

General information

Solvents were dried by reflux under N₂ over sodium or CaH₂ and freshly distilled prior to use. Air-sensitive compounds were handled under a N₂ atmosphere using standard Schlenk and glovebox techniques. NMR spectra were recorded on Bruker SPECT NMR (400 MHz for ¹H, 376 MHz for ¹⁹F, 100 MHz for ¹³C) and Bruker DMX500 NMR (500 MHz for ¹H, 160 MHz for ¹¹B, 471 MHz for ¹⁹F) spectrometers. Most assignments were based on a series of 2D NMR experiments. HRMS analyses were performed at Bruker micrOTOF II. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Center: CCDC 1543215 (**3**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre at www.ccdc.cam.ac.uk/data_request/cif.

Detection of intermediate **4** by ³¹P NMR and ¹⁹F NMR.

A solution of 1,2,2,6,6-pentamethylpiperidine (8 mg, 0.05 mmol) in CD₂Cl₂ was added to the mixed solution of **1** (33 mg, 0.05 mmol) and diethyl phosphite (69 mg, 0.5 mmol) in CD₂Cl₂ in a J-Young valve capped NMR tube. Then the reaction was followed by ³¹P and ¹⁹F NMR analysis.

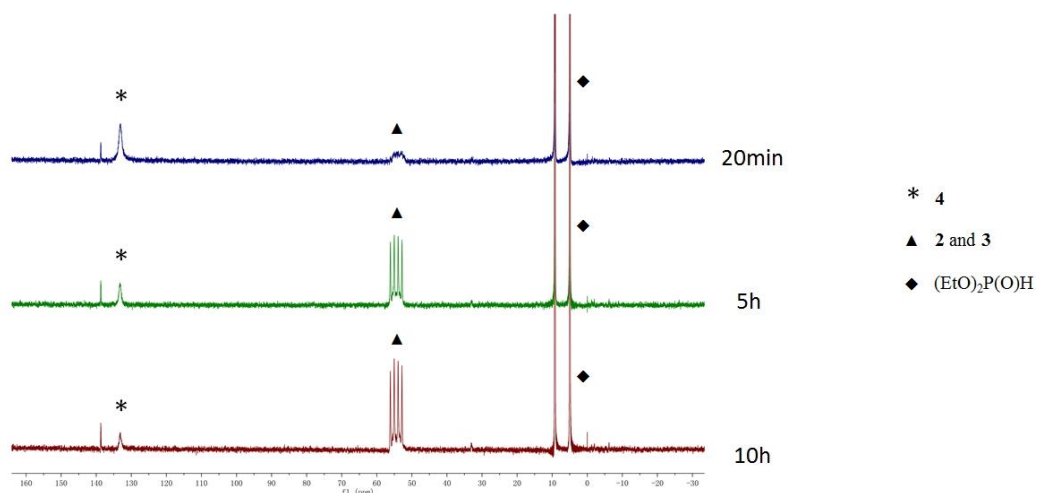


Figure S1: Intermediate **4** monitored by ³¹P NMR.

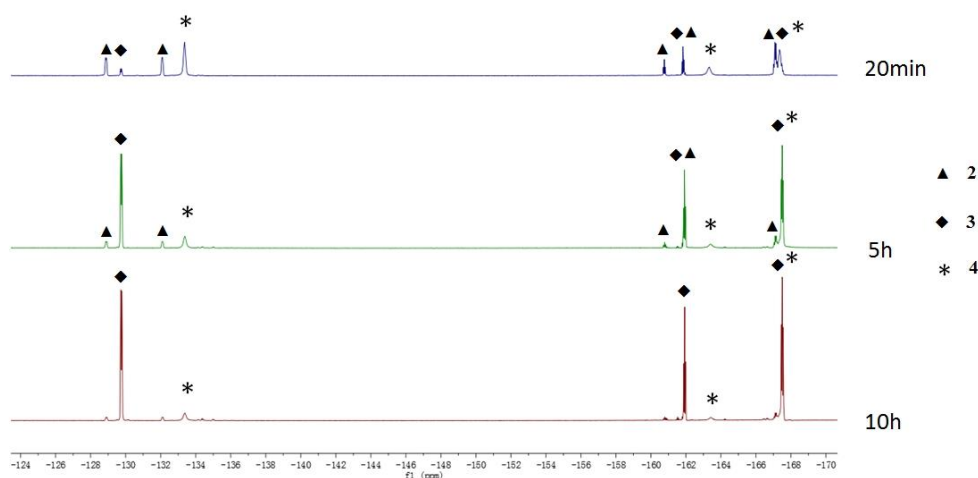
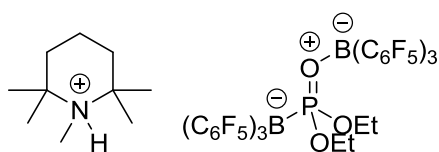


Figure S2: Intermediate **4** monitored by ^{19}F NMR.

Table S1: Hydrophosphonylation of 1-phenylprop-2-yn-1-one catalysed by $\text{B}(\text{C}_6\text{F}_5)_3$ and different bases^a.

Entry	Base	Yield (%) ^b
1	Pyridine	0
2	Et_3N	0
3	2,2,6,6-Tetramethylpiperidine	26(>20:1)
4	2,6-Lutidine	31(3:1)
5	1,2,2,6,6-Pentamethylpiperidine	67 ^c (11:1)
6	$n\text{-BuLi}^d$	0
7	MeMgBr^d	0
8	Me_3Al^d	0

^a1-Phenylprop-2-one (0.3 mmol, 1 equiv.), diethyl phosphite (0.3 mmol, 1 equiv.), $\text{B}(\text{C}_6\text{F}_5)_3$ (0.03 mmol, 0.1 equiv.) and base (0.09 mmol, 0.3 equiv.) were mixed in CD_2Cl_2 (0.5 mL) in a J-Young valve capped NMR tube. ^bYields were determined by ^{31}P NMR analysis, and the rate of diethyl (Z)-(3-oxo-3-phenylprop-1-en-1-yl)phosphonate to diethyl (E)-(3-oxo-3-phenylprop-1-en-1-yl)phosphonate is given in parentheses. ^cIsolated yield. ^dWithout addition of $\text{B}(\text{C}_6\text{F}_5)_3$, and the base was added in 10 mol%.



Synthesis of **2**:

A solution of 1,2,2,6,6-pentamethylpiperidine (36 mg, 0.23 mmol) in CH₂Cl₂ (1 mL) was added to the mixture of diethyl phosphite (28 mg, 0.20 mmol) and B(C₆F₅)₃ (205 mg, 0.40 mmol) in CH₂Cl₂ (2 mL). The resulting mixture was stirred for 5 minutes at room temperature. Afterwards, hexane (3 mL) was added to the reaction mixture and a white precipitate appeared. The solid was filtered and dried under vacuum, producing **2** (175 mg, 65%) as a white solid.

¹H NMR (400 MHz, C₆D₆): δ 3.69 (m, 2H, CH₂CH₃), 3.52 (m, 2H, CH₂CH₃), 2.88 (s, 3H, NHCH₃), 2.02-1.70 (m, 6H, CH₂CH₂CH₂), 1.49 (s, 6H, C(CH₃)₂), 1.44 (s, 6H, C(CH₃)₂), 0.90 (t, ³J_{HH} = 7.0 Hz, 6H, CH₂CH₃).

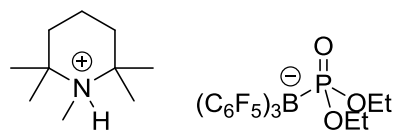
¹³C NMR (100 MHz, C₆D₆): δ 149.97 (d, ¹J_{CF} = 238.1 Hz, CF), 147.50 (d, ¹J_{CF} = 250.2 Hz, CF), 137.10 (d, ¹J_{CF} = 265.6 Hz, CF), 63.56 (d, ²J_{CP} = 11.5 Hz, CH₂CH₃), 39.28 (CH₂CH₂CH₂), 31.31 (C(CH₃)₂), 30.95 (NCH₃), 20.05 (C(CH₃)), 15.91 (CH₂CH₂CH₂), 15.46 (d, ³J_{CP} = 7.9 Hz, CH₂CH₃).

³¹P NMR (162 MHz, CD₂Cl₂): δ 53.75 (q, ¹J_{PB} = 175.3 Hz).

¹¹B NMR (160 MHz, CD₂Cl₂): δ -2.62 (s, OB), -15.06 (d, ¹J_{BP} = 175.5 Hz, PB).

¹⁹F NMR (376 MHz, CD₂Cl₂): δ -128.80 (d, ³J_{FF} = 19.7 Hz, 6F, *o*-C₆F₅), -132.03 (d, ³J_{FF} = 14.9 Hz, 6F, *o*-C₆F₅), -160.59 (td, ³J_{FF} = 20.4 Hz, ⁴J_{FF} = 3.6 Hz, 3F, *p*-C₆F₅), -161.65 (t, ³J_{FF} = 20.3 Hz, 3F, *p*-C₆F₅), -166.77--167.15 (m, 12F, *m*-C₆F₅).

HRMS (ESI) m/z Calcd for [C₄₀H₁₀B₂F₃₀O₃P, M]⁺: 1161.0082; Found: 1161.0094.



Synthesis of **3**:

A solution of 1,2,2,6,6-pentamethylpiperidine (155 mg, 1.0 mmol) in CH₂Cl₂ (2 mL) was added to the mixture of diethyl phosphite (138mg, 1.0 mmol) and B(C₆F₅)₃ (512 mg, 1.0 mmol) in CH₂Cl₂ (4 mL). The resulting mixture was stirred for 3 days at room temperature. Afterwards, hexane (30 mL) was added to the reaction mixture and a white precipitate appeared. The solid was filtered and dried under vacuum, producing **3** (602 mg, 75%) as a white solid.

¹H NMR (400 MHz, CD₂Cl₂): δ 10.09 (bs, 1H, NH), 3.82 (m, 4H, CH₂CH₃), 2.44 (d, ³J_{HH} = 5.0 Hz, 3H, NHCH₃), 1.86-1.53 (m, 6H, CH₂CH₂CH₂), 1.28 (s, 6H, C(CH₃)₂), 1.26 (s, 6H, C(CH₃)₂), 1.04 (t, ³J_{HH} = 7.0 Hz, 6H, CH₂CH₃).

¹³C NMR (100 MHz, CD₂Cl₂): δ 63.69 (C(CH₃)₂), 59.86(d, ²J_{CP} = 9.7 Hz, CH₂CH₃), 37.68(CH₂CH₂CH₂), 28.86 (NCH₃), 28.81 (C(CH₃)), 20.76 (CH₂CH₂CH₂), 16.42 (d, ³J_{CP} = 6.1 Hz, CH₂CH₃).

³¹P NMR (162 MHz, CD₂Cl₂): δ 54.67 (q, ¹J_{PB} = 179.5 Hz).

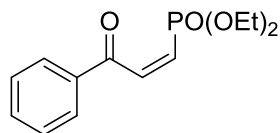
¹¹B NMR (160 MHz, CD₂Cl₂): δ -16.59 (d, ¹J_{BP} = 178.7 Hz).

¹⁹F NMR (376 MHz, CD₂Cl₂): δ -129.73 (d, ³J_{FF} = 20.4 Hz, 6F, *o*-C₆F₅), -161.75 (td, ³J_{FF} = 20.4 Hz, ⁴J_{FF} = 3.7 Hz, 3F, *p*-C₆F₅), -167.39 (td, ³J_{FF} = 22.1 Hz, ⁴J_{FF} = 6.2 Hz, 6F, *m*-C₆F₅).

HRMS (ESI) m/z Calcd for [C₂₀H₁₀BF₁₅O₃P, M]⁺: 649.0220; Found: 649.0234.

Representative procedure for (*Z*)-vinylphosphonates synthesis

The solution of $B(C_6F_5)_3$ (51 mg, 0.10 mmol) in CH_2Cl_2 (0.5 mL) was added to mixed solution of ynone (1.0 mmol), diethyl phosphite (138mg, 1.0 mmol) and 1,2,2,6,6-pentamethylpiperidine (47 mg, 0.30 mmol) in CH_2Cl_2 (1.5 mL). The resulting mixture was stirred at room temperature for 24 h. The product was purified by column chromatography on silica gel (20-50% ethyl acetate and 1% Et_3N in petroleum ether) to provide (Z)-vinylphosphonate as yellow oil.



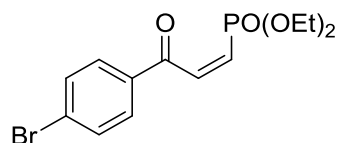
Characterization of diethyl (Z)-(3-oxo-3-phenylprop-1-en-1-yl)phosphonate (**6a**):

1H NMR (400 MHz, C_6D_6): δ 7.86 (d, $^3J_{HH} = 7.2$ Hz, 2H, *H*-*o*-Ph), 7.08 (t, $^3J_{HH} = 7.2$ Hz, 1H, *H*-*p*-Ph), 7.02 (t, $^3J_{HH} = 7.2$ Hz, 2H, *H*-*m*-Ph), 6.48 (dd, $^3J_{HP} = 47.7$ Hz, $^3J_{HH} = 14.3$ Hz, 1H, *CHC*(O)), 5.84 (dd, $^2J_{HP} = 16.7$ Hz, $^3J_{HH} = 14.4$ Hz, 1H, *CHP*(O)), 3.92 (m, 4H, CH_2), 0.96 (t, $^3J_{HH} = 7.0$ Hz, 6H, CH_3).

^{13}C NMR (100 MHz, C_6D_6): δ 145.11 (*CHC*(O)), 133.29 (*C*-*p*-Ph), 129.37 (*C*-*o*-Ph), 128.62 (*C*-*m*-Ph), 125.36 ($^1J_{CP} = 183.9$ Hz, *CHP*(O)), 61.91(d, $^2J_{CP} = 5.4$ Hz, CH_2), 16.28 (d, $^3J_{CP} = 6.0$ Hz, CH_3).

^{31}P NMR (161.83 MHz, C_6D_6): δ 13.12 (dm, $^3J_{PH} = 47.7$ Hz).

HRMS (ESI) m/z Calcd for $[C_{13}H_{17}O_4P, M+H]^+$: 269.0937; Found: 269.0947.



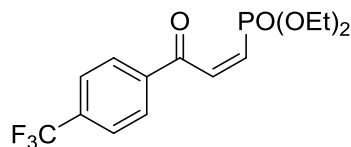
Characterization of diethyl (Z)-(3-(4-bromophenyl)-3-oxoprop-1-en-1-yl)phosphonate (**6b**):

1H NMR (400 MHz, C_6D_6): δ 7.53 (d, $^3J_{HH} = 8.3$ Hz, 2H, *H*-2,6- C_6H_4), 7.18 (d, $^3J_{HH} = 8.4$ Hz, 2H, *H*-3,5- C_6H_4), 6.45 (dd, $^3J_{HP} = 47.6$ Hz, $^3J_{HH} = 14.3$ Hz, 1H, *CHC*(O)), 5.85 (dd, $^2J_{HP} = 16.5$ Hz, $^3J_{HH} = 14.4$ Hz, 1H, *CHP*(O)), 3.89 (m, 4H, CH_2), 0.96 (t, $^3J_{HH} = 7.1$ Hz, 6H, CH_3).

^{13}C NMR (100 MHz, C_6D_6): δ 192.19 (*C*(O)), 144.75 (*CHC*(O)), 135.31 (*C*-1- C_6H_4), 131.99 (*C*-3,5- C_6H_4), 130.83 (*C*-2,6- C_6H_4), 128.66 (*C*-4- C_6H_4), 125.70 (d, $^1J_{CP} = 183.3$ Hz, *CHP*(O)), 61.96 (d, $^2J_{CP} = 5.2$ Hz, CH_2), 16.30 (d, $^3J_{CP} = 6.0$ Hz, CH_3).

^{31}P NMR (162 MHz, C_6D_6): δ 12.94 (dm, $^3J_{PH} = 47.3$ Hz).

HRMS (ESI) m/z Calcd for $[C_{13}H_{16}BrO_4P, M+H]^+$: 347.0042, 349.0022; Found: 347.0045, 349.0026.



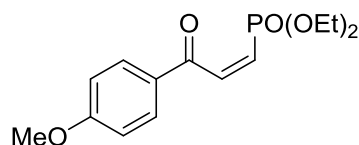
Characterization of diethyl (Z)-(3-oxo-3-(4-(trifluoromethyl)phenyl)prop-1-en-1-yl)phosphonate (**6c**):

¹H NMR (400 MHz, C₆D₆): δ 7.70 (d, ³J_{HH} = 8.1 Hz, 2H, *H*-3,5-C₆H₄), 7.26 (d, ³J_{HH} = 8.2 Hz, 2H, *H*-2,6-C₆H₄), 6.43 (dd, ³J_{HP} = 47.4 Hz, ³J_{HH} = 14.3 Hz, 1H, *CHC*(O)), 5.85 (dd, ²J_{HP} = 16.3 Hz, ³J_{HH} = 14.3 Hz, 1H, *CHP*(O)), 3.88 (m, 4H, CH₂), 0.96 (t, ³J_{HH} = 7.1 Hz, 6H, CH₃).

¹³C NMR (100 MHz, C₆D₆): δ 192.36 (C(O)), 144.68 (*CHC*(O)), 139.09 (C-1-C₆H₄), 134.66 (q, ²J_{CF} = 32.7 Hz, C-4-C₆H₄), 129.60 (C-2,6-C₆H₄), 126.12 (d, ¹J_{CP} = 182.9 Hz, *CHP*(O)), 125.65 (q, ³J_{CF} = 3.4 Hz, C-3,5-C₆H₄), 62.00 (d, ²J_{CP} = 5.3 Hz, CH₂), 16.26 (d, ³J_{CP} = 6.0 Hz, CH₃).

³¹P NMR (162 MHz, C₆D₆): δ 12.84 (dm, ³J_{PH} = 47.6 Hz).

HRMS (ESI) *m/z* Calcd for [C₁₄H₁₆F₃O₄P, M+H]⁺: 337.0811; Found: 337.0811.



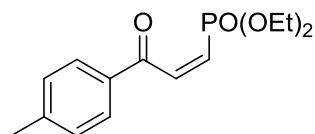
Characterization of diethyl (Z)-(3-(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)phosphonate (**6d**):

¹H NMR (400 MHz, C₆D₆): δ 7.90 (d, ³J_{HH} = 8.5 Hz, 2H, *H*-2,6-C₆H₄), 6.71-6.55 (m, 3H, *CHC*(O), *H*-3,5-C₆H₄), 5.87 (dd, ²J_{HP} = 16.6 Hz, ³J_{HH} = 14.6 Hz, 1H, *CHP*(O)), 3.96 (m, 4H, CH₂), 3.18 (s, 3H, OCH₃), 1.00 (t, ³J_{HH} = 7.2 Hz, 6H, CH₂CH₃).

¹³C NMR (100 MHz, C₆D₆): δ 191.56 (d, ³J_{CP} = 8.4 Hz, C(O)), 164.10 (C-1-C₆H₄), 145.41 (*CHC*(O)), 131.73 (C-2,6-C₆H₄), 129.90 (C-4-C₆H₄), 124.82 (d, ¹J_{CP} = 184.0 Hz, *CHP*(O)), 114.06 (C-3,5-C₆H₄), 61.88 (d, ²J_{CP} = 5.3 Hz, CH₂), 54.97 (OCH₃), 16.34 (d, ³J_{CP} = 6.0 Hz, CH₂CH₃).

³¹P NMR (162 MHz, C₆D₆): δ 13.32 (dm, ³J_{PH} = 48.1 Hz).

HRMS (ESI) *m/z* Calcd for [C₁₄H₁₉O₅P, M+H]⁺: 299.1043; Found: 299.1061.



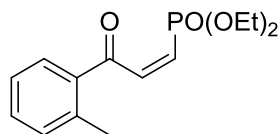
Characterization of diethyl (Z)-(3-oxo-3-(p-tolyl)prop-1-en-1-yl)phosphonate (**6e**):

¹H NMR (400 MHz, C₆D₆): δ 7.84 (d, ³J_{HH} = 8.0 Hz, 2H, *H*-2,6-C₆H₄), 6.87 (d, ³J_{HH} = 8.0 Hz, 2H, *H*-3,5-C₆H₄), 6.54 (dd, ³J_{HP} = 47.9 Hz, ³J_{HH} = 14.3 Hz, 1H, *CHC*(O)), 5.86 (dd, ²J_{HP} = 16.8 Hz, ³J_{HH} = 14.3 Hz, 1H, *CHP*(O)), 3.95 (m, 4H, CH₂), 1.95 (s, 3H, 4-CH₃-C₆H₄), 0.99 (t, ³J_{HH} = 7.2 Hz, 6H, CH₂CH₃).

¹³C NMR (100 MHz, C₆D₆): δ 145.31 (*CHC*(O)), 144.10 (C-1-C₆H₄), 134.36 (C-4-C₆H₄), 129.57 (C-2,6-C₆H₄), 129.42 (C-3,5-C₆H₄), 125.10 (d, ¹J_{CP} = 184.0 Hz, *CHP*(O)), 61.90 (d, ²J_{CP} = 5.4 Hz, CH₂), 21.45 (4-CH₃-C₆H₄), 16.32 (d, ³J_{CP} = 6.0 Hz, CH₂CH₃).

³¹P NMR (161.83 MHz, C₆D₆): δ 13.25 (dm, ³J_{PH} = 48.0 Hz).

HRMS (ESI) *m/z* Calcd for [C₁₄H₁₉O₄P, M+H]⁺: 283.1094; Found: 283.1109.



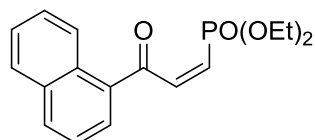
Characterization of diethyl (Z)-(3-oxo-3-(o-tolyl)prop-1-en-1-yl)phosphonate (**6f**):

¹H NMR (400 MHz, C₆D₆): δ 7.50 (d, ³J_{HH} = 7.3 Hz, 2H, *H*-6-C₆H₄), 7.04 (m, 1H, *H*-5-C₆H₄), 6.96-6.90 (m, 2H, *H*-3,4-C₆H₄), 6.62 (dd, ³J_{HP} = 48.0 Hz, ³J_{HH} = 14.2 Hz, 1H, *CHC*(O)), 5.79 (dd, ²J_{HP} = 16.5 Hz, ³J_{HH} = 14.2 Hz, 1H, *CHP*(O)), 3.90 (m, 4H, CH₂), 2.72 (s, 3H, 2-CH₃-C₆H₄), 0.97 (t, ³J_{HH} = 7.1 Hz, 6H, CH₂CH₃).

¹³C NMR (100 MHz, C₆D₆): δ 195.21 (C(O)), 147.48 (*CHC*(O)), 140.44 (C-1-C₆H₄), 136.12 (C-2-C₆H₄), 132.32 (C-3-C₆H₄), 132.14 (C-5-C₆H₄), 131.77 (C-6-C₆H₄), 125.48 (C-4-C₆H₄), 124.23 (d, ¹J_{CP} = 183.3 Hz, *CHP*(O)), 61.78 (d, ²J_{CP} = 5.2 Hz, CH₂), 21.89 (2-CH₃-C₆H₄), 16.34 (d, ³J_{CP} = 6.0 Hz, CH₂CH₃).

³¹P NMR (162 MHz, C₆D₆): δ 13.53 (dm, ³J_{PH} = 48.0 Hz).

HRMS (ESI) *m/z* Calcd for [C₁₄H₁₉O₄P, M+H]⁺: 283.1094; Found: 283.1115.



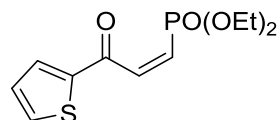
Characterization of diethyl (Z)-(3-(naphthalen-1-yl)-3-oxoprop-1-en-1-yl)phosphonate (**6g**):

¹H NMR (400 MHz, C₆D₆): δ 9.53 (d, ³J_{HH} = 8.7 Hz, 1H, *H*-8-Naph), 7.70 (d, ³J_{HH} = 7.2 Hz, 1H, *H*-2-Naph), 7.58 (d, ³J_{HH} = 8.2 Hz, 1H, *H*-4-Naph), 7.52 (d, ³J_{HH} = 8.1 Hz, 1H, *H*-5-Naph), 7.40 (dd, ³J_{HH} = 8.4, 6.9 Hz, 1H, *H*-7-Naph), 7.21 (m, 1H, *H*-6-Naph), 7.05 (m, 1H, *H*-3-Naph), 6.65 (dd, ³J_{HP} = 47.8 Hz, ³J_{HH} = 14.2 Hz, 1H, *CHC*(O)), 5.87 (dd, ²J_{HP} = 16.5 Hz, ³J_{HH} = 14.2 Hz, 1H, *CHP*(O)), 3.91 (m, 4H, CH₂), 0.94 (t, ³J_{HH} = 7.1 Hz, 6H, CH₃).

¹³C NMR (100 MHz, C₆D₆): δ 146.71 (*CHC*(O)), 134.39 (C-4-Naph), 134.06 (C-1-Naph), 132.27 (C-2-Naph), 131.34 (C-9-Naph), 128.74 (C-7-Naph), 128.53 (C-5-Naph), 127.20 (C-8-Naph), 126.82 (C-6-Naph), 124.89 (d, ¹J_{CP} = 184.1 Hz, *CHP*(O)), 124.27 (C-3-Naph), 61.88 (d, ²J_{CP} = 5.3 Hz, CH₂), 16.32 (d, ³J_{CP} = 5.9 Hz, CH₃).

³¹P NMR (162 MHz, C₆D₆): δ 13.40 (dm, *J* = 47.9 Hz).

HRMS (ESI) *m/z* Calcd for [C₁₇H₁₉O₄P, M+H]⁺: 319.1094; Found: 319.1092.



Characterization of diethyl (Z)-(3-oxo-3-(thiophen-2-yl)prop-1-en-1-yl)phosphonate (**6h**):

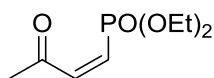
¹H NMR (400 MHz, C₆D₆): δ 7.26 (d, ³J_{HH} = 3.8 Hz, 1H, *H*-3-C₄H₃S), 6.87 (d, ³J_{HH} = 4.9 Hz, 1H, *H*-5-C₄H₃S), 6.52 (dd, ³J_{HH} = 4.9, 3.8 Hz, 1H, *H*-4-C₄H₃S), 6.47 (dd, ³J_{HP}

= 47.1 Hz, $^3J_{\text{HH}} = 14.1$ Hz, 1H, $\text{CHC}(\text{O})$), 5.85 (dd, $^2J_{\text{HP}} = 16.0$ Hz, $^3J_{\text{HH}} = 14.1$ Hz, 1H, $\text{CHP}(\text{O})$), 3.97 (m, 4H, CH_2), 1.00 (t, $^3J_{\text{HH}} = 7.1$ Hz, 6H, CH_3).

^{13}C NMR (100 MHz, C_6D_6): δ 144.14 ($\text{C-2-C}_4\text{H}_3\text{S}$), 142.79 ($\text{CHC}(\text{O})$), 134.47 ($\text{C-5-C}_4\text{H}_3\text{S}$), 134.00 ($\text{C-3-C}_4\text{H}_3\text{S}$), 126.69 (d, $^1J_{\text{CP}} = 184.5$ Hz, $\text{CHP}(\text{O})$), 62.09 (d, $^2J_{\text{CP}} = 5.7$ Hz, CH_2), 16.33 (d, $^3J_{\text{CP}} = 6.2$ Hz, CH_3).

^{31}P NMR (162 MHz, C_6D_6): δ 12.65 (dm, $J = 45.1$ Hz).

HRMS (ESI) m/z Calcd for $[\text{C}_{11}\text{H}_{15}\text{O}_4\text{PS}, \text{M}+\text{H}]^+$: 275.0501; Found: 275.0516.



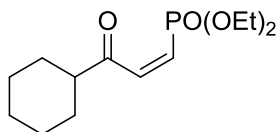
Characterization of diethyl (Z)-(3-oxobut-1-en-1-yl)phosphonate (**6i**):

^1H NMR (400 MHz, C_6D_6): δ 6.11 (dd, $^3J_{\text{HP}} = 48.3$ Hz, $^3J_{\text{HH}} = 14.3$ Hz, 1H, $\text{CHC}(\text{O})$), 5.58 (dd, $^2J_{\text{HP}} = 15.9$ Hz, $^3J_{\text{HH}} = 14.4$ Hz, 1H, $\text{CHP}(\text{O})$), 3.96 (m, 4H, CH_2), 2.09 (s, 3H, $\text{C}(\text{O})\text{CH}_3$), 1.03 (t, $^3J_{\text{HH}} = 7.1$ Hz, 6H, CH_2CH_3).

^{13}C NMR (100 MHz, C_6D_6): δ 200.16 ($\text{C}(\text{O})$), 147.30 ($\text{CHC}(\text{O})$), 123.16 (d, $^1J_{\text{CP}} = 182.9$ Hz, $\text{CHP}(\text{O})$), 61.89 (d, $^2J_{\text{CP}} = 5.2$ Hz, CH_2), 30.00 ($\text{C}(\text{O})\text{CH}_3$), 16.36 (d, $^2J_{\text{CP}} = 6.1$ Hz, CH_2CH_3).

^{31}P NMR (162 MHz, C_6D_6): δ 13.37 (dm, $^3J_{\text{PH}} = 48.5$ Hz).

HRMS (ESI) m/z Calcd for $[\text{C}_8\text{H}_{15}\text{O}_4\text{P}, \text{M}+\text{H}]^+$: 207.0781; Found: 207.0788.



Characterization of diethyl (Z)-(3-cyclohexyl-3-oxoprop-1-en-1-yl)phosphonate (**6j**):

^1H NMR (400 MHz, C_6D_6): δ 6.26 (dd, $^3J_{\text{HP}} = 48.1$ Hz, $^3J_{\text{HH}} = 14.2$ Hz, 1H, $\text{CHC}(\text{O})$), 5.69 (dd, $^2J_{\text{HP}} = 16.1$ Hz, $^3J_{\text{HH}} = 14.2$ Hz, 1H, $\text{CHP}(\text{O})$), 4.05 (m, 4H, CH_2CH_3), 2.49 (tt, $^3J_{\text{HH}} = 11.2$, 3.5 Hz, 1H, $H\text{-1-Cy}$), 1.94-1.81 (m, 2H, $H\text{-2,6-Cy}$), 1.64-1.55 (m, 2H, $H\text{-3,5-Cy}$), 1.47-1.32 (m, 3H, $H\text{-2,3,4-Cy}$), 1.17-0.97 (m, 9H, CH_2CH_3 , $H\text{-4,5,6-Cy}$).

^{13}C NMR (100 MHz, C_6D_6): δ 204.76 ($\text{C}(\text{O})$), 146.74 ($\text{CHC}(\text{O})$), 124.49 (d, $^1J_{\text{CP}} = 184.1$ Hz, $\text{CHP}(\text{O})$), 61.88 (d, $^2J_{\text{CP}} = 5.4$ Hz, CH_2), 50.26 (C-1-Cy), 28.17 (C-2,6-Cy), 26.20 (C-3,5-Cy), 25.80 (C-4-Cy), 16.45 (d, $^3J_{\text{CP}} = 6.2$ Hz, CH_3).

^{31}P NMR (162 MHz, C_6D_6): δ 13.63 (dm, $^3J_{\text{PH}} = 49.1$ Hz).

HRMS (ESI) m/z Calcd for $[\text{C}_{13}\text{H}_{23}\text{O}_4\text{P}, \text{M}+\text{H}]^+$: 275.1407; Found: 275.1408.

Attempt of hydrophosphonylation of phenylacetylene via the procedure reported by A. I. Kuraashin et al.

Under Ar atmosphere, $\text{Mo}(\text{CO})_6$ (528 mg, 2.0 mmol) was added into the mixture of phenylacetylene (2.0 g, 20 mmol) and diethyl phosphite (2.8 g, 20 mmol). The mixture was heated to reflux and stirred for 10 h. The resulting black reaction mixture was analyzed by ^{31}P NMR (Figure S53), but no signal for *O,O*-diethyl-(*Z*)-2-phenylvinylphosphonate was observed ($\delta = 2.56$ ppm, singlet, as reported by A. I. Kuraashin et al.).

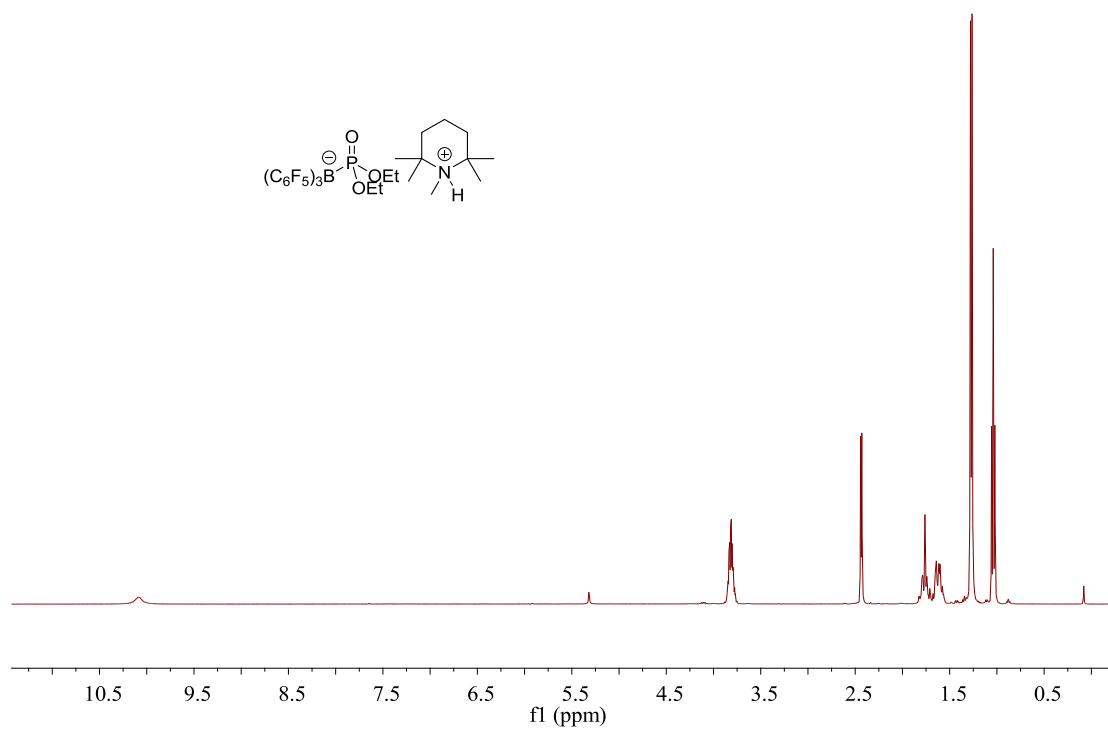


Figure S3: ¹H NMR spectrum for **3** in CD₂Cl₂

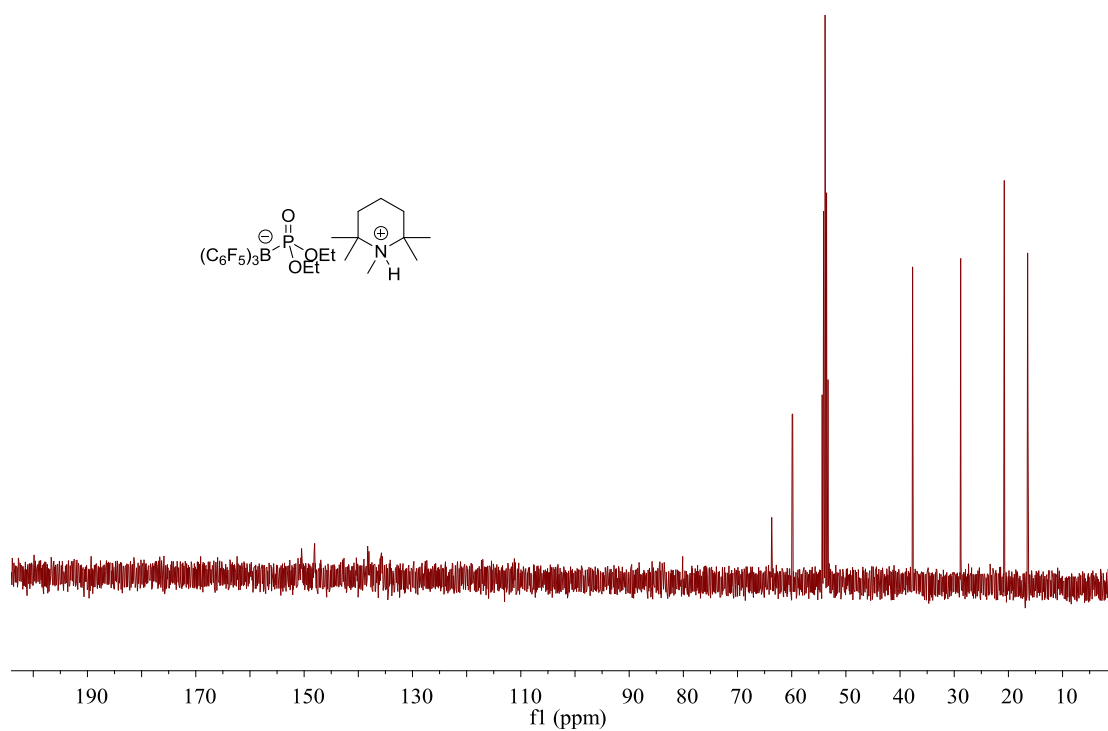


Figure S4: ^{13}C NMR spectrum for **3** in CD_2Cl_2

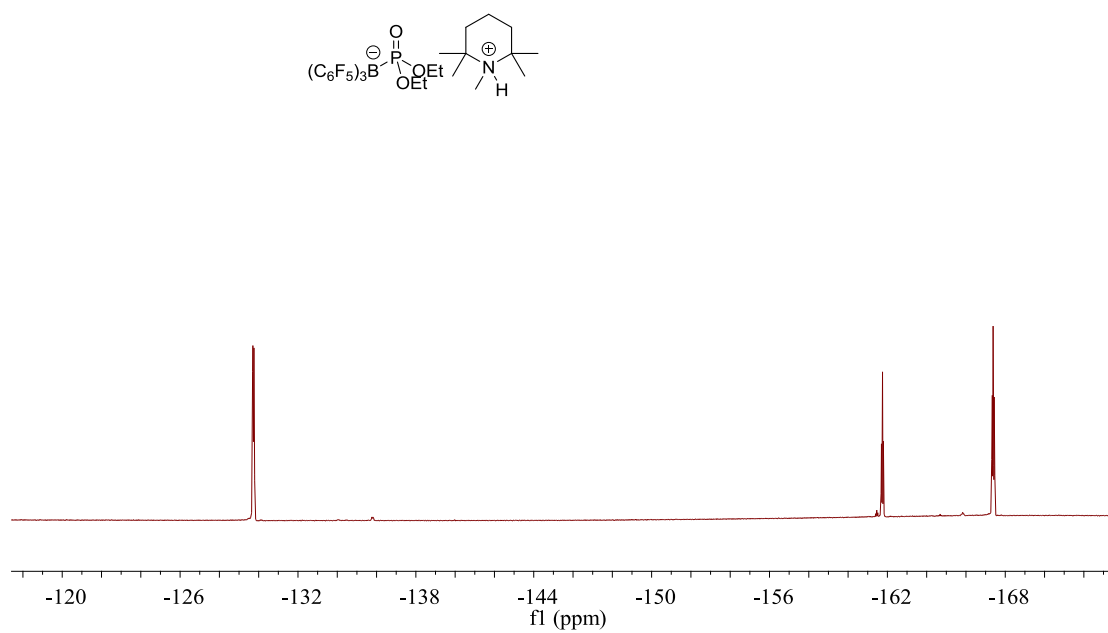


Figure S5: ^{19}F NMR spectrum for **3** in CD_2Cl_2

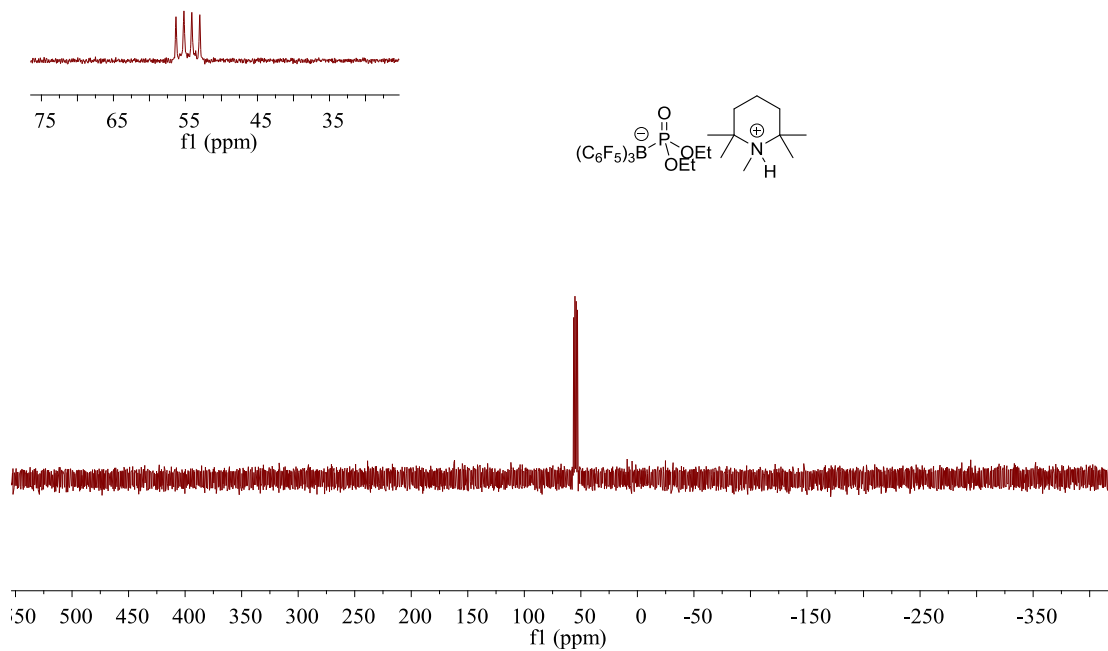


Figure S6: ^{31}P NMR spectrum for **3** in CD_2Cl_2

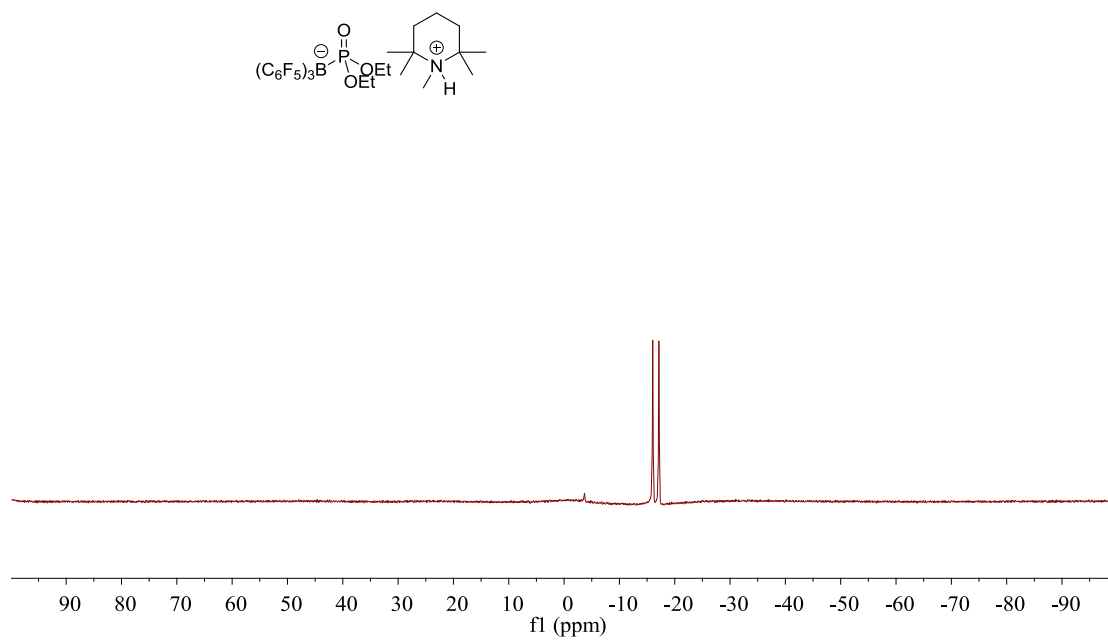
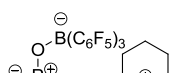


Figure S7: ^{11}B NMR spectrum for **3** in CD_2Cl_2



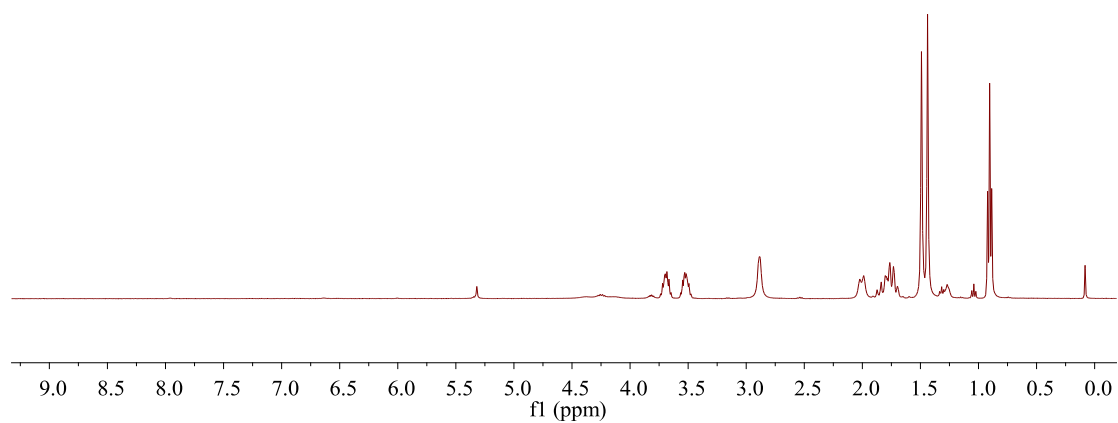


Figure S8: ^1H NMR spectrum for **2** in CD_2Cl_2

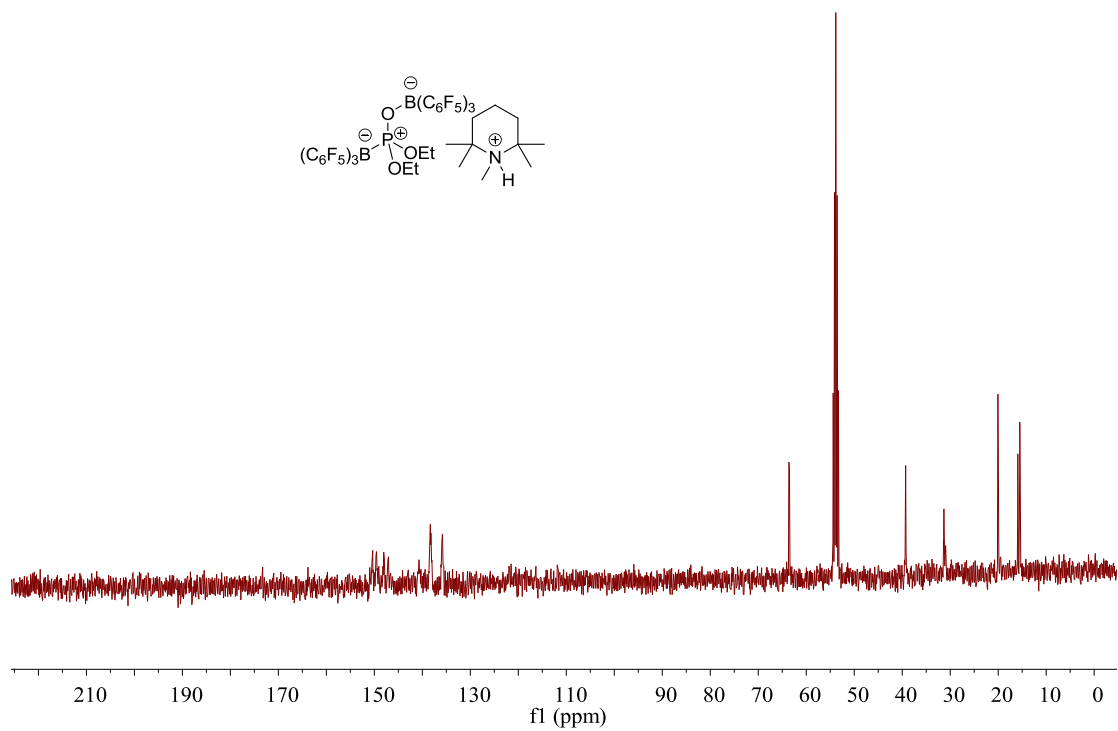


Figure S9: ^{13}C NMR spectrum for **2** in CD_2Cl_2

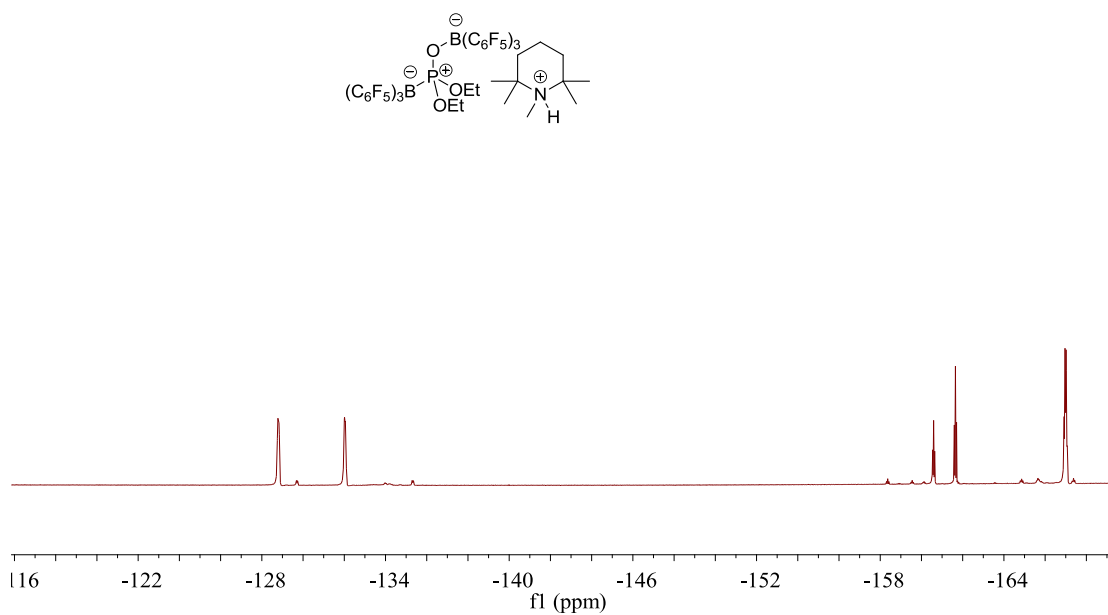


Figure S10: ^{19}F NMR spectrum for **2** in CD_2Cl_2

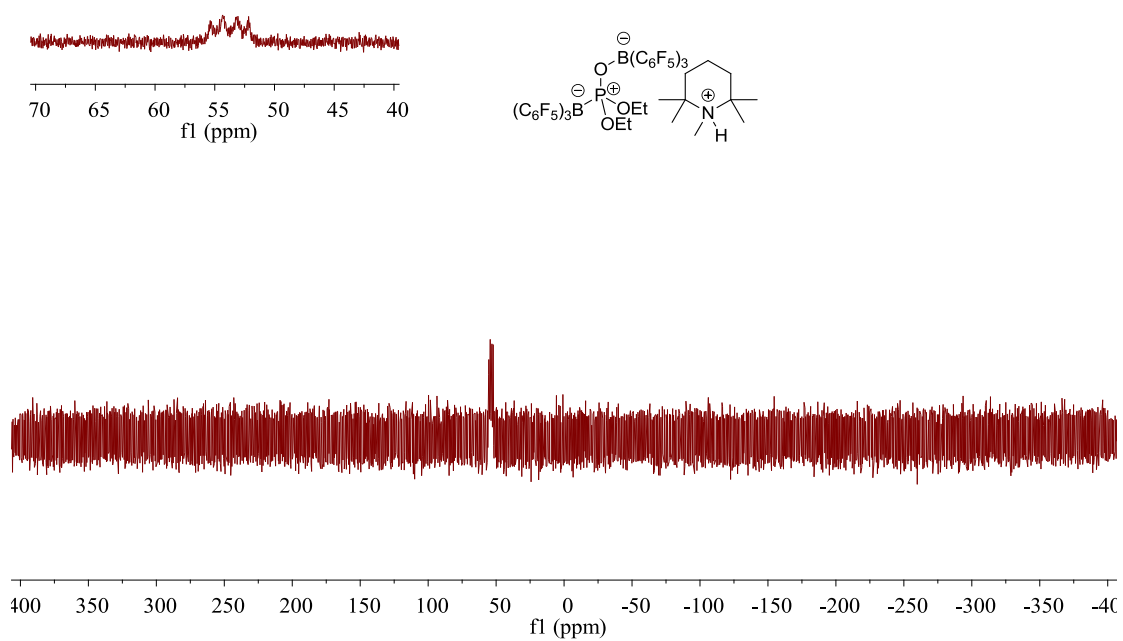


Figure S11: ^{31}P NMR spectrum for **2** in CD_2Cl_2

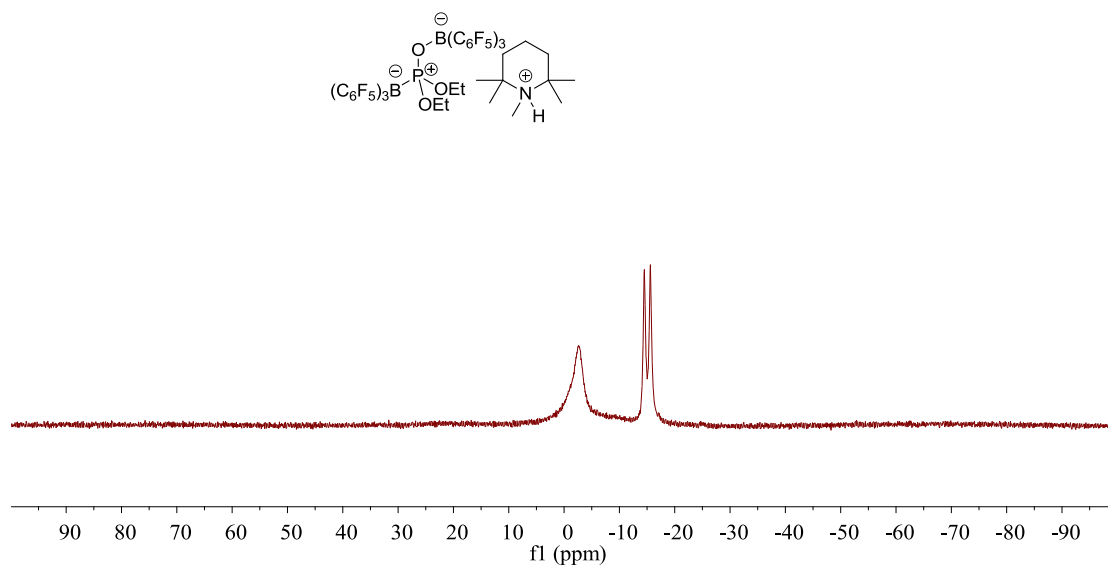


Figure S12: ^{11}B NMR spectrum for **2** in CD_2Cl_2

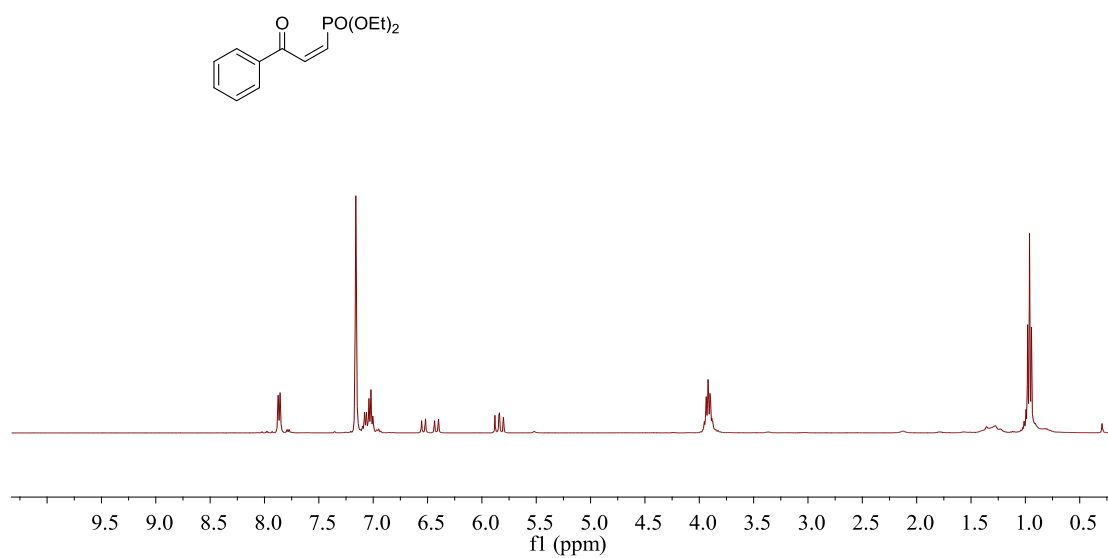


Figure S13: ^1H NMR spectrum for **6a** in C_6D_6

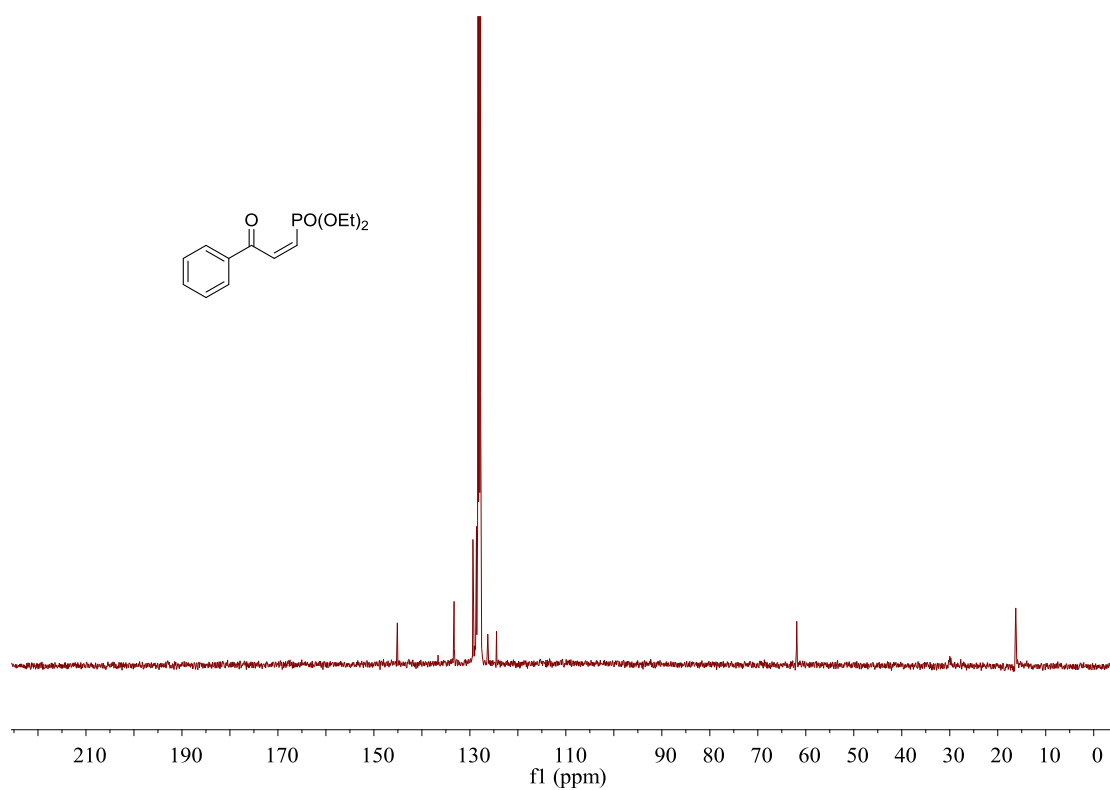


Figure S14: ¹³C NMR spectrum for **6a** in C₆D₆

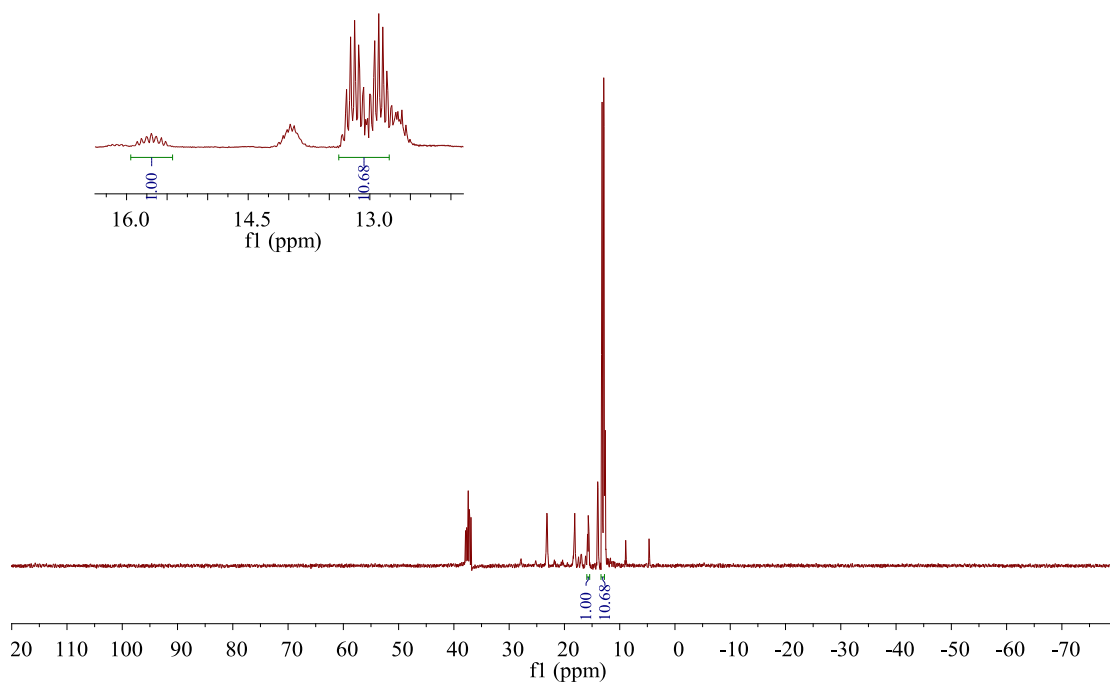


Figure S15: ³¹P NMR spectrum for crude **6a** in C₆D₆

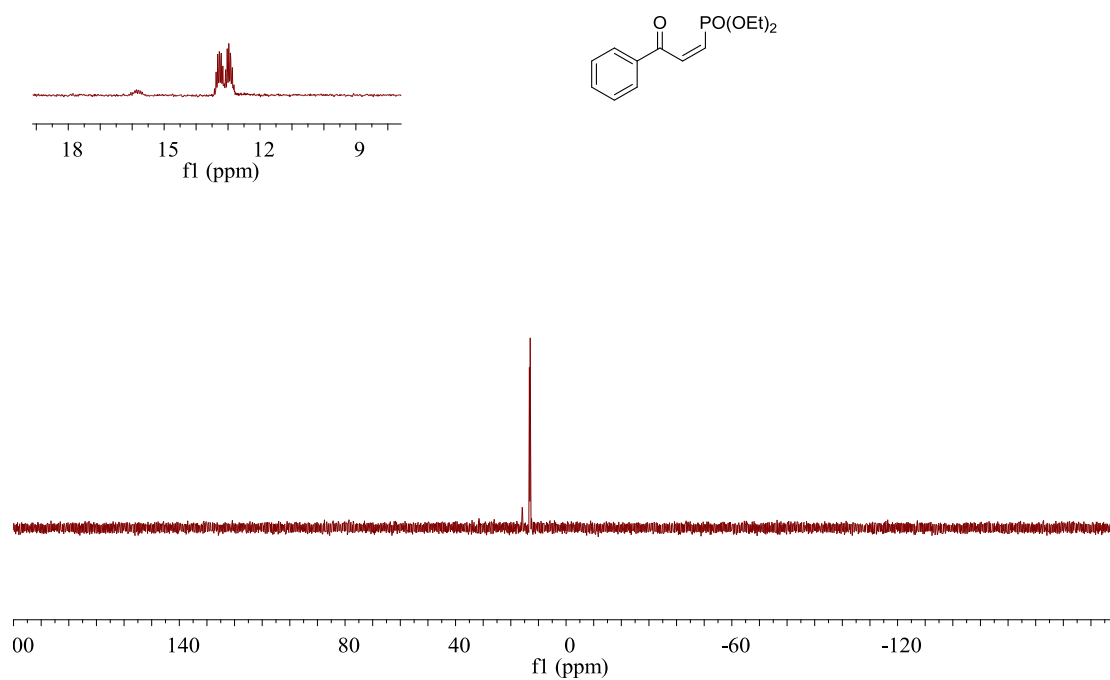


Figure S16: ^{31}P NMR spectrum for **6a** in C_6D_6

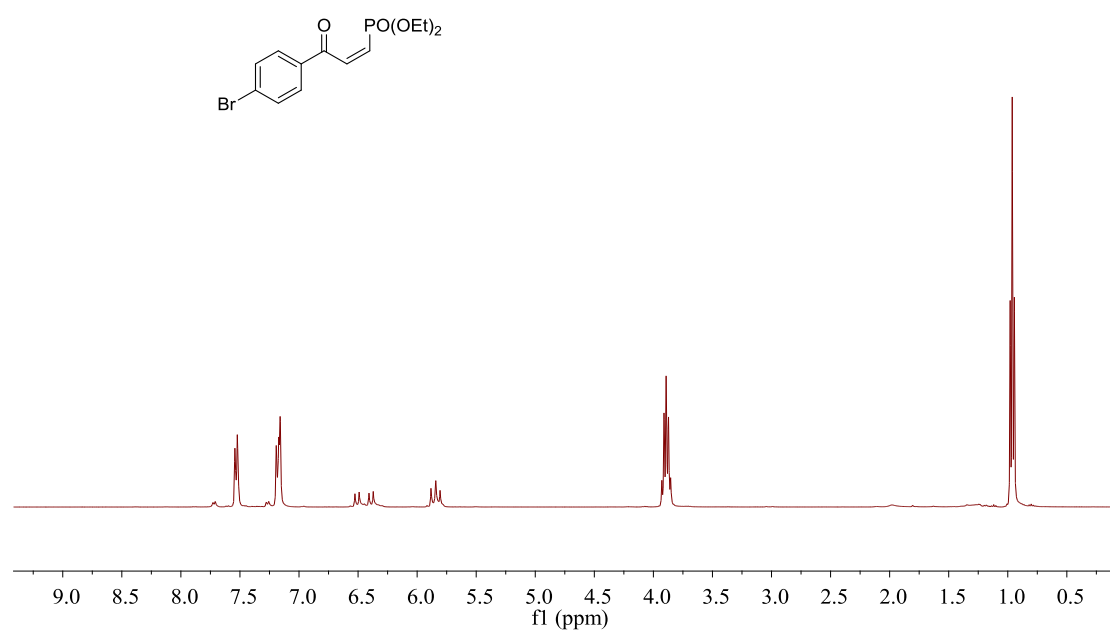


Figure S17: ^1H NMR spectrum for **6b** in C_6D_6

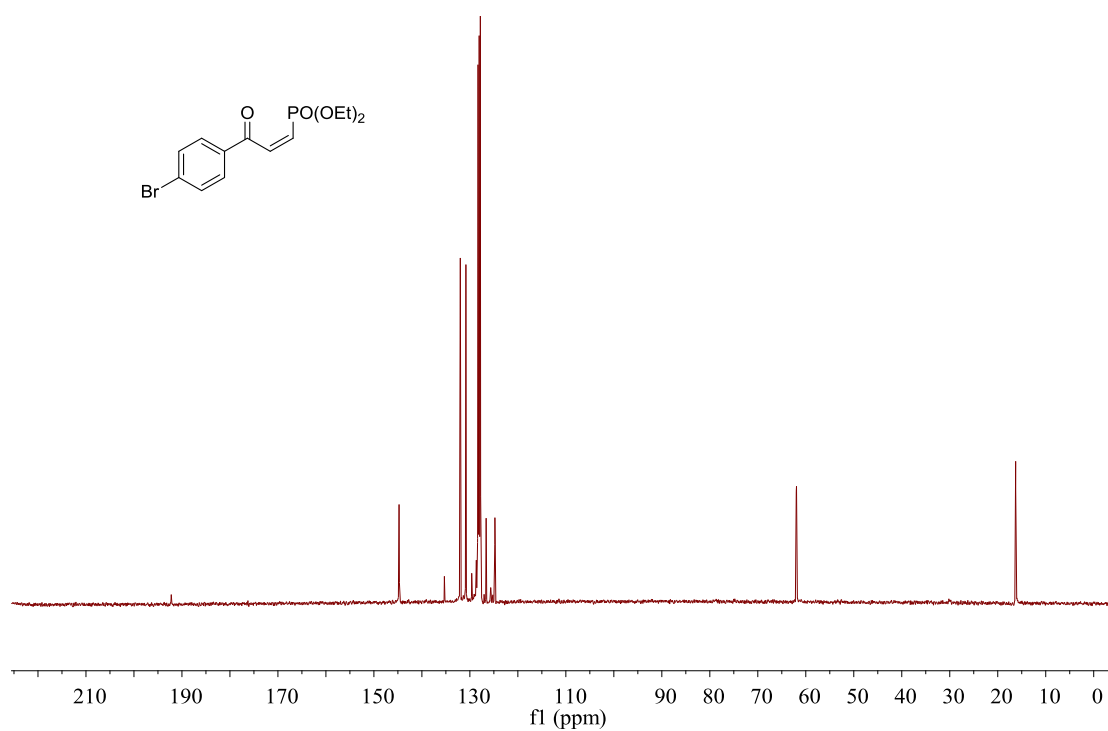


Figure S18: ^{13}C NMR spectrum for **6b** in C_6D_6

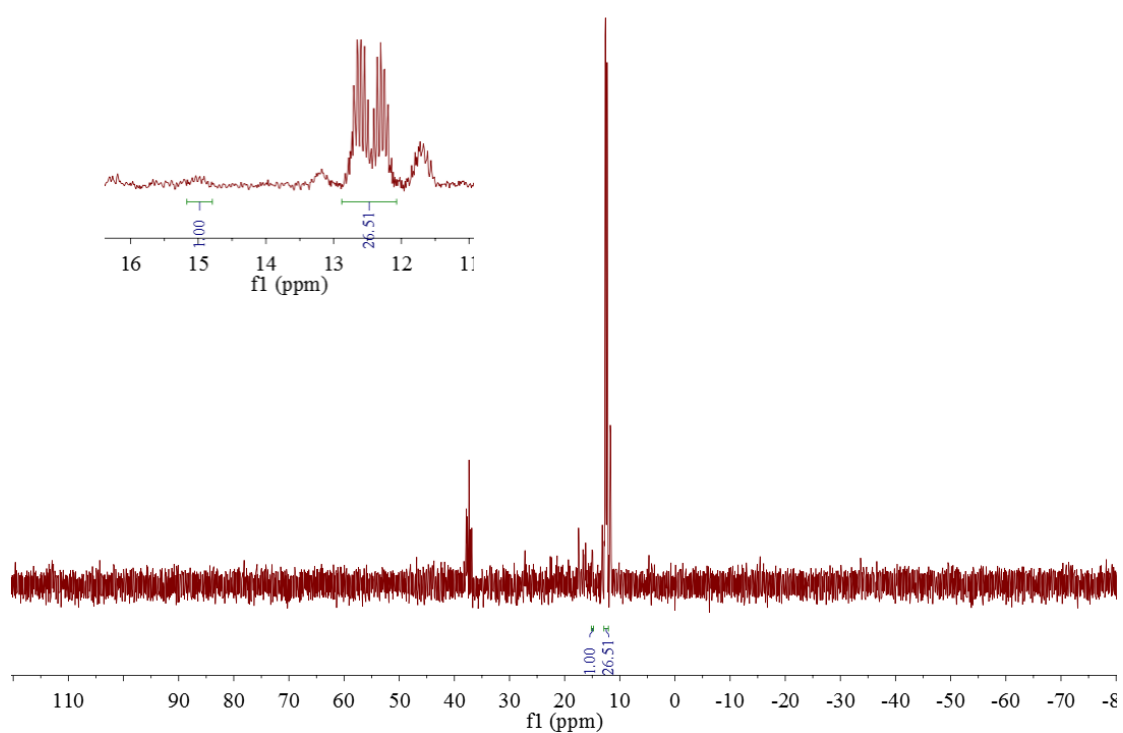


Figure S19: ^{31}P NMR spectrum for crude **6b** in C_6D_6

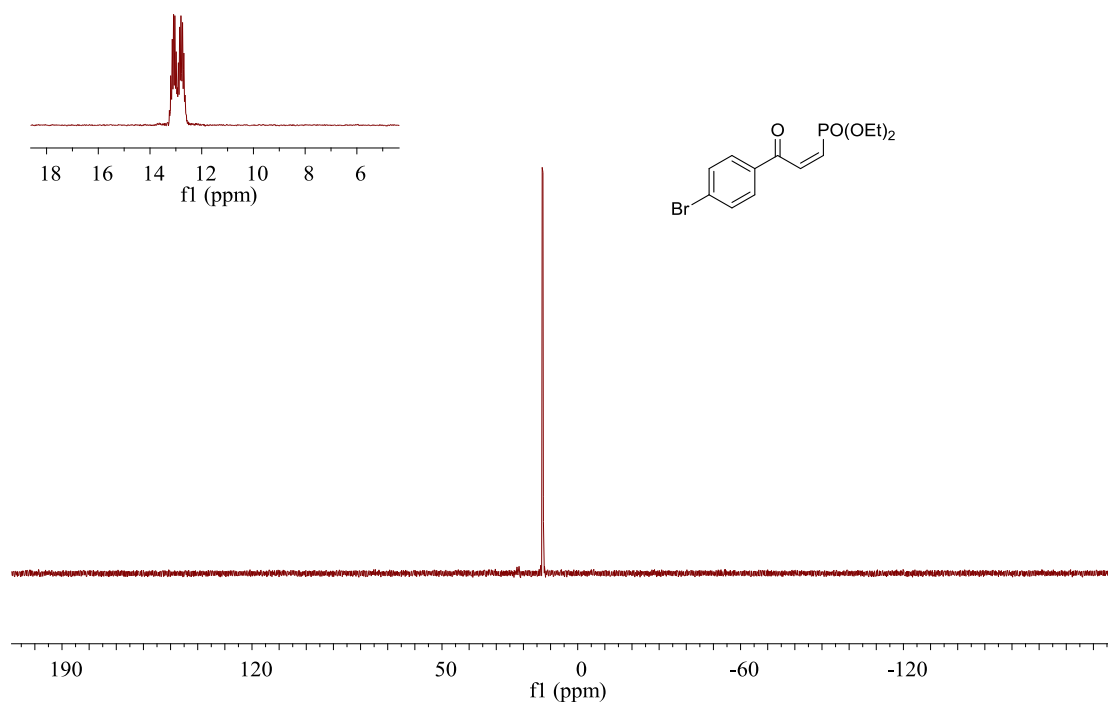


Figure S20: ^{31}P NMR spectrum for **6b** in C_6D_6

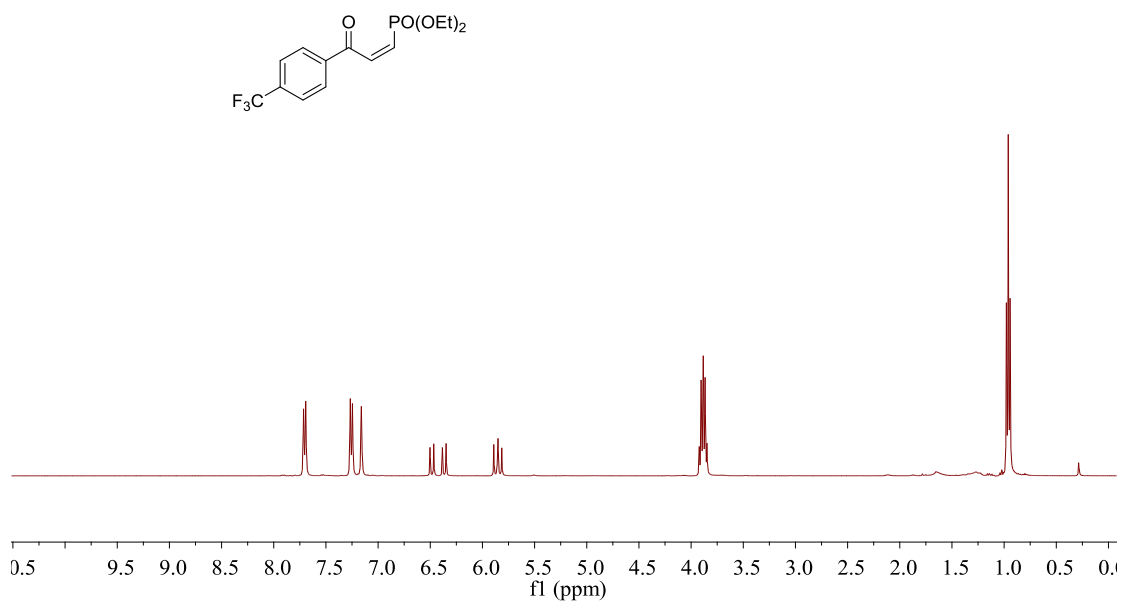


Figure S21: ^1H NMR spectrum for **6c** in C_6D_6

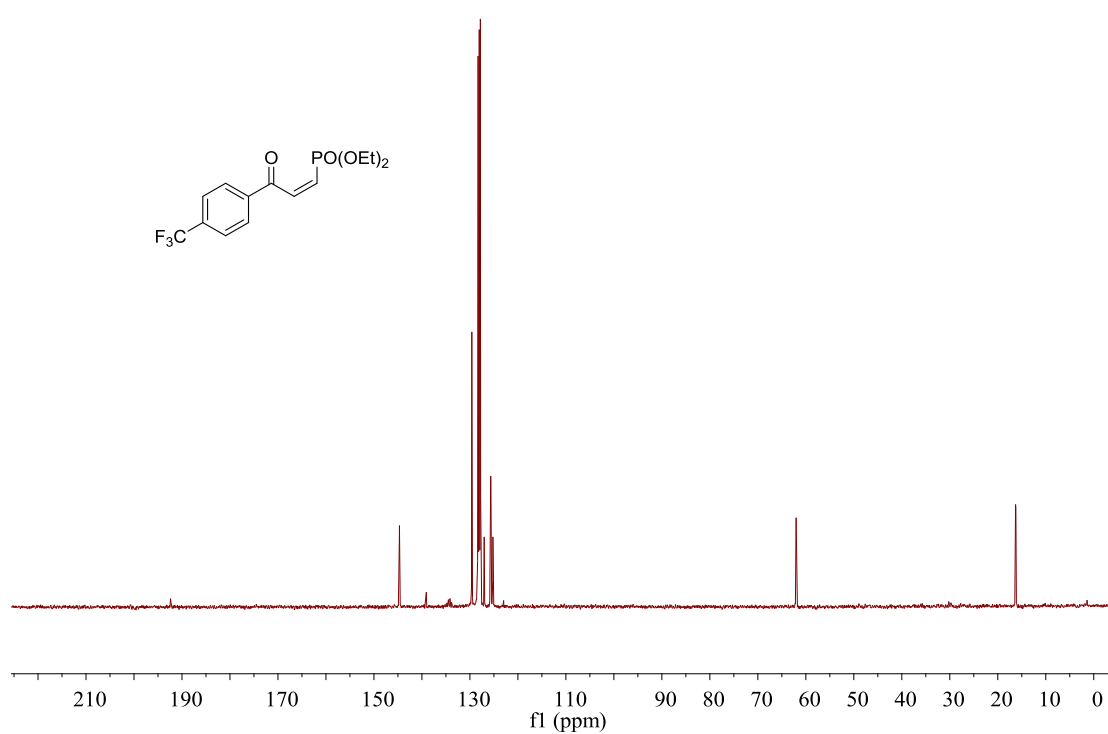


Figure S22: ^{13}C NMR spectrum for **6c** in C_6D_6

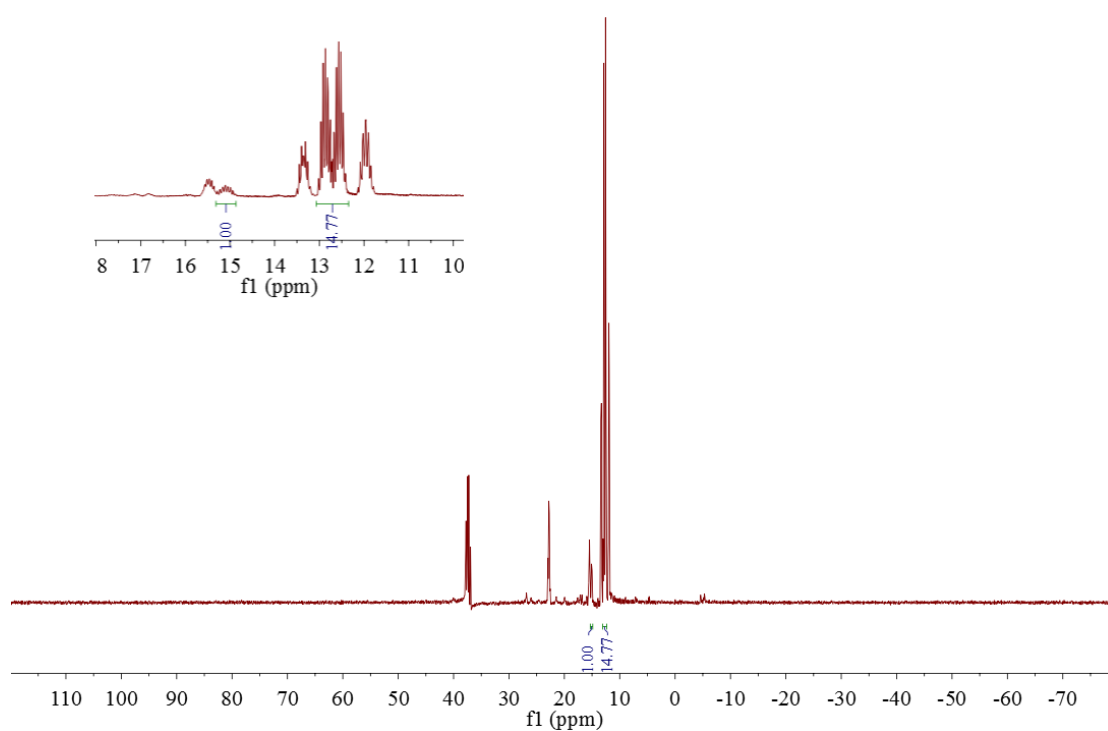


Figure S23: ^{31}P NMR spectrum for crude **6c** in C_6D_6

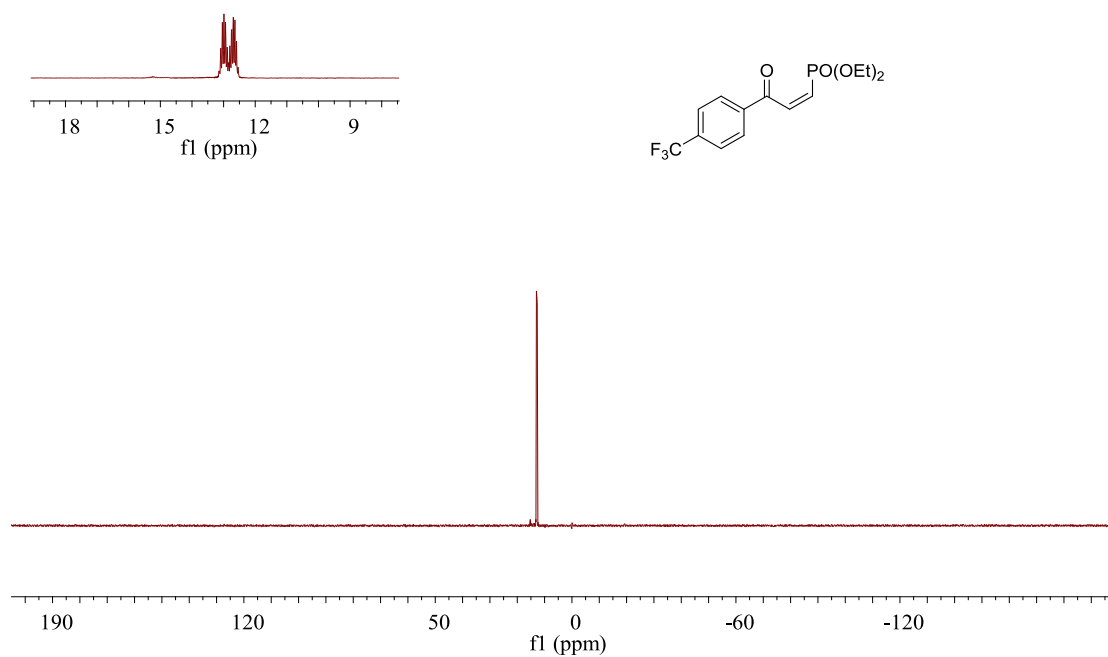


Figure S24: ^{31}P NMR spectrum for **6c** in C_6D_6

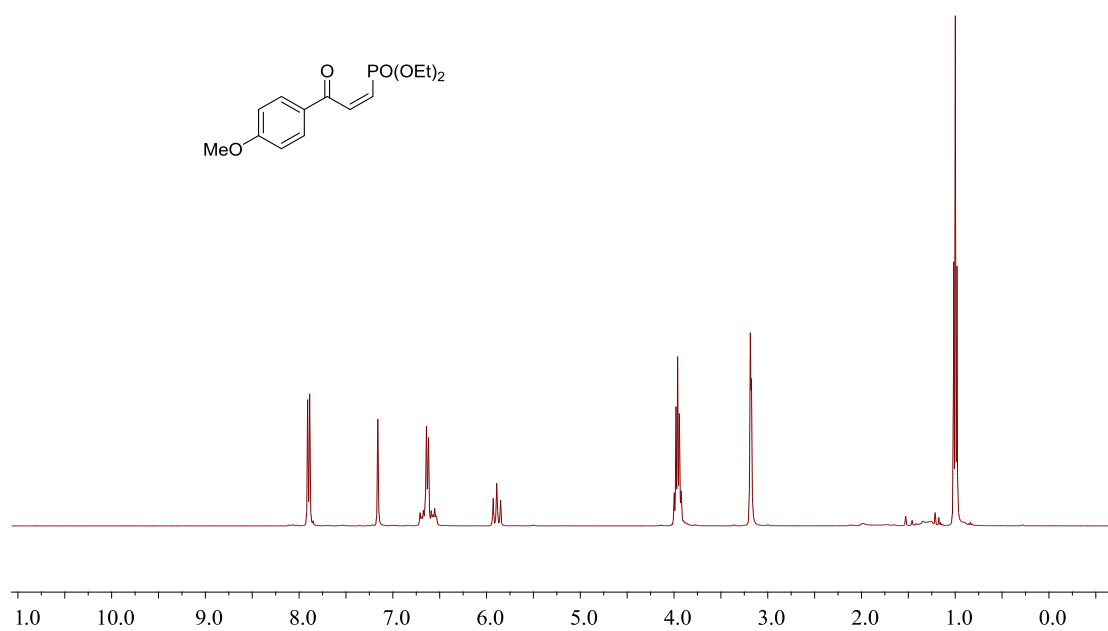


Figure S25: ^1H NMR spectrum for **6d** in C_6D_6

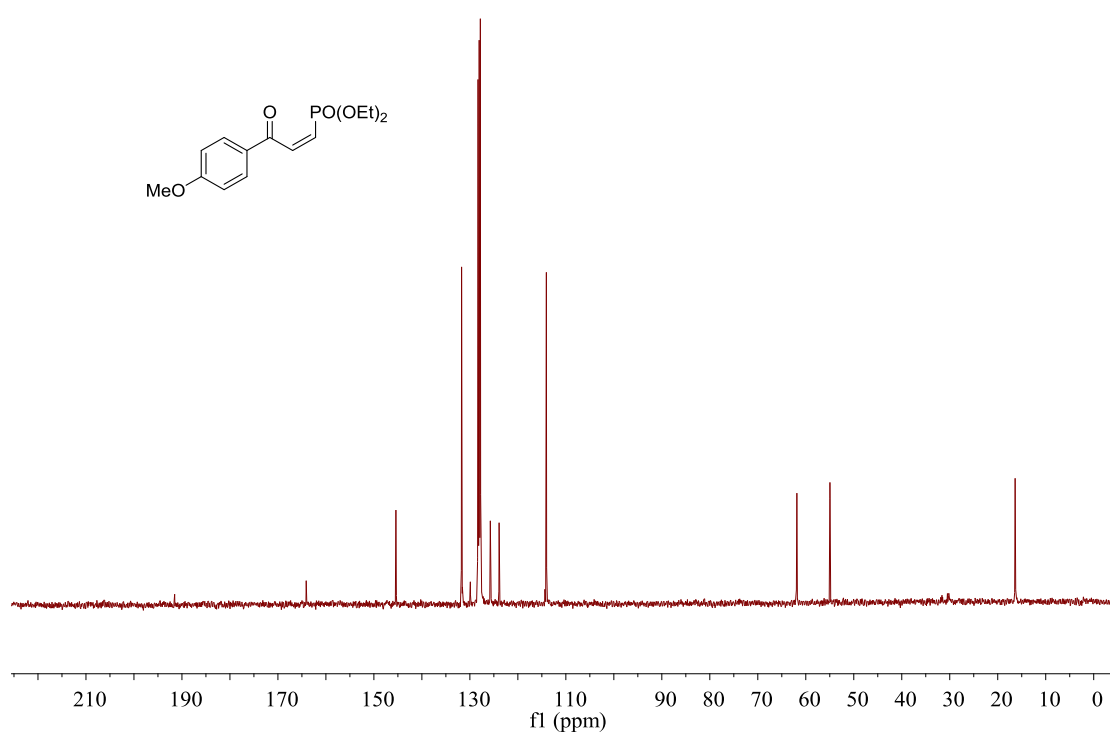


Figure S26: ^{13}C NMR spectrum for **6d** in C_6D_6

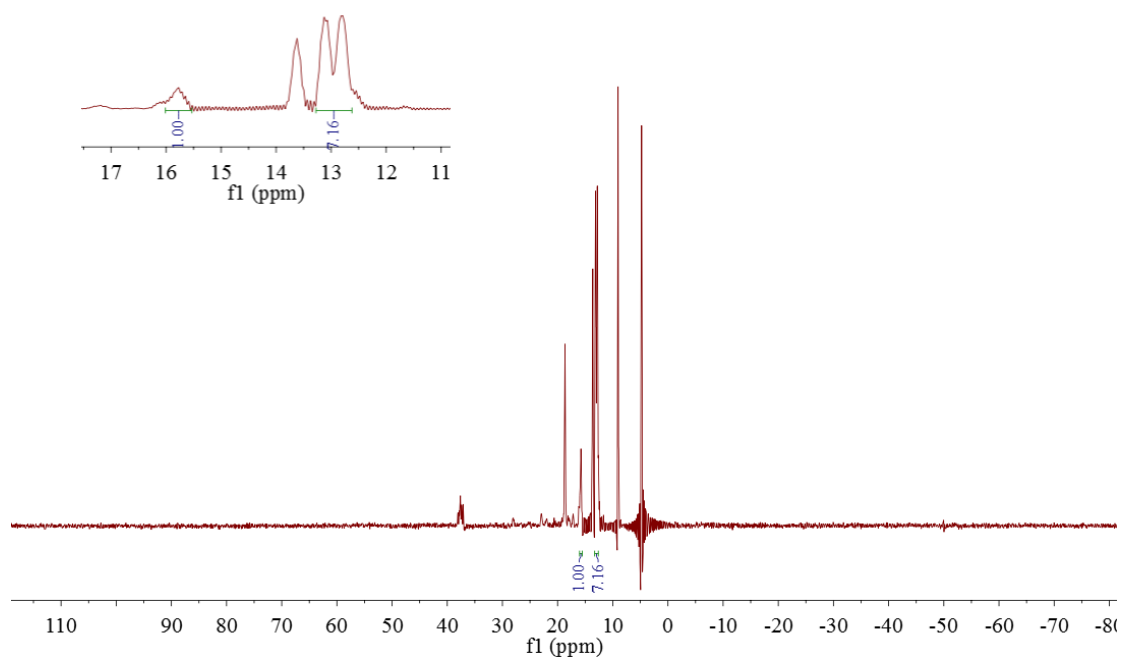


Figure S27: ^{31}P NMR spectrum for crude **6d** in C_6D_6

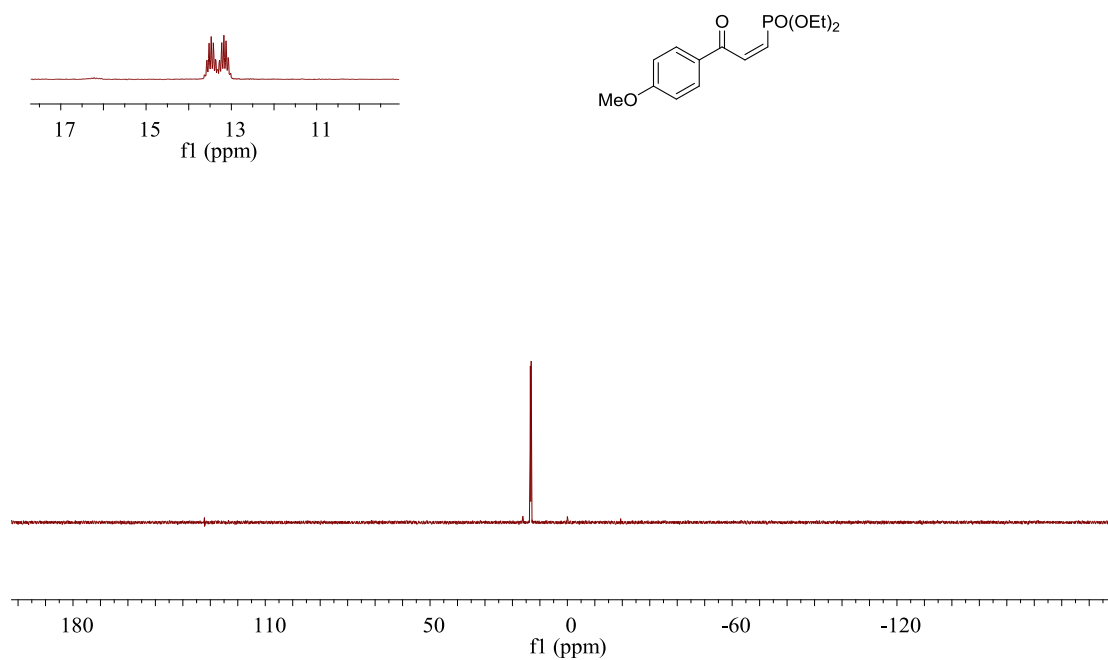


Figure S28: ^{31}P NMR spectrum for **6d** in C_6D_6

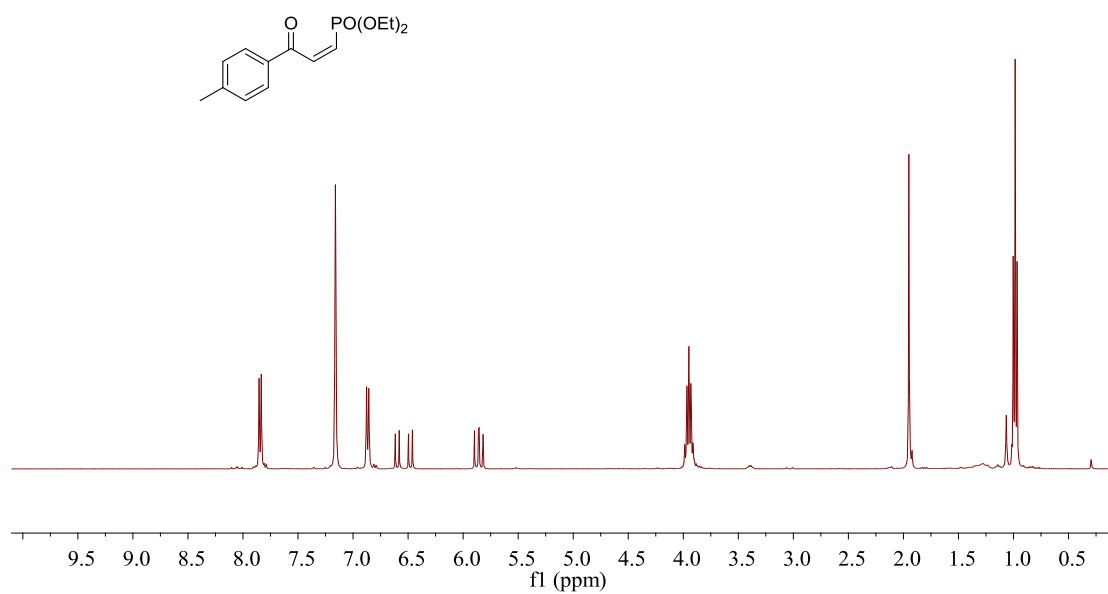


Figure S29: ^1H NMR spectrum for **6e** in C_6D_6

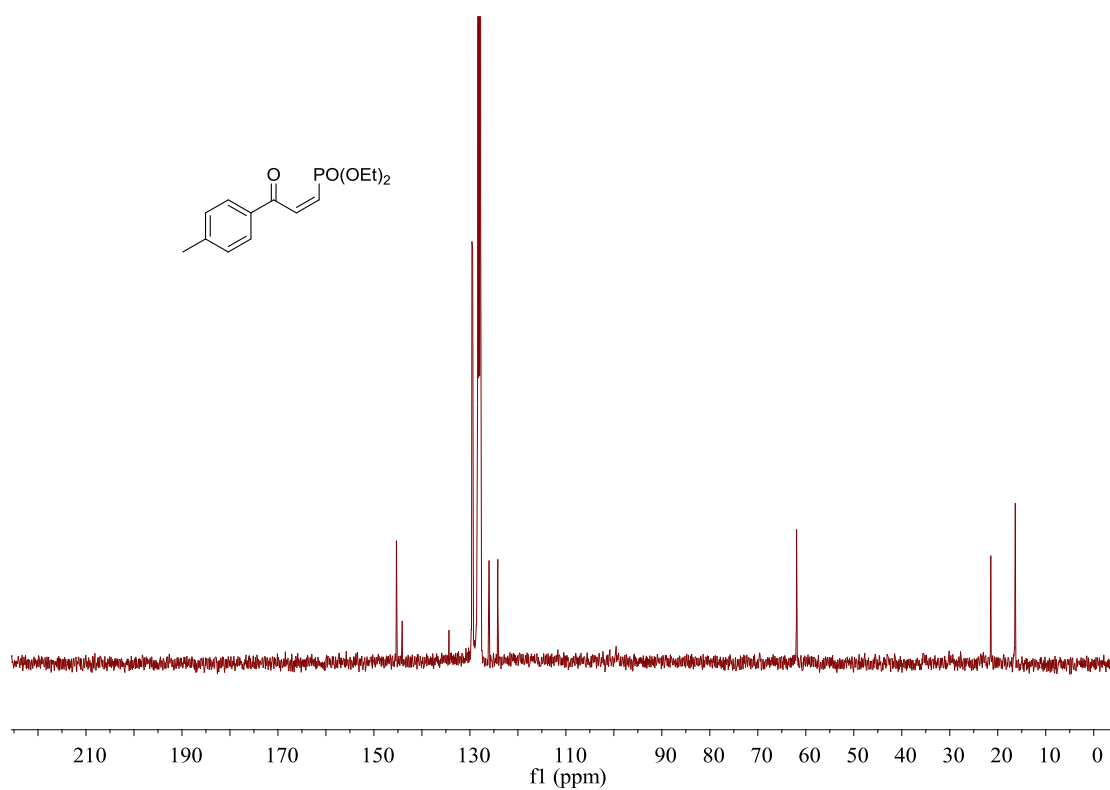


Figure S30: ¹³C NMR spectrum for **6e** in C₆D₆

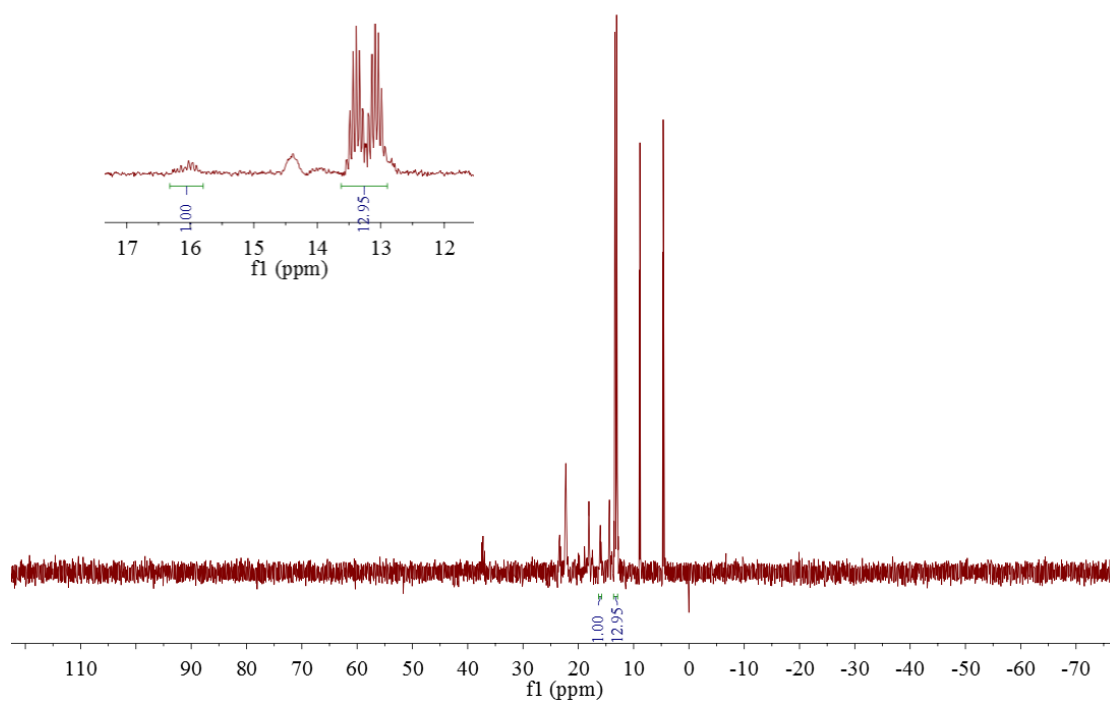


Figure S31: ³¹P NMR spectrum for crude **6e** in C₆D₆

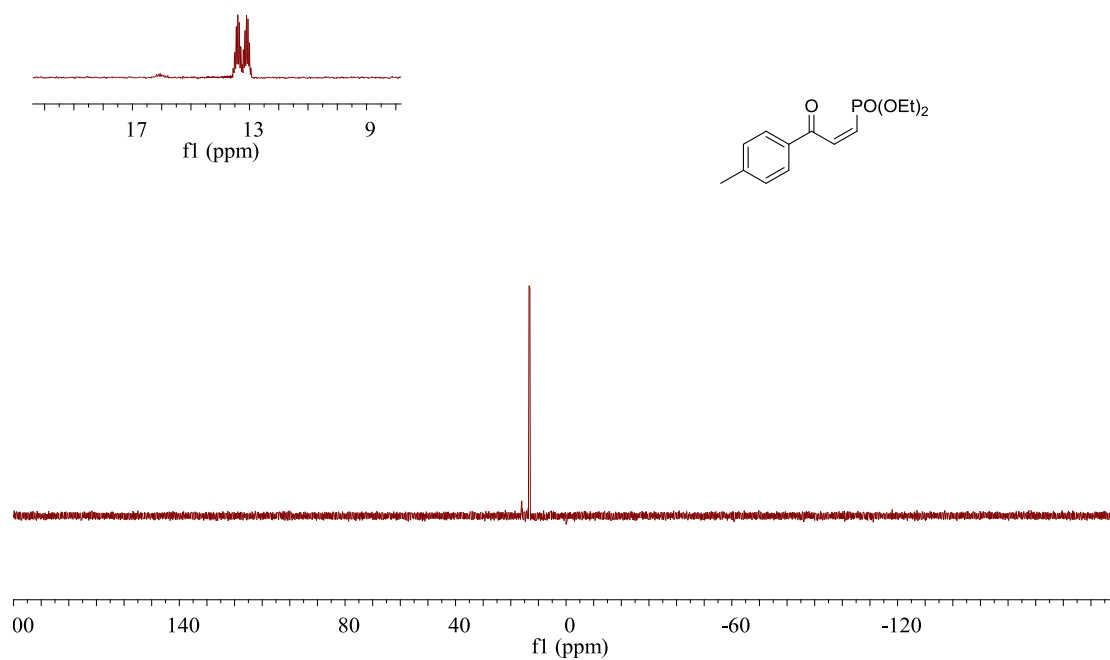


Figure S32: ³¹P NMR spectrum for **6e** in C₆D₆

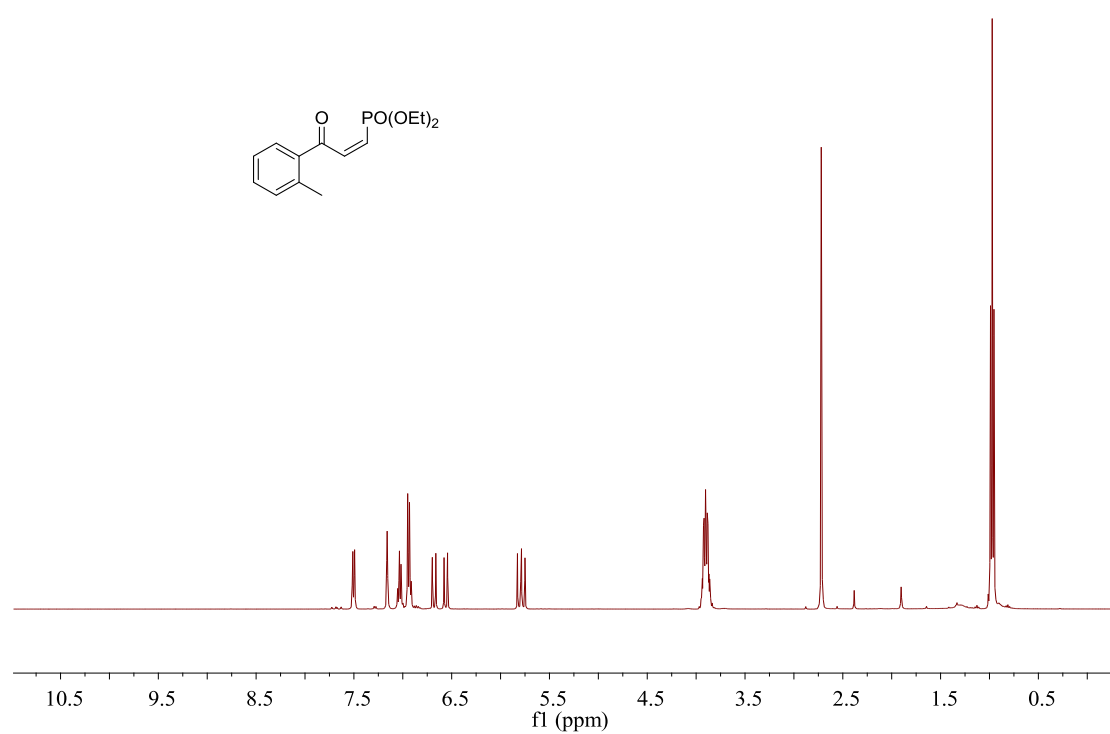


Figure S33: ¹H NMR spectrum for **6f** in C₆D₆

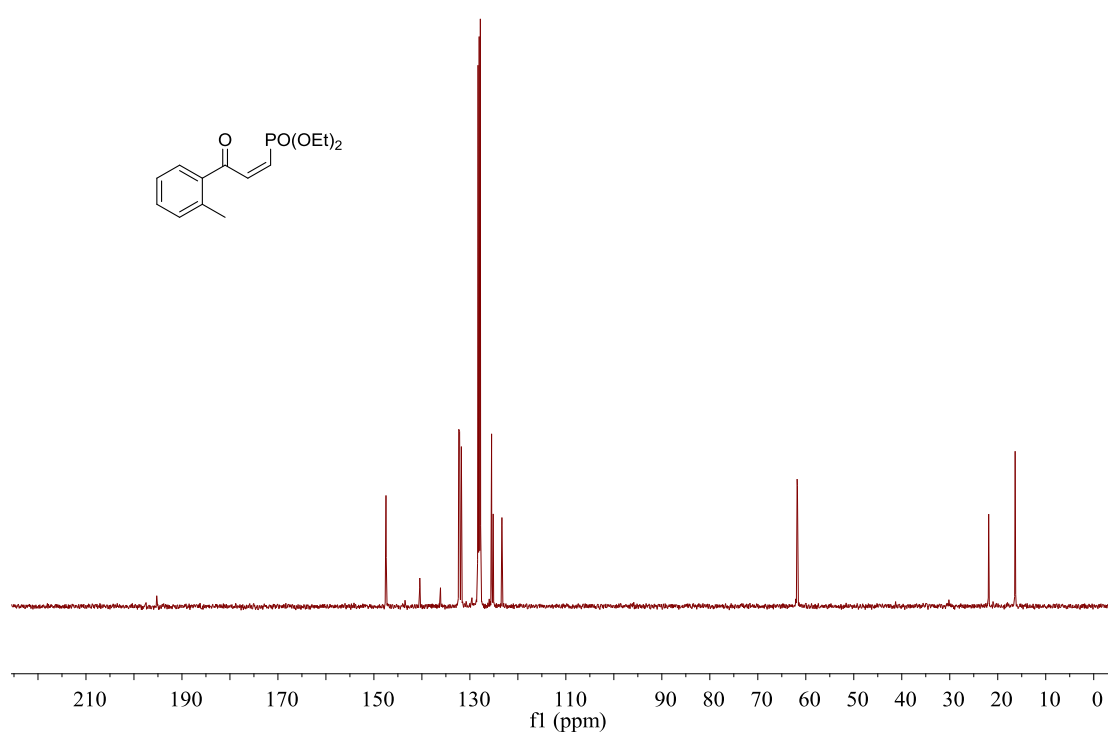


Figure S34: ^{13}C NMR spectrum for **6f** in C_6D_6

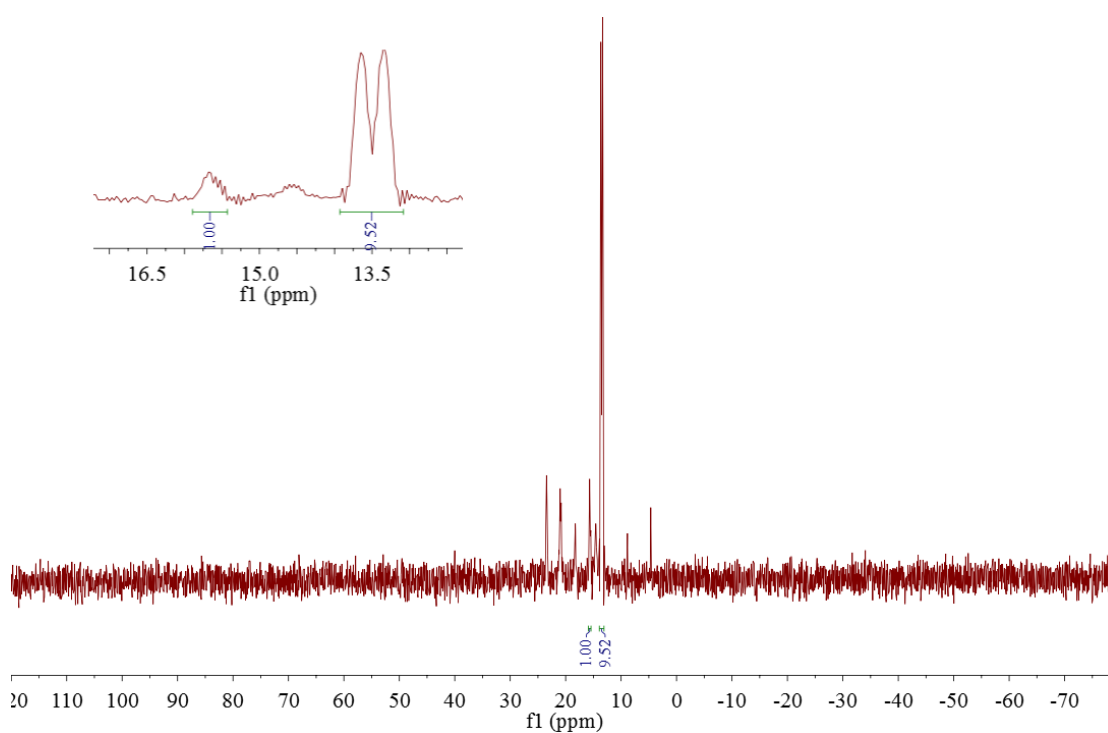


Figure S35: ^{31}P NMR spectrum for crude **6f** in C_6D_6

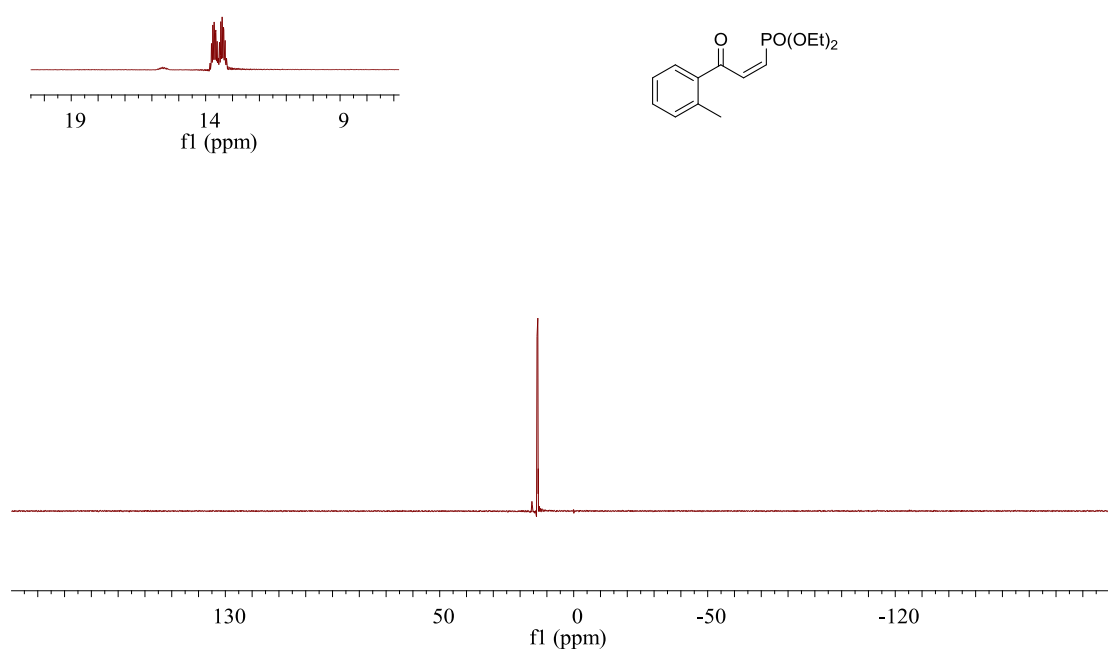


Figure S36: ^{31}P NMR spectrum for **6f** in C_6D_6

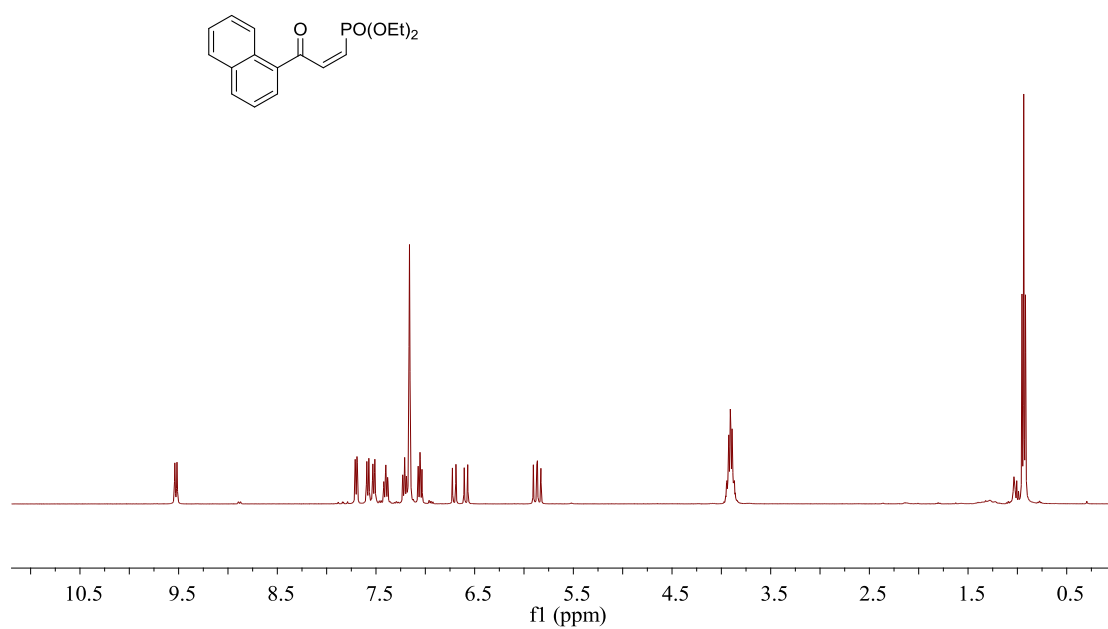


Figure S37: ^1H NMR spectrum for **6g** in C_6D_6

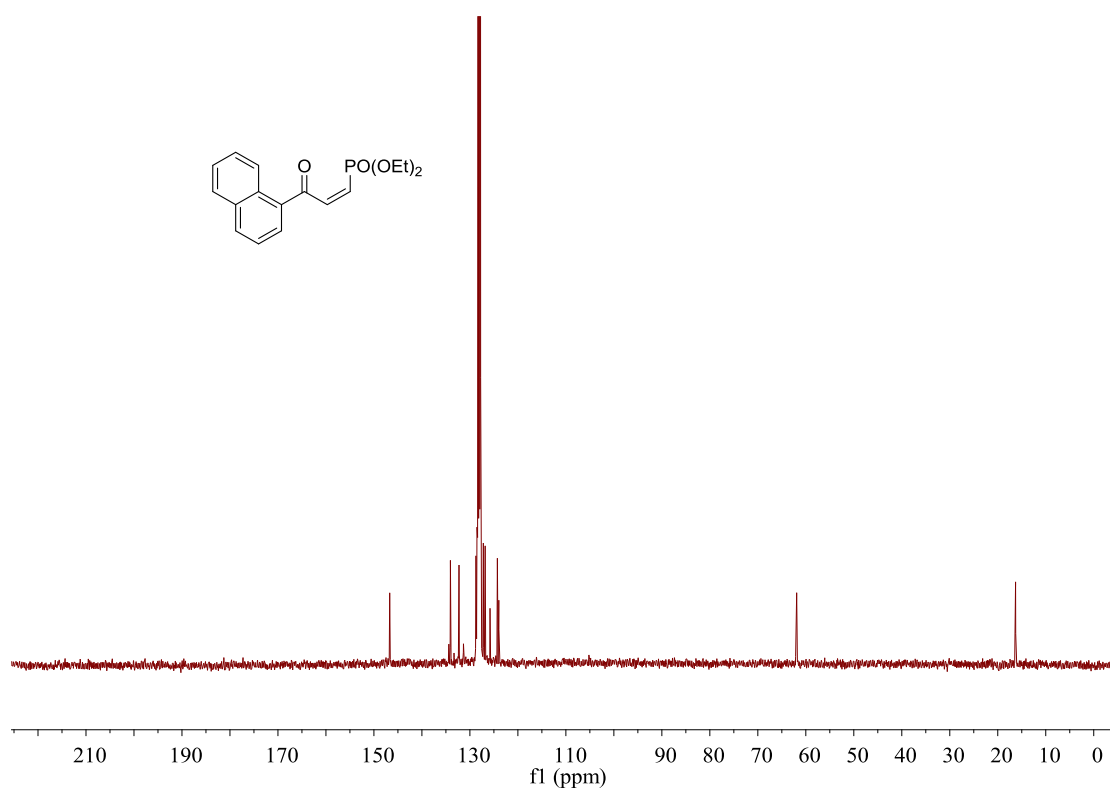


Figure S38: ^{13}C NMR spectrum for **6g** in C_6D_6

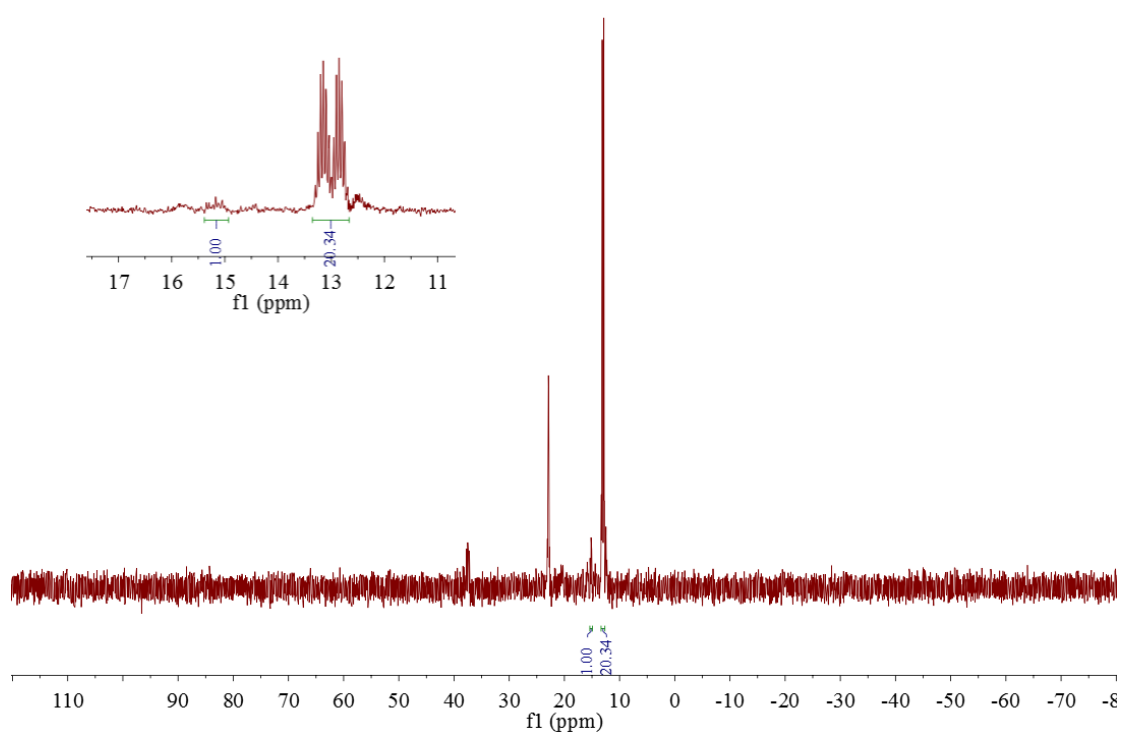


Figure S39: ^{31}P NMR spectrum for crude **6g** in C_6D_6

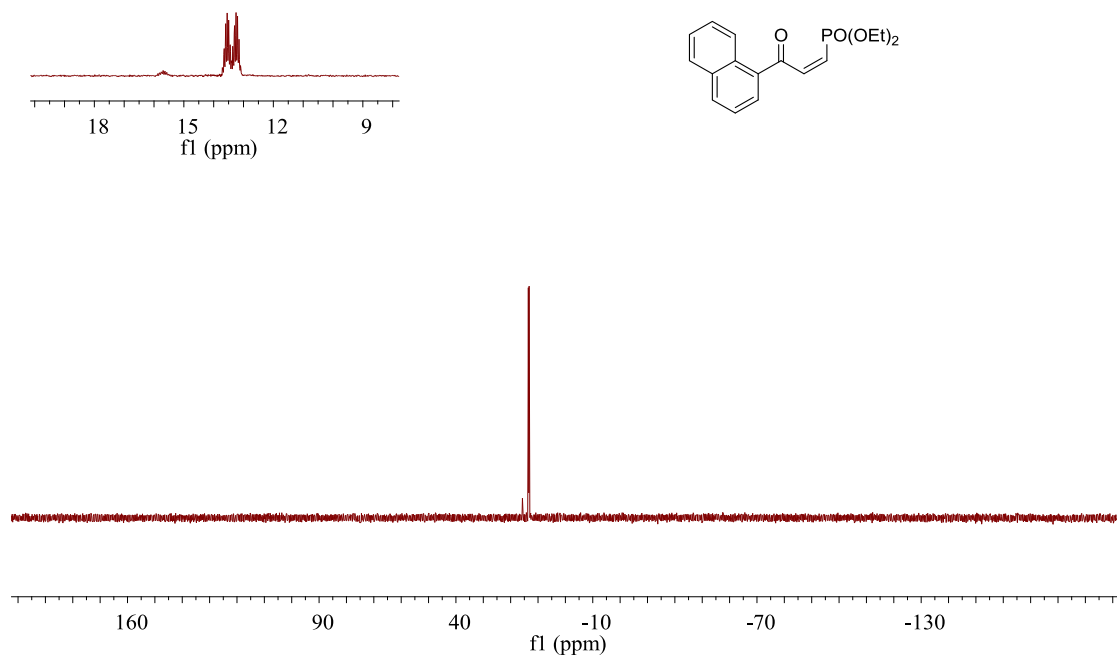


Figure S40: ^{31}P NMR spectrum for **6g** in C_6D_6

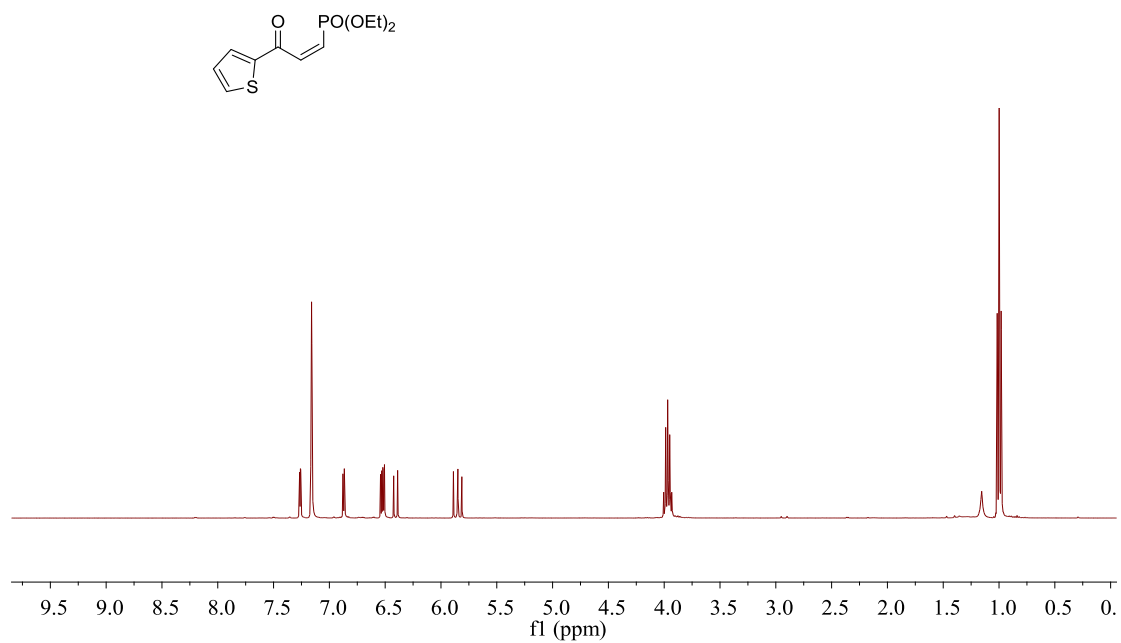


Figure S41: ^1H NMR spectrum for **6h** in C_6D_6

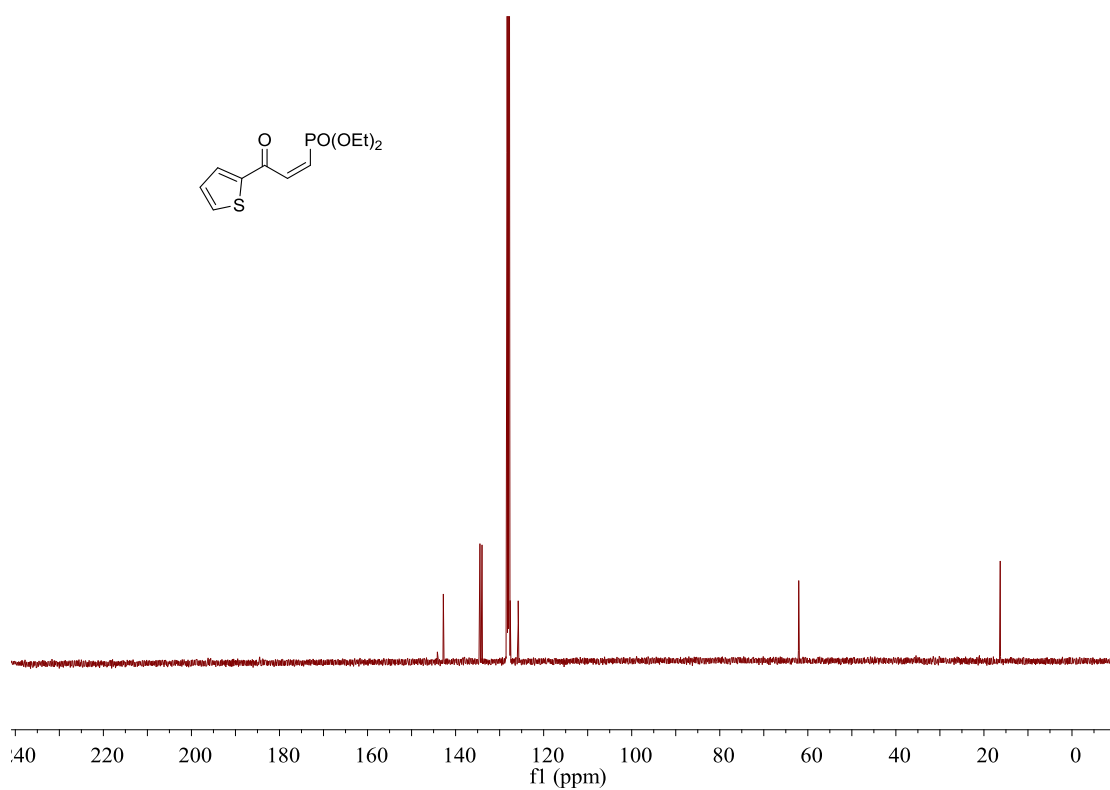


Figure S42: ^{13}C NMR spectrum for **6h** in C_6D_6

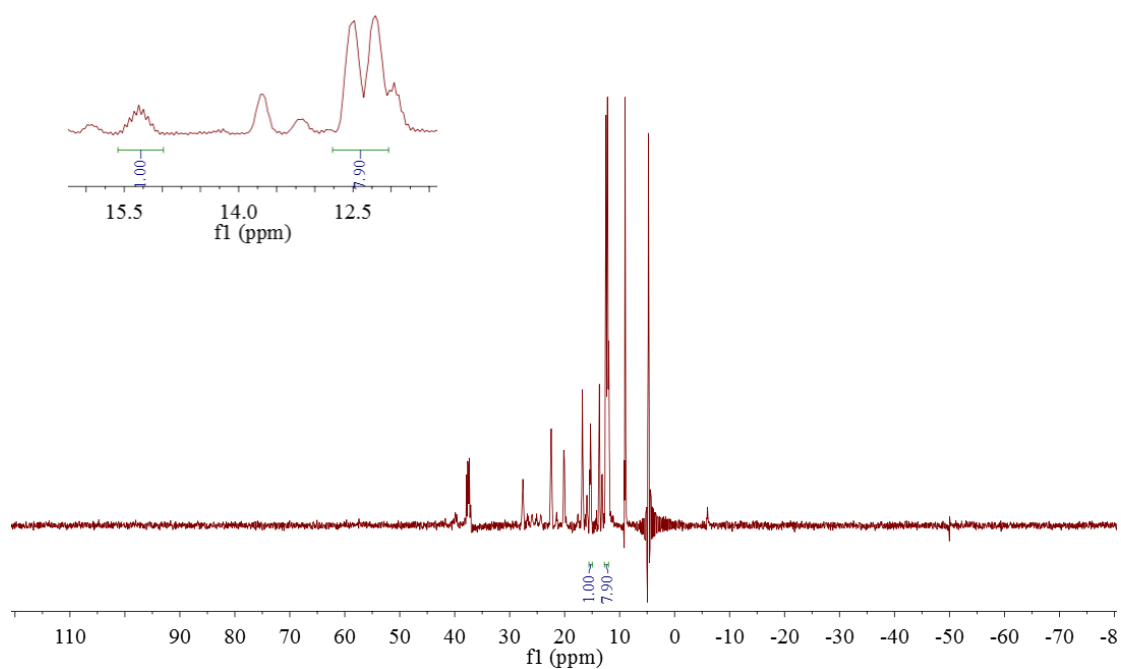


Figure S43: ^{31}P NMR spectrum for crude **6h** in C_6D_6

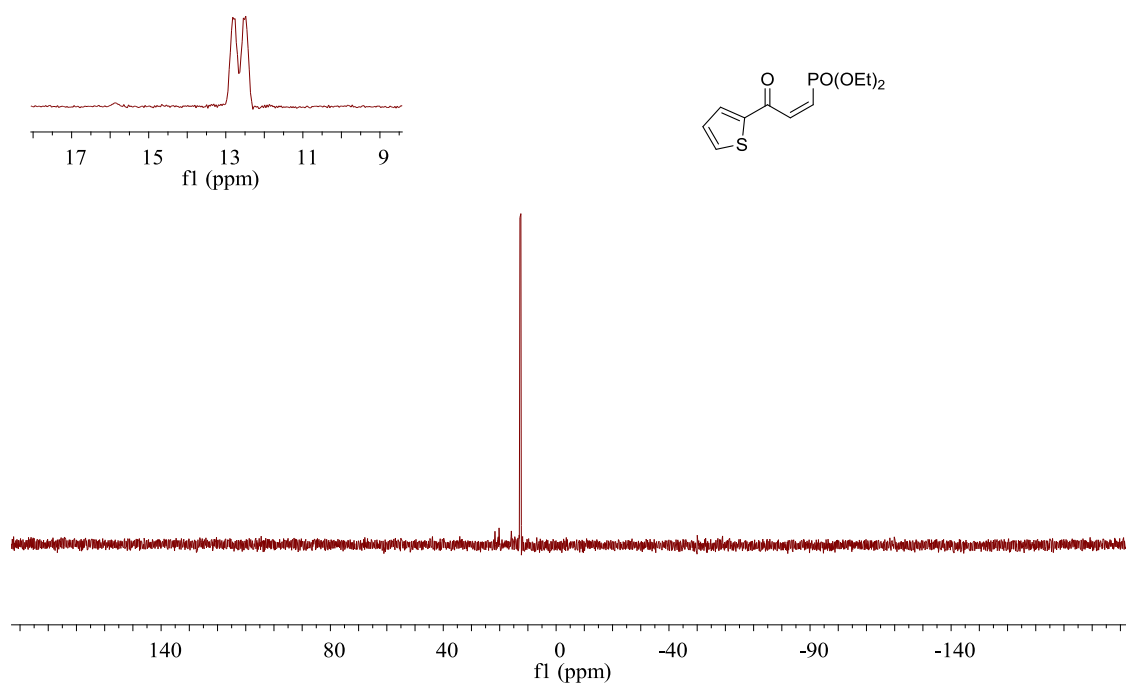


Figure S44: ^{31}P NMR spectrum for **6h** in C_6D_6

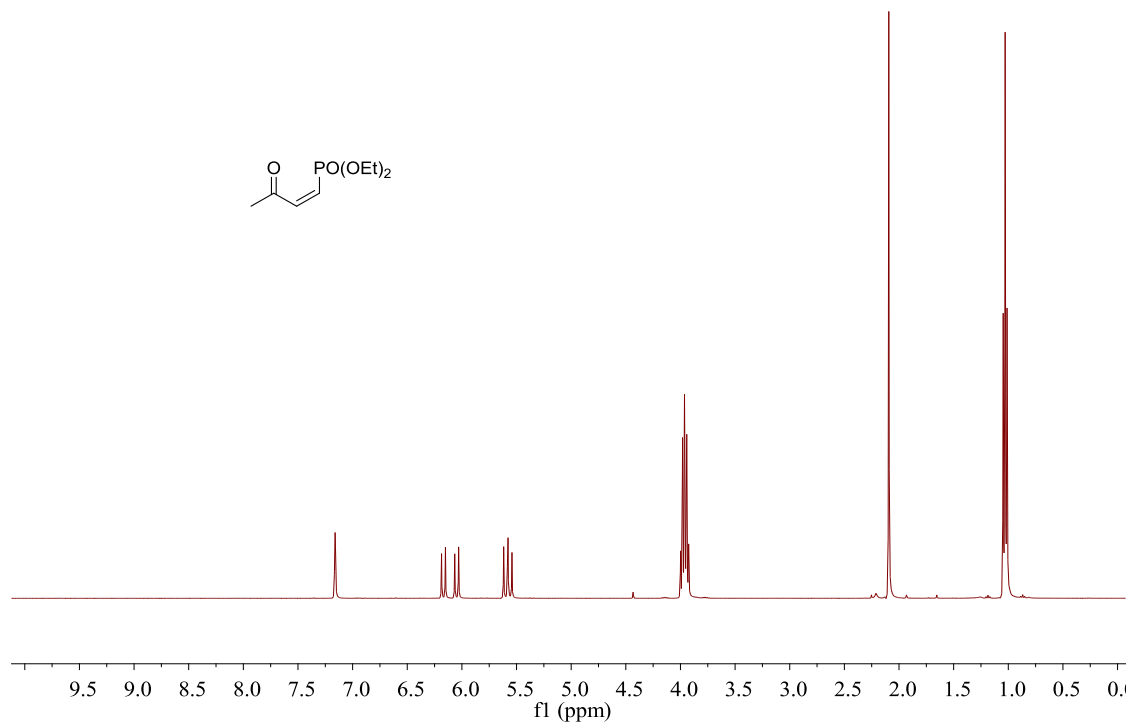


Figure S45: ^1H NMR spectrum for **6i** in C_6D_6

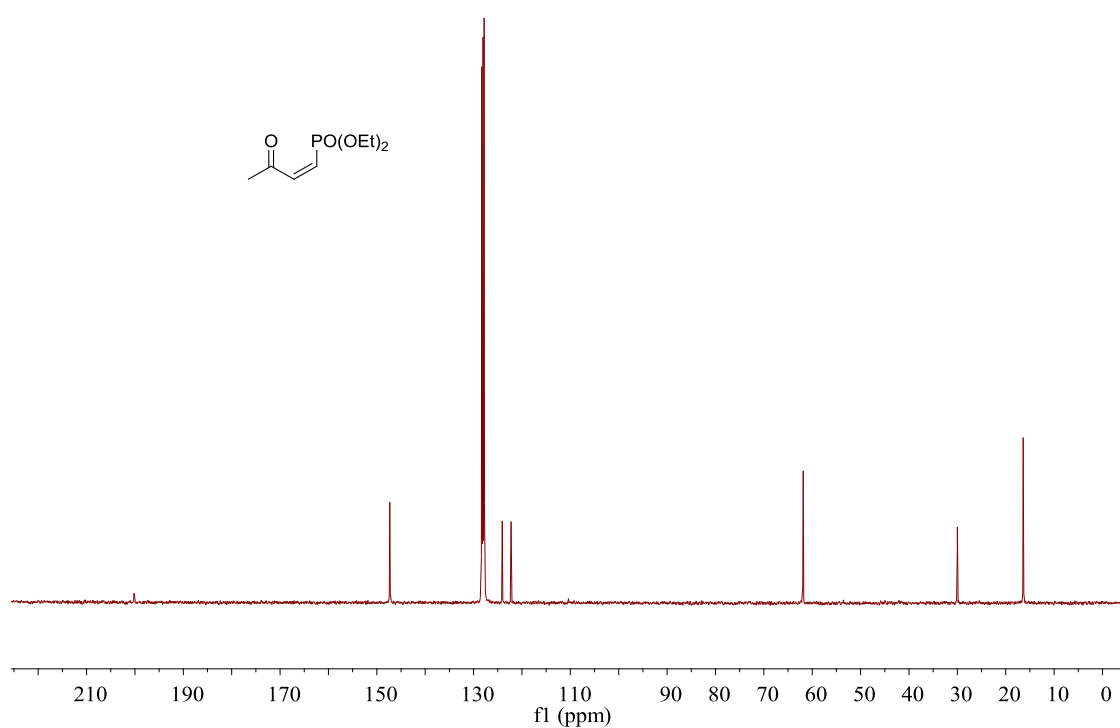


Figure S46: ^{13}C NMR spectrum for **6i** in C_6D_6

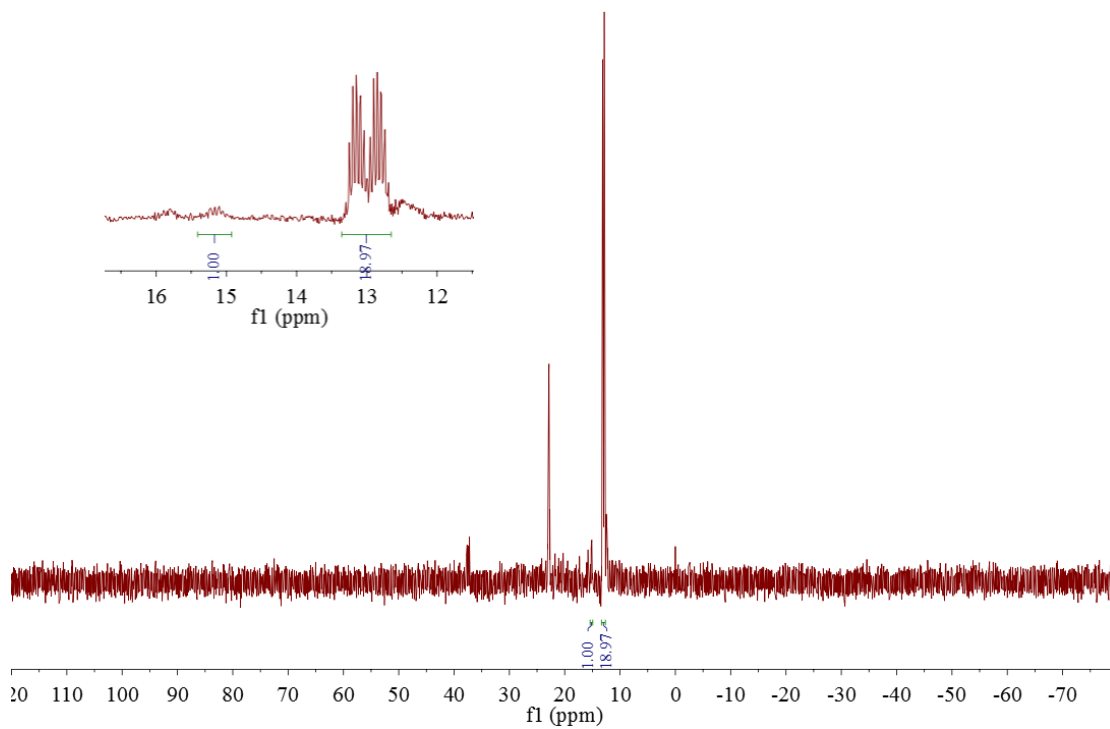


Figure S47: ^{31}P NMR spectrum for crude **6i** in C_6D_6

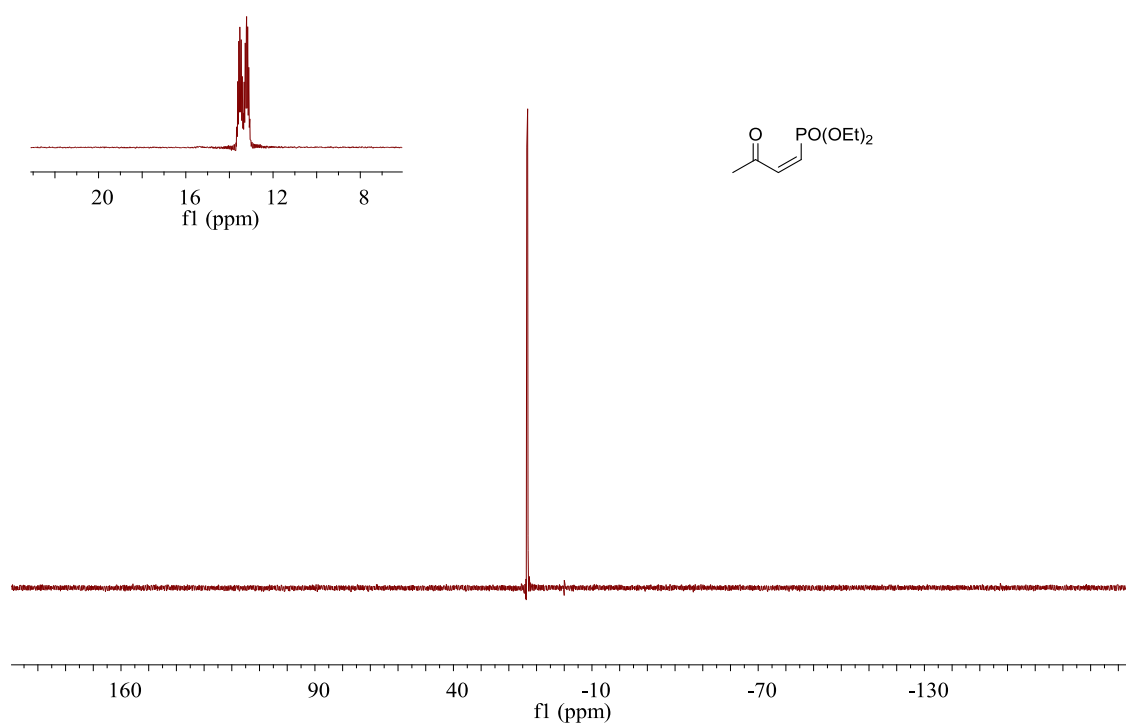


Figure S48: ^{31}P NMR spectrum for **6i** in C_6D_6

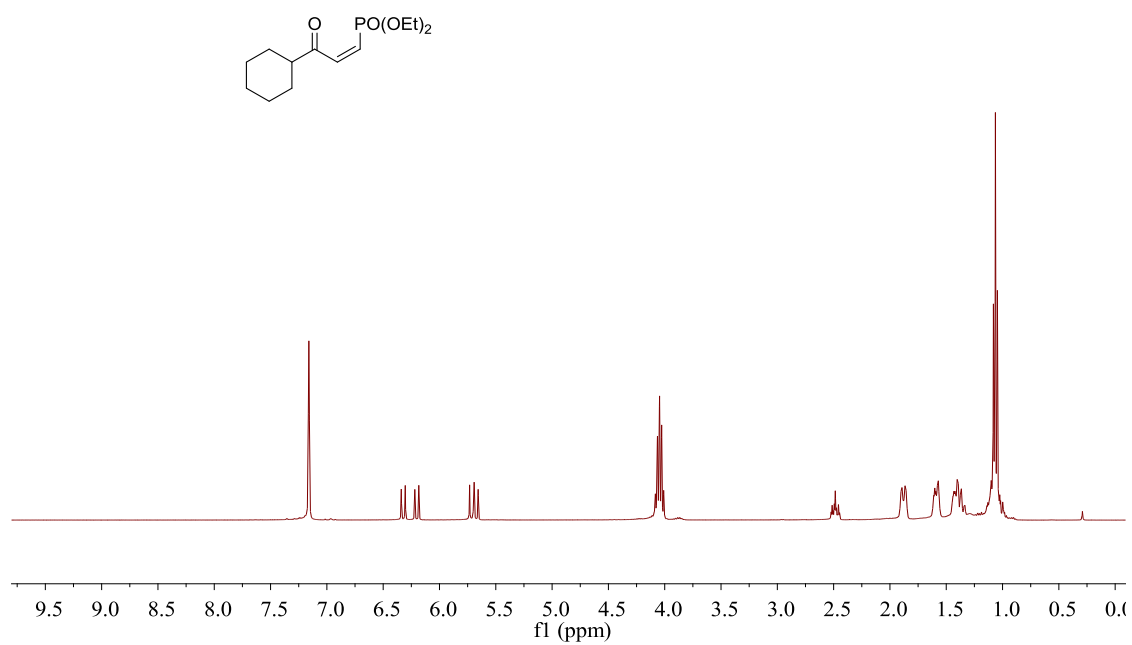


Figure S49: ^1H NMR spectrum for **6j** in C_6D_6

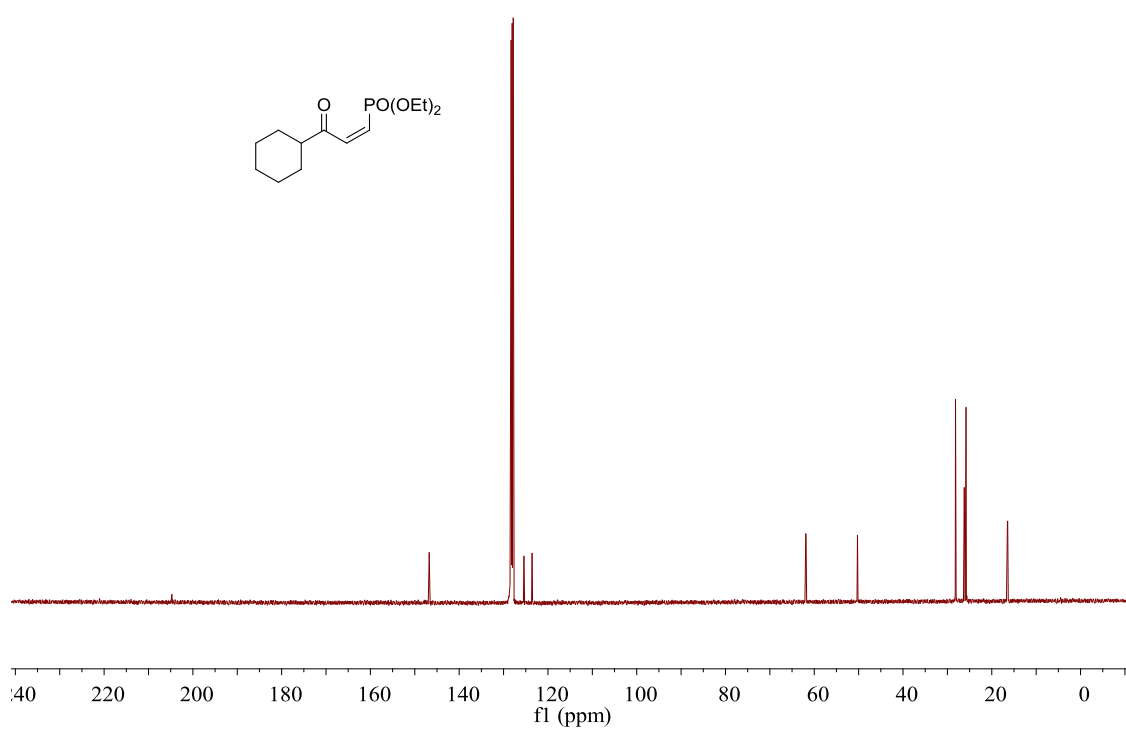


Figure S50: ¹³C NMR spectrum for **6j** in C₆D₆

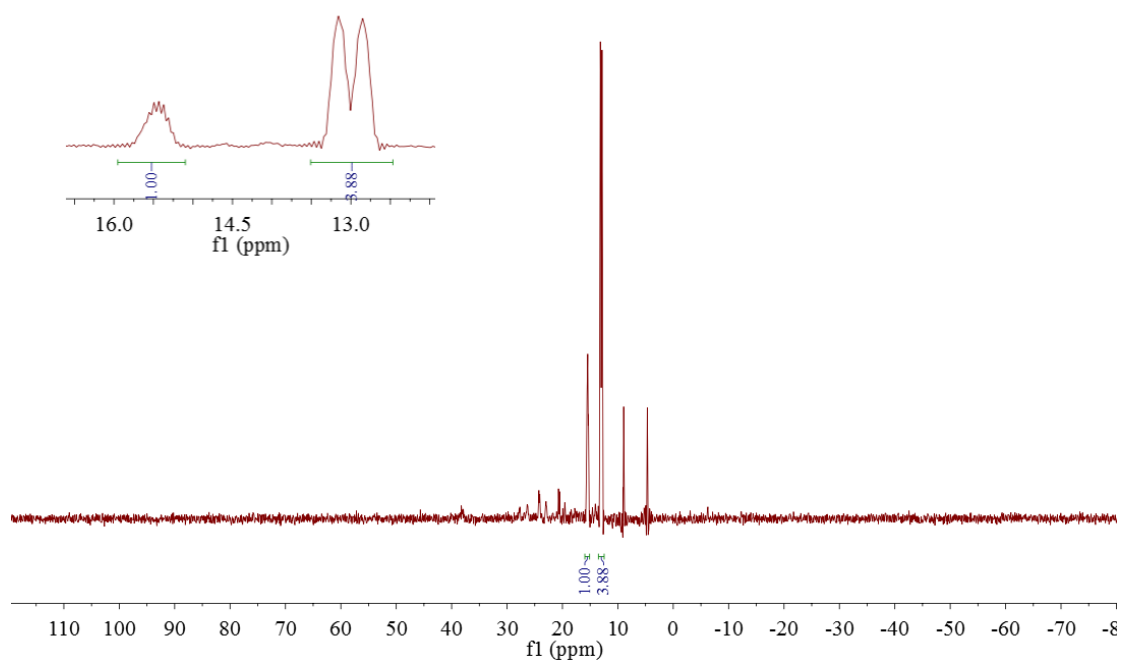


Figure S51: ³¹P NMR spectrum for crude **6j** in C₆D₆

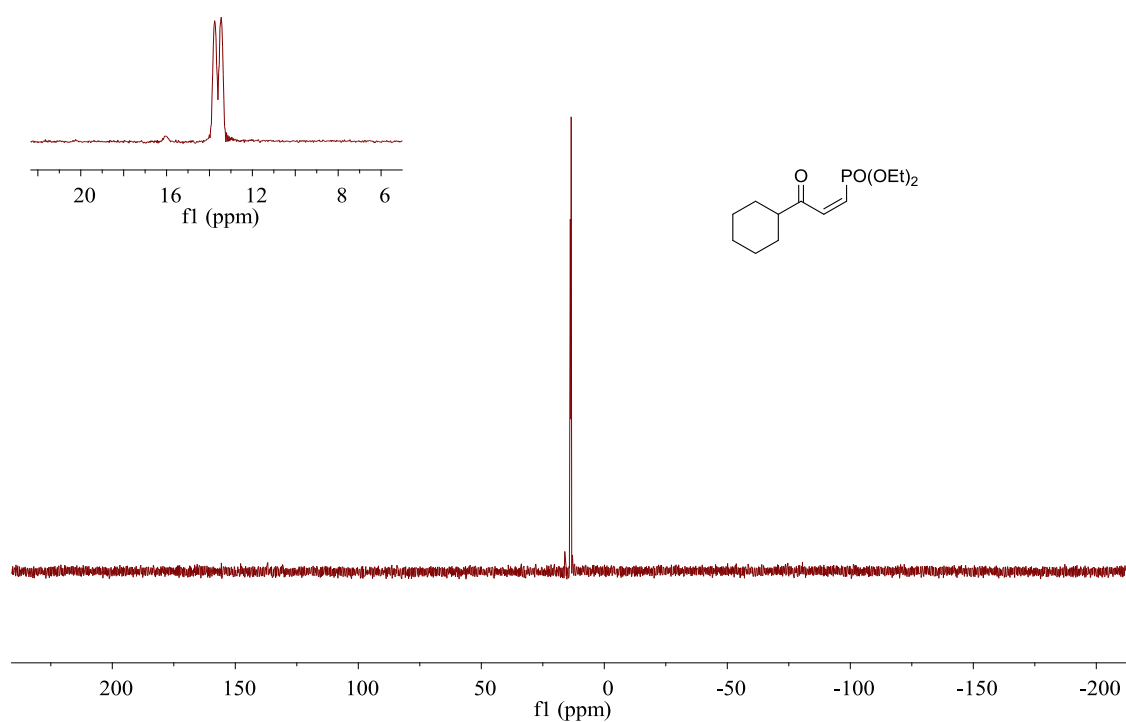


Figure S52: ^{31}P NMR spectrum for **6j** in C_6D_6

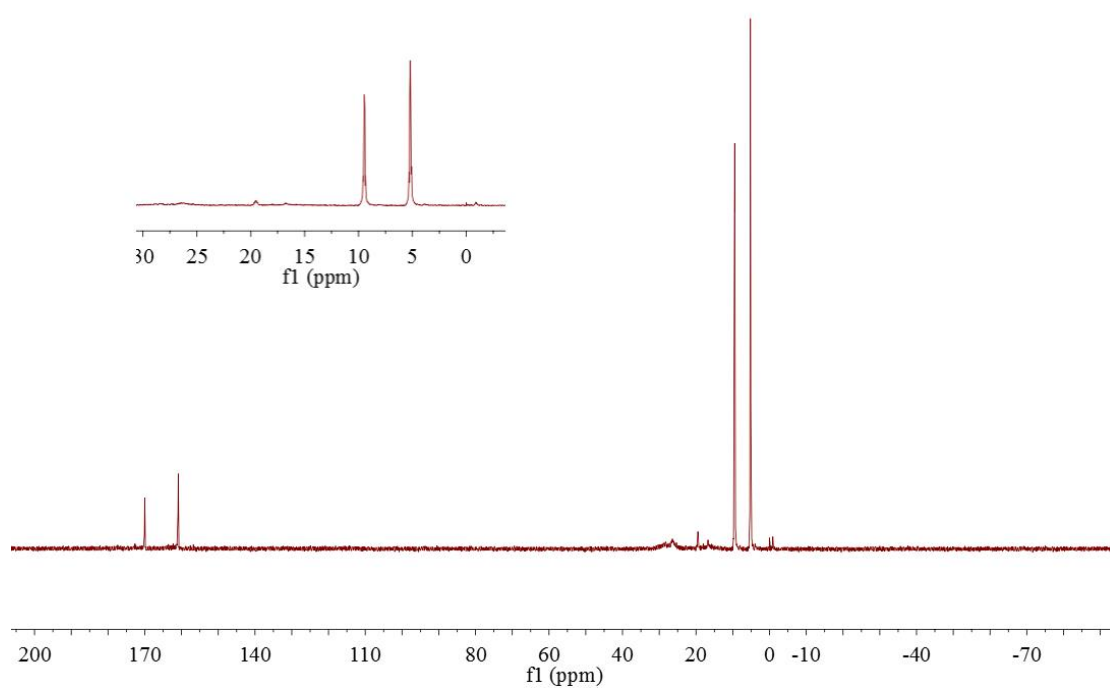


Figure S53: ^{31}P NMR spectrum for the crude product of hydrophosphonylation of phenylacetylene by following Kuramshin's method (in CDCl_3)

II. Computation details

Quantum chemical calculations were all performed at the density functional theory (DFT) level using the hybrid meta-GGA M06-2x functional,¹ which has been proven to give reliable results to the structural and energetic properties of non-covalent systems and reaction energy barriers.² The M06-2x functional has a mean absolute error in energy barriers of about 1.3 kcal/mol. The 6-31+G(d,p) basis set³ was employed in all the calculations. All the DFT calculations were performed with a pruned (99,590) integration grid.

Full geometry optimization were carried out in the dichloromethane solution which was modelled by the polarizable continuum solvation model (IEFPCM)⁴ with radii and non-electrostatic terms for Truhlar and coworkers' SMD solvation model.⁵ This solvation model is by far the most reliable one in predicting solvation free energies. The convergence criteria used for the geometry optimization are 4.50×10^{-4} au. for gradients, and 1.80×10^{-3} au. for displacements. Harmonic vibrational analyses were carried out to confirm if the optimized structure is a local minima or a first order transition state and to provide zero-point vibrational energy corrections and thermal corrections to various thermodynamic properties. Transition states were further confirmed by IRC calculations.⁶

NMR chemical shift of ^{31}P was calculated using the Gauge-Independent Atomic Orbital (GIAO) method⁷ using phosphoric acid as reference, for which the geometry was fully optimized in the water solution with the 6-31+G(d,p) basis set. To obtain accurate chemical shift, the ^{31}P chemical shifts of two known species (δ_1^{Cal} and δ_2^{Cal}) were computed by the same computational method. A scaling factor was obtained by the following Eq:

$$s = \left(\frac{\delta_1^{\text{Exp}}}{\delta_1^{\text{Cal}}} + \frac{\delta_2^{\text{Exp}}}{\delta_2^{\text{Cal}}} \right) / 2,$$

where δ_1^{Exp} and δ_2^{Exp} are the two experimental chemical shifts of the two known species. The final chemical shift of an unknown species was obtained by multiplying the directly computed chemical shift by the scaling factor s .

All the calculations were performed by using the Gaussian 09 program.⁷

The equation for the calculation of the ratio of Z-6i and E-6i:

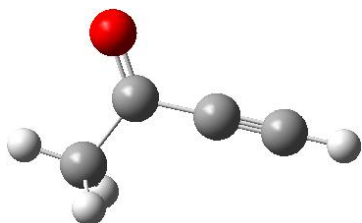
$$\begin{aligned} \frac{\frac{d[Z-6i]}{dt}}{\frac{d[E-6i]}{dt}} &= \frac{k_{Z-7 \rightarrow Z-6i}[Z-7]}{k_{E-7 \rightarrow E-6i}[E-7]} = \frac{k_{Z-7 \rightarrow Z-6i} \int_0^t [\text{IM1}] k_{\text{IM1} \rightarrow Z-7}}{k_{E-7 \rightarrow E-6i} \int_0^t [\text{IM1}] k_{\text{IM1} \rightarrow E-7}} = \frac{k_{Z-7 \rightarrow Z-6i}}{k_{E-7 \rightarrow E-6i}} \cdot \frac{k_{\text{IM1} \rightarrow Z-7}}{k_{\text{IM1} \rightarrow E-7}} \\ &= \frac{e^{-[-28.7 - (-53.7)] \cdot \frac{4180}{8.314 \cdot 298.15}}}{e^{-[-33.6 - (-55.1)] \cdot \frac{4180}{8.314 \cdot 298.15}}} \cdot \frac{e^{-0 \cdot \frac{4180}{8.314 \cdot 298.15}}}{e^{-6.1 \cdot \frac{4180}{8.314 \cdot 298.15}}} = 80.5 \end{aligned}$$

References:

1. a) Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101; b) Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A* **2006**, *110*, 5121.

2. Zhao, Y.; Truhlar, D. G. *Theo. Chem. Acc.* **2008**, *120*, 215.
3. a) McLean, A. D.; Chandler, G. S. *J. Chem. Phys.* 1980, *72*, 5639-5648. b) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. *J. Chem. Phys.* **1980**, *72*, 650-654.
4. Scalmani, G.; Frisch, M. J.; Map, V. *J. Chem. Phys.* **2010**, *132*, 114110.
5. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.
6. a) Hratchian, H. P.; Schlegel, H. B. *J. Chem. Phys.* **2004**, *120*, 9918-9924. (b) Hratchian, H. P.; Schlegel, H. B. *J. Chem. Theory and Comput.* **2005**, *1*, 61-69.
7. Wolinski, K.; Hilton, J. F.; Pulay, P. *J. Am. Chem. Soc.*, **1990**, *112*, 8251-60.
8. Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

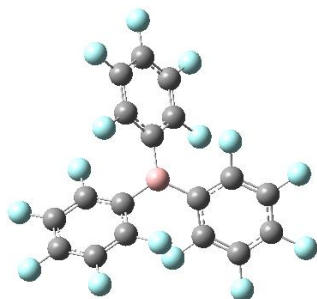
Geometries and Cartesian coordinates of the important intermediates and transition states involved in the reaction



5i

Charge = 0 Multiplicity = 1

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H,0,0.3438317407,-2.6222551592,-1.3385332293
H,0,4.4653933638,-0.6792446004,-0.8544111801
C,0,1.0078980772,-1.888753803,-0.9242370968
C,0,1.7509143924,-1.0588025923,-0.4566963485
C,0,2.6656638543,-0.062425226,0.1080109481
O,0,2.2384543793,1.0059325107,0.5012760676



B(C₆F₅)₃

Charge = 0 Multiplicity = 1

X

B,1,2.

C,2,r1,1,a1

C,2,r1,1,a1,3,120.,0

C,2,r1,1,a1,4,120.,0

C,3,r2,2,a2,1,d2,0

C,6,r3,3,a3,2,d3,0

C,7,r4,6,a4,3,d4,0

C,8,r5,7,a5,6,d5,0

C,9,r6,8,a6,7,d6,0

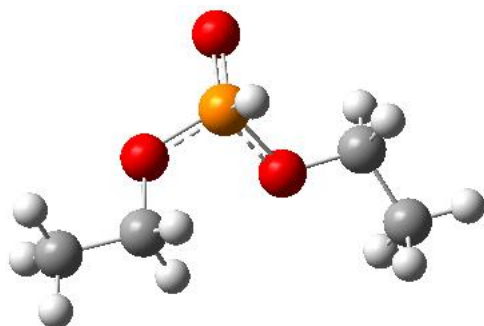
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C,12,r4,11,a4,4,d4,0
C,13,r5,12,a5,11,d5,0
C,14,r6,13,a6,12,d6,0
C,5,r2,2,a2,1,d2,0
C,16,r3,5,a3,2,d3,0
C,17,r4,16,a4,5,d4,0
C,18,r5,17,a5,16,d5,0
C,19,r6,18,a6,17,d6,0
F,6,r7,3,a7,2,d7,0
F,7,r8,6,a8,3,d8,0
F,8,r9,7,a9,6,d9,0
F,9,r10,8,a10,7,d10,0
F,10,r11,9,a11,8,d11,0
F,11,r7,4,a7,2,d7,0
F,12,r8,11,a8,4,d8,0
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F,14,r10,13,a10,12,d10,0
F,15,r11,14,a11,13,d11,0
F,16,r7,5,a7,2,d7,0
F,17,r8,16,a8,5,d8,0
F,18,r9,17,a9,16,d9,0
F,19,r10,18,a10,17,d10,0
F,20,r11,19,a11,18,d11,0

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a3=123.0737591
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r4=1.38667701
a4=119.19847219
d4=0.84493799
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a5=119.92813118
d5=-0.41195433
r6=1.38428994
a6=119.20062494
d6=-0.39779235
r7=1.34107419
a7=120.24544892

d7=0.39216588
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a8=120.89175527
d8=180.6748909
r9=1.32938813
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d9=-180.40774749
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d11=-179.97953845



(EtO)₂P(O)H

Charge = 0 Multiplicity = 1

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O,0,0.972898908,1.9393389201,-0.9873492234

O,0,-1.224656335,0.8981368647,-0.1540359459

O,0,0.8614231521,-0.4125634665,0.1607299191

C,0,-1.9848262473,0.0988436362,0.78474948

C,0,-3.4505336682,0.3644788542,0.5372574137

H,0,-1.6985730581,0.3787998768,1.805760887

H,0,-1.7316800491,-0.9522739693,0.6221591855

H,0,-4.0506960376,-0.2332166182,1.2293790119

H,0,-3.6840072313,1.4210776495,0.6950849252

H,0,-3.7232406802,0.0902975895,-0.485697714

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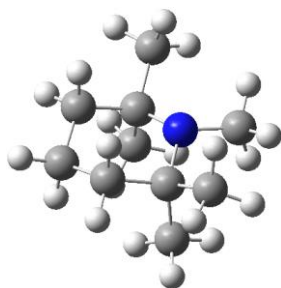
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H,0,2.778597489,-0.3529287113,-0.6188040179

H,0,3.5569102458,-2.3097274736,0.7258194987

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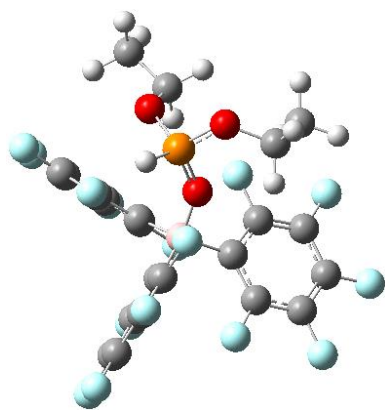
H,0,2.089226734,-2.7254390806,-0.1833887968



PMP

Charge = 0 Multiplicity = 1

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C,0,-2.155562194,-0.0409859652,0.
C,0,-1.4217039757,0.4515172126,-1.2391659015
C,0,0.0555981753,0.0273084193,-1.2774289774
H,0,-1.9081609266,0.088613842,2.1527826645
H,0,-2.2195916668,-1.1361116458,0.
H,0,-3.1866551608,0.3305858071,0.
H,0,-1.9081609266,0.088613842,-2.1527826645
H,0,-1.4643964478,1.5495845248,-1.2633092974
H,0,-1.4643964478,1.5495845248,1.2633092974
C,0,0.7094705194,0.8031768825,2.4329732338
H,0,0.063296189,0.7459687479,3.315482792
H,0,1.682068564,0.3922797384,2.720223364
H,0,0.836897809,1.8585341029,2.1683158195
C,0,0.1594477052,-1.4739333347,1.6170796091
H,0,1.1844917386,-1.8411757859,1.4984456833
H,0,-0.1243915181,-1.6297153799,2.6642129689
H,0,-0.496938706,-2.0961863258,1.0049541336
C,0,0.1594477052,-1.4739333347,-1.6170796091
H,0,-0.1243915181,-1.6297153799,-2.6642129689
H,0,1.1844917386,-1.8411757859,-1.4984456833
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H,0,0.063296189,0.7459687479,-3.315482792
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C,0,2.1472215341,0.2018546585,0.
H,0,2.598945862,0.6729512438,0.8744001747
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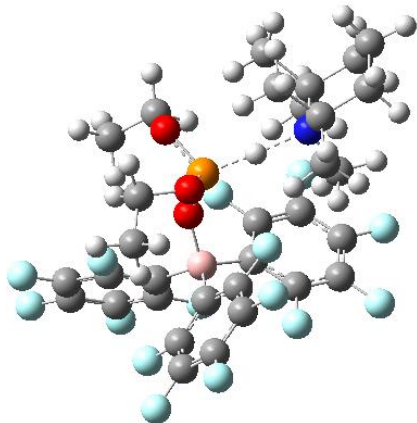


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H,0,1.4216095242,-0.2611232042,3.3138761522
H,0,1.076014277,-0.9129087034,4.9328715411
H,0,0.4888808476,1.5205034357,4.812175581
H,0,-0.6288170555,1.1963063819,3.4734161093
H,0,-0.9590599462,0.534884896,5.0949197218
C,0,-3.0737028894,-0.6394810151,2.0731638124
C,0,-4.476438833,-1.135862949,1.8229008326
H,0,-2.7853844659,0.149844977,1.3736265539
H,0,-2.9445624489,-0.2843449033,3.099956004
H,0,-5.176692555,-0.3027584729,1.9307707595
H,0,-4.5695886139,-1.5425526094,0.8113208451
H,0,-4.7458477565,-1.9144464303,2.5416016696
C,0,-1.1125094842,0.0619690853,-0.9723859771
C,0,1.4132077917,-0.8243326085,-0.8611608944
C,0,0.8155215008,1.6083218384,0.2245712497
C,0,-1.7882590618,1.1454761058,-1.5172068017
C,0,-1.7717916713,-1.1536649578,-1.1041547933
C,0,1.6642330587,-0.6413643002,-2.2159441885
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C,0,-3.0477614363,1.045409239,-2.0934424891
C,0,-3.0353119268,-1.3045156394,-1.649577542
C,0,2.5791741251,-1.3853446019,-2.9397562004
C,0,3.1069435996,-2.5856204465,-0.9396866313
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C,0,3.3062483838,-2.37355302,-2.2922491817
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F,0,-1.2435021354,2.0020403246,1.3265085433
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F,0,2.7778221923,-1.1567581214,-4.2426378971
F,0,3.8098306219,-3.5274612504,-0.2995377656
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F,0,-0.4755938783,4.415225229,2.1959789186
F,0,-4.902272353,-0.2914754308,-2.6783034702
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F,0,1.9830786959,5.3943691968,1.5293890716
P,0,-0.6166926865,-1.6615582424,1.9951902032
H,0,-0.1866322487,-2.9026100132,1.5643750276
O,0,-0.0227801928,-0.4634616681,1.2604185461
O,0,-0.2333694454,-1.5155916204,3.5127576466
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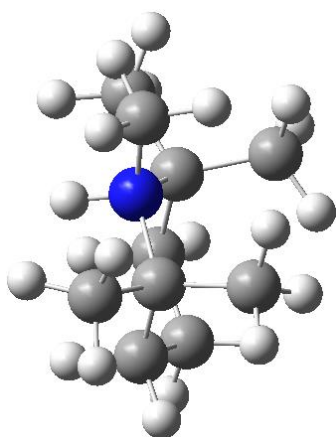
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H,0,0.9930341942,2.7205678699,-4.0224611559
H,0,1.4982647365,1.4602225658,-2.8771213472
H,0,1.1597447147,1.040490625,-4.5755534581
C,0,0.3419548094,-2.6120236308,-2.7246233024
C,0,1.0937052898,-3.7323373145,-2.0472278739

H,0,1.0189145614,-1.8086108125,-3.0264503774
H,0,-0.2060638709,-2.9614899009,-3.602825934
H,0,1.764449297,-4.2006357095,-2.7744671923
H,0,1.7005964198,-3.3522561397,-1.2205246163
H,0,0.4047209406,-4.494773312,-1.6705954316
C,0,1.4441553608,-1.3770412478,0.8744545646
C,0,0.3406544046,1.0842188881,1.3619891943
C,0,2.627895782,0.8637572499,-0.1171879738
C,0,2.6531174411,-2.0178713755,1.1088275008
C,0,0.3293361857,-2.1798176348,1.0736871213
C,0,-0.0430710763,0.7624396032,2.6560200929
C,0,-0.1576707266,2.2978465663,0.8980186612
C,0,3.2137252737,1.9917730987,0.4347469831
C,0,3.3005553569,0.3340842825,-1.2133736964
C,0,2.7498586879,-3.3547756975,1.4812088033
C,0,0.3666167509,-3.5144250342,1.4292107086
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C,0,4.9850435641,2.0239752003,-1.1795248497
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H,0,-6.5700413394,-1.9259011581,-0.5332541641
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H,0,-4.8465039027,-2.7352512571,-2.2232241034
H,0,-4.9167076808,-1.0928440898,-2.8336358011
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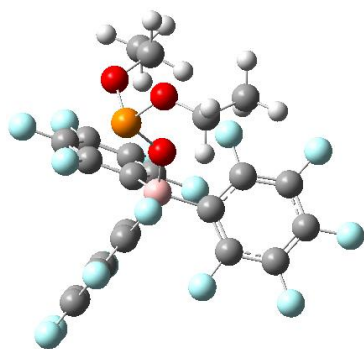
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H,0,-4.2419683338,0.4880102919,1.6051385555
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N,0,-3.6770560714,-0.0572092785,-0.4064585365



[HPMP]⁺

Charge = 1 Multiplicity = 1

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C,0,-1.4473381325,0.4071269865,-1.2438931207
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H,0,-1.9306221829,0.039843414,2.1550427345
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H,0,1.2359332656,-1.8159163075,1.5134281428
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H,0,-0.4345506509,-2.1184891249,0.9869233255
C,0,0.198016748,-1.4859549037,-1.6092494133
H,0,-0.0983337481,-1.6487125051,-2.6500435716
H,0,1.2359332656,-1.8159163075,-1.5134281428
H,0,-0.4345506509,-2.1184891249,-0.9869233255
C,0,0.6903408307,0.8061747258,-2.455316589
H,0,1.6701926774,0.41041263,-2.7326895736
H,0,0.0463603078,0.7375031405,-3.3364853147
H,0,0.7883845136,1.8668754972,-2.1963995649
N,0,0.7039308377,0.4365122908,0.
H,0,0.5878025737,1.4588567891,0.
C,0,2.1800878145,0.2099891324,0.
H,0,2.3899753016,-0.8566280183,0.
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H,0,2.6088878357,0.6755907246,0.8841311736

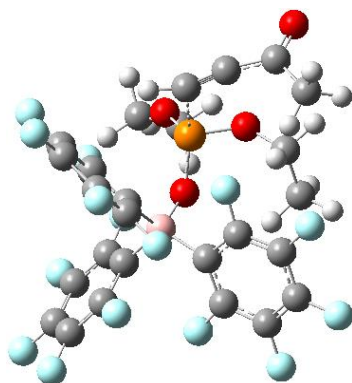


[B(C₆F₅)₃-O-P(OEt)₂]⁻

Charge = -1 Multiplicity = 1

C,0,0.8932803435,1.7803182391,3.6385240897
 C,0,0.2472452814,3.0883750975,3.2230960777
 H,0,1.6032923902,1.4468333159,2.8758831133
 H,0,1.4370158127,1.903804023,4.5810593962
 H,0,1.0100006811,3.869785767,3.129027386
 H,0,-0.2623527754,2.9805859928,2.2616399232
 H,0,-0.4843311504,3.411330343,3.9718232941
 C,0,-2.7725955498,0.8603483876,2.7422749102
 C,0,-3.9112908945,0.6959312481,1.7570136566
 H,0,-2.0858083551,1.639439963,2.3988313363
 H,0,-3.1466672367,1.1410685229,3.7330315187
 H,0,-4.5215893433,1.6051424334,1.7369413345
 H,0,-3.5244624732,0.5227375261,0.7481667686
 H,0,-4.5529626878,-0.1453869873,2.038154826
 C,0,-1.2894024874,-0.5141672008,-0.6290689847
 C,0,1.2443796311,-1.2462126922,-0.0523691515
 C,0,0.7315864533,1.361435665,-0.6371266784
 C,0,-2.0111955652,0.1179428417,-1.6323952118
 C,0,-1.9109850475,-1.6462981221,-0.1129680195
 C,0,1.2830483203,-2.1450193422,-1.1108867071
 C,0,2.2356630588,-1.4450754423,0.8995387054
 C,0,1.9381390968,1.5248298939,-1.2988083159
 C,0,0.0189787817,2.5416054863,-0.440479542
 C,0,-3.262754556,-0.3046772532,-2.0655551805
 C,0,-3.1558234693,-2.108113431,-0.5067755809
 C,0,2.1882444666,-3.1898375973,-1.2094699143
 C,0,3.1606395303,-2.4788458313,0.8509663033
 C,0,2.427895396,2.760614691,-1.7120987236
 C,0,0.4681214769,3.792988544,-0.8216052415
 C,0,-3.8429387939,-1.4246588612,-1.496567702
 C,0,3.1350767149,-3.3622316191,-0.2136219718
 C,0,1.6916584122,3.9030095626,-1.4669439335
 F,0,-3.6970502442,-3.1992345364,0.052275281

F,0,-1.5235383367,1.2054832004,-2.2677648209
F,0,-1.283976671,-2.3765252094,0.8381600504
F,0,0.4191280435,-2.018105659,-2.1435135666
F,0,2.3719395454,-0.5929782852,1.943674567
F,0,2.7326846407,0.4701196306,-1.5844280252
F,0,-1.2040044925,2.4990554142,0.1311947922
F,0,-3.9102702655,0.3599379498,-3.0333767902
F,0,2.163854495,-4.0267710211,-2.2564701791
F,0,4.08512879,-2.6190832949,1.8116622405
F,0,3.6098355749,2.8499397124,-2.3394854422
F,0,-0.2644232852,4.8923460484,-0.592103072
F,0,-5.0467493637,-1.8457913316,-1.9012458985
F,0,4.0192207633,-4.3638064443,-0.2855774354
F,0,2.1466949184,5.1016704304,-1.8499927038
P,0,-0.4259535392,-0.4493476775,2.7913665152
O,0,-0.1186672353,0.3781353333,1.4395116684
O,0,-0.0916340174,0.769827326,3.8771229482
O,0,-2.0711105336,-0.385316018,2.8812543397
B,0,0.1445807508,-0.0204387322,0.0400657505



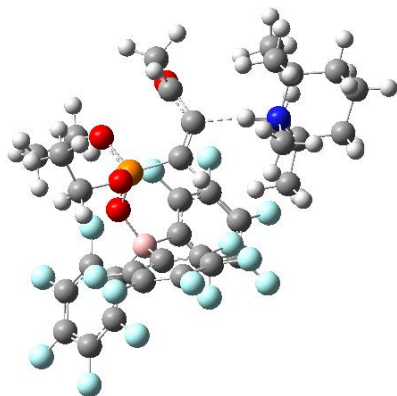
TS2

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H,0,-3.0723376294,0.5744054211,-1.0627752301
H,0,-3.9958589377,0.3566097665,-2.5541342244
H,0,-2.8977589902,2.5861082939,-2.555913287
H,0,-1.3023971883,1.8219550067,-2.3441651886
H,0,-2.2239759948,1.5677686939,-3.8445202547
C,0,-0.1127136025,-1.9364108645,-3.8651797659
C,0,0.9361627358,-2.8841956156,-4.4011978467
H,0,0.2843149947,-0.9218231892,-3.7670034408
H,0,-0.994929932,-1.9100751303,-4.5115863597

H,0,1.252993516,-2.5595633447,-5.3976136159
H,0,1.8103977777,-2.9013938833,-3.7451675227
H,0,0.5349313713,-3.8992235804,-4.4811467315
C,0,-0.1901115713,1.705058459,0.2714916481
C,0,2.1455570465,0.3664488955,-0.2760352345
C,0,0.39133755,-0.8144551056,1.2404306108
C,0,-1.5261069709,1.7130123011,0.6532412059
C,0,0.3230414115,2.9594718128,-0.0194255102
C,0,2.9430016179,0.9552749018,0.6980256525
C,0,2.8395797558,-0.1619172051,-1.3539999831
C,0,0.0093548475,-0.5212943477,2.5431663877
C,0,0.7462116986,-2.1435269822,1.0367023645
C,0,-2.3168054943,2.8448394305,0.7265818058
C,0,-0.4236473335,4.1316438332,0.0497134816
C,0,4.3204089532,1.0533783306,0.6224857602
C,0,4.2243755251,-0.0911419843,-1.4734122996
C,0,-0.0807882966,-1.473703953,3.5505519756
C,0,0.6657898969,-3.1322624947,2.0041970024
C,0,-1.7538945596,4.075599071,0.4230320816
C,0,4.968975539,0.5208876837,-0.4821600773
C,0,0.2402421957,-2.7926015455,3.2780570399
C,0,-5.4980656412,-0.3412021338,0.1014460441
H,0,-6.2735872533,-0.6239355826,0.8233563652
H,0,-4.6983162986,0.1727856575,0.6393029077
H,0,-1.8872046619,-2.97413748,0.6811220491
H,0,-5.9503684473,0.3303283985,-0.6343736455
F,0,0.1331571849,5.3124611371,-0.2519655759
F,0,-2.1373601536,0.5385648001,0.9454500686
F,0,1.6002803108,3.1135261606,-0.4306565572
F,0,2.349717204,1.4869749634,1.7916187782
F,0,2.2052407034,-0.7847981442,-2.3666428136
F,0,-0.3144999037,0.7362425593,2.9051861257
F,0,1.1830434534,-2.5354511898,-0.1832713856
F,0,-3.6096188287,2.7620975166,1.0723718687
F,0,5.0300564479,1.6509874346,1.5899169483
F,0,4.8427416446,-0.6140266127,-2.5424759392
F,0,-0.4750587749,-1.127611959,4.7829171256
F,0,0.970177317,-4.4053183949,1.7157445734
F,0,-2.4895013836,5.1901866349,0.4868645576
F,0,6.3007816367,0.598364423,-0.5852170187
F,0,0.1441438277,-3.7245715697,4.2310352308
P,0,-1.195318123,-1.416708905,-1.4826911071
O,0,-0.1518287095,-0.2298765881,-1.2534341507
O,0,-2.2912956597,-0.7324846926,-2.4843147834

O,0,-0.5245796235,-2.4145463428,-2.5658909232
B,0,0.5315617927,0.2526355696,-0.0167921503
C,0,-2.6129796109,-2.4400630465,0.094003652
C,0,-3.8094985535,-2.1592119995,-0.1085466274
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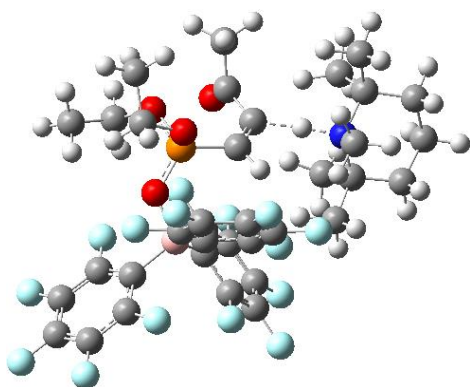
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C,0,-3.1144506194,0.7567223825,0.0837173147
C,0,-2.3698006695,-2.0303665735,-1.3354266528
C,0,-0.4977896861,-1.0332470373,-2.3022392363
C,0,-0.6389728578,2.2025657911,-1.3978852423
C,0,0.1990084595,1.934999297,0.7681323347
C,0,-4.1257908407,0.7676689416,-0.8660684859
C,0,-3.4249206382,1.3996176983,1.2768256105
C,0,-2.273400551,-3.1187305502,-2.183413834
C,0,-0.3560479323,-2.1055304729,-3.1757908819
C,0,0.1336130698,3.3329830582,-1.5960579823
C,0,0.9843085755,3.0725985957,0.6231284494
C,0,-5.3712632215,1.3422972355,-0.6489926204
C,0,-4.6555560127,1.9799672384,1.5416381879
C,0,-1.2482570378,-3.1592845009,-3.1169376131
C,0,0.9623164116,3.7668276904,-0.5718686268
C,0,-5.6385220334,1.9506776628,0.5654211848
C,0,-0.5523750845,-0.8676235524,3.9416907043
C,0,-1.9040154383,-1.4322423564,4.3122316964
H,0,-0.6296601186,0.1439639117,3.5456578236
H,0,0.139118468,-0.8736145145,4.785272775
H,0,-2.3371727982,-0.8244078781,5.1130852963

H,0,-2.5869346643,-1.4069343959,3.4569027866
H,0,-1.8149606062,-2.4628198844,4.6701861124
C,0,-1.5497904173,-3.8159944411,1.3963375249
C,0,-1.0427873143,-4.8505037511,2.3749163818
H,0,-2.0221166223,-4.2817588622,0.5288040367
H,0,-2.2690075052,-3.1322507023,1.8571921619
H,0,-1.8864759072,-5.4412039105,2.745318326
H,0,-0.3348127528,-5.5262375081,1.8861754093
H,0,-0.5471062519,-4.3751037125,3.2262267463
C,0,3.2754358437,-2.0917173234,3.281827932
H,0,2.863918987,-2.1789600305,4.2918544287
H,0,2.9946585505,-2.9688019297,2.6918757333
H,0,1.3690349862,-1.1923072392,-0.4982866279
H,0,4.369167693,-2.0595069218,3.3660056875
C,0,5.9489518786,-0.5289745518,-0.0214924767
C,0,7.0647859225,-0.0669719881,-0.9658362325
C,0,6.9737312944,1.4089702829,-1.344401879
C,0,5.6089849337,1.712134738,-1.9550063268
C,0,4.4307958226,1.3324789719,-1.0508229162
H,0,8.0175329565,-0.2855087633,-0.4699418577
H,0,7.1557336919,2.0464970579,-0.4719332599
H,0,7.7583895836,1.6468443693,-2.0695035283
H,0,5.5115449842,2.7797893467,-2.1825995638
H,0,5.5113845215,1.1746802406,-2.9078051971
H,0,7.0364329318,-0.675878822,-1.8789745314
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H,0,6.937452753,-2.289802845,0.6775007159
H,0,5.1728432861,-2.4313649753,0.7321102185
H,0,6.0499707752,-2.581221459,-0.8142209706
C,0,6.1045260378,0.0789745059,1.3828840424
H,0,5.1667871289,0.0498978016,1.9466239804
H,0,6.8421048376,-0.5145710508,1.9302237059
H,0,6.4681849394,1.1050594364,1.3738689118
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C,0,3.1214152374,1.5190884368,-1.8257601425
H,0,2.2555768041,1.1735601627,-1.2468259509
H,0,3.003937221,2.5913685651,-2.0093824652
H,0,3.1241794379,1.0262134717,-2.8005126517
F,0,-3.3708491125,-2.0702686302,-0.4288496429
F,0,0.4557657265,-0.0812751765,-2.4148096156
F,0,-1.444389301,1.822401353,-2.4137615844

F,0,0.2836478709,1.3268802941,1.9672982981
 F,0,-3.9413457977,0.1996952334,-2.0757024076
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 F,0,-3.137150935,-4.1384873558,-2.0940421169
 F,0,0.6566612912,-2.1322246287,-4.052993455
 F,0,0.1114136408,3.9936624078,-2.7606483863
 F,0,1.7806250523,3.4842530169,1.6185038126
 F,0,-6.3120028622,1.315031185,-1.601498276
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 F,0,-1.1240900346,-4.2021800275,-3.9408318355
 F,0,1.7649960401,4.821112528,-0.7550752894
 F,0,-6.8294989455,2.5127460875,0.7930443122
 P,0,-0.1028056263,-1.5939201136,1.3887086338
 O,0,-1.3166361627,-0.6544511049,1.1508337926
 O,0,0.0943546738,-1.7162308228,2.9468483289
 O,0,-0.4283629091,-3.056101235,0.8622628198
 C,0,1.4137003209,-1.1529020461,0.5915126638
 C,0,2.5309862606,-0.8260996391,1.2548370948
 C,0,2.7846376807,-0.790317216,2.6673857973
 O,0,2.7937245831,0.2479585372,3.3410290606
 H,0,3.8504423864,-0.3246095945,0.1739805551
 N,0,4.5779816062,-0.1422337768,-0.6213975766
 B,0,-1.6134364833,0.1434473437,-0.1179282893
 C,0,4.1495948593,-1.0908803932,-1.6881154787
 H,0,4.8507410252,-1.079177715,-2.5246909379
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TS3'

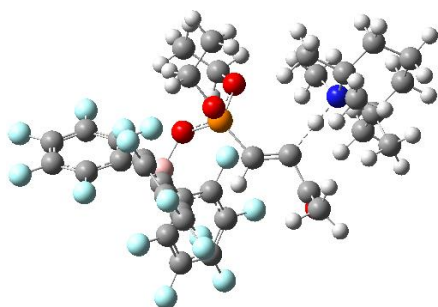
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C,0,-2.3242610961,1.9381157476,1.4409328848
C,0,-0.5085152095,0.7756773876,2.3269689912
C,0,-0.7439318702,-2.3426641448,1.0950450102
C,0,0.1268787824,-1.8860729232,-1.0254950449
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C,0,-4.7166297114,-1.6750350854,-1.8506586841
C,0,-1.187371371,2.8408736864,3.3378383656
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C,0,-0.4809213193,1.2569735244,-3.9048562309
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H,0,-1.6732824151,2.9725062144,-4.4564205638
C,0,-1.3793254672,3.9780948902,-1.0808801153
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C,0,5.854799999,0.4186855056,-0.0161624783
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C,0,5.5137881632,-1.9713235382,1.7118423559
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H,0,6.4233947711,-1.0861836669,-1.5343696591
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C,0,3.0310196343,-1.7585738211,1.5934185511
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H,0,2.9110124732,-2.8429854209,1.6784320374
H,0,3.029683736,-1.3576781361,2.6095339254
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F,0,-1.5498410456,-2.0416800433,2.1365097531
F,0,0.2463442127,-1.1624506557,-2.1564242611
F,0,-4.003681441,-0.2809967506,1.9327726223
F,0,-2.520338609,-1.221472462,-2.4700572525
F,0,-3.0208342527,3.9906205235,2.3944802366
F,0,0.6619566846,1.6514716817,4.1888707182
F,0,-0.0635119599,-4.2827083441,2.2778585197
F,0,1.6737186248,-3.3874256561,-2.0125536868
F,0,-6.4092383842,-1.2395705859,1.3135238255
F,0,-4.9587329059,-2.151642712,-3.0785233261
F,0,-1.0347369612,3.7925894492,4.2608698316
F,0,1.5902493974,-4.9553852591,0.214231339
F,0,-6.9260761133,-2.1808567344,-1.1935104904
P,0,-0.0496336425,1.6933530428,-1.2829778632
O,0,-1.2953600239,0.7800501716,-1.1557714337
O,0,0.1859662029,1.9652766838,-2.8156155598
O,0,-0.3129878748,3.1032686729,-0.6090031267
C,0,1.4321007983,1.1042383756,-0.5173018135
C,0,2.5575307521,0.8166987087,-1.1873068473
C,0,2.7809551407,0.9562289759,-2.6216609427
O,0,2.7407754402,-0.0009059234,-3.3928532128
H,0,3.6601417083,0.3142818309,-0.324754218
N,0,4.4907511748,-0.004629816,0.5399853176
B,0,-1.6381757488,-0.1344179758,0.0242249022
C,0,4.0799695206,0.8465460479,1.6837416934

H,0,4.7952999377,0.7989346856,2.5098928317
H,0,3.9830223436,1.8762902147,1.3439377837
H,0,3.1007771216,0.5341508459,2.0373314906



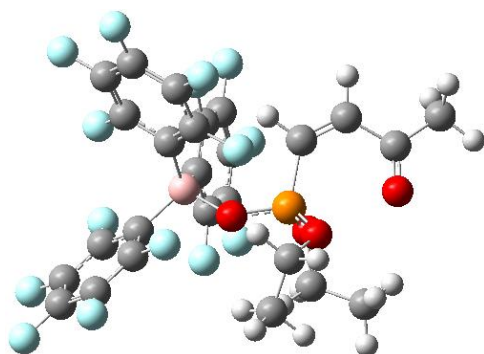
TS3

Charge = 0 Multiplicity = 1

C,0,-1.8289719021,1.0828945477,1.3505171327
C,0,-1.6070700119,-1.5400415124,0.52006268
C,0,-3.242336908,0.035402771,-0.770427708
C,0,-2.0878787434,2.4230179369,1.0764365519
C,0,-1.3874629116,0.8431471172,2.6437064929
C,0,-2.4762638526,-2.11683397,1.4390096307
C,0,-0.6600556732,-2.4078655115,-0.0035340497
C,0,-4.464573959,0.5497917616,-0.363689366
C,0,-3.247386158,-0.5695278196,-2.0224656541
C,0,-1.9112677445,3.453132741,1.9824188719
C,0,-1.1945106542,1.8416116664,3.5916326282
C,0,-2.3998433436,-3.4312317825,1.8617619369
C,0,-0.5375350168,-3.7339175565,0.3933398881
C,0,-5.6072575959,0.5100876548,-1.1515454013
C,0,-4.3601716214,-0.6267256196,-2.8464807137
C,0,-1.4558998072,3.1579833983,3.2588770161
C,0,-1.4110264354,-4.2491019753,1.3341943887
C,0,-5.5535953022,-0.0796207656,-2.403045303
C,0,0.8444555125,0.1242683626,-3.1527664688
C,0,-0.0663166227,1.0491021702,-3.9261541429
H,0,0.3203778646,-0.7648824509,-2.8042202267
H,0,1.7110074172,-0.1745213106,-3.7451564558
H,0,-0.4190764511,0.5295899836,-4.8228917153
H,0,-0.9383295066,1.3321194958,-3.3291711879
H,0,0.467627398,1.9527822097,-4.2370032774
C,0,0.2887734287,3.5175924281,-1.0918180894
C,0,1.4501833806,4.1891705961,-1.7869548109
H,0,-0.2476836327,4.2091780187,-0.4393048899
H,0,-0.4225466121,3.0916018251,-1.8057841949

H,0,1.0702801264,5.0105135662,-2.402922445
H,0,2.1522807978,4.6010315653,-1.0560902519
H,0,1.9815485545,3.4853921705,-2.4342428522
C,0,3.3016586917,-0.5666364871,3.2053275894
H,0,3.7845182645,-1.2478316518,3.9102205422
H,0,3.9383585149,0.3038195815,3.0167730007
H,0,0.7089567125,-0.1475952581,1.5189803139
H,0,2.3673219239,-0.1937947271,3.6462806088
C,0,5.781224786,-1.4041894079,-0.6051393086
C,0,7.0608254208,-1.2948267004,-1.4518310565
C,0,7.7074733433,0.0894881597,-1.404927856
C,0,6.6963886334,1.1665051665,-1.793886148
C,0,5.4341189724,1.1355607524,-0.9223748383
H,0,7.7579079196,-2.060198244,-1.0907830005
H,0,8.1103710806,0.2938775002,-0.4060607466
H,0,8.5593665001,0.1163588086,-2.0919239934
H,0,7.1403244556,2.1657587004,-1.7154295403
H,0,6.4040939057,1.0299073758,-2.8439810951
H,0,6.8315720599,-1.548801314,-2.4945539653
C,0,5.0916805346,-2.7458638812,-0.8909911004
H,0,5.7553885366,-3.5439585879,-0.5467551659
H,0,4.1468544945,-2.8318566396,-0.3405450913
H,0,4.907009953,-2.9123018353,-1.9539590318
C,0,6.1344701062,-1.3931956091,0.8989990431
H,0,5.3706112848,-0.9082913994,1.5077911534
H,0,6.227965037,-2.4241986899,1.2506281996
H,0,7.0868373951,-0.8995880669,1.1028065278
C,0,5.7410739823,1.5476622454,0.5261032177
H,0,6.004645412,2.609208537,0.5256126033
H,0,4.8548734414,1.4253092932,1.1595389287
H,0,6.571483952,1.0130535903,0.9800294647
C,0,4.4164640378,2.1668934118,-1.431355064
H,0,3.4488641023,2.0425715985,-0.9321121821
H,0,4.7916810152,3.1657492933,-1.1913428579
H,0,4.2647593793,2.1330939568,-2.5127094428
F,0,-2.5089405796,2.7775240281,-0.1578067583
F,0,-1.0600282694,-0.4044929169,3.0487761718
F,0,-3.4466255811,-1.3481910983,1.9814248959
F,0,0.2187179976,-2.0051599302,-0.9510323884
F,0,-4.5990473578,1.1340515573,0.8437775182
F,0,-2.1241886066,-1.1609587764,-2.4850300495
F,0,-2.1514829123,4.7237121328,1.6344356725
F,0,-0.7348518534,1.5382589277,4.8116691793
F,0,-3.255848511,-3.9189266072,2.7679360723

F,0,0.4213910774,-4.5123210499,-0.1254781333
F,0,-6.7592801777,1.033974571,-0.7141908578
F,0,-4.3009845303,-1.2173945996,-4.047057923
F,0,-1.2656628217,4.1338426503,4.1498197632
F,0,-1.3091082715,-5.5220224882,1.7265269088
F,0,-6.6439069404,-0.1249701442,-3.1743213295
P,0,0.6818641506,0.9380370086,-0.61072199
O,0,-0.7833749201,0.511526779,-0.8631910141
O,0,1.4192894365,0.8144559975,-1.9998694364
O,0,0.7791820961,2.4667124051,-0.2064157592
C,0,1.4246967419,0.0365530824,0.7123707583
C,0,2.6756188836,-0.4567151733,0.7347080571
C,0,2.9587351177,-1.2867953682,1.9229572746
O,0,2.9205346063,-2.5104808224,1.8591398162
H,0,3.8535110791,-0.3045362898,-0.180684685
N,0,4.8233393338,-0.2640667628,-0.9707796941
B,0,-1.8599866431,0.0196684668,0.0992434166
C,0,4.1607402396,-0.5495067997,-2.267908918
H,0,4.8713996391,-0.8754029773,-3.0306071473
H,0,3.4089227026,-1.3267355645,-2.111382038
H,0,3.6400603649,0.3334585533,-2.61723358



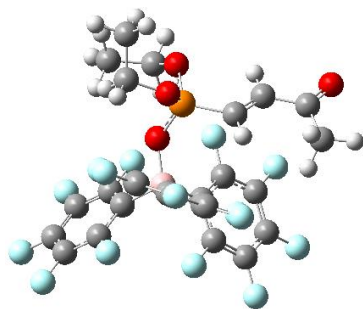
Z-7

Charge = 0 Multiplicity = 1

C,0,-1.882031866,-0.9864577142,-1.286208111
C,0,-1.5781834551,1.628121427,-0.4686303866
C,0,-3.2143275107,0.0950450924,0.8723647247
C,0,-2.1517010517,-2.3237513076,-1.0125090392
C,0,-1.4930177496,-0.7350989516,-2.5940954841
C,0,-2.5264028961,2.2715492418,-1.255920544
C,0,-0.535389212,2.436187044,-0.0440647291
C,0,-4.4518655533,-0.4256900328,0.5233258712
C,0,-3.1733926147,0.7328486106,2.1077750015
C,0,-2.0364617494,-3.3455316611,-1.9366237992

C,0,-1.3710023185,-1.7247015475,-3.562567356
C,0,-2.4624965178,3.6061159912,-1.6116920703
C,0,-0.4227714764,3.7817175661,-0.3749732168
C,0,-5.5685598266,-0.3531550257,1.3455286055
C,0,-4.2597124415,0.8256685824,2.9635968139
C,0,-1.6427268797,-3.0397827236,-3.2309800402
C,0,-1.3962541644,4.3717448507,-1.1598484937
C,0,-5.4708149749,0.2755162872,2.5750204264
C,0,0.9142303468,-0.0318508324,3.1280474189
C,0,-0.0055750149,-0.8598145356,3.9934279269
H,0,0.4167515428,0.855222929,2.7384494164
H,0,1.820241796,0.2594322175,3.6603726604
H,0,-0.2864829989,-0.27045296,4.8723606525
H,0,-0.920890236,-1.1265258151,3.4555664523
H,0,0.4943924468,-1.7713212411,4.3360392366
C,0,0.1029760847,-3.5602985466,1.4156587564
C,0,1.3345699327,-4.1618416896,2.0496037768
H,0,-0.4882073625,-4.3043956765,0.8804829551
H,0,-0.5437338068,-3.0652788424,2.1456455963
H,0,1.0225266552,-4.9127614902,2.7826892939
H,0,1.9569075341,-4.6499266052,1.294795236
H,0,1.9319513483,-3.3997471803,2.5566176222
C,0,4.6051076088,-2.1606321332,-1.6374893295
H,0,5.199960298,-2.9214536711,-1.130466648
H,0,4.2218051642,-2.5523871676,-2.5871176855
H,0,0.7639864399,0.4042611818,-1.2826581493
H,0,5.2309720658,-1.2927232956,-1.876525136
F,0,-2.50753906,-2.6815592297,0.2406456883
F,0,-1.1573789097,0.5117954545,-2.9912395844
F,0,-3.5690188348,1.5532850492,-1.7266265787
F,0,0.4720423264,1.9438417168,0.7215850862
F,0,-4.6304373645,-1.0443183437,-0.660856665
F,0,-2.0291293796,1.3216390766,2.5210804022
F,0,-2.2725848252,-4.6170777826,-1.5902259616
F,0,-0.970285834,-1.4168511126,-4.8021654274
F,0,-3.4059993051,4.1658014041,-2.3771442943
F,0,0.6146466944,4.5051284106,0.0632412148
F,0,-6.7362467102,-0.883159918,0.9603641178
F,0,-4.1571030716,1.4506019265,4.1435351982
F,0,-1.5111463135,-4.0074588453,-4.1406227053
F,0,-1.3120019992,5.6640059593,-1.4861500058
F,0,-6.5352005159,0.3554985221,3.378473078
P,0,0.6117027808,-1.0589334338,0.6772336713
O,0,-0.7655132356,-0.4061420603,0.9059121378

O,0,1.4213236257,-0.8179917234,2.0002725626
O,0,0.4870722874,-2.5972900495,0.3863846802
C,0,1.3637197955,-0.3636259456,-0.7982903357
C,0,2.5341341696,-0.6982469227,-1.3477769934
C,0,3.4609517144,-1.7275373709,-0.7722906229
O,0,3.2592164407,-2.1603080345,0.3464357306
H,0,2.8416796025,-0.208267859,-2.2691618946
B,0,-1.8588869249,0.0744801774,-0.0401982442

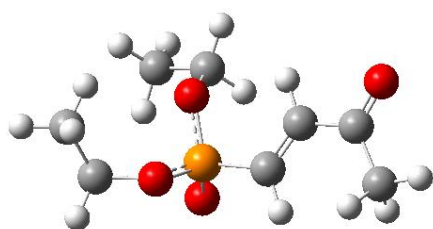


E-7

Charge = 0 Multiplicity = 1

C,0,-2.0435831302,-1.0734645367,-1.1759518978
C,0,-1.6479345028,1.5632245218,-0.4654259849
C,0,-3.295154817,0.1210425943,0.9676949564
C,0,-2.3632483417,-2.3853214322,-0.8360280674
C,0,-1.6605699688,-0.9044420901,-2.4989240859
C,0,-2.4993076654,2.1480532681,-1.3962963478
C,0,-0.653631771,2.4028998838,0.0140592892
C,0,-4.5588930222,-0.3554368215,0.6497855144
C,0,-3.204912372,0.7750047773,2.191611171
C,0,-2.3100941286,-3.452911265,-1.7137515601
C,0,-1.5922265269,-1.9437805821,-3.4199636333
C,0,-2.360792022,3.4388397623,-1.8726856713
C,0,-0.4641124035,3.7019977511,-0.4417237406
C,0,-5.6541056128,-0.2290367884,1.4938465418
C,0,-4.2675815325,0.9187543551,3.0691515298
C,0,-1.9179243011,-3.2285414451,-3.0253914437
C,0,-1.3208165938,4.2237099859,-1.394168169
C,0,-5.5063505644,0.4099804474,2.713256599
C,0,1.0126494512,-0.1198393318,3.1177224346
C,0,0.2510101534,-1.1152591474,3.9589159598
H,0,0.4073531502,0.7504884473,2.8657152555
H,0,1.9378940741,0.2006937314,3.5963649466
H,0,0.0051515547,-0.6501197583,4.9188161301
H,0,-0.6857907921,-1.4083301456,3.4742143258
H,0,0.8534709122,-2.0080567033,4.1525740289

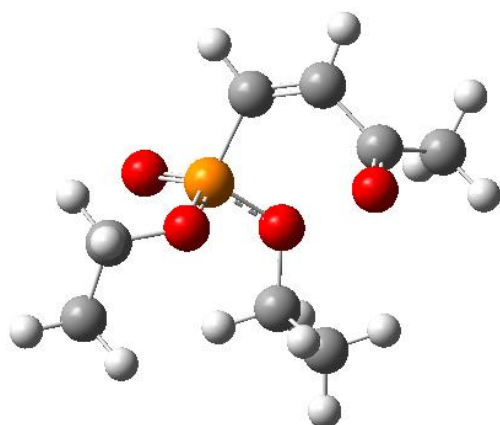
C,0,0.1928449287,-3.5243000594,1.0735005776
C,0,1.4125707717,-4.2031411032,1.6486299232
H,0,-0.3950153699,-4.1991105864,0.4488521003
H,0,-0.4574780335,-3.1095400096,1.8488445895
H,0,1.091674419,-5.0269210458,2.2935530092
H,0,2.0382029888,-4.6111151229,0.8497124634
H,0,2.0079892203,-3.5053865874,2.2445078743
C,0,2.3049444462,1.4097677902,-3.1408876374
H,0,2.8837461066,2.0058422187,-3.8476820181
H,0,2.2811737385,0.366188777,-3.4733660545
H,0,0.8997859384,-0.3644239038,-1.7783636782
H,0,1.2707689561,1.772712893,-3.1152489859
F,0,-2.7179646778,-2.6716319224,0.4355324931
F,0,-1.2704901205,0.3028742807,-2.9637593247
F,0,-3.5144220677,1.4115795094,-1.8954437347
F,0,0.2189412552,1.9938925777,0.9667306375
F,0,-4.7829591414,-0.9856080672,-0.5201819617
F,0,-2.0309298335,1.326121245,2.569238578
F,0,-2.6040125421,-4.6935625967,-1.3061489695
F,0,-1.18714407,-1.7115745717,-4.6741625204
F,0,-3.2031225289,3.9318263002,-2.7872343928
F,0,0.5523461128,4.4404221376,0.0232181184
F,0,-6.8491106346,-0.7173562917,1.1405845539
F,0,-4.1173286093,1.5542421804,4.2379162475
F,0,-1.8439897897,-4.2409955285,-3.8908421148
F,0,-1.1535886225,5.4686193538,-1.8459049176
F,0,-6.5498651091,0.5389813827,3.536972385
P,0,0.5725310666,-0.938147985,0.5988823278
O,0,-0.8473320366,-0.4607776472,0.9525457495
O,0,1.4700894076,-0.7404890431,1.8686562146
O,0,0.6143849208,-2.4506216286,0.1709570242
C,0,1.306199457,-0.1152681233,-0.7997204104
C,0,2.29998873,0.7611545547,-0.6364303776
C,0,2.9168510563,1.5198762892,-1.7731474107
O,0,3.8848336271,2.2197153987,-1.5383650674
H,0,2.7159364476,0.9842365541,0.3441782176
B,0,-1.967190915,0.0382957325,0.025264801



E-6i

Charge = 0 Multiplicity = 1

C,0,-0.6621656297,-0.1451540763,3.9017898829
 C,0,0.6945435074,0.155397272,4.4987476572
 H,0,-0.6108989939,-0.9689847111,3.1828839614
 H,0,-1.3936748647,-0.3979556155,4.6721904186
 H,0,1.0584203994,-0.7180867304,5.0488390321
 H,0,1.4160731141,0.3964170848,3.7126506094
 H,0,0.6274404004,0.9987632556,5.1930239671
 C,0,-0.0345126263,3.6846936092,2.1609052701
 C,0,-0.6124268341,4.4290378613,3.3426810285
 H,0,0.29974169,4.3665213401,1.3764174023
 H,0,0.8141377082,3.0580663304,2.4554414185
 H,0,0.1503786458,5.0885672506,3.7680977825
 H,0,-1.4642296138,5.0408802423,3.0319916216
 H,0,-0.9426613184,3.7306902864,4.1171432309
 C,0,-4.8616974568,-0.2794172106,-0.6107663078
 H,0,-5.8348830328,-0.6768946796,-0.9026504925
 H,0,-4.7715610123,0.7574875954,-0.9517396719
 H,0,-2.5016433808,0.877396335,-0.2148580252
 H,0,-4.0684393244,-0.8588373156,-1.0958484302
 P,0,-0.9672857738,1.2734718003,1.6835337569
 O,0,0.2628831306,0.6388986254,1.1402218627
 O,0,-1.1929914645,1.0362731349,3.252273681
 O,0,-1.0644955006,2.8599507923,1.5538272463
 C,0,-2.474735498,0.7421612646,0.8655408492
 C,0,-3.4747651088,0.1579065027,1.5321143012
 C,0,-4.7202695433,-0.3562049473,0.8849231024
 O,0,-5.5920574772,-0.8293154796,1.5948087228
 H,0,-3.4373251416,0.0291071829,2.6124841222



Z-6i

Charge = 0 Multiplicity = 1

C,0,-0.4490336074,0.2978099456,-3.6892872027
C,0,-0.1278120785,-1.1380282864,-4.0402639601
H,0,0.3419314128,0.7458511844,-3.0814019196
H,0,-0.5928687751,0.9054512588,-4.5848307613
H,0,0.7795991478,-1.1741301019,-4.6516804408
H,0,0.0433134853,-1.7286947538,-3.1350082206
H,0,-0.9478976017,-1.5861161494,-4.6103793932
C,0,-3.155186289,-1.9174363055,-1.6726886089
C,0,-4.2437237876,-1.93691471,-2.7209250804
H,0,-3.3840370168,-2.5831539075,-0.8376406034
H,0,-2.1877910128,-2.2144207075,-2.0917393656
H,0,-4.3529427335,-2.9524371247,-3.1150279814
H,0,-5.1997164899,-1.6278674741,-2.2869343578
H,0,-3.9985024935,-1.2621413138,-3.5458163467
C,0,-5.7404673332,0.9719946638,-0.3071702191
H,0,-6.6068569387,0.5272638234,-0.8009903721
H,0,-5.2128711994,0.2140884549,0.2825044784
H,0,-1.5702877073,2.5603914456,-0.383370275
H,0,-6.0649345148,1.7581539466,0.3843053426
P,0,-1.770632029,0.3182913195,-1.3772990008
O,0,-0.4918254448,-0.1149069295,-0.7529772144
O,0,-1.7068429368,0.3761500718,-2.9795001139
O,0,-3.0561196323,-0.5898696677,-1.1019032424
C,0,-2.3471929176,1.9131100773,-0.7861156404
C,0,-3.6200078711,2.3147860598,-0.7748909552
C,0,-4.7947485576,1.5470015588,-1.3221189832
O,0,-4.9698419119,1.4692488352,-2.522237488
H,0,-3.876469166,3.2817427864,-0.3399250741