0.188106
C25	-5.31566	-0.665458	-0.321712
C26	-3.042965	0.399943	-0.228779
H27	-3.111185	0.424734	-1.327215
H28	-2.926119	1.447747	0.098656
H29	-5.331623	-0.652876	-1.416041
H30	-6.19417	-1.081249	0.176253

Atom	**Phosphoric acid diethyl ester(5)** Total atom =20		
	X	Y	Z
P1	-0.016816	0.735036	0.089136
O2	0.298388	1.829525	-1.054434
H3	0.118109	2.716467	-0.717927
O4	-1.388550	0.100019	-0.447077
O5	1.016230	-0.448120	-0.264916
O6	0.008869	1.244037	1.478840
C7	-2.011914	-0.940351	0.319900
C8	-3.407638	-1.137389	-0.193774
H9	-2.007155	-0.657253	1.385908
H10	-1.411201	-1.860445	0.221290
H11	-3.910342	-1.940827	0.359634
	-4.001705	-0.221171	-0.081386
	-3.400796	-1.407597	-1.257749
	2.379870	-0.323778	0.160412

O108	-3.824683	0.518378	1.473390	3.090885	-1.609394	-0.144080
O109	-3.728658	0.211919	-1.167716	2.403500	-0.087235	1.237256
O110	-5.930038	0.712681	0.055218	2.843560	0.525743	-0.370540
O111	-4.727849	-1.560458	0.081926	4.143808	-1.547714	0.159200
C112	-6.701530	0.463506	-1.124623	2.630677	-2.450135	0.391380
C113	-8.118893	0.884494	-0.865564	3.057064	-1.833588	-1.218175
H114	-6.639519	-0.606246	-1.389877			
H115	-6.261436	1.024830	-1.967156			
H116	-8.736996	0.730185	-1.759349			
H117	-8.558532	0.307128	-0.041512			
H118	-8.170225	1.947084	-0.594098			
C119	-5.242200	-2.313869	1.185865			
C120	-5.187849	-3.767944	0.816614			
H121	-6.276295	-1.987943	1.400105			
H122	-4.640825	-2.099196	2.085749			
H123	-5.571678	-4.389654	1.635839			
H124	-5.787804	-3.972842	-0.080268			
H125	-4.154236	-4.078994	0.608353			
C126	-1.529445	1.116360	-1.606937			
H127	-1.392707	0.263317	-2.292397			
H128	-1.048819	1.942802	-2.154026			
C129	-2.999278	1.419444	-1.440425			
H130	-3.424832	1.849290	-2.361412			
H131	-3.155135	2.144661	-0.626056			

Atom	**Ruthenium carbide (4)** Total atom =105		
	X	Y	Z
Ru1	-0.522810	-0.027735	-0.023831
Cl2	-0.294556	0.126721	-2.433979
Cl3	0.015851	0.642648	2.248814
P4	1.623817	-1.227534	0.017042
N5	-1.759527	2.780135	-0.231085
N6	-3.326742	1.266700	-0.235950
C7	-1.996159	1.455479	-0.151603
C8	-2.980343	3.572830	-0.399466
H9	-2.955830	4.105447	-1.365165
H10	-3.052022	4.337904	0.389935
C11	-4.079133	2.522655	-0.321017
H12	-4.727405	2.636334	0.564647
H13	-4.741025	2.518510	-1.200994
C14	-0.499876	3.432221	-0.060235
C15	0.298957	3.723386	-1.179618
C16	1.518793	4.377505	-0.960893
H17	2.151915	4.602453	-1.826178
C18	1.937171	4.769227	0.311294

Atom	**TS1a** Total atom =125		
	X	Y	Z
Ru1	-0.634606	-0.515615	0.140481
Cl2	-0.770792	-0.449531	-2.242574
Cl3	-1.323888	-0.370582	2.442501
P4	-0.687505	1.976095	0.179563
N5	-2.366931	-3.000686	-0.271054
N6	-0.319329	-3.588458	0.192757
C7	-1.137046	-2.537337	0.024279
C8	-2.441501	-4.464489	-0.248110
H9	-2.881159	-4.841743	-1.184579
H10	-3.097814	-4.794249	0.575764
C11	-0.988168	-4.870462	-0.053212
H12	-0.832757	-5.554628	0.794906
H13	-0.550316	-5.356413	-0.941514
C14	-3.554066	-2.224962	-0.438898
C15	-3.997289	-1.922732	-1.741738
C16	-5.187532	-1.200852	-1.878086
H17	-5.533825	-0.950528	-2.886168
C18	-5.958574	-0.819780	-0.777665

C19	1.087777	4.509957	1.393161	C19	-5.507771	-1.176529	0.497567
H20	1.383637	4.833644	2.396273	H20	-6.113091	-0.915321	1.372193
C21	-0.137613	3.862768	1.234437	C21	-4.323489	-1.892105	0.696039
C22	-0.139439	3.444904	-2.582430	C22	-3.295151	-2.421947	-2.964034
H23	-1.044417	2.831064	-2.636311	H23	-2.283241	-2.785348	-2.756664
H24	0.634533	2.906621	-3.146353	H24	-3.200868	-1.631609	-3.719727
H25	-0.324209	4.391285	-3.115392	H25	-3.872800	-3.239440	-3.425663
C26	3.244842	5.467000	0.521058	C26	-7.260960	-0.104153	-0.956544
H27	3.752026	5.685604	-0.427615	H27	-7.385124	0.713100	-0.232057
H28	3.933723	4.861527	1.129813	H28	-8.111869	-0.786013	-0.803392
H29	3.114216	6.418117	1.057728	H29	-7.364310	0.317160	-1.964940
C30	-1.061426	3.716304	2.402322	C30	-3.972658	-2.367891	2.070974
H31	-0.502389	3.548781	3.330959	H31	-4.132547	-1.581514	2.819643
H32	-1.756238	2.875607	2.292107	H32	-2.929246	-2.687616	2.168092
H33	-1.653623	4.636354	2.543872	H33	-4.618689	-3.214992	2.354136
C34	-4.028325	0.029972	-0.110612	C34	1.080666	-3.557357	0.470006
C35	-4.314527	-0.459003	1.174665	C35	1.499590	-3.621521	1.813475
C36	-5.026349	-1.656229	1.274762	C36	2.868999	-3.586617	2.070463
H37	-5.253117	-2.052362	2.269607	H37	3.211664	-3.597380	3.109445
C38	-5.444502	-2.364238	0.143300	C38	3.814459	-3.506754	1.039260
C39	-5.135795	-1.844029	-1.117419	C39	3.355867	-3.487681	-0.279118
H40	-5.449477	-2.388635	-2.013554	H40	4.081770	-3.423065	-1.094158
C41	-4.425699	-0.650343	-1.271667	C41	1.994303	-3.495988	-0.594797
C42	-3.814609	0.254305	2.388846	C42	0.496132	-3.656040	2.921458
H43	-4.213816	-0.189335	3.309067	H43	0.981159	-3.797485	3.894855
H44	-4.084177	1.321871	2.389930	H44	-0.239792	-4.465898	2.796862
H45	-2.713134	0.214398	2.448010	H45	-0.080793	-2.717458	2.969360
C46	-6.171422	-3.665375	0.280302	C46	5.266631	-3.360609	1.349667
H47	-5.466111	-4.507113	0.364574	H47	5.556912	-3.920146	2.249316
H48	-6.810383	-3.873370	-0.587995	H48	5.484281	-2.296695	1.531646
H49	-6.800968	-3.691701	1.179828	H49	5.903150	-3.681062	0.514776
C50	-4.048217	-0.135949	-2.622638	C50	1.541733	-3.335394	-2.007994
H51	-4.380659	0.900841	-2.785652	H51	0.595755	-3.851214	-2.225578
H52	-4.481442	-0.750227	-3.421397	H52	2.300183	-3.697984	-2.714040
H53	-2.953309	-0.132270	-2.750414	H53	1.376066	-2.266830	-2.223292
C54	-1.449803	-1.366823	0.171706	C54	1.001104	-0.720331	0.471713
C55	1.963262	-2.052437	1.644063	H55	1.894876	-0.873448	1.124871
H56	2.109449	-1.176860	2.303466	C56	0.173218	2.708135	1.647676
C57	0.768399	-2.812500	2.225255	H57	-0.492691	2.395371	2.474184
H58	0.539363	-3.695553	1.602975	C58	1.540126	2.097798	1.955977
H59	-0.127892	-2.176685	2.205964	H59	2.245416	2.267295	1.123955
C60	1.062908	-3.254356	3.652046	H60	1.448188	1.009085	2.060296
H61	1.162409	-2.353682	4.284621	C61	2.116922	2.662004	3.246111
H62	0.206161	-3.813863	4.058569	H62	1.489287	2.329567	4.092803
C63	2.335885	-4.082274	3.742152	H63	3.112408	2.225476	3.419375
H64	2.547959	-4.361106	4.786355	C64	2.171239	4.181605	3.233501

H65	2.189712	-5.034617	3.200027
C66	3.519088	-3.343393	3.135761
H67	4.427304	-3.965902	3.166914
H68	3.743563	-2.448302	3.743693
C69	3.228150	-2.909952	1.704129
H70	3.088053	-3.811846	1.081124
H71	4.097354	-2.378058	1.283302
C72	1.788295	-2.442313	-1.375482
H73	1.403585	-1.841907	-2.221848
C74	0.844355	-3.636824	-1.226021
H75	1.197249	-4.284154	-0.401466
H76	-0.166205	-3.298891	-0.944806
C77	0.798403	-4.450138	-2.511845
H78	0.356190	-3.827595	-3.309864
H79	0.124950	-5.313036	-2.392367
C80	2.187755	-4.906447	-2.931042
H81	2.576194	-5.620502	-2.181649
H82	2.146146	-5.461914	-3.881107
C83	3.147303	-3.730973	-3.041363
H84	2.825073	-3.072662	-3.868356
H85	4.158470	-4.077440	-3.307377
C86	3.195147	-2.916564	-1.753407
H87	3.886714	-2.069415	-1.880021
H88	3.620429	-3.538899	-0.947898
C89	3.083096	-0.105427	-0.219082
H90	3.965383	-0.773892	-0.165773
C91	3.091815	0.573292	-1.591517
H92	2.245840	1.282389	-1.640627
H93	2.910445	-0.144102	-2.406608
C94	4.404988	1.311988	-1.809606
H95	5.232693	0.578537	-1.835066
H96	4.406549	1.799742	-2.797344
C97	4.657447	2.333262	-0.710786
H98	3.899754	3.130599	-0.794920
H99	5.634518	2.823827	-0.848513
C100	4.558520	1.709990	0.673691
H101	4.670084	2.479523	1.454491
H102	5.401489	1.009948	0.823103
C103	3.247582	0.958509	0.867497
H104	2.395633	1.661470	0.819268
H105	3.207119	0.519926	1.876176

Atom	**Styrene(6)** Total atom =16		
	X	Y	Z
C1	2.25940	0.26786	0.00000
H65	2.562919	4.566118	4.188190
H66	2.883787	4.517864	2.458166
C67	0.801313	4.774402	2.940059
H68	0.846602	5.874391	2.907752
H69	0.108268	4.522913	3.763713
C70	0.236094	4.237164	1.631546
H71	0.887060	4.565476	0.801340
H72	-0.757398	4.673759	1.432313
C73	-0.102880	2.756622	-1.401028
H74	-0.515851	2.061475	-2.154758
C75	1.416794	2.658752	-1.508175
H76	1.886419	3.312347	-0.750870
H77	1.750009	1.635619	-1.290489
C78	1.907499	3.078030	-2.883075
H79	1.531962	2.357001	-3.631484
H80	3.005764	3.006999	-2.915854
C81	1.430250	4.477628	-3.234009
H82	1.888890	5.204307	-2.537174
H83	1.766567	4.772627	-4.240667
C84	-0.084698	4.573576	-3.133561
H85	-0.537434	3.916207	-3.897750
H86	-0.431415	5.592366	-3.369196
C87	-0.604976	4.158064	-1.759937
H88	-1.705660	4.198378	-1.772538
H89	-0.278366	4.897096	-1.007846
C90	-2.439669	2.578875	0.314758
H91	-2.387194	3.638625	0.002908
C92	-3.323426	1.836886	-0.692274
H93	-3.404956	0.775067	-0.378720
H94	-2.859228	1.808584	-1.692001
C95	-4.711427	2.456500	-0.756417
H96	-4.627521	3.478369	-1.171106
H97	-5.344116	1.897093	-1.463779
C98	-5.360265	2.521036	0.618141
H99	-5.551915	1.491131	0.969779
H100	-6.343384	3.015647	0.561192
C101	-4.464567	3.218331	1.630321
H102	-4.932751	3.215348	2.626941
H103	-4.354113	4.282852	1.352472
C104	-3.087655	2.569552	1.698186
H105	-3.176193	1.532629	2.062344
H106	-2.462333	3.099145	2.433636
P107	3.726376	0.236534	3.783252
O108	3.685266	-0.205	3.750187
O109	2.529721	-0.383875	-0.995752
O110	5.064434	-0.889689	-0.789826

C2	1.35271	1.33070	0.00000
C3	-0.01560	1.08779	0.00000
C4	-0.51645	-0.22671	0.00000
C5	0.41021	-1.28290	0.00000
C6	1.78173	-1.04119	0.00000
H7	3.33439	0.46253	0.00000
H8	1.71930	2.36018	0.00000
H9	-0.70998	1.93149	0.00000
H10	0.03895	-2.31190	0.00000
H11	2.48161	-1.88029	0.00000
C12	-1.94800	-0.53346	0.00000
C13	-2.96716	0.33642	0.00000
H14	-2.18469	-1.60442	0.00000
H15	-4.00273	-0.00803	0.00000
H16	-2.81782	1.41939	0.00000
O111	4.150375	1.476976	-0.519640
C112	5.225619	-0.912234	-2.203285
C113	6.508153	-1.625894	-2.527531
H114	5.235165	0.121489	-2.596065
H115	4.355333	-1.412197	-2.666406
H116	6.672427	-1.662488	-3.612624
H117	7.368170	-1.119473	-2.068493
H118	6.492688	-2.658418	-2.151264
C119	5.187860	2.121020	0.206186
C120	5.138397	3.593016	-0.097868
H121	6.166386	1.689357	-0.078041
H122	5.060480	1.926713	1.286301
H123	5.928399	4.133629	0.440496
H124	5.269148	3.780006	-1.172915
H125	4.170088	4.022444	0.197537

Atom	**P1a** Total atom =125		
	X	Y	Z
Ru1	-0.796896	-0.493938	0.243209
Cl2	-1.152185	-0.416607	-2.143233
Cl3	-1.519509	-0.317961	2.541144
P4	-0.749597	1.966269	0.152154
N5	-2.552835	-2.996229	-0.149517
N6	-0.501623	-3.568549	0.314305
C7	-1.328722	-2.520085	0.153294
C8	-2.614408	-4.460242	-0.125767
H9	-3.068531	-4.843779	-1.052175
H10	-3.251020	-4.794632	0.712307
C11	-1.154323	-4.853114	0.039241
H12	-0.981571	-5.559997	0.864792
H13	-0.723088	-5.308250	-0.869073
C14	-3.721445	-2.225684	-0.432634
C15	-4.100390	-2.043300	-1.779867
C16	-5.245213	-1.290854	-2.043983
H17	-5.539840	-1.133942	-3.086798
C18	-6.030214	-0.745670	-1.021293
C19	-5.650942	-0.990263	0.299304
H20	-6.271027	-0.603297	1.115147
C21	-4.516591	-1.746703	0.623917
C22	-3.360128	-2.693601	-2.905744
H23	-2.324766	-2.941626	-2.645509
H24	-3.321066	-2.038956	-3.785344
H25	-3.870569	-3.620031	-3.218490
C26	-7.259750	0.044458	-1.345967
H27	-7.779634	0.387608	-0.442200

Atom	**GII** Total atom =117		
	X	Y	Z
Ru1	0.049711	-0.419465	0.093424
Cl2	-0.293875	-0.439259	-2.334889
Cl3	-0.205389	-0.456244	2.545228
P4	-1.092405	1.765518	0.143392
N5	-0.422011	-3.403358	0.244819
N6	1.698889	-2.991017	0.537706
C7	0.507009	-2.417551	0.231146
C8	0.108112	-4.684277	0.712093
H9	-0.227920	-5.508532	0.064716
H10	-0.258396	-4.897800	1.732106
C11	1.606075	-4.448825	0.667054
H12	2.130621	-4.799145	1.568387
H13	2.091096	-4.936882	-0.198473
C14	-1.801311	-3.277705	-0.099355
C15	-2.161471	-3.454615	-1.452813
C16	-3.513669	-3.384083	-1.789195
H17	-3.802083	-3.511759	-2.837375
C18	-4.508267	-3.192826	-0.821995
C19	-4.116302	-3.084775	0.513338
H20	-4.882006	-2.972696	1.288440
C21	-2.772676	-3.133038	0.906085
C22	-1.125069	-3.770213	-2.481606
H23	-0.427684	-2.931186	-2.617117
H24	-1.583898	-3.984194	-3.454603
H25	-0.525990	-4.648680	-2.193313
C26	-5.951058	-3.122404	-1.213980
H27	-6.228983	-3.942029	-1.892003

H28	-7.974620	-0.548953	-1.935317	H28	-6.178957	-2.187307	-1.749147
H29	-7.025123	0.933510	-1.950512	H29	-6.616514	-3.166280	-0.341928
C30	-4.260324	-2.105262	2.053701	C30	-2.417972	-3.120703	2.358271
H31	-4.336511	-1.229062	2.710396	H31	-3.090318	-2.465353	2.928328
H32	-3.267510	-2.536558	2.221130	H32	-1.395873	-2.769906	2.542571
H33	-5.014406	-2.831810	2.397592	H33	-2.524092	-4.129912	2.789794
C34	0.883323	-3.527533	0.660831	C34	2.995183	-2.407365	0.421457
C35	1.231718	-3.604274	2.018666	C35	3.704780	-2.076932	1.589811
C36	2.589545	-3.572242	2.347484	C36	4.996497	-1.562936	1.448409
H37	2.877378	-3.622426	3.402253	H37	5.552300	-1.284116	2.349730
C38	3.584418	-3.466254	1.370422	C38	5.591791	-1.384785	0.194294
C39	3.193767	-3.391375	0.028544	C39	4.857235	-1.732146	-0.942855
H40	3.956957	-3.284826	-0.748486	H40	5.297357	-1.579721	-1.933624
C41	1.849979	-3.415141	-0.354105	C41	3.560533	-2.245345	-0.856249
C42	0.173544	-3.659851	3.073232	C42	3.070684	-2.232546	2.933662
H43	0.606303	-3.820794	4.068165	H43	3.733777	-1.878603	3.732826
H44	-0.556944	-4.464210	2.894062	H44	2.824342	-3.282647	3.155870
H45	-0.400840	-2.718863	3.104547	H45	2.120211	-1.676922	2.996581
C46	5.027034	-3.372306	1.751170	C46	6.981372	-0.842709	0.075211
H47	5.218280	-3.791300	2.747750	H47	7.214475	-0.135565	0.883254
H48	5.352066	-2.320715	1.760995	H48	7.137189	-0.326648	-0.881681
H49	5.675564	-3.889848	1.030776	H49	7.733473	-1.645757	0.131935
C50	1.448532	-3.243216	-1.782624	C50	2.768236	-2.557801	-2.082411
H51	2.318299	-3.270133	-2.448749	H51	2.344590	-3.574057	-2.059908
H52	0.955160	-2.269574	-1.938702	H52	3.378683	-2.468627	-2.989700
H53	0.733341	-4.011170	-2.115504	H53	1.907423	-1.874599	-2.186574
C54	0.829051	-0.631126	0.416925	C54	1.747892	0.242009	0.346072
H55	2.694937	-0.482617	0.656623	H55	2.084400	0.179979	1.403566
C56	-0.041006	2.748153	1.679949	C56	2.762037	0.888073	-0.479337
H57	-0.543862	2.168450	2.477816	C57	3.852243	1.477633	0.197150
C58	1.458970	2.484951	1.820725	H58	3.886022	1.416253	1.289537
H59	2.001052	3.035298	1.030079	C59	4.865565	2.130389	-0.497022
H60	1.682826	1.419506	1.659990	H60	5.694241	2.588665	0.048906
C61	1.974386	2.934051	3.179914	C61	4.826256	2.187471	-1.890259
H62	1.510703	2.308592	3.963175	H62	5.623230	2.693589	-2.441097
H63	3.058699	2.751482	3.250491	C63	3.761418	1.598227	-2.578437
C64	1.653043	4.397641	3.440359	H64	3.727040	1.645492	-3.669995
H65	2.000896	4.702379	4.439794	C65	2.735818	0.965156	-1.887356
H66	2.211977	5.025794	2.721463	H66	1.890491	0.527479	-2.423472
C67	0.164139	4.668476	3.285044	C67	-0.825739	2.763134	1.687136
H68	-0.057103	5.735239	3.446604	H68	-1.244796	2.079047	2.447534
H69	-0.390398	4.121693	4.069012	C69	0.634474	2.957069	2.098098
C70	-0.347447	4.231230	1.917199	H70	1.159797	3.616283	1.386253
H71	0.134235	4.849420	1.141891	H71	1.151086	1.986876	2.078712
H72	-1.426104	4.437497	1.840840	C72	0.715050	3.557500	3.494952
C73	0.138793	2.583080	-1.356982	H73	0.302539	2.828742	4.215775

H74	-0.563666	2.295528	-2.161583
C75	1.446050	1.842250	-1.650009
H76	2.190197	2.063745	-0.864653
H77	1.290681	0.755247	-1.638439
C78	2.011621	2.247254	-3.002216
H79	1.318715	1.898667	-3.789646
H80	2.958232	1.713480	-3.169039
C81	2.195988	3.751891	-3.114393
H82	2.980018	4.074677	-2.404722
H83	2.565289	4.028882	-4.114543
C84	0.905203	4.493140	-2.799202
H85	0.149683	4.261287	-3.571642
H86	1.056212	5.583709	-2.841434
C87	0.356617	4.095292	-1.433776
H88	-0.570507	4.651281	-1.214989
H89	1.087615	4.397034	-0.660941
C90	-2.448387	2.701183	0.029344
H91	-2.282162	3.791211	-0.086695
C92	-3.243774	2.217318	-1.185133
H93	-3.433000	1.132358	-1.083213
H94	-2.668292	2.324809	-2.117063
C95	-4.567019	2.963816	-1.290664
H96	-4.366101	4.031375	-1.496897
H97	-5.135438	2.594734	-2.159634
C98	-5.391534	2.841270	-0.017796
H99	-5.701450	1.789048	0.105287
H100	-6.321251	3.427517	-0.096835
C101	-4.592307	3.251098	1.209483
H102	-5.183637	3.096203	2.125582
H103	-4.375018	4.334988	1.170293
C104	-3.283265	2.479358	1.294267
H105	-3.491709	1.399381	1.395909
H106	-2.731385	2.751552	2.206659
P107	4.347765	-0.107882	-0.693280
O108	3.655695	-0.227927	0.736679
O109	3.648474	-0.629241	-1.888555
O110	5.777298	-0.782734	-0.328780
O111	4.701027	1.465778	-0.871921
C112	6.755479	-0.877861	-1.371639
C113	6.582761	-2.131037	-2.187572
H114	7.731255	-0.856556	-0.863637
H115	6.708080	0.022658	-2.009711
H116	7.366549	-2.203998	-2.953548
H117	6.647033	-3.025203	-1.552404
H118	5.606658	-2.132679	-2.690642
C119	5.307621	2.196826	0.196540

H74	1.767357	3.706057	3.784270
C75	-0.056520	4.865198	3.590886
H76	-0.009012	5.273075	4.612916
H77	0.425795	5.620066	2.942718
C78	-1.502930	4.687186	3.154723
H79	-2.043707	5.646184	3.191342
H80	-2.019844	4.020012	3.868442
C81	-1.597768	4.081861	1.759145
H82	-1.182584	4.796749	1.025473
H83	-2.655437	3.942217	1.480983
C84	-0.803835	2.849845	-1.348410
H85	-0.656997	2.097424	-2.146484
C86	0.498699	3.645961	-1.234400
H87	0.381392	4.433172	-0.467405
H88	1.323239	3.004464	-0.889955
C89	0.853828	4.306199	-2.558385
H90	1.038746	3.521258	-3.313902
H91	1.799231	4.863768	-2.463575
C92	-0.269413	5.215979	-3.030680
H93	-0.374112	6.058853	-2.322917
H94	-0.024661	5.669648	-4.003988
C95	-1.587732	4.461884	-3.110521
H96	-1.518833	3.695460	-3.903249
H97	-2.404661	5.135848	-3.413520
C98	-1.941596	3.772144	-1.796700
H99	-2.880497	3.214000	-1.929325
H100	-2.143990	4.533740	-1.021621
C101	-2.935027	1.521929	0.140123
H102	-3.360413	2.532903	-0.007563
C103	-3.389780	0.649529	-1.031694
H104	-3.033430	-0.386409	-0.868273
H105	-2.920515	0.960352	-1.978401
C106	-4.907429	0.667041	-1.143739
H107	-5.235601	1.692500	-1.398159
H108	-5.233259	0.033080	-1.984254
C109	-5.572430	0.224086	0.151586
H110	-5.365976	-0.847824	0.303528
H111	-6.668316	0.315508	0.078464
C112	-5.050891	0.992102	1.357374
H113	-5.485316	0.588655	2.286006
H114	-5.390392	2.043232	1.301027
C115	-3.528452	0.976283	1.438708
H116	-3.156628	-0.050837	1.608402
H117	-3.201009	1.559381	2.312930

C120	5.025170	3.659436	0.002603
H121	6.393595	1.994668	0.199991
H122	4.912321	1.840086	1.162866
H123	5.496693	4.253180	0.797133
H124	5.410228	4.013368	-0.963240
H125	3.944005	3.859193	0.024137