Supporting Information

Insight into fragmentation of phosphirane to form phosphinidene complex: an illustration with 1-phenylselenylphosphirane $W(CO)_5$ complex.

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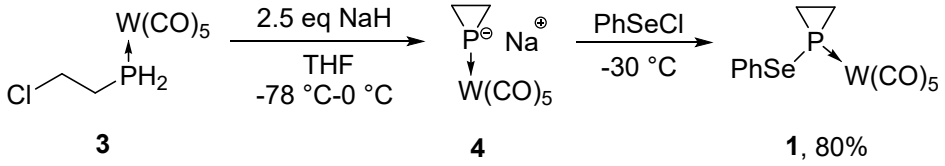
General information

All reactions were performed under nitrogen using solvents dried by standard methods except for special statement. Tetrahydrofuran (THF), toluene were dried with sodium and distilled before use. NMR spectra were obtained using Bruker AV300 spectrometer. All spectra were recorded in $CDCl_3$. All coupling constants (*J* values) were reported in hertz (Hz). Chemical shifts were expressed in parts per million (ppm) downfield from internal TMS (^1H). HRMS spectra were obtained on an Agilent 1290-6540 UHPLC Q-T of HR-MS spectrometer. X-ray crystallographic analyses were performed on an Oxford diffraction Gemini E diffractometer. Silica gel (200-300 mesh) was used for the chromatographic separations. All commercially available reagents were used without further purification. 2-chloroethylphosphine $W(CO)_5$ complex **3** and 1-phenoxylphosphirane complex **10** were prepared according to literature method (*Dalton Trans.* **2016**, *45*, 8284).

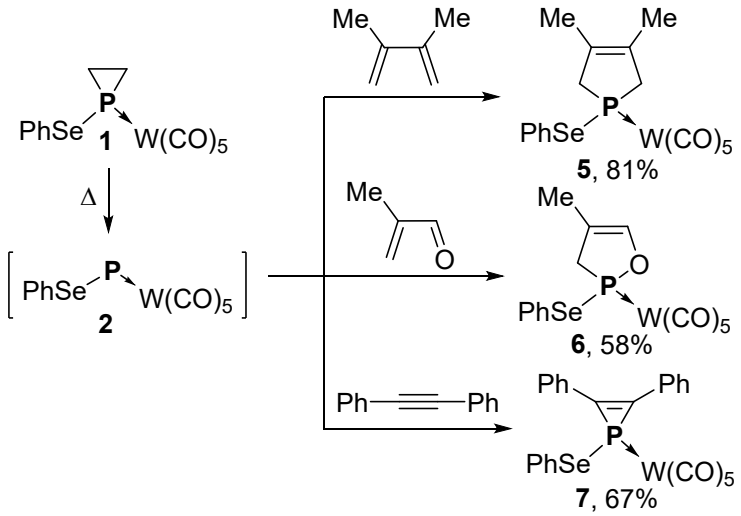
Experimental Procedures and Characterization Data



Scheme S1. The preparation of 1-phenylselenylphosphoriane $W(CO)_5$ complex **1**.

NaH (2 mmol, 80 mg) was added to the solution of 2-chloroethylphosphine $W(CO)_5$ complex **3** (1 mmol, 420 mg) in THF (20 mL) at -78 °C under nitrogen. Then the mixture was stirred vigorously in an ice bath for 5 min, produced phosphiranide complex **4**. Phenylselenenyl chloride (1.2 mmol, 230 mg) was added to the solution of **4** at -30 °C. The solution was stirred for 15 min. The solvent was removed by rotary evaporation. Purification was performed via column chromatography on silica using 30/1 petroleum ether/dichloromethane, to give pure **1** (yellow oil, 432 mg, 80%).

1: ^{31}P NMR ($CDCl_3$; 121 MHz): δ -183.0 (J_{PSe} = 297.7 Hz, J_{PW} = 262.6 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 1.55–1.62 (m, 2H, CH_2), 1.81–1.89 (m, 2H, CH_2), 7.32-7.44 (m, 3H, Ph), 7.60-7.63 (m, 2H, Ph). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 13.5 (d, J = 19.5 Hz, CH_2), 125.5 (d, J = 2.3 Hz, C), 129.5 (d, J = 2.3 Hz, CH), 129.8 (s, CH), 136.1 (d, J = 4.5 Hz, CH), 195.2 (d, J = 7.5 Hz, CO *cis*), 197.5 (d, J = 37.5 Hz, CO *trans*). HRMS (ESI) m/z: $[M-H]^-$ Calcd for $C_{13}H_8O_5PSeW$ 538.8789; Found 538.8793.



Scheme S2. Thermal decomposition of **1** with different trapping reagents**.**

A solution of phosphirane $W(CO)_5$ complex **1** (0.5 mmol, 270 mg) and 2,3-dimethyl-1,3-butadiene (2 mmol, 234 μL) in toluene (10 mL) was stirred for 1 h at 90 °C under nitrogen. The solution was cooled to room temperature. All volatile were removed by rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether/dichloromethane: 15/1), to give pure **5** (yellow oil, 240 mg, 81%).

5: ^{31}P NMR ($CDCl_3$; 121 MHz): δ 14.4 (J_{PSe} = 303.7 Hz, J_{PW} = 233.5 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 1.30 (s, 6H, CH_3), 3.05-3.35 (m, 4H, CH_2), 7.24-7.31 (m, 2H, Ph), 7.35-7.40 (m, 1H, Ph), 7.55 (d, J= 7.2 Hz, 2H, Ph). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 15.3 (d, J = 8.3 Hz, CH_3), 47.2 (d, J = 18.8 Hz, CH_2), 128.1 (d, J = 2.3 Hz, C), 129.1 (s, CH), 129.3 (d, J = 1.5 Hz, CH), 129.7 (s, C), 136.3 (s, CH), 196.1 (d, J = 6.0 Hz, CO *cis*), 199.3 (d, J = 24.8 Hz, CO *trans*). HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{16}O_5PSeW$ 594.9404; Found 594.9409.

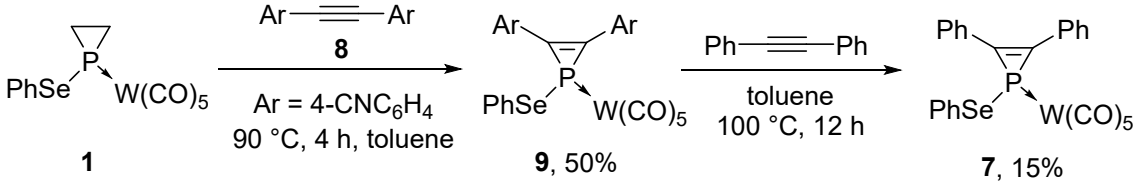
A solution of phosphirane $W(CO)_5$ complex **1** (0.5 mmol, 270 mg) and methacrylaldehyde (1.5 mmol, 125 μL) in toluene (10 mL) was stirred for 3 h at 90 °C under nitrogen. The solution was cooled to room temperature. The solvent was removed by rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether/dichloromethane: 30/1), to give pure **6** (yellow oil, 170 mg, 58%).

6: ^{31}P NMR ($CDCl_3$; 121 MHz): δ 145.4 (J_{PSe} = 367.8 Hz, J_{PW} = 295.2 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 1.40 (s, 3H, CH_3), 3.19-3.53 (m, 1H, CH_2), 5.95 (d, J = 17.4 Hz, 1H, CH), 7.29-7.40 (m, 3H, Ph), 7.64 (d, J= 6.9 Hz, 2H, Ph). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 12.2 (d, J = 8.3 Hz, CH_3), 46.0 (d, J = 13.5 Hz, CH_2), 116.4 (s, C), 127.6 (s, C), 129.3 (d, J = 1.5 Hz, =CH), 129.4 (s, CH), 136.5 (d, J = 2.3 Hz, CH), 140.5 (d, J = 9.8 Hz, CH), 195.0 (d, J = 7.5 Hz, CO *cis*), 198.9 (d, J = 33.8 Hz, CO *trans*). HRMS (ESI) m/z: $[M-H]^-$ Calcd for $C_{15}H_{10}O_6PSeW$ 580.8895; Found 580.8893.

A solution of phosphirane $W(CO)_5$ complex **1** (0.5 mmol, 270 mg) and 1,2-diphenylethyne (2 mmol, 356 mg) in toluene (10 mL) was stirred for 3 h at 90 °C under nitrogen. The

solution was cooled to room temperature. The solvent was removed by rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether/dichloromethane: 20/1), to give pure **7** (yellow oil, 231 mg, 67%).

7: ^{31}P NMR ($CDCl_3$; 121 MHz): δ -144.5 (J_{PSe} = 304.9 Hz, J_{PW} = 277.1 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 6.77 (t, *J*= 7.5 Hz, 1H, CH), 7.06 (d, *J*= 7.5 Hz, 1H, CH), 7.27-7.30 (m, 5H, CH), 7.40-7.44 (m, 3H, CH), 7.49-7.52 (m, 3H, CH), 7.61-7.64 (m, 2H, CH). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 89.7 (s, C), 123.5 (s, C), 128.5 (s, CH), 128.8 (d, *J*= 3.0 Hz, CH), 129.2 (s, CH), 130.1 (d, *J*= 5.3 Hz, CH), 131.1 (s, CH), 131.8 (s, CH), 132.7 (d, *J*= 18.8 Hz, C), 195.8 (d, *J* = 7.5 Hz, CO *cis*), 198.1 (d, *J* = 39.0 Hz, CO *trans*). HRMS (ESI) m/z: $[M-H]^-$ Calcd for $C_{25}H_{14}O_5PSeW$ 688.9259; Found 688.9256.

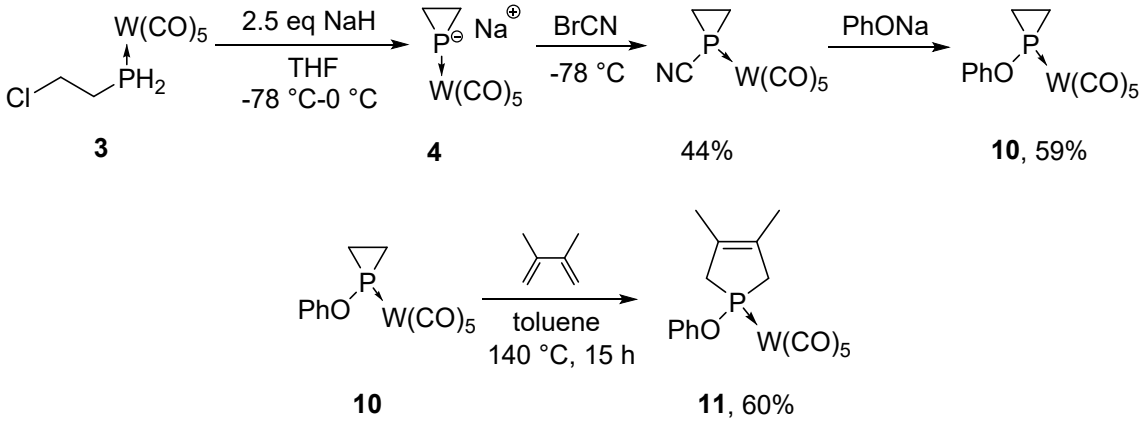


Scheme S3. Reversible cycloadditions of phosphinidene complex**2** with alkynes.

A solution of phosphirane $W(CO)_5$ complex **1** (0.5 mmol, 270 mg) and alkyne **8** (2 mmol, 456 mg) in toluene (10 mL) was stirred for 4 h at 90 °C under nitrogen. The solution was cooled to room temperature. The solvent was removed by rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether/dichloromethane: 1/1), to give pure **9** (yellow oil, 185 mg, 50%).

9: ^{31}P NMR ($CDCl_3$; 121 MHz): δ -137.6 (J_{PSe} = 303.7 Hz, J_{PW} = 275.9 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 6.90 (t, *J*= 7.8 Hz, 2H, CH), 7.08 (d, *J*= 7.5 Hz, 2H, CH), 7.15 (t, *J*= 7.2 Hz, 1H, CH), 7.67 (d, *J*= 8.1 Hz, 4H, CH), 7.80 (d, *J*= 8.1 Hz, 4H, CH). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 114.7 (s, C), 117.9 (s, C), 126.9 (s, C), 129.1 (s, CH), 129.3 (s, CH), 130.0 (d, *J*= 4.5 Hz, CH), 130.7 (d, *J*= 4.5 Hz, C), 132.9 (s, CH), 135.3 (d, *J*= 18.8 Hz, C), 137.6 (d, *J*= 2.3 Hz, CH), 195.1 (d, *J* = 7.5 Hz, CO *cis*), 196.9 (d, *J* = 40.5 Hz, CO *trans*). HRMS (ESI) m/z: $[M-H]^-$ Calcd for $C_{27}H_{12}N_2O_5PSeW$ 738.9164; Found 738.9166.

A solution of phosphirene $W(CO)_5$ complex **9** (0.5 mmol, 370 mg) and 1,2-diphenylethyne (2 mmol, 356 mg) in toluene (10 mL) was stirred for 12 h at 100 °C under nitrogen. The solution was cooled to room temperature. The solvent was removed by rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether/dichloromethane: 20/1), to give pure **7** (yellow oil, 52 mg, 15%).



Scheme S4. Synthesis and thermal decomposition of **10**.

A solution of 1-cyanophosphirane $W(CO)_5$ complex (0.5 mmol, 205 mg) and sodium benzenolate.(0.6 mmol, 70 mg) in THF (10 mL) was stirred for 1 h at room temperature under nitrogen. The solvent was removed by rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether), to give pure **10** (white oil, 140 mg, 59%).

10: ^{31}P NMR ($CDCl_3$; 121 MHz): δ -42.8 (J_{PW} = 309.8 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 1.07–1.16 (m, 2H, CH_2), 1.77–1.86 (m, 2H, CH_2), 7.03-7.07 (m, 2H, CH), 7.13-7.18 (m, 1H, CH), 7.31-7.36 (m, 2H, CH). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 11.0 (d, J = 13.5 Hz, CH_2), 120.0 (d, J = 7.5 Hz, CH), 124.6 (s, CH), 130.1 (s, CH), 152.9 (d, J = 6.8 Hz, C), 194.4 (d, J = 9.0 Hz, CO *cis*), 197.6 (d, J = 38.3 Hz, CO *trans*). HRMS (APCI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{10}O_6PW$ 476.9719; Found 476.9717.

A solution of phosphirane $W(CO)_5$ complex **10** (0.5 mmol, 238 mg) and 2,3-dimethyl-1,3-butadiene (2 mmol, 234 μL) in toluene (10 mL) was stirred for 15 h at 140 °C under nitrogen. The solution was cooled to room temperature. All volatile were removed by

rotary evaporation. The residues were purified by chromatography on silica gel (petroleum ether), to give pure **11** (white oil, 159 mg, 60%).

11: ^{31}P NMR ($CDCl_3$; 121 MHz): δ 135.8 (J_{PW} = 269.8 Hz). ^{1}H NMR ($CDCl_3$; 300 MHz): δ 1.69 (s, 6H, CH_3), 2.94-3.05 (m, 2H, CH_2), 3.20 (dd, *J* = 17.4, 10.8 Hz, 2H, CH_2), 6.95 (d, *J*= 8.4 Hz, 2H, CH), 7.13 (t, *J*= 7.5 Hz, 1H, CH), 7.29 (t, *J*= 7.8 Hz, 2H, CH). ^{13}C NMR ($CDCl_3$; 75 MHz): δ 15.8 (d, *J* = 8.3 Hz, CH_3), 49.2 (d, *J* = 24.8 Hz, CH_2), 121.0 (d, *J* = 4.5 Hz, CH), 124.5 (d, *J* = 1.5 Hz, CH), 129.0 (s, C), 129.8 (s, CH), 154.0 (d, *J* = 8.3 Hz, C), 195.9 (d, *J* = 7.5 Hz, CO *cis*), 199.1 (d, *J* = 26.3 Hz, CO *trans*). HRMS (ESI) m/z: $[M-H]^-$ Calcd for $C_{17}H_{14}O_6PW$ 529.0043; Found 529.0042.

DFT calculations

Computational Methods

All of the calculations were carried out by using Gaussian09.[1] The optimized structures were illustrated using CYLView.[2] The density functional theory (DFT) calculations were performed with the B3LYP [3] functional. All geometry optimizations and frequency calculations were performed at B3LYP/6-31G(d, p)[4]/LanL2DZ[5] level. The further single-point energies were obtained at the MP2[6]/6-311+G(d, p)/SDD [7]/SMD[8] toluene level. Then, frequency calculations were carried out to identify all of the stationary points as minima (zero imaginary frequency) or transition state (only one frequency), and to provide corrections for free energies.

References

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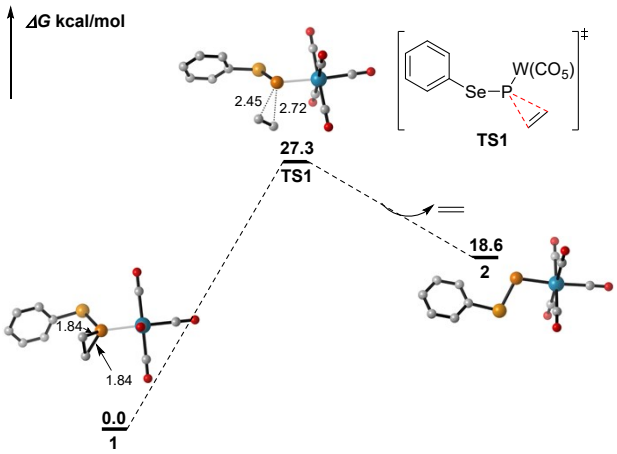


Figure S1. Free energy profile (kcal/mol) for the reverse [1+2] cycloaddition of **1** computed at the MP2/6-311+G(d, p)/SDD/$SMD_{toluene}$//B3LYP/6-31G(d, p)/LanL2DZ level (distance: Å)

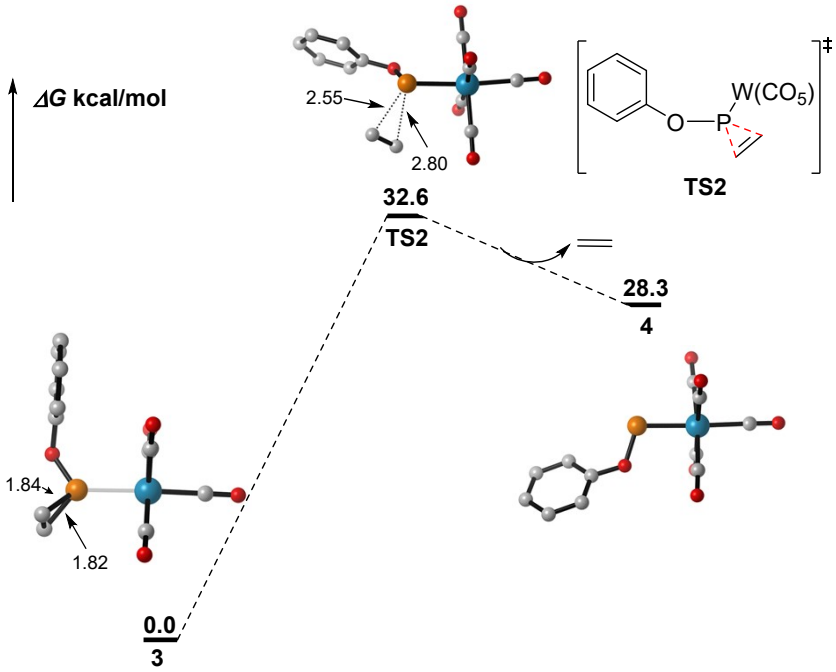
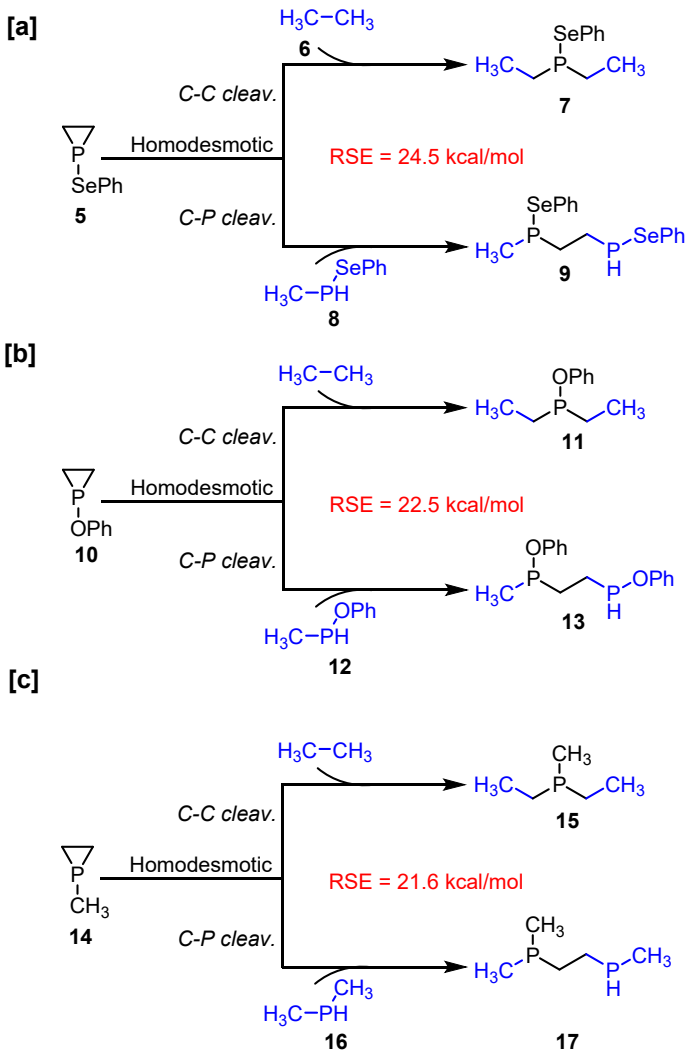


Figure S2. Free energy profile (kcal/mol) for the reverse [1+2] cycloaddition of **10** computed at the MP2/6-311+G(d, p)/SDD/$SMD_{toluene}$//B3LYP/6-31G(d, p)/LanL2DZ level (distance: Å)



Scheme 5 The RSE values calculated at the MP2/6-311+G(d, p)/$SMD_{toluene}$//B3LYP/6-31G(d, p) level.

Energies, Cartesian coordinates, and representative vibrational frequencies of the listed compounds

1

Zero-point correction= 0.189904
Thermal correction to Energy= 0.213744
Thermal correction to Enthalpy= 0.214689
Thermal correction to Gibbs Free Energy= 0.130688
Sum of electronic and zero-point Energies= -3684.953751
Sum of electronic and thermal Energies= -3684.929911
Sum of electronic and thermal Enthalpies= -3684.928967
Sum of electronic and thermal Free Energies= -3685.012967

Cartesian coordinates

P	-0.585415	0.531691	0.007280
C	-1.418620	1.980668	-0.756638
C	-1.420031	1.981216	0.768551
H	-2.375835	1.817323	-1.244352
H	-0.770597	2.685088	-1.272660
H	-0.773136	2.686085	1.285499
H	-2.378108	1.818379	1.254722
Se	-2.022146	-1.264337	0.003745
C	-3.761578	-0.426721	0.001433
C	-4.408408	-0.150663	1.213390
C	-4.409552	-0.163722	-1.212789
C	-5.690545	0.401815	1.207370
H	-3.910939	-0.375115	2.151255
C	-5.691923	0.388204	-1.211568
H	-3.912627	-0.397797	-2.148582
C	-6.331875	0.672521	-0.003306
H	-6.188760	0.614671	2.148646
H	-6.191229	0.590229	-2.154646
H	-7.330528	1.099134	-0.005154
W	1.903037	0.018737	-0.000725
C	2.159397	1.583623	-1.306028
O	2.285481	2.468607	-2.038299
C	2.123728	1.298326	1.592333
O	2.233804	2.023711	2.484559
C	1.626733	-1.549135	1.311187
O	1.491263	-2.425452	2.049127
C	1.655519	-1.260244	-1.599299
O	1.532642	-1.974109	-2.497280
C	3.890874	-0.330774	-0.011458
O	5.031670	-0.525652	-0.017696

Vibrational frequencies

12.6475	18.1224	31.8425
48.3385	55.3736	57.5010
58.8240	67.5800	75.7508
79.4334	88.3202	89.6976
91.2538	101.4817	159.2836
177.7724	191.5143	224.7560
246.2474	251.8806	307.8015

364.0584	370.0817	391.3898
391.9182	411.2421	414.9595
422.5355	425.6635	432.5677

TS1

Zero-point correction= 0.187796
Thermal correction to Energy= 0.212285
Thermal correction to Enthalpy= 0.213230
Thermal correction to Gibbs Free Energy= 0.127967
Sum of electronic and zero-point Energies= -3684.918697
Sum of electronic and thermal Energies= -3684.894208
Sum of electronic and thermal Enthalpies= -3684.893264
Sum of electronic and thermal Free Energies= -3684.978526

Cartesian coordinates

P	0.606678	0.374419	0.644297
C	1.513759	2.651572	0.670707
C	0.677975	2.894535	-0.373640
H	2.538686	2.329302	0.518646
H	1.247953	2.946626	1.681134
H	-0.301263	3.333155	-0.221591
H	0.964911	2.665185	-1.394250
Se	1.902000	-0.530009	-0.950618
C	3.664148	-0.353076	-0.161824
C	4.677473	0.248310	-0.917405
C	3.945691	-0.855588	1.113574
C	5.968056	0.350540	-0.393655
H	4.458612	0.635120	-1.908089
C	5.234689	-0.740297	1.634986
H	3.162528	-1.333547	1.692813
C	6.247538	-0.140270	0.882852
H	6.751287	0.818464	-0.983015
H	5.448972	-1.130015	2.625909
H	7.251174	-0.058632	1.289463
W	-1.817133	-0.093816	0.069957
C	-1.995828	-0.737132	2.019508
O	-2.100555	-1.093492	3.112442
C	-2.368977	1.785095	0.683113
O	-2.677878	2.844854	1.029892
C	-1.567046	0.576658	-1.860731
O	-1.398140	0.969146	-2.933397

C	-1.288519	-1.998627	-0.526108
O	-1.015873	-3.069541	-0.855126
C	-3.762894	-0.572231	-0.262312
O	-4.870004	-0.840489	-0.463269

Vibrational frequencies

-144.2957	18.7750	22.8741
26.5253	41.4308	54.1591
57.9481	61.2256	73.9705
77.4620	83.5604	88.1048
89.3146	90.6848	106.5278
107.6214	121.6288	156.4206
183.6323	217.4653	248.3470
296.3777	315.9057	364.4773
368.8016	389.3451	391.9760
414.7291	416.7597	420.8467

2

Zero-point correction= 0.134320
Thermal correction to Energy= 0.155764
Thermal correction to Enthalpy= 0.156708
Thermal correction to Gibbs Free Energy= 0.077002
Sum of electronic and zero-point Energies= -3606.381051
Sum of electronic and thermal Energies= -3606.359606
Sum of electronic and thermal Enthalpies= -3606.358662
Sum of electronic and thermal Free Energies= -3606.438369

Cartesian coordinates

P	-0.607382	0.792300	0.278418
Se	-1.959750	-0.861216	-0.258050
C	-3.730349	-0.101117	-0.052028
C	-4.740533	-0.953060	0.407382
C	-4.020492	1.224621	-0.384978
C	-6.042896	-0.470405	0.543003
H	-4.512067	-1.982802	0.665846
C	-5.323621	1.700877	-0.239081
H	-3.236434	1.879761	-0.749981
C	-6.335932	0.856406	0.222733
H	-6.824953	-1.131615	0.904456
H	-5.548185	2.731890	-0.496286
H	-7.349788	1.230424	0.329110

W	1.726814	0.066475	0.028570
C	2.098387	1.955958	-0.717131
O	2.311234	3.012498	-1.125734
C	2.083625	0.794826	1.931574
O	2.291545	1.203045	2.988665
C	1.316974	-1.810156	0.783166
O	1.067324	-2.854416	1.200930
C	1.352380	-0.681978	-1.860170
O	1.121430	-1.107002	-2.905329
C	3.729112	-0.379235	-0.165878
O	4.847150	-0.637929	-0.281214

Vibrational frequencies

7.2871	22.5967	26.3085
36.0779	59.6186	62.5516
66.9088	75.1777	85.4603
86.2901	88.1278	90.0930
110.4405	115.9275	186.7790
248.4366	302.0541	340.6418
361.9086	382.7691	383.9788
387.2639	400.9640	408.8022
413.5741	418.0669	432.9400
441.5259	478.8315	484.8777

CH_2=CH_2

Zero-point correction= 0.051138
Thermal correction to Energy= 0.054181
Thermal correction to Enthalpy= 0.055125
Thermal correction to Gibbs Free Energy= 0.028956
Sum of electronic and zero-point Energies= -78.542669
Sum of electronic and thermal Energies= -78.539625
Sum of electronic and thermal Enthalpies= -78.538681
Sum of electronic and thermal Free Energies= -78.564851

Cartesian coordinates

C	-0.664938	0.000000	0.000003
C	0.664938	0.000000	-0.000004
H	-1.238866	-0.922486	-0.000010
H	-1.238865	0.922486	0.000024
H	1.238866	0.922486	0.000011

H	1.238865	-0.922486	-0.000022

Vibrational frequencies

829.9293	960.8094	976.4461
1068.4359	1240.5150	1388.8650
1483.7182	1716.2534	3147.5597
3163.3425	3222.5782	3248.4466

3

Zero-point correction= 0.192966
Thermal correction to Energy= 0.215681
Thermal correction to Enthalpy= 0.216626
Thermal correction to Gibbs Free Energy= 0.136423
Sum of electronic and zero-point Energies= -1361.239397
Sum of electronic and thermal Energies= -1361.216682
Sum of electronic and thermal Enthalpies= -1361.215738
Sum of electronic and thermal Free Energies= -1361.295941

Cartesian coordinates

P	0.483681	1.611953	-0.134099
C	0.616356	3.094268	0.945475
C	0.150900	3.369514	-0.483246
H	1.616329	3.425844	1.210588
H	-0.114009	3.189717	1.745086
H	-0.887665	3.650555	-0.635813
H	0.851593	3.867251	-1.147754
C	2.929941	0.529562	-0.349515
C	3.681405	-0.142457	-1.315426
C	3.147821	0.306240	1.011553
C	4.660537	-1.048230	-0.909980
H	3.486641	0.052516	-2.364607
C	4.124403	-0.612495	1.403095
H	2.569518	0.843743	1.755972
C	4.883571	-1.289467	0.448309
H	5.245197	-1.572552	-1.660015
H	4.289969	-0.793111	2.460931
H	5.642200	-2.000929	0.759062
W	-1.152691	-0.305818	0.000284
C	-0.017647	-1.275855	1.421938
O	0.586165	-1.835501	2.230274

C	-2.135428	0.693499	1.500842
O	-2.674796	1.266842	2.347087
C	-2.300405	0.655264	-1.411034
O	-2.945273	1.198761	-2.199437
C	-0.136162	-1.295649	-1.498974
O	0.422927	-1.851898	-2.340054
C	-2.512800	-1.799298	0.081240
O	-3.294098	-2.651035	0.125903
O	2.003723	1.457687	-0.813606

Vibrational frequencies

13.2923	22.1800	40.0660
49.4095	51.9128	63.2247
74.7796	76.1490	83.1395
87.4344	90.2065	92.9169
94.0211	152.9662	159.9513
183.5957	247.0934	261.7392
290.3034	364.4610	391.0183
392.9480	401.0074	412.3579
417.4325	423.4290	425.8461
431.1971	447.6555	496.6590
501.4945	534.7147	537.7568
548.8542	558.6260	592.0044
594.0472	622.6726	626.1790
654.7927	686.5147	702.4150
727.9290	772.4277	773.7519
787.3513	836.3978	891.2282
910.9922	935.8158	967.5647
993.5162	1016.0947	1022.2823
1049.1603	1050.1678	1050.8088
1104.7617	1185.0493	1192.3054
1203.4456	1238.5090	1334.1662
1360.1366	1442.2766	1458.7990
1496.1197	1532.0439	1645.3187
1652.5234	2044.8682	2048.8536
2053.9952	2077.8782	2154.5857
3143.1369	3146.6893	3190.0309
3197.9238	3208.4034	3215.7165
3221.4004	3228.3145	3241.1248

TS2

Zero-point correction= 0.190683
Thermal correction to Energy= 0.214166
Thermal correction to Enthalpy= 0.215110
Thermal correction to Gibbs Free Energy= 0.132992
Sum of electronic and zero-point Energies= -1361.196699
Sum of electronic and thermal Energies= -1361.173217
Sum of electronic and thermal Enthalpies= -1361.172272
Sum of electronic and thermal Free Energies= -1361.254390

Cartesian coordinates

P	0.814056	0.326780	0.839779
C	1.818208	2.664543	0.903747
C	1.049353	2.917453	-0.181146
H	2.832000	2.287329	0.810060
H	1.505976	2.965122	1.899085
H	0.075911	3.385947	-0.087973
H	1.381751	2.667236	-1.183624
C	3.240072	-0.333688	-0.136451
C	4.058159	0.011688	-1.215312
C	3.790813	-0.796340	1.061324
C	5.442571	-0.095866	-1.086240
H	3.597879	0.351090	-2.137534
C	5.178341	-0.894968	1.177781
H	3.141295	-1.082842	1.881834
C	6.007294	-0.545130	0.110065
H	6.079813	0.171599	-1.923958
H	5.609627	-1.257793	2.106121
H	7.085257	-0.629972	0.206411
W	-1.463102	-0.139799	-0.026825
C	-1.956036	-0.696821	1.892073
O	-2.226589	-1.002294	2.972461
C	-2.138598	1.755073	0.389569
O	-2.503648	2.827162	0.623890
C	-0.856580	0.461213	-1.900606
O	-0.475598	0.818810	-2.929736
C	-0.762397	-2.033849	-0.458459
O	-0.368081	-3.089442	-0.701594
C	-3.321937	-0.705236	-0.675860
O	-4.363456	-1.024477	-1.059564
O	1.869076	-0.237596	-0.338575

Vibrational frequencies

-100.6141	17.0796	25.9902
33.2770	44.7099	61.7317
62.7910	71.4124	76.8350
83.7248	86.3290	87.4316
88.7353	95.8201	107.9625
128.7555	135.1909	168.0030
203.8455	273.1865	336.7738
366.3155	388.1114	393.6886
394.0221	413.3471	415.4516
421.0702	424.1192	426.6941
441.7197	449.4796	495.2583
505.2556	510.2281	520.0185
542.8512	568.4112	586.6355
593.9375	614.0911	625.7680
701.9658	728.7067	780.6781
831.1620	840.7650	875.2144
919.3284	970.2819	974.2311
994.8726	1000.6316	1015.8987
1034.6198	1049.3229	1103.2842
1183.8913	1187.9681	1226.0846
1240.3572	1332.8826	1355.8621
1358.9913	1480.8359	1494.7848
1527.0925	1637.1209	1642.8044
1648.7836	2042.2839	2047.0313
2059.5617	2077.1022	2146.0395
3167.1007	3179.6060	3188.6335
3196.6634	3208.1082	3214.5684
3218.4345	3251.6891	3278.9268

4

Zero-point correction= 0.137142
Thermal correction to Energy= 0.157616
Thermal correction to Enthalpy= 0.158560
Thermal correction to Gibbs Free Energy= 0.082385
Sum of electronic and zero-point Energies= -1282.655061
Sum of electronic and thermal Energies= -1282.634587
Sum of electronic and thermal Enthalpies= -1282.633643
Sum of electronic and thermal Free Energies= -1282.709818

Cartesian coordinates

P	-0.857520	0.755214	0.645106
C	-3.347440	-0.060627	-0.013202
C	-4.126031	-1.214454	0.095730
C	-3.935222	1.203057	-0.090009
C	-5.513853	-1.096156	0.147069
H	-3.633563	-2.180079	0.141483
C	-5.325943	1.306048	-0.034821
H	-3.314434	2.086016	-0.199982
C	-6.117844	0.162505	0.085129
H	-6.123547	-1.990382	0.235618
H	-5.789583	2.286101	-0.096610
H	-7.199232	0.250555	0.121800
W	1.334522	-0.005639	-0.003655
C	1.971927	1.928968	0.295933
O	2.316416	3.015289	0.474577
C	1.802790	-0.425688	1.970084
O	2.065430	-0.658190	3.067047
C	0.569891	-1.906322	-0.258910
O	0.110308	-2.953596	-0.391267
C	0.872884	0.356894	-1.989814
O	0.601303	0.548261	-3.091858
C	3.259786	-0.568300	-0.569669
O	4.315965	-0.889445	-0.895974
O	-1.971569	-0.247152	-0.091714

Vibrational frequencies

11.6646	19.3068	34.5161
51.1923	63.0445	67.8140
73.3345	84.2478	84.9103
86.7078	89.0527	106.8296
120.0114	141.6112	252.4507
351.7158	363.7511	371.6907
378.0454	391.4009	398.3421
409.0502	417.9418	421.3094
422.8896	436.1138	466.3780
493.3149	498.3517	511.6689
527.4517	564.8032	578.4253
590.3892	599.5377	625.9302
700.4184	735.7047	779.7523
837.5898	885.3185	919.2696

969.1550	994.8570	1016.2235
1049.1199	1104.3923	1183.7036
1187.4512	1221.7017	1334.6161
1359.7249	1496.2015	1525.8506
1643.2320	1648.6038	2062.6053
2072.6291	2080.6046	2092.3678
2159.2942	3189.4755	3197.8240
3208.9774	3215.9385	3220.4791

5

Zero-point correction= 0.147201
Thermal correction to Energy= 0.157291
Thermal correction to Enthalpy= 0.158235
Thermal correction to Gibbs Free Energy= 0.109801
Sum of electronic and zero-point Energies= -3050.864312
Sum of electronic and thermal Energies= -3050.854222
Sum of electronic and thermal Enthalpies= -3050.853278
Sum of electronic and thermal Free Energies= -3050.901712

Cartesian coordinates

P	-2.390425	0.498912	-0.000217
C	-1.466927	1.932478	0.752811
C	-1.466499	1.932605	-0.752478
H	-0.522921	1.721227	1.247353
H	-2.083511	2.663141	1.271486
H	-2.082838	2.663355	-1.271326
H	-0.522221	1.721494	-1.246563
Se	-0.909614	-1.274422	0.000019
C	0.836749	-0.464783	0.000010
C	1.487084	-0.198504	-1.211430
C	1.487149	-0.198592	1.211430
C	2.774037	0.341761	-1.209017
H	0.983452	-0.424121	-2.145728
C	2.774099	0.341687	1.208984
H	0.983567	-0.424262	2.145741
C	3.417502	0.613674	-0.000024
H	3.274364	0.546067	-2.151176
H	3.274477	0.545928	2.151131
H	4.419712	1.031871	-0.000035

Vibrational frequencies

48.0864	65.6270	73.3132
189.5047	230.2030	231.5858
243.6145	301.8599	347.5829
428.2615	493.8061	627.6230
630.3765	637.5986	677.5201
723.4381	773.1696	796.0680
798.9524	872.9747	910.1744
953.0881	997.3740	1012.8403
1015.0613	1020.9370	1037.4757
1042.9041	1078.1988	1088.1738
1096.8580	1187.6398	1201.7288
1210.9161	1326.8171	1351.1873
1456.9594	1476.9287	1477.6696
1513.1926	1628.4713	1635.0752
3132.4324	3132.4552	3182.2848
3190.8343	3202.2754	3209.0071
3213.3042	3214.0850	3226.2738

6

Zero-point correction= 0.074927
Thermal correction to Energy= 0.078405
Thermal correction to Enthalpy= 0.079349
Thermal correction to Gibbs Free Energy= 0.051813
Sum of electronic and zero-point Energies= -79.763814
Sum of electronic and thermal Energies= -79.760336
Sum of electronic and thermal Enthalpies= -79.759392
Sum of electronic and thermal Free Energies= -79.786928

Cartesian coordinates

C	-0.765291	-0.000002	0.000003
C	0.765290	0.000002	-0.000004
H	-1.164643	-0.643118	-0.791300
H	-1.164553	-0.363810	0.952603
H	-1.164725	1.006835	-0.161231
H	1.164642	0.643127	0.791293
H	1.164726	-1.006833	0.161242
H	1.164553	0.363800	-0.952606

Vibrational frequencies

311.4089	827.2671	827.5947
1004.3057	1225.9801	1226.2138

1418.8820	1440.3548	1516.5419
1516.8501	1521.1514	1521.6593
3043.3123	3044.5346	3098.7568
3098.8833	3122.5902	3122.7064

7

Zero-point correction= 0.225538
Thermal correction to Energy= 0.239859
Thermal correction to Enthalpy= 0.240803
Thermal correction to Gibbs Free Energy= 0.182692
Sum of electronic and zero-point Energies= -3130.655871
Sum of electronic and thermal Energies= -3130.641549
Sum of electronic and thermal Enthalpies= -3130.640605
Sum of electronic and thermal Free Energies= -3130.698716

Cartesian coordinates

P	-2.077431	-0.444392	0.038399
Se	-0.143535	-1.638889	-0.168783
C	1.350861	-0.407280	-0.137803
C	1.755392	0.242005	-1.309414
C	2.089429	-0.236655	1.039048
C	2.873379	1.078367	-1.295553
H	1.199121	0.083981	-2.227375
C	3.211871	0.592449	1.047375
H	1.781739	-0.756529	1.940643
C	3.601717	1.255889	-0.118167
H	3.179099	1.583705	-2.207274
H	3.781457	0.719403	1.963589
H	4.474461	1.902162	-0.110353
C	-1.855116	0.950255	-1.190303
C	-3.075901	1.881103	-1.224191
H	-1.724559	0.466936	-2.164405
H	-0.939488	1.515419	-0.988027
H	-2.959262	2.641366	-2.003932
H	-3.995813	1.325970	-1.434596
H	-3.214791	2.406704	-0.273819
C	-1.990270	0.433630	1.699533
C	-1.025592	1.605278	1.901253
H	-1.792026	-0.361283	2.427045
H	-3.022816	0.757968	1.887435
H	-1.111994	1.996723	2.921362

H	0.011493	1.303193	1.744441
H	-1.239583	2.432125	1.217219

Vibrational frequencies

27.3058	50.2350	58.8565
95.7222	112.3001	137.5826
151.9965	195.1796	207.9376
241.2327	246.8701	255.8291
273.8012	298.3561	385.8043
406.5160	427.3188	492.6638
600.1983	630.5399	669.8995
674.4019	720.5886	722.3074
770.8763	776.8506	871.2356
948.0004	985.5927	988.3537
993.7801	999.1615	1013.9393
1014.9508	1027.0767	1042.2358
1047.7367	1071.3023	1087.1334
1097.1729	1186.6919	1202.4836
1266.5081	1278.6148	1284.3980
1301.1936	1326.9046	1350.8798
1423.4585	1428.1120	1472.3634
1477.2255	1483.7009	1511.8780
1514.1619	1516.1480	1517.8883
1522.8314	1629.6085	1635.0661
3032.5490	3043.6801	3048.1941
3056.0237	3086.8581	3099.2393
3110.3011	3111.4903	3122.1968
3150.2613	3180.2032	3188.8791
3200.5784	3207.7409	3212.4351

8

Zero-point correction= 0.138989
Thermal correction to Energy= 0.148885
Thermal correction to Enthalpy= 0.149829
Thermal correction to Gibbs Free Energy= 0.101885
Sum of electronic and zero-point Energies= -3012.791408
Sum of electronic and thermal Energies= -3012.781512
Sum of electronic and thermal Enthalpies= -3012.780568
Sum of electronic and thermal Free Energies= -3012.828512

Cartesian coordinates

P	-2.311290	0.544861	0.713925
Se	-1.048964	-0.977720	-0.423053
C	0.754358	-0.347244	-0.142784
C	1.373645	0.457577	-1.105110
C	1.460119	-0.734113	1.001822
C	2.690868	0.881680	-0.916430
H	0.824737	0.741381	-1.997002
C	2.774783	-0.307009	1.187322
H	0.975939	-1.367772	1.737988
C	3.391069	0.502002	0.229442
H	3.168109	1.506710	-1.665713
H	3.319460	-0.609782	2.076994
H	4.415682	0.831438	0.374519
H	-1.536743	0.599317	1.907438
C	-1.751707	2.181943	0.014338
H	-0.665087	2.283945	-0.029695
H	-2.166449	2.299108	-0.989753
H	-2.160325	2.976192	0.648540

Vibrational frequencies

45.0268	66.5624	83.2739
181.9525	205.4794	236.5478
244.7682	301.5869	366.7203
426.1755	490.7217	630.5080
674.2454	676.9539	720.1882
722.4717	773.0407	799.7561
869.8393	905.0254	948.6489
993.3458	1013.7107	1015.5908
1042.8358	1046.2043	1088.0969
1097.5763	1187.0959	1201.5832
1327.7249	1339.6755	1351.1830
1477.9684	1479.8891	1490.4041
1514.1039	1630.4541	1636.0211
2378.7175	3049.0796	3132.6964
3154.3035	3181.0915	3189.5974
3201.0048	3207.5905	3212.2368

9

Zero-point correction= 0.289117
Thermal correction to Energy= 0.310401
Thermal correction to Enthalpy= 0.311345

Thermal correction to Gibbs Free Energy= 0.233566
Sum of electronic and zero-point Energies= -6063.691832
Sum of electronic and thermal Energies= -6063.670548
Sum of electronic and thermal Enthalpies= -6063.669604
Sum of electronic and thermal Free Energies= -6063.747382

Cartesian coordinates

P	-1.473975	-2.095857	0.635265
Se	-2.553437	-1.239727	-1.190226
C	-3.635988	0.189569	-0.471885
C	-4.944109	-0.077739	-0.049726
C	-3.145034	1.499875	-0.422279
C	-5.748143	0.955316	0.434018
H	-5.325568	-1.091603	-0.110258
C	-3.952633	2.530250	0.062854
H	-2.139171	1.713333	-0.767821
C	-5.252628	2.259416	0.493189
H	-6.762020	0.741483	0.759912
H	-3.564700	3.543936	0.100784
H	-5.879787	3.062899	0.867955
C	-2.830513	-2.256106	1.900882
H	-3.404776	-1.335785	2.038820
H	-3.507286	-3.060743	1.603217
H	-2.369979	-2.534604	2.855141
C	-0.602909	-0.568117	1.299634
C	0.491994	-0.087843	0.337188
H	-0.171839	-0.858922	2.266692
H	-1.335302	0.224545	1.495238
H	1.279872	-0.839856	0.235218
H	0.050776	0.066318	-0.654131
P	1.193981	1.557323	0.894427
Se	3.008862	1.852974	-0.451673
C	4.023745	0.228747	-0.199447
C	4.932938	0.130881	0.859303
C	3.886600	-0.830041	-1.103340
C	5.691217	-1.028658	1.020298
H	5.040880	0.962629	1.548035
C	4.648624	-1.988703	-0.939022
H	3.189249	-0.740083	-1.929667
C	5.548901	-2.089614	0.122578
H	6.396068	-1.102006	1.843526

H	4.537723	-2.810153	-1.640855
H	6.141425	-2.990963	0.248710
H	1.867506	1.073805	2.053212

Vibrational frequencies

12.2630	18.8876	26.0272
35.0301	45.4436	59.2737
71.2432	88.4021	91.5612
134.6817	153.0940	182.6627
202.2103	206.1379	216.5232
228.6813	244.2562	246.6782
274.8964	300.4642	304.8715
328.7173	363.1286	397.9821
426.7900	428.4079	489.9430
493.2288	630.2005	630.5025
663.4805	676.3645	676.8744
688.0875	705.7917	721.3889
721.9038	738.4373	761.1399
772.8761	775.4269	836.5211
870.7687	872.0108	898.6092
920.1430	949.9823	950.7777
983.0367	994.6677	995.9227
1013.7863	1014.4586	1016.1482
1017.9019	1025.6372	1043.0110
1043.0354	1087.6739	1088.9036
1098.3459	1099.0985	1130.3826
1187.2102	1187.5667	1202.1128
1204.4083	1208.4574	1305.8690
1310.2042	1328.1438	1328.1834
1340.2250	1352.0068	1352.5564
1473.7395	1477.9950	1478.3187
1479.8277	1484.7452	1498.9410
1514.6000	1515.1175	1629.5433
1630.7921	1635.1308	1635.8401
2364.5025	3030.2717	3043.7529
3055.4618	3079.0158	3116.5356
3125.8622	3147.0226	3181.4913
3182.3042	3190.4298	3191.7755
3201.4947	3203.0969	3208.4068
3211.0499	3213.2960	3215.4976

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Zero-point correction= 0.149808
Thermal correction to Energy= 0.159048
Thermal correction to Enthalpy= 0.159993
Thermal correction to Gibbs Free Energy= 0.113983
Sum of electronic and zero-point Energies= -726.688181
Sum of electronic and thermal Energies= -726.678941
Sum of electronic and thermal Enthalpies= -726.677997
Sum of electronic and thermal Free Energies= -726.724006

Cartesian coordinates

P	-1.932802	0.106470	0.753545
C	-2.713020	0.819096	-0.794345
C	-3.281855	-0.501768	-0.368490
H	-2.079612	0.835386	-1.676327
H	-3.322843	1.710013	-0.665042
H	-4.281903	-0.521714	0.056682
H	-3.028492	-1.379185	-0.956030
C	0.625943	-0.343551	0.030427
C	1.626804	-1.314597	-0.095236
C	0.967085	1.012067	0.087184
C	2.962192	-0.927302	-0.162676
H	1.335824	-2.358976	-0.136748
C	2.311900	1.385058	0.027167
H	0.193663	1.768655	0.168617
C	3.313902	0.424079	-0.098719
H	3.732854	-1.686550	-0.260677
H	2.571239	2.438927	0.074229
H	4.356436	0.722385	-0.147440
O	-0.670355	-0.805561	0.060960

Vibrational frequencies

37.8460	41.8785	130.1730
209.2109	257.0727	271.4934
379.4124	424.0252	512.7068
553.1137	604.4960	626.7895
642.8160	701.0088	714.9584
768.9719	780.7547	804.8753
832.7333	881.9054	899.2518
911.5647	961.9257	986.2821
1003.5696	1014.0934	1028.7503

1051.2203	1089.0751	1105.4020
1183.2343	1194.4999	1215.0978
1262.4063	1332.5697	1362.4543
1449.0212	1470.4479	1496.3247
1534.2024	1640.9382	1655.8948
3137.5700	3142.5862	3180.3821
3187.8874	3202.4954	3208.9193
3214.0832	3222.6498	3237.2458

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Zero-point correction= 0.228500
Thermal correction to Energy= 0.241728
Thermal correction to Enthalpy= 0.242672
Thermal correction to Gibbs Free Energy= 0.188223
Sum of electronic and zero-point Energies= -806.474332
Sum of electronic and thermal Energies= -806.461103
Sum of electronic and thermal Enthalpies= -806.460159
Sum of electronic and thermal Free Energies= -806.514609

Cartesian coordinates

P	1.689376	0.211929	-0.972841
C	-1.046195	-0.147401	-0.721938
C	-1.412808	-1.356828	-0.121917
C	-1.890883	0.964243	-0.630497
C	-2.609035	-1.439002	0.592523
H	-0.769517	-2.222853	-0.232287
C	-3.084581	0.871044	0.085022
H	-1.604588	1.884530	-1.129056
C	-3.446279	-0.327629	0.703834
H	-2.889341	-2.380004	1.057243
H	-3.735903	1.737640	0.154195
H	-4.376377	-0.397279	1.259357
C	1.995382	-1.199595	0.215110
C	3.426758	-1.153756	0.771167
H	1.854846	-2.117692	-0.367312
H	1.261833	-1.215869	1.027572
H	3.632116	-2.034552	1.387849
H	4.168060	-1.132989	-0.034638
H	3.593154	-0.270815	1.396836
C	1.568340	1.671107	0.203504
C	0.950818	1.527596	1.600595

H	1.051126	2.452665	-0.367039
H	2.606143	2.021924	0.288710
H	0.976039	2.489927	2.124585
H	-0.090230	1.201265	1.557036
H	1.502301	0.811028	2.216559
O	0.096324	-0.058067	-1.491428

Vibrational frequencies

33.4229	63.7335	74.8657
111.6043	113.7766	163.7303
181.7842	200.7549	241.4636
260.3456	264.6523	344.6559
422.6172	426.7422	430.4473
464.0347	562.5595	592.4764
630.1384	671.0517	690.5334
707.0519	726.0600	782.3941
787.7017	843.9236	882.3270
916.4877	967.3723	984.1881
987.6291	989.4943	996.8902
1017.0829	1024.8941	1046.0831
1049.8651	1067.7060	1099.5778
1183.6781	1188.5828	1244.0781
1267.6132	1278.5033	1287.0501
1305.9127	1324.1720	1355.6630
1425.5868	1428.8383	1468.5581
1487.6701	1491.9459	1514.4306
1517.3846	1519.1934	1523.7985
1531.1005	1639.2790	1649.9917
3032.4140	3045.0174	3047.7448
3052.2356	3073.9513	3098.9497
3108.7052	3114.2917	3120.3812
3147.0454	3181.1312	3188.9570
3203.8656	3211.8712	3217.9791

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Zero-point correction= 0.141849
Thermal correction to Energy= 0.150787
Thermal correction to Enthalpy= 0.151731
Thermal correction to Gibbs Free Energy= 0.106661
Sum of electronic and zero-point Energies= -688.609419
Sum of electronic and thermal Energies= -688.600481

Sum of electronic and thermal Enthalpies= -688.599537
Sum of electronic and thermal Free Energies= -688.644606

Cartesian coordinates

P	-2.393498	-0.424193	-0.114665
C	0.265757	-0.116741	-0.518300
C	0.939906	1.104218	-0.597494
C	0.894858	-1.238746	0.028334
C	2.248521	1.200557	-0.122422
H	0.434532	1.956751	-1.039219
C	2.201962	-1.130128	0.503319
H	0.365420	-2.185437	0.064761
C	2.882496	0.087261	0.432060
H	2.772206	2.150016	-0.186312
H	2.692058	-2.003850	0.923108
H	3.900535	0.165674	0.800832
H	-1.904737	-1.394446	0.819438
C	-2.318150	1.004772	1.074150
H	-1.332733	1.132849	1.529289
H	-2.599199	1.927513	0.559599
H	-3.053312	0.821174	1.865903
O	-1.008049	-0.209313	-1.051913

Vibrational frequencies

29.5893	73.1993	128.4872
203.8651	219.7469	313.5211
409.8485	424.6332	478.2586
557.3359	628.5672	666.4024
704.1841	712.5601	733.7286
781.1677	840.7692	868.0784
889.7301	914.4904	959.2349
965.9620	989.6342	1017.2884
1046.9703	1048.9509	1100.0667
1184.0008	1187.6280	1243.7715
1326.6791	1336.5578	1356.9628
1471.8813	1488.8164	1493.3329
1531.6330	1642.8477	1650.8788
2321.2140	3047.1922	3129.5672
3147.7564	3181.8193	3189.6644
3202.6036	3209.3515	3214.0565

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Zero-point correction= 0.294632
Thermal correction to Energy= 0.313951
Thermal correction to Enthalpy= 0.314895
Thermal correction to Gibbs Free Energy= 0.242141
Sum of electronic and zero-point Energies= -1415.325251
Sum of electronic and thermal Energies= -1415.305932
Sum of electronic and thermal Enthalpies= -1415.304988
Sum of electronic and thermal Free Energies= -1415.377743

Cartesian coordinates

P	-1.443144	1.979767	0.031187
C	-3.354410	0.125364	0.685708
C	-4.687308	0.528068	0.552673
C	-3.006601	-1.217587	0.507437
C	-5.664992	-0.410705	0.223693
H	-4.943577	1.568540	0.722934
C	-3.992682	-2.148938	0.177396
H	-1.976366	-1.527456	0.644444
C	-5.322084	-1.750569	0.030505
H	-6.698875	-0.093058	0.123640
H	-3.717219	-3.190571	0.040772
H	-6.085732	-2.478747	-0.224596
C	-2.627145	2.462757	-1.318974
H	-3.141302	1.613398	-1.777923
H	-3.372223	3.159661	-0.925723
H	-2.052317	2.988984	-2.088825
C	-0.489262	0.672947	-0.914969
C	0.610577	0.024020	-0.059860
H	-0.045848	1.189669	-1.776510
H	-1.183622	-0.077218	-1.315531
H	1.376357	0.757983	0.211011
H	0.187739	-0.361732	0.874699
P	1.359801	-1.423591	-0.976715
C	3.771994	-0.813461	0.098724
C	4.587367	-0.388815	-0.953807
C	3.998299	-0.357155	1.399332
C	5.627845	0.504591	-0.698299
H	4.412205	-0.768426	-1.955363
C	5.044180	0.533779	1.643657
H	3.360046	-0.713241	2.201274

C	5.859370	0.970061	0.597763
H	6.264588	0.830834	-1.515573
H	5.219864	0.887186	2.655503
H	6.671979	1.663349	0.791426
H	1.897029	-0.629162	-2.042222
O	2.770472	-1.746315	-0.113732
O	-2.402154	1.050220	1.077934

Vibrational frequencies

11.1087	19.4795	22.0855
30.6486	36.3450	82.9177
93.2205	98.7910	132.8537
137.6666	182.7349	195.1416
211.4026	234.4054	261.1382
298.3421	338.0811	371.4742
408.7432	424.5578	426.3892
432.2069	468.7065	478.9430
555.9020	567.9615	628.6976
630.0675	652.8103	672.2569
691.9334	703.5780	705.4299
706.8939	713.6816	735.7940
780.2711	784.1574	802.3061
839.8136	845.2924	862.6085
880.5927	898.4606	912.3544
914.4974	920.6996	949.5618
965.5802	968.8282	989.0230
990.0854	991.6554	1017.2848
1017.3843	1025.1987	1048.9587
1049.7694	1100.2100	1100.9448
1119.2071	1184.1922	1184.4957
1187.7885	1188.8565	1200.8109
1237.4248	1242.1745	1299.9533
1304.8198	1325.7508	1327.1503
1338.9443	1355.6257	1357.0634
1467.9214	1474.0073	1483.7652
1490.4514	1492.5209	1493.4694
1530.2651	1531.3980	1640.3215
1643.2083	1649.6757	1650.6784
2309.7227	3029.1601	3045.6478
3057.2136	3077.2249	3110.9972
3128.7652	3141.5712	3182.2565

3182.9472	3190.2595	3191.2509
3202.6600	3204.8516	3209.2120
3212.5337	3214.6265	3217.8540

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Zero-point correction= 0.092470
Thermal correction to Energy= 0.097736
Thermal correction to Enthalpy= 0.098680
Thermal correction to Gibbs Free Energy= 0.064553
Sum of electronic and zero-point Energies= -459.777835
Sum of electronic and thermal Energies= -459.772569
Sum of electronic and thermal Enthalpies= -459.771624
Sum of electronic and thermal Free Energies= -459.805751

Cartesian coordinates

P	0.217860	-0.734558	-0.000263
C	-1.127868	0.329668	0.750455
C	-1.127762	0.330311	-0.750248
H	-0.819727	1.237779	1.261777
H	-1.926662	-0.204483	1.258115
H	-1.926473	-0.203409	-1.258491
H	-0.819546	1.238863	-1.260741
C	1.649173	0.476378	0.000196
H	2.271034	0.305373	0.884335
H	2.271064	0.306036	-0.884051
H	1.321162	1.520068	0.000582

Vibrational frequencies

148.0360	270.3615	273.4016
594.3660	643.4080	685.6334
777.5078	804.5661	852.2112
943.2779	968.9948	1011.7609
1033.2028	1086.1788	1211.7427
1342.4831	1463.6265	1483.8454
1484.8496	1495.7091	3043.3315
3127.6309	3131.1935	3135.1789
3138.1238	3212.0986	3226.7342

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Zero-point correction= 0.170940
Thermal correction to Energy= 0.180191

Thermal correction to Enthalpy= 0.181135
Thermal correction to Gibbs Free Energy= 0.137413
Sum of electronic and zero-point Energies= -539.568215
Sum of electronic and thermal Energies= -539.558964
Sum of electronic and thermal Enthalpies= -539.558020
Sum of electronic and thermal Free Energies= -539.601742

Cartesian coordinates

P	-0.099301	-0.692880	-0.648441
C	1.303316	-0.406007	0.565246
C	2.409806	0.496530	0.006422
H	1.713589	-1.398643	0.788417
H	0.922254	-0.005797	1.512866
H	3.244083	0.579536	0.711223
H	2.805532	0.103668	-0.935870
H	2.043385	1.510353	-0.186735
C	-0.926587	0.995955	-0.706218
C	-1.270468	1.709981	0.605708
H	-1.834387	0.851935	-1.305775
H	-0.273326	1.629172	-1.318850
H	-1.752976	2.673591	0.406141
H	-1.959113	1.122997	1.221063
H	-0.377773	1.911756	1.206055
C	-1.268319	-1.635546	0.462342
H	-2.233604	-1.752714	-0.039683
H	-0.861950	-2.637351	0.631619
H	-1.432686	-1.160783	1.435142

Vibrational frequencies

68.4376	102.6822	177.2998
184.7843	206.0360	230.1869
263.2411	270.1489	340.2689
390.2126	597.2113	657.5887
682.2877	716.1176	772.6459
889.7375	903.2334	987.8672
992.8032	1001.3735	1043.6234
1061.2562	1069.7135	1272.6425
1282.8423	1291.6623	1304.2507
1341.3729	1426.3537	1426.9513
1476.1337	1480.0215	1484.8689
1491.8492	1514.1745	1517.7545

1521.4319	1523.3323	3035.6483
3040.5003	3040.9101	3042.3829
3045.8368	3076.7280	3079.0118
3105.8174	3108.2577	3116.0532
3122.1038	3126.2632	3129.9693

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Zero-point correction= 0.084163
Thermal correction to Energy= 0.089302
Thermal correction to Enthalpy= 0.090247
Thermal correction to Gibbs Free Energy= 0.056937
Sum of electronic and zero-point Energies= -421.703653
Sum of electronic and thermal Energies= -421.698514
Sum of electronic and thermal Enthalpies= -421.697569
Sum of electronic and thermal Free Energies= -421.730879

Cartesian coordinates

P	-0.000004	-0.659872	-0.112727
H	0.000040	-1.083937	1.248871
C	-1.435514	0.531867	0.021855
H	-1.327151	1.245810	0.843493
H	-1.527060	1.087055	-0.916430
H	-2.361411	-0.033048	0.162835
C	1.435512	0.531868	0.021843
H	2.361368	-0.033054	0.163078
H	1.527244	1.086928	-0.916496
H	1.327035	1.245927	0.843370

Vibrational frequencies

185.0253	193.5759	251.5475
648.4815	697.2336	723.9352
730.7811	836.8642	977.0493
1023.1236	1036.6686	1332.7821
1349.8474	1479.8878	1485.7882
1493.0995	1494.7340	2367.4592
3047.3503	3049.0418	3132.5666
3133.1715	3136.3687	3136.8746

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Zero-point correction= 0.179412
Thermal correction to Energy= 0.190858

Thermal correction to Enthalpy= 0.191803
Thermal correction to Gibbs Free Energy= 0.141649
Sum of electronic and zero-point Energies= -881.511128
Sum of electronic and thermal Energies= -881.499681
Sum of electronic and thermal Enthalpies= -881.498737
Sum of electronic and thermal Free Energies= -881.548891

Cartesian coordinates

P	-1.937686	0.129174	-0.609175
C	-3.152603	-1.094058	0.106839
H	-3.030778	-1.229755	1.187411
H	-4.172604	-0.750692	-0.090189
H	-3.028463	-2.063349	-0.385373
C	-0.352780	-0.585340	0.105200
C	0.891422	0.242773	-0.246616
H	-0.254312	-1.596165	-0.310458
H	-0.447011	-0.696764	1.193615
H	0.991434	0.341830	-1.333461
H	0.798958	1.257659	0.159338
P	2.458582	-0.481026	0.500232
H	2.524305	-1.634876	-0.336592
C	3.752919	0.529886	-0.396215
H	3.766649	1.541484	0.020132
H	4.738117	0.087967	-0.222122
H	3.579961	0.595631	-1.474180
C	-2.213812	1.550316	0.569571
H	-1.481880	2.340537	0.379285
H	-3.206643	1.975499	0.393604
H	-2.142053	1.247322	1.620461

Vibrational frequencies

40.3620	66.4133	94.7156
109.5920	176.5091	188.4724
197.7467	199.6883	221.8851
270.7354	290.7280	336.5592
641.6683	664.3087	690.9944
693.3999	700.1698	723.3686
729.1998	794.9943	833.2978
878.0357	909.2192	917.7135
972.4365	999.8627	1026.1599
1035.6010	1130.8415	1210.0510

1304.1697	1310.0295	1330.9682
1342.3064	1349.4213	1473.2418
1478.7614	1483.3163	1484.9047
1487.2579	1488.4369	1491.1226
1494.8309	2360.8627	3025.3059
3035.2383	3036.8849	3041.5475
3048.6082	3071.5143	3094.6920
3119.6868	3120.2262	3132.2213
3132.4484	3133.5797	3136.5877

NMR Spectra

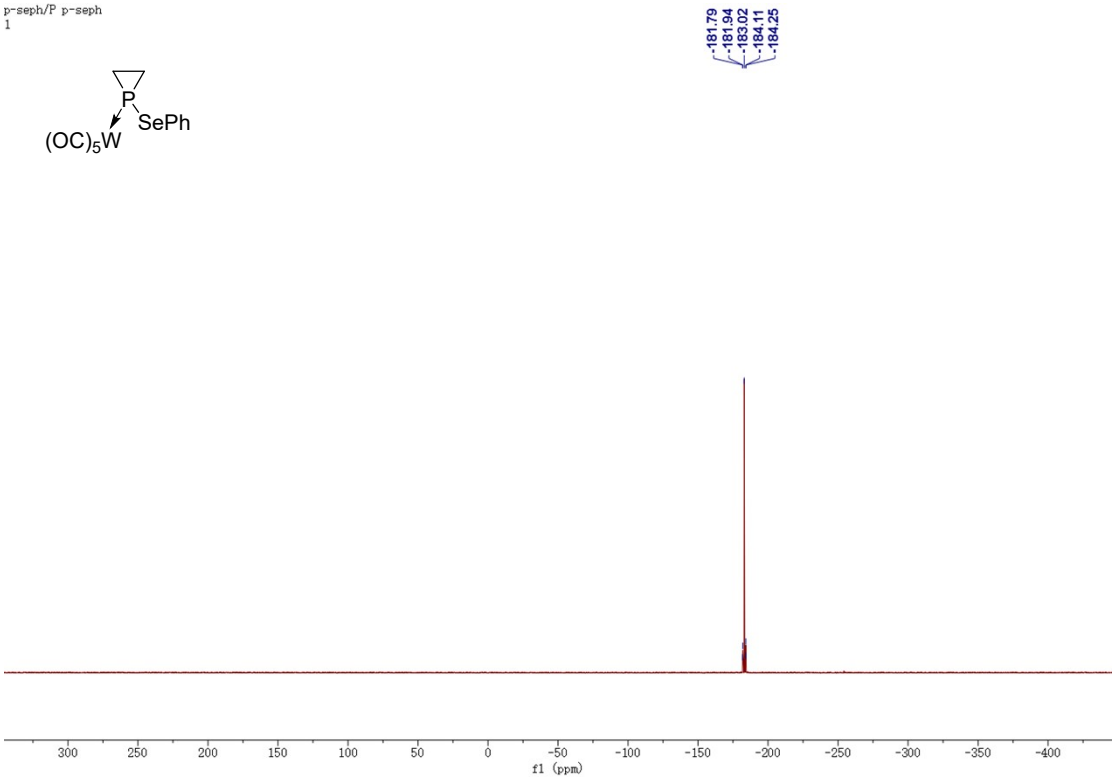

Figure S3. ^{31}P $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **1**

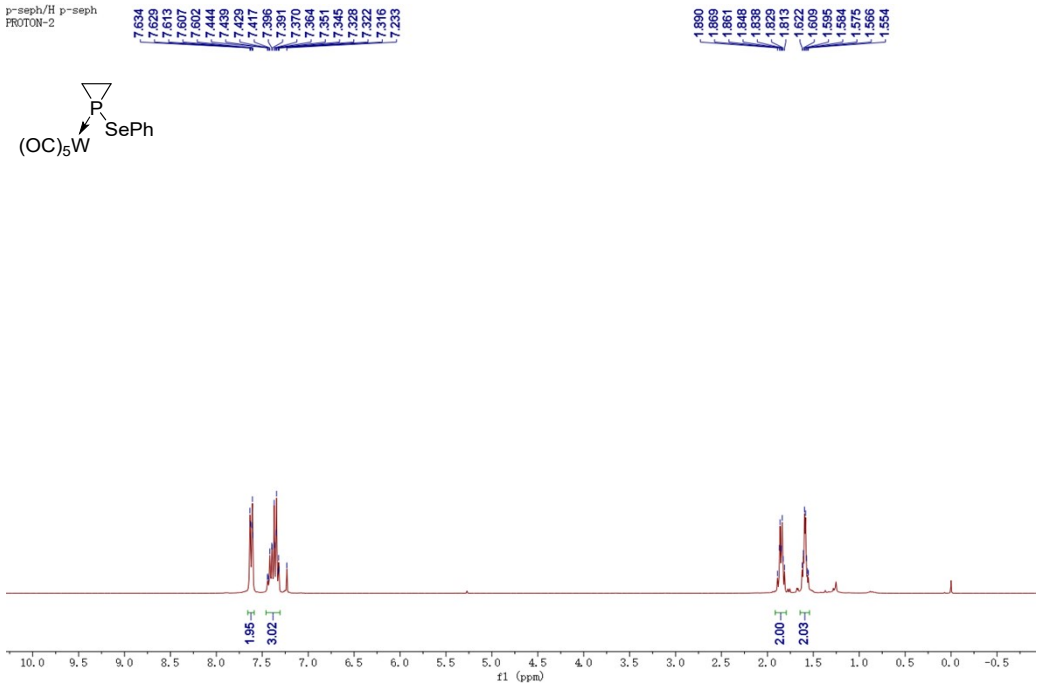

Figure S4. ^{1}H NMR ($CDCl_3$) of Compound **1**

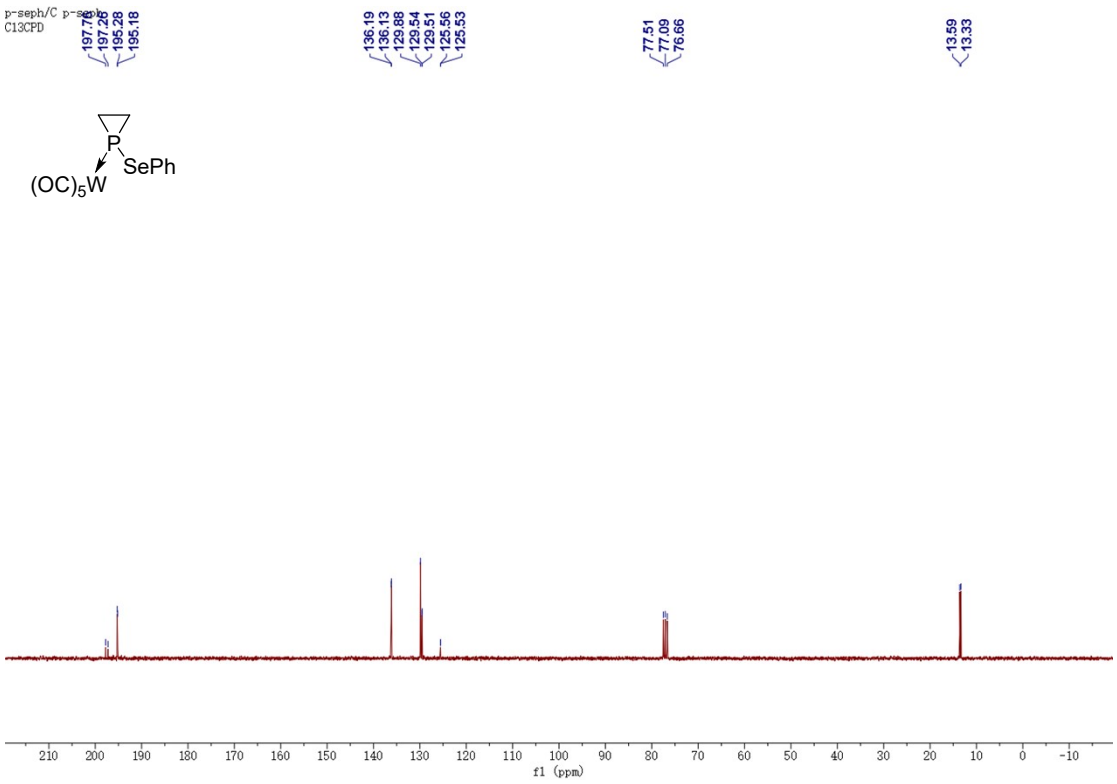

Figure S5. ^{13}C $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **1**

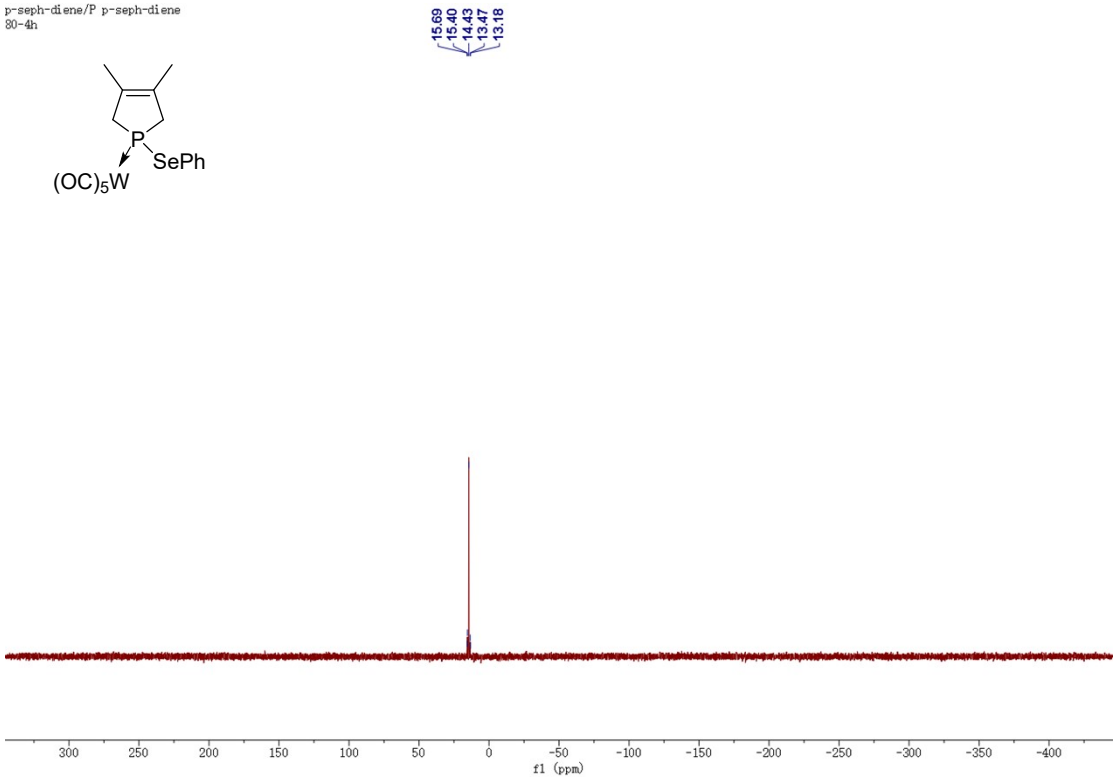

Figure S6. ^{31}P $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **5**

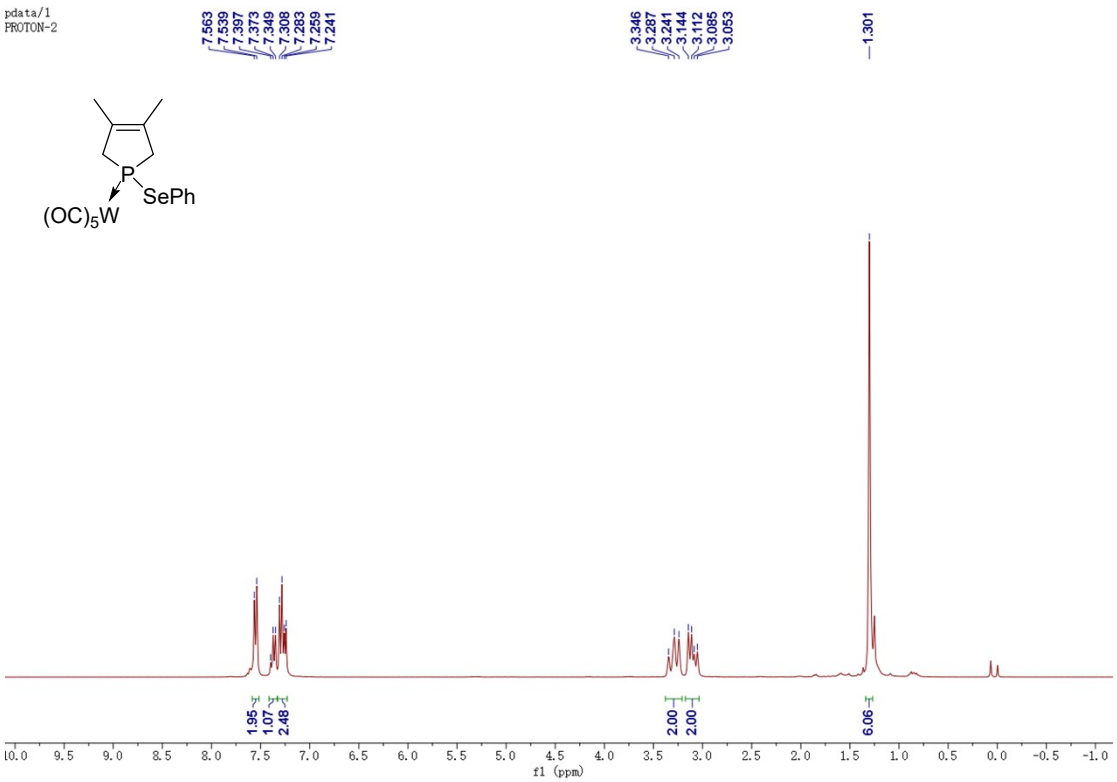

Figure S7. ^{1}H NMR ($CDCl_3$) of Compound **5**

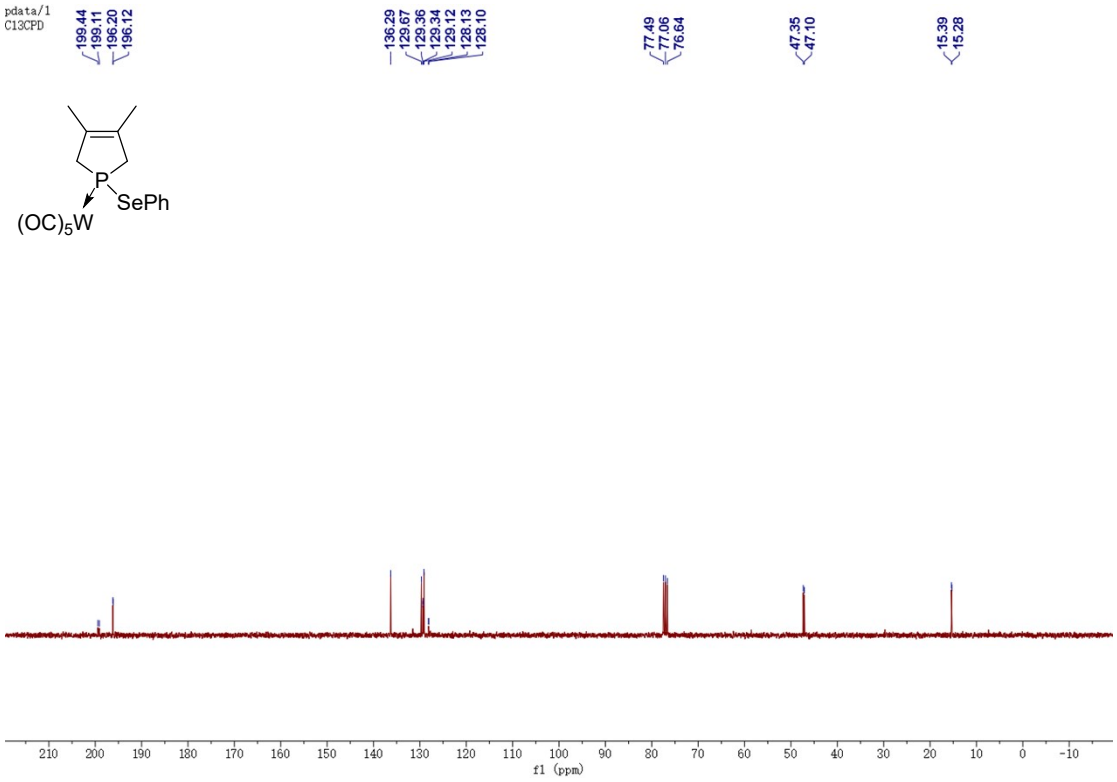

Figure S8. ^{13}C {^{1}H} NMR ($CDCl_3$) of Compound **5**

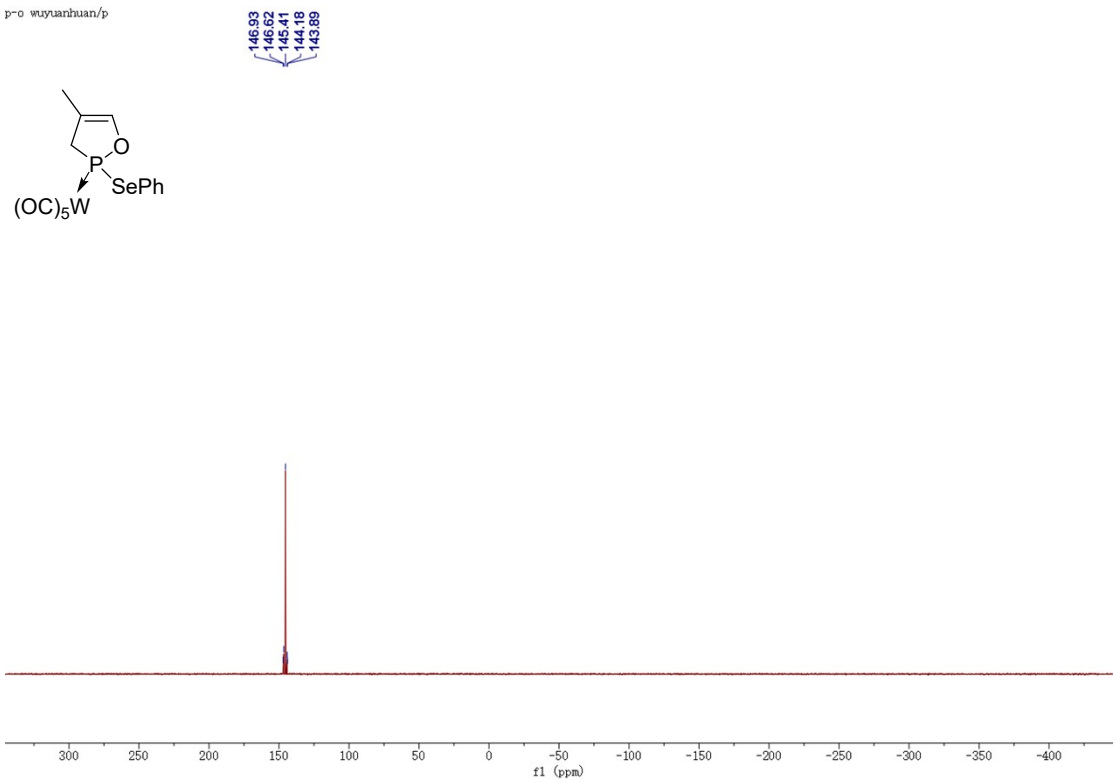

Figure S9. ^{31}P $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **6**

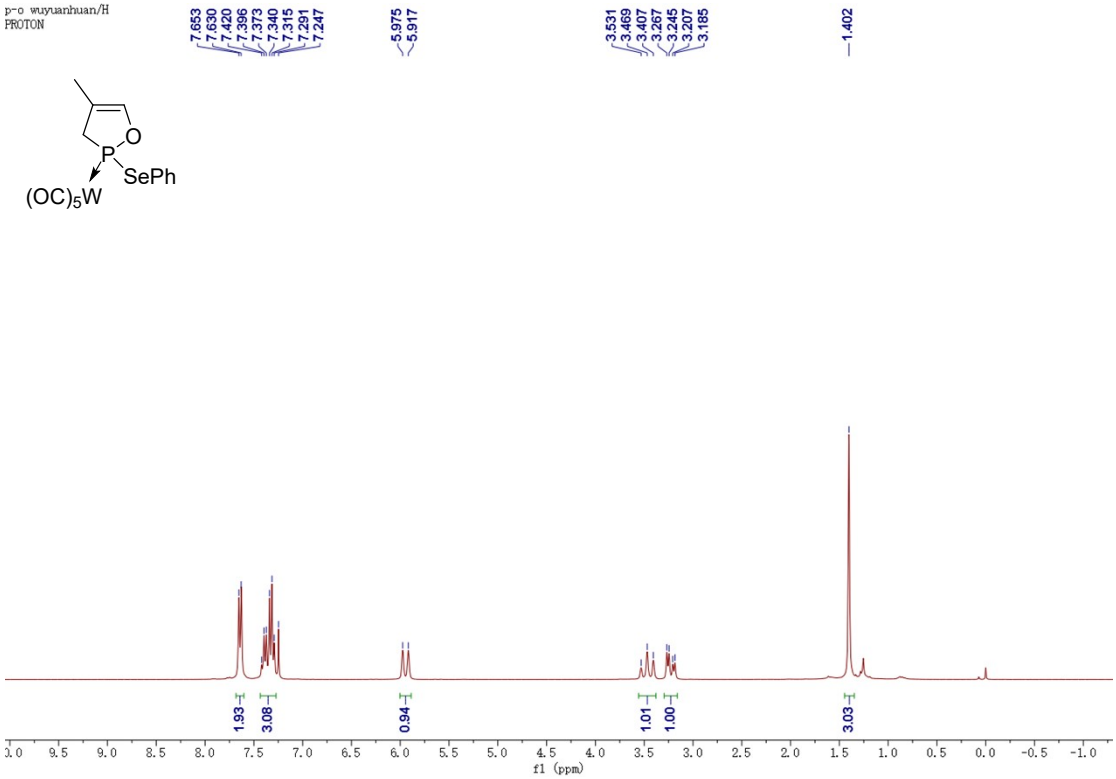

Figure S10. ^{1}H NMR ($CDCl_3$) of Compound **6**

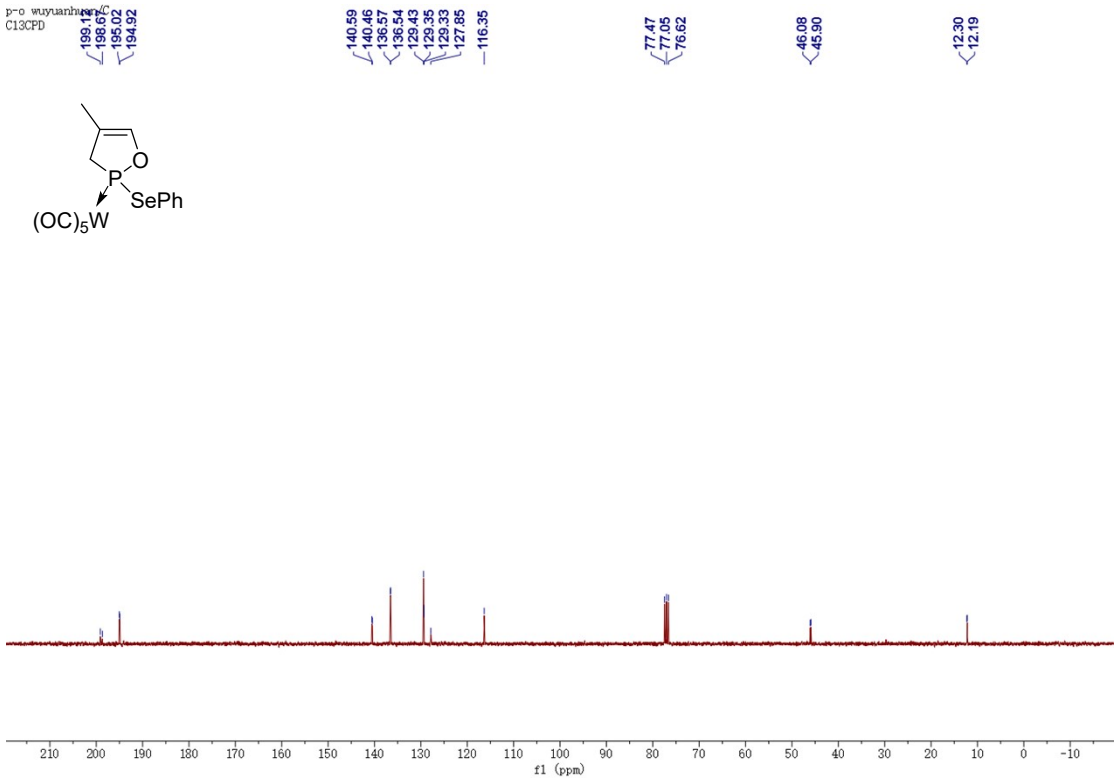

Figure S11. ^{13}C {^{1}H} NMR ($CDCl_3$) of Compound **6**

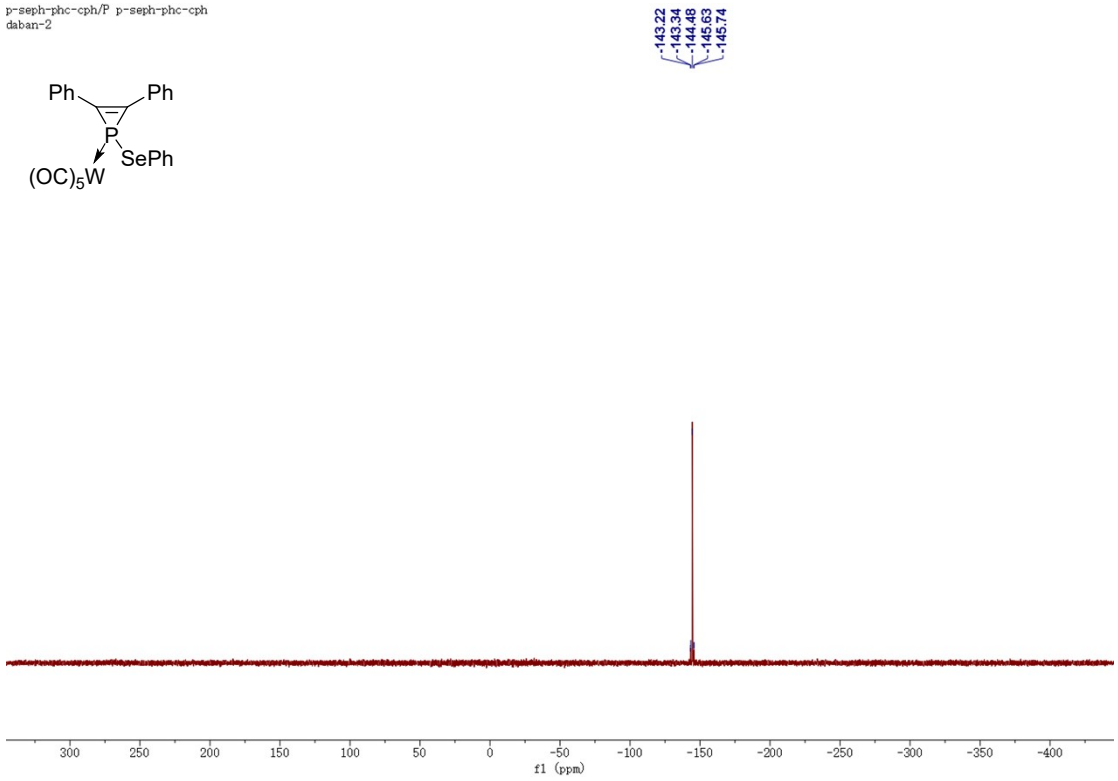

Figure S12. ^{31}P {^{1}H} NMR ($CDCl_3$) of Compound **7**

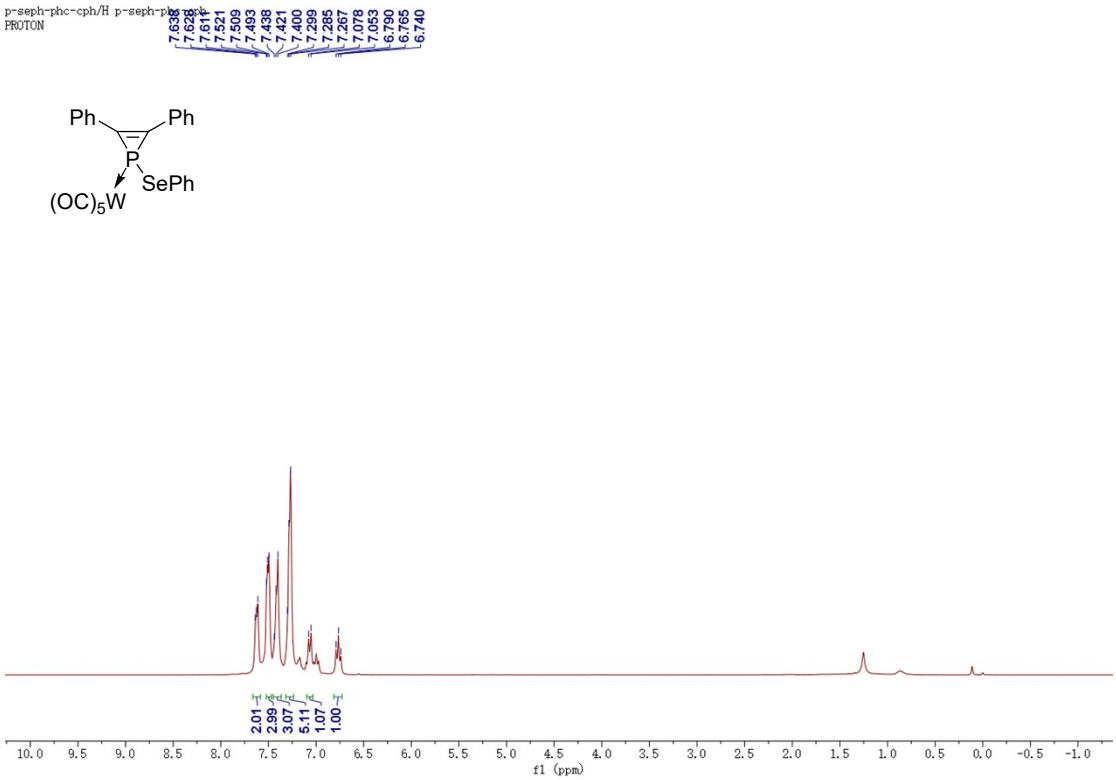

Figure S13. ^{1}H NMR ($CDCl_3$) of Compound **7**

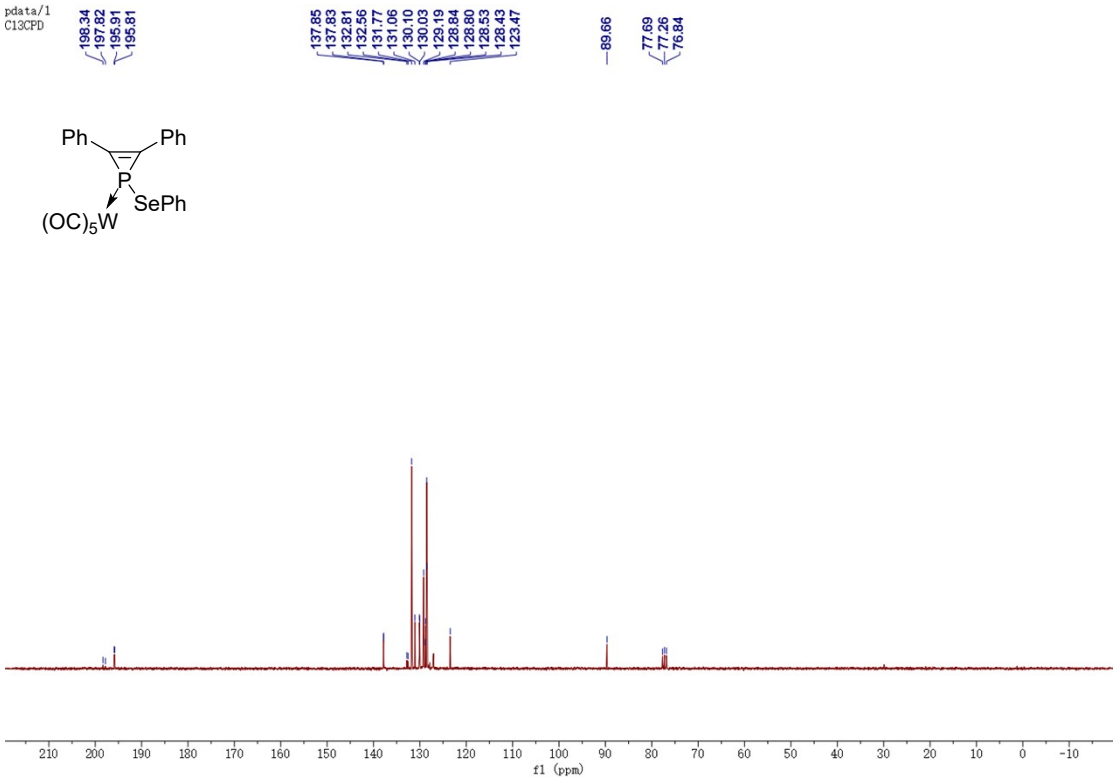

Figure S14. ^{13}C $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **7**

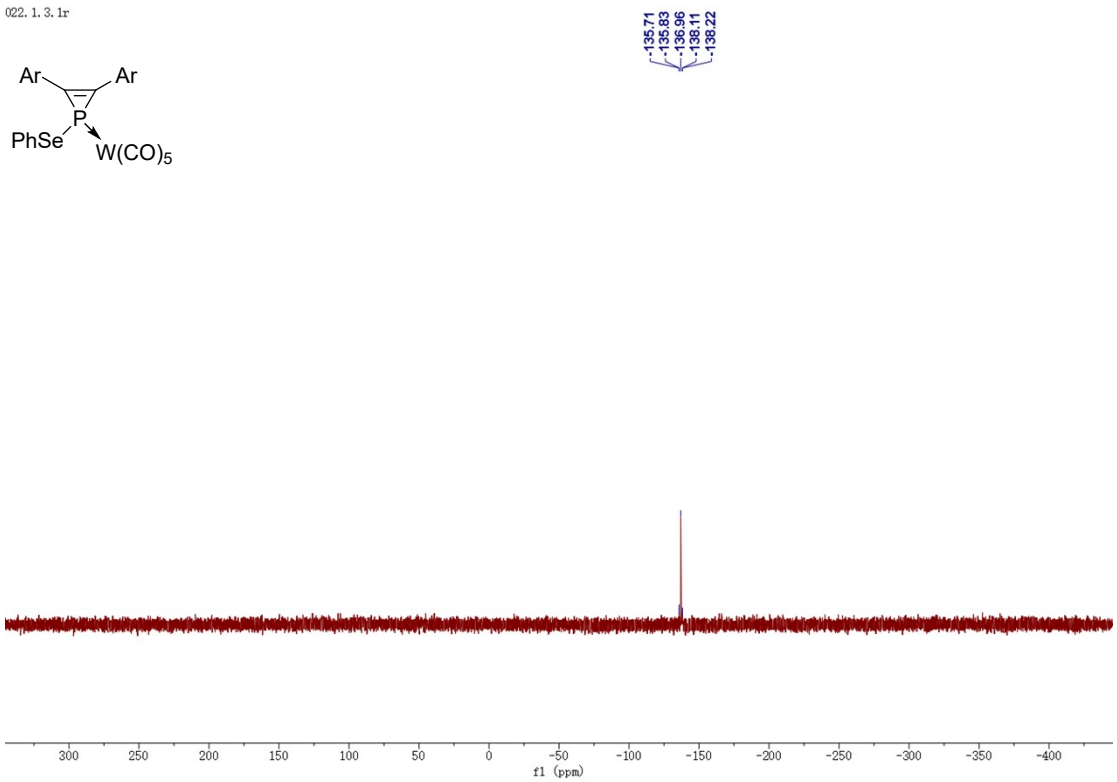

Figure S15. ^{31}P $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **9**

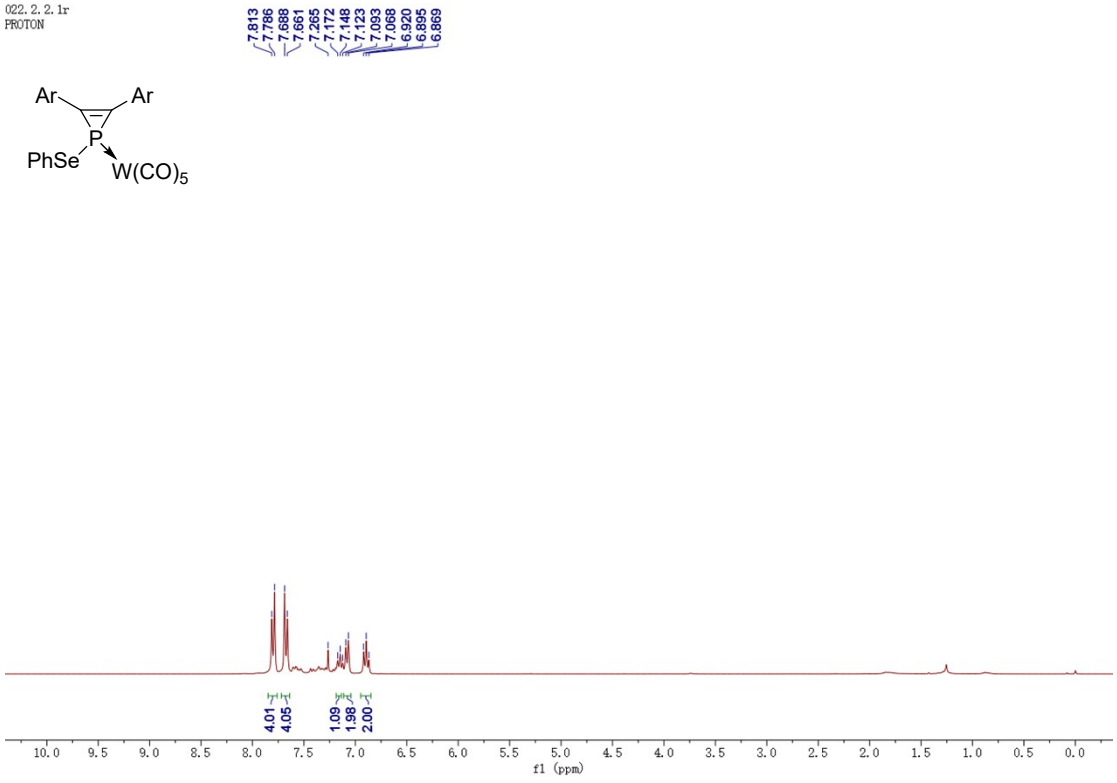

Figure S16. ^{1}H NMR ($CDCl_3$) of Compound **9**

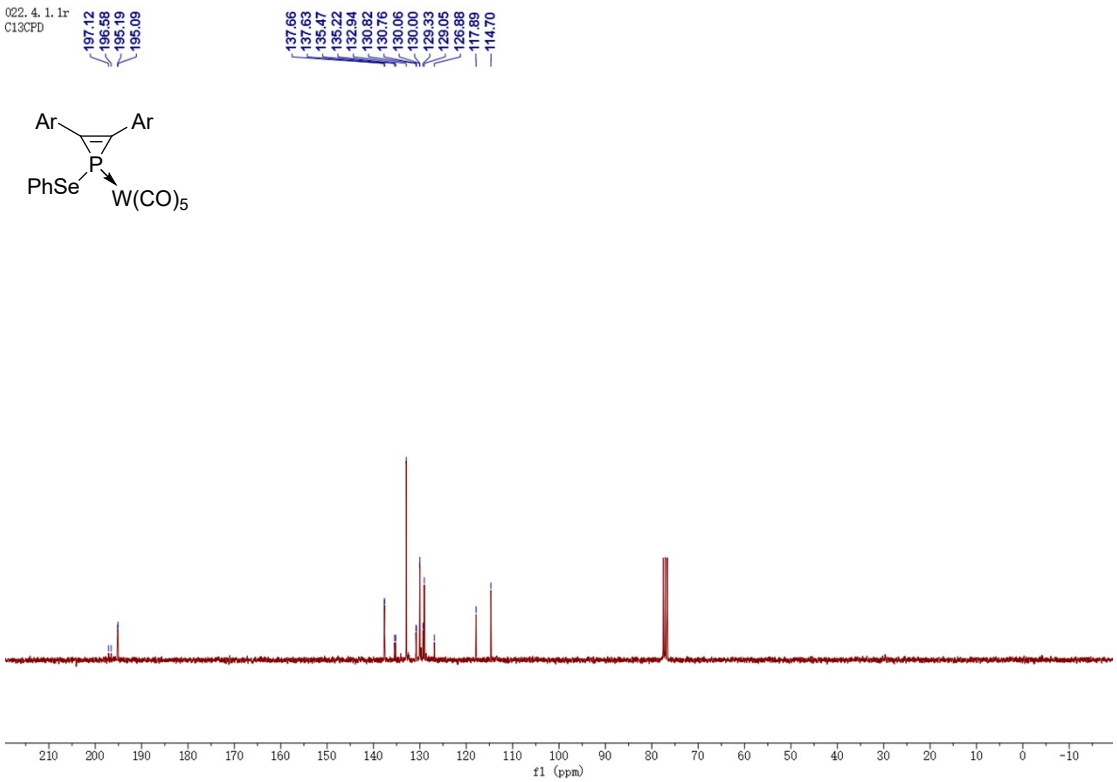

Figure S17. ^{13}C $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **9**

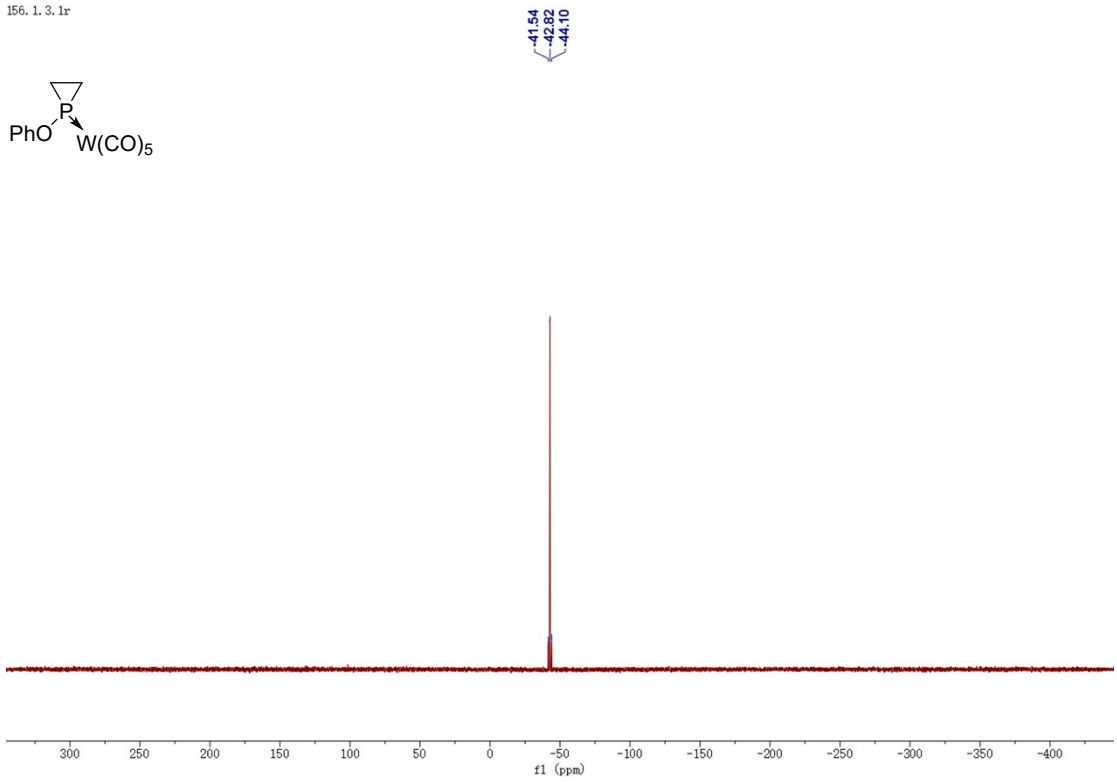

Figure S18. ^{31}P $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **10**

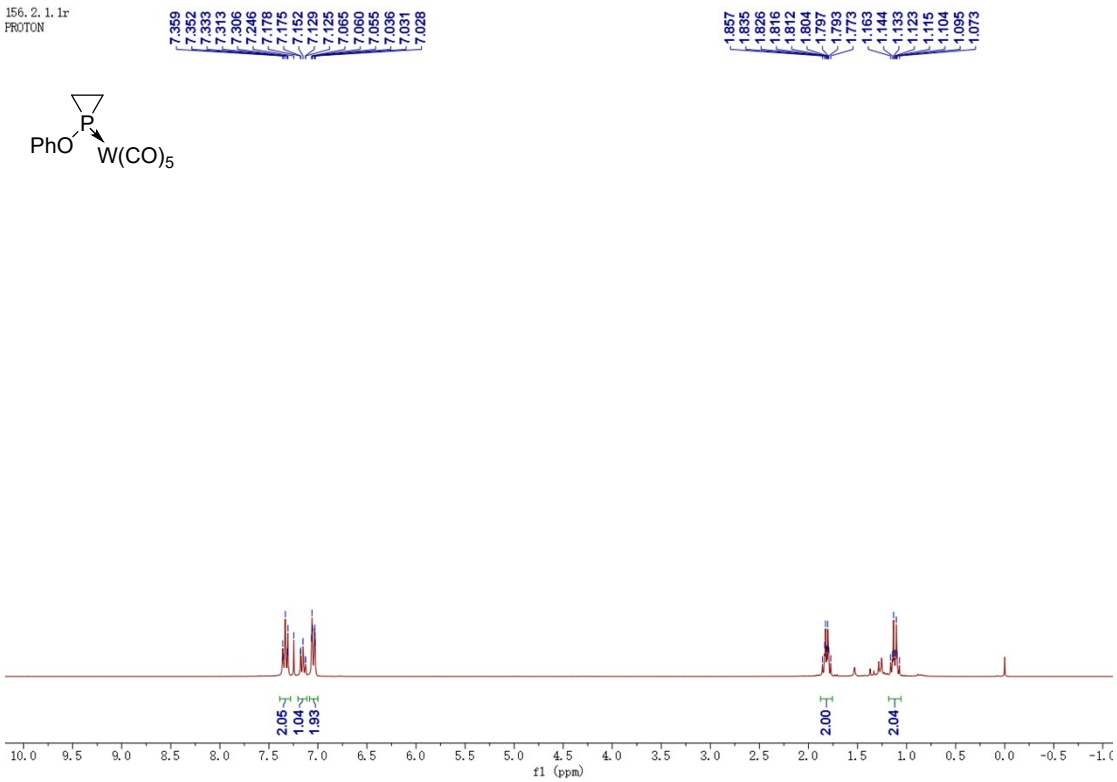

Figure S19. ^{1}H NMR ($CDCl_3$) of Compound **10**

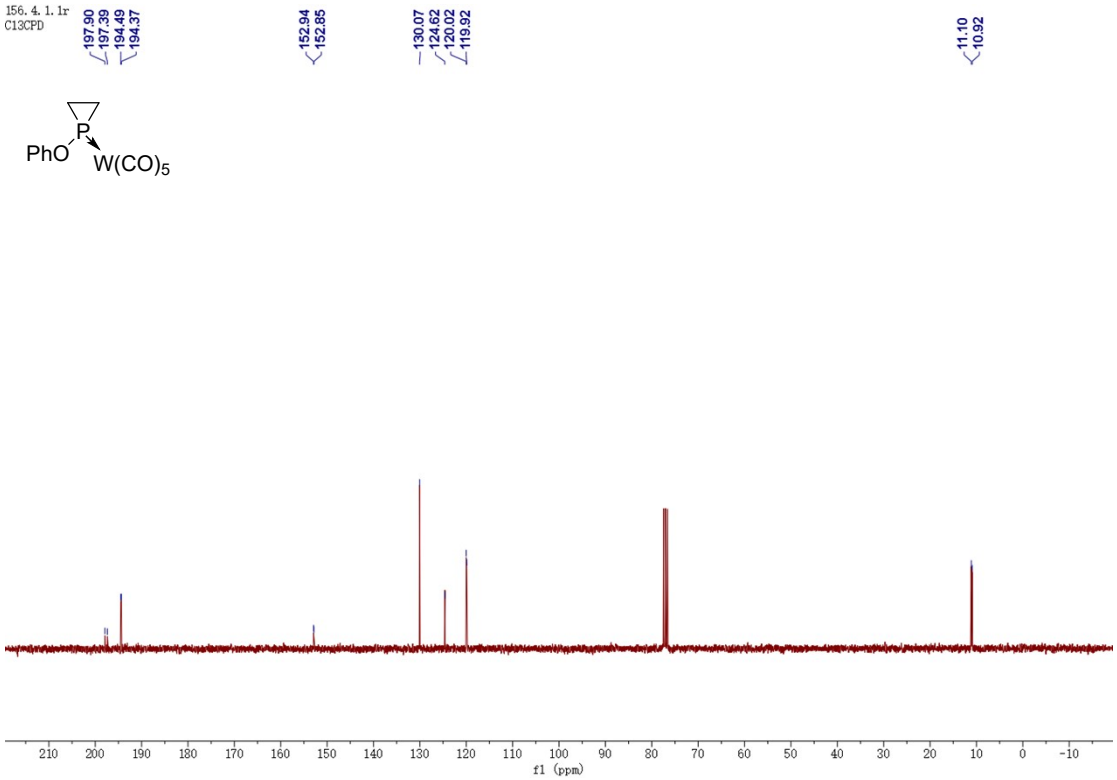

Figure S20. ^{13}C {^{1}H} NMR ($CDCl_3$) of Compound **10**

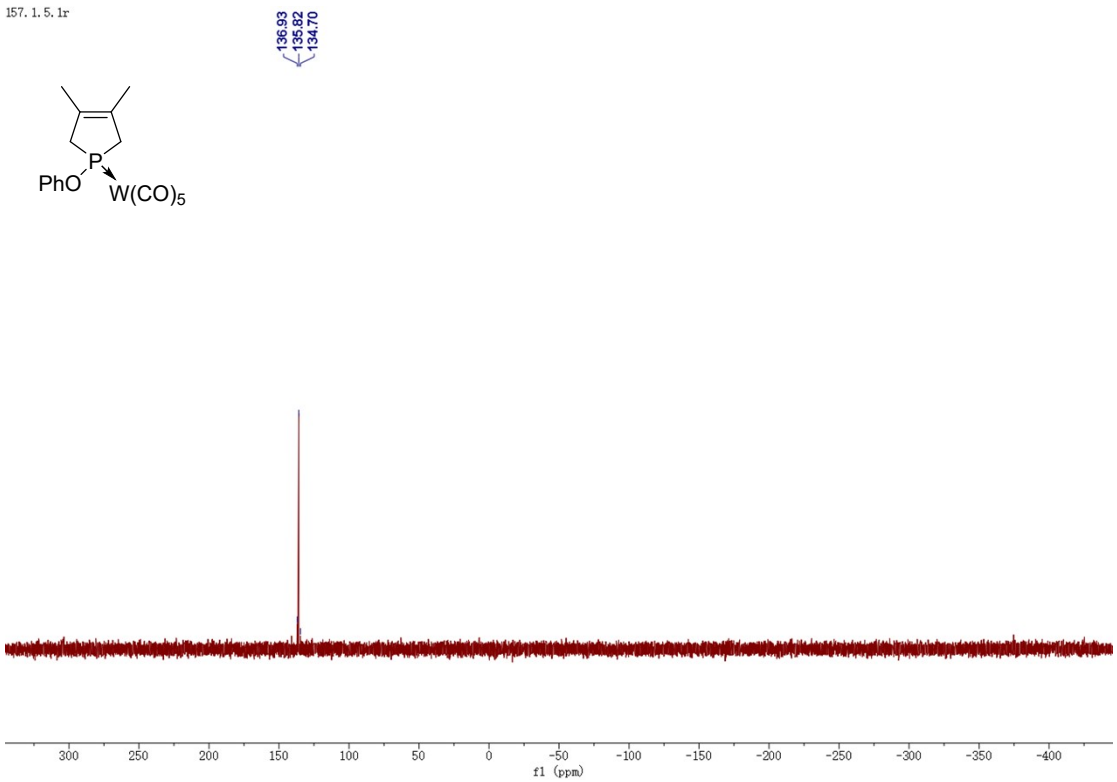

Figure S21. ^{31}P $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **11**

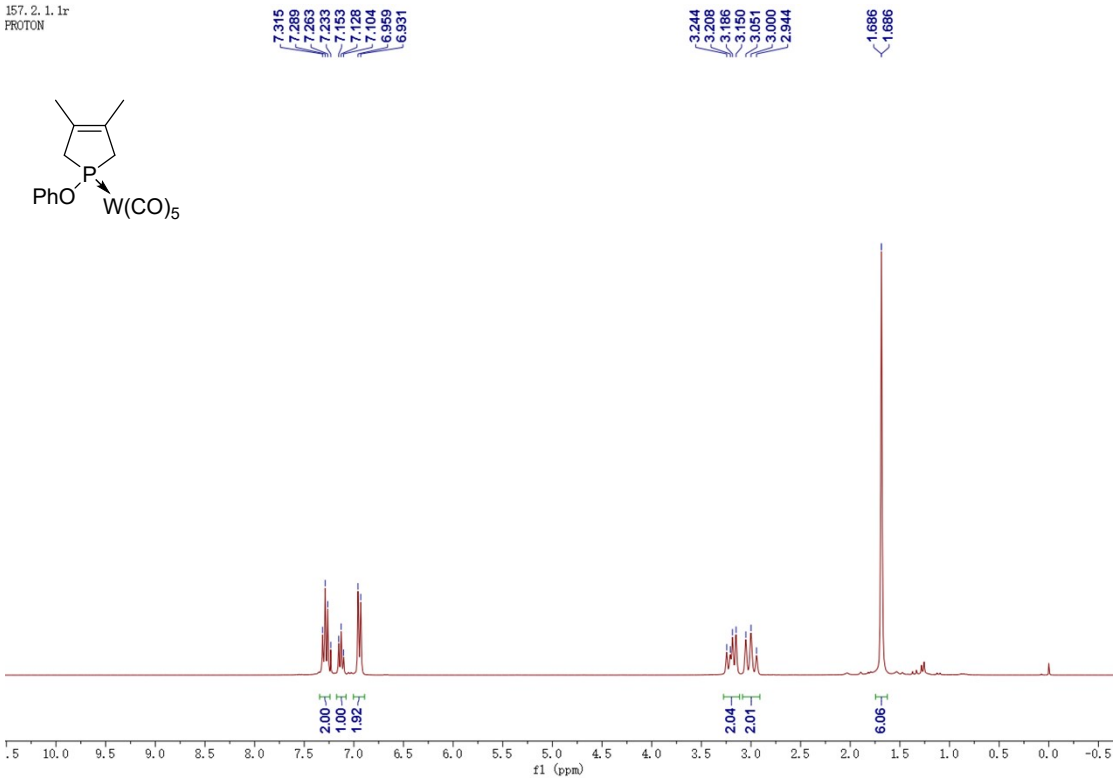

Figure S22. ^{1}H NMR ($CDCl_3$) of Compound **11**

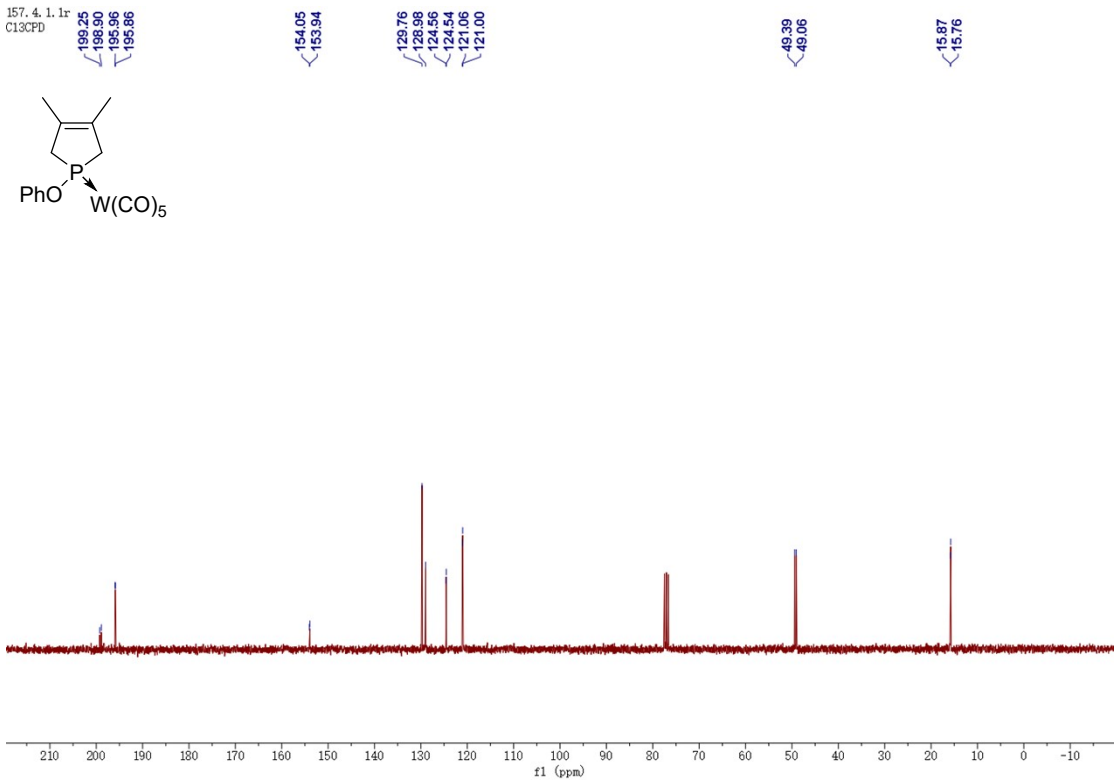

Figure S22. ^{13}C $\{^{1}H\}$ NMR ($CDCl_3$) of Compound **11**