Electronic Supplementary Information (ESI)

Competitive or sequential reactions of an electrophilic terminal phosphinidene metal(0) complex with allyl halides? [2+1]-Cycloaddition *vs* C-X bond insertion

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The transiently generated electrophilic terminal phosphinidene complex $[(CO)_5WPCH(SiMe_3)_2]$ reacted in toluene with allyl halides (X = F, Cl, Br, I) resulting in the formation of stable C-X insertion products **3a-c** and diastereomeric phosphirane complexes **4a,a',b,b'** as well as a methylene phosphirane complex **5** as observed by $^{31}P\{^1H\}$ NMR spectroscopy. DFT calculations revealed that a novel rearrangement of transient phosphirane complexes was responsible.

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Experimental Procedures

All manipulations were carried out under an inert atmosphere of dry nitrogen using standard Schlenk techniques. Solvents were dried and degassed according to standard protocols. Tetrahydrofuran (THF), diethyl ether, petrol ether and n-pentane were dried over sodium wire/benzophenone, CH_2Cl_2 over CaH_2, toluene over sodium and further purified by subsequent distillation. All spectra were recorded on a Bruker Avance 300 spectrometer at 25 °C. The ^{1}H and ^{13}C NMR spectra were referenced to the residual proton resonances and the ^{13}C NMR signals of the deuterated solvents; ^{31}P NMR spectra were referenced to 85% H_3PO_4 and ^{19}F NMR spectra to $CFCl_3$ as an external standard, respectively. Melting points were determined in one-side melted off capillaries using a Büchi Type S apparatus and are uncorrected. Elemental analyses were carried out on a Vario EL gas chromatograph. Mass spectrometric data were collected on a Kratos Concept 1H Spectrometer. IR spectra of all compounds were recorded on a Thermo Nicolet 380 FT-IR spectrometer with an attenuated total reflection (ATR) attachment or a Bruker Alpha Diamond ATR FTIR spectrometer. X-ray data were collected with a Bruker X8-KappaApexII and Nonius KappaCCD diffractometer. CCDC 1917784-1917786 contain the supplementary crystallographic data.

*Synthesis of Complex **3a**.* 2*H*-Azaphosphirene complex **1** (0.5 g, 0.80 mmol) was dissolved in 3 mL of toluene followed by addition of allyl fluoride as toluene solution (1.26 mmol) and was heated at 75°C for 15h. The excess of toluene was removed in vacuo and the product 3a was isolated by column chromatography (Silica gel: 2x5 cm, T = -20°C) as fraction-1 using petrol ether as eluent and after evaporation of the latter in vacuo as light yellow solid. X-ray suitable single-crystals were grown in petrol ether at -25°C.
Yield of **3a** = 0.210 g ca. 46% (m.p. = 95°C). **^{1}H NMR** ($CDCl_3$) δ: 0.22 (s, 9H, $SiMe_3$), 0.24 (s, 9H, $SiMe_3$), 1.95 (d, $^{2}J_{P,H}$ = 12.0 Hz, 1H, PCH), 2.75 (m, 1H, =CH_2), 3.27 (m, 1H, =CH_2), 5.33 (m, 2H, PCH_2), 5.82 (m, 1H, =CH); **^{31}P NMR:** δ: 192.3 ppm (d, $^{1}J_{W,P}$ = 290 Hz, $^{1}J_{P,F}$ = 827.7 Hz; **^{13}C NMR:** δ: 2.00 (d, $^{3}J_{P,C}$ = 3.6 Hz, $SiMe_3$), 2.35 (d, $^{3}J_{P,C}$ = 2.4 Hz, $SiMe_3$), 32.6 (dd, $^{1}J_{P,C}$ = 4.77 Hz), 43.6 (dd, $^{1}J_{P,C}$ = 13.7 Hz), 121.7 (d, 4.8 Hz), 128.8 (d, 11.3 Hz) 196.1 (d, $^{2}J_{P,C}$ = 8.3 Hz, *cis*-CO), 198.8 (d, $^{2}J_{P,C}$ = 28.6 Hz, *trans*-CO); **^{19}F NMR:** δ: -118.51 ppm (d, $^{1}J_{P,F}$ = 827.7 Hz). Mass (EI, 70 eV): 572 (40%) [M^+], 488 (70) [M^+-3CO], 432 (50) [M^+-5CO], 73 (100) [$SiMe_3$]. IR (KBr) data (cm^{-1}): *ν*(CO) 1915 and 2064. Anal. Calcd. for $C_{15}H_{24}FO_5PSi_2W$: C, 31.37; H, 4.21; Found: C, 31.53; H, 4.32.

*Synthesis of Complex **3b**.* 2*H*-Azaphosphirene complex **1** (0.617g, 1mmol) was dissolved in 3 mL of toluene followed by addition of allyl chloride (0.5 g, 6.5 mmol) and was heated at 75°C for 6h. The excess of toluene (and allyl chloride) was removed in *vacuo* and the product **3b** was isolated by column chromatography (neutral aluminum oxide: 2x5 cm, T = -20°C) as Fraction-1 with 2-5% diethylether in petrol ether which on evaporation afforded the light yellow solid. Suitable crystals were grown in diethylether at -25^{0}C and data was collected.
Yield of **3b** = 0.30 g ca. 51% (m.p. = 72-75°C). **^{1}H NMR** ($CDCl_3$): δ: 0.28 (s, 9H, $SiMe_3$), 0.29 (s, 9H, $SiMe_3$), 1.85 (d, $^{2}J_{P,H}$ = 12.0 Hz, 1H, PCH), 3.04 (m, 1H, =CH_2), 3.35 (m, 1H, =CH_2), 5.33 (m, 2H, PCH_2), 5.90 (m, 1H, =CH); **^{31}P NMR:** δ: 118 ppm ($^{1}J_{W,P}$ = 277 Hz); **^{13}C NMR:** δ: 2.1 (d, $^{3}J_{P,C}$ = 3.2 Hz, $SiMe_3$), 2.8 (d, $^{3}J_{P,C}$ = 2.6 Hz, $SiMe_3$), 29.9 (d, $^{1}J_{P,C}$ = 16.8 Hz), 45.25 (d, $^{1}J_{P,C}$ = 14.9 Hz), 121.34 (d, 12.3 Hz), 128.73 (d, 5.2 Hz) 196.05 (d, $^{2}J_{P,C}$ = 7.8 Hz, *cis*-CO), 198.20 (d, $^{2}J_{P,C}$ = 31.7 Hz, *trans*-CO). Mass (EI, 70 eV): 590 (8%) [M^+], 506 (6) [M^+-3CO], 450 (15) [M^+-5CO], 231 (100) [M^+-($W(CO)_5$+Cl)], 73 (50) [$SiMe_3$]. IR (KBr) data (cm^{-1}): ν(CO) 1909, 1939, 1989 and 2074. Anal. Calcd. for $C_{15}H_{24}ClO_5PSi_2W$: C, 30.50; H, 4.09 Found: C, 30.69; H, 4.15.

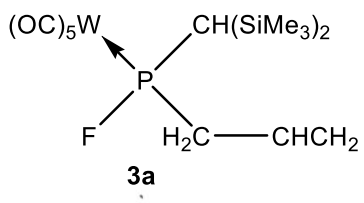
*Synthesis of Complex **3c***. 2*H*-azaphosphirene complex **1** (0.617 g, 1 mmol) was dissolved in 3 mL of toluene followed by addition of allyl bromide (0.2 mL, 1.64 mmol) and was heated at 75°C for 2 h. The excess of toluene and allyl bromide was removed in vacuo and the product was isolated by column chromatography (Silica gel:2x5 cm, Temp. = -30°C) as fraction-2 with 10% diethylether in petrol ether on evaporation afforded the light yellow solid. Suitable crystals were grown in n-pentane at -25°C and data was collected.

Yield of **3c** = 0.120 g ca. 24% (m.p. =70-72°C). **^{1}H NMR:** δ: 0.31 (s, 9H, $SiMe_3$), 0.32 (s, 9H, $SiMe_3$), 1.93 (d, $^{2}J_{P,H}$ = 10.7 Hz, 1H, PCH), 3.18 (m, 1H, $=CH_2$), 3.44 (m, 1H, $=CH_2$), 5.37 (m, 2H, PCH_2), 5.96 (m, 1H, =CH); **^{31}P NMR:** δ: 102.4 ppm, $^{1}J_{W,P}$ = 274.6 Hz; **^{13}C NMR:** δ: 3.33 (d, $^{3}J_{P,C}$ = 3.6 Hz, $SiMe_3$), 3.77 (d, $^{3}J_{P,C}$ = 2.4 Hz, $SiMe_3$), 31.02 (d, $^{1}J_{P,C}$ = 21.5 Hz), 46.45 (d, $^{1}J_{P,C}$ = 11.9 Hz), 122.27 (d, 12.5 Hz), 130.52 (d, 5.9 Hz) 197.49 (d, $^{2}J_{P,C}$ = 6.8 Hz, *cis*-CO), 199.30 (d, $^{2}J_{P,C}$ = 31.6 Hz, *trans*-CO). Mass (EI, 70 eV): 633.90 (36%) [M^+], 550 (22) [M^+-3CO], 494 (70) [M^+-5CO], 231 (100) [M^+-($W(CO)_5$+Br)], 73 (45) [$SiMe_3$]. IR (KBr) data (cm^{-1}): *ν*(CO) 1930 and 2073. Anal. Calcd. for $C_{15}H_{24}BrO_5PSi_2W$: C, 28.36; H, 3.81; Found: C, 28.43; H, 3.89.

Table S1: Product ratios obtained from NMR integration of the corresponding signals from the reaction with allyl-X.

	3 / %	**4,4' / %**	**5 / %**
X = F	19	75	6
X = Cl	17	80	3

NMR/MS/IR Spectra



3a

Figure S1: ^{1}H NMR Spectrum of **3a** in $CDCl_3$ at 300.1 MHz.

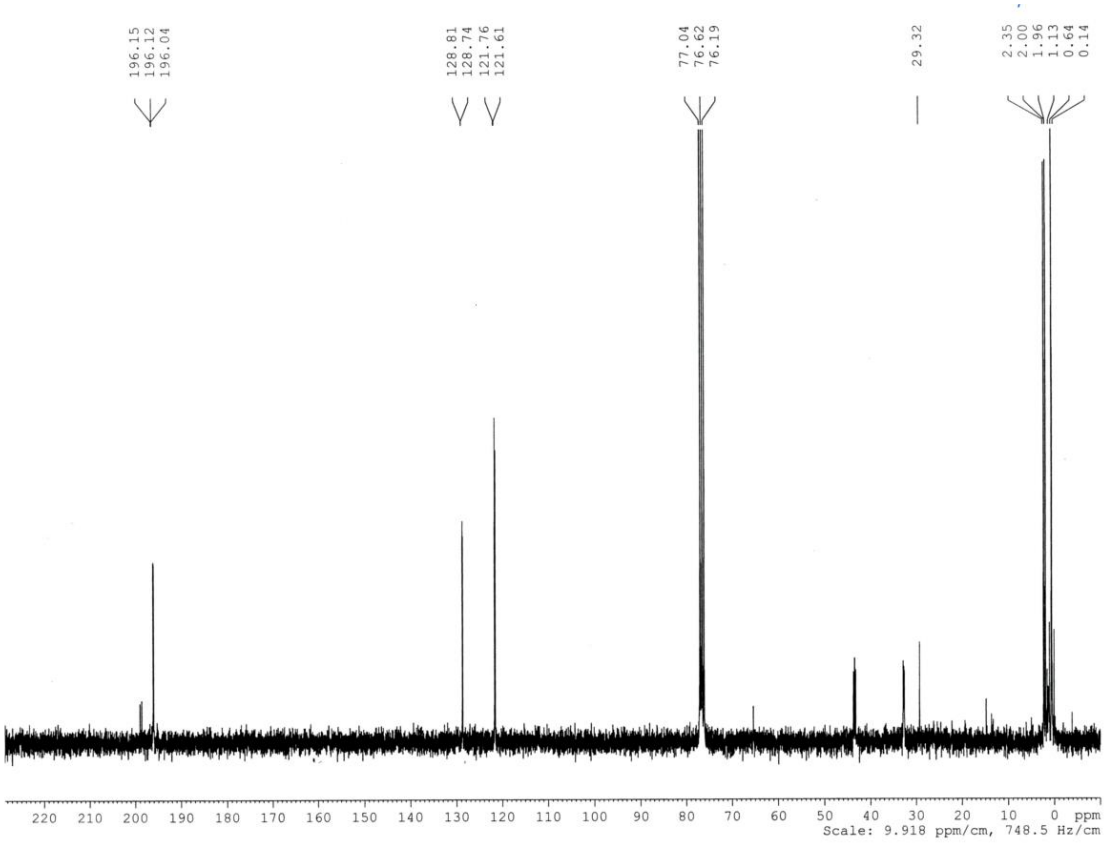


Figure S2: $^{13}C\{^{1}H\}$ NMR Spectrum of **3a** in $CDCl_3$ at 75.5 MHz.

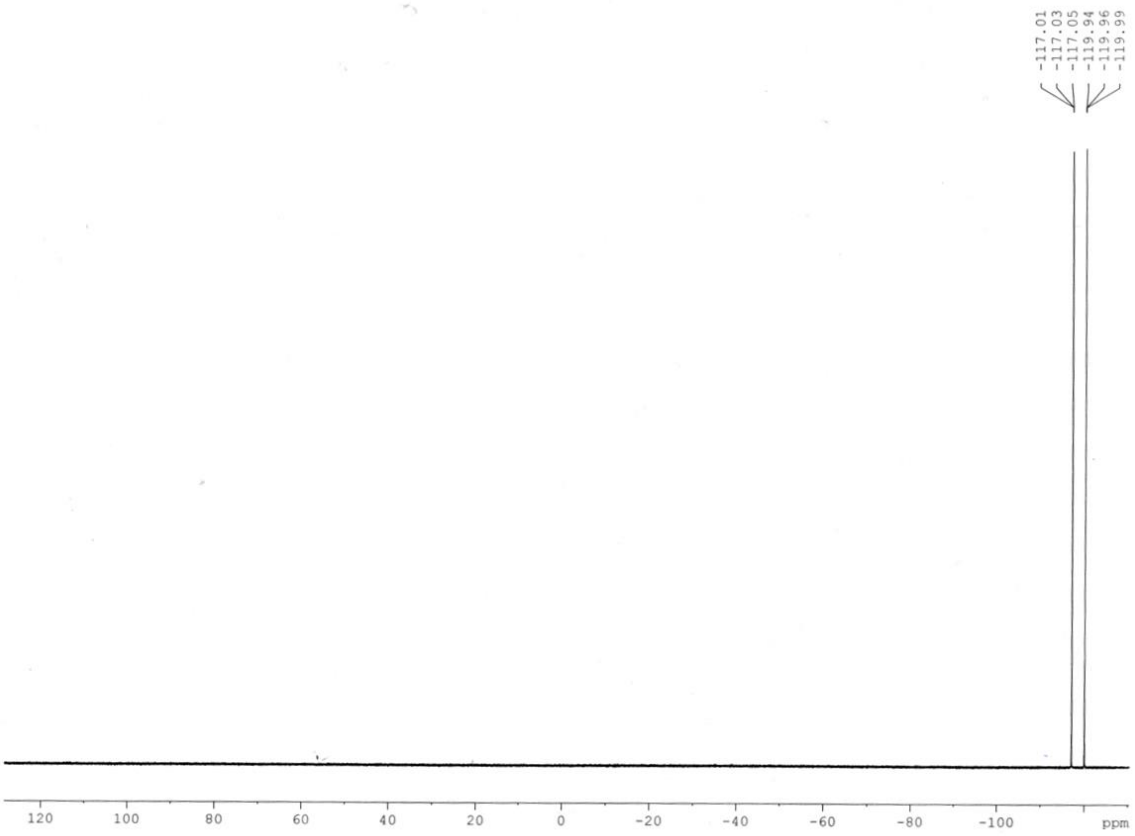


Figure S3: $^{19}F\{^{1}H\}$ NMR Spectrum of **3a** in $CDCl_3$ at 282.4 MHz.

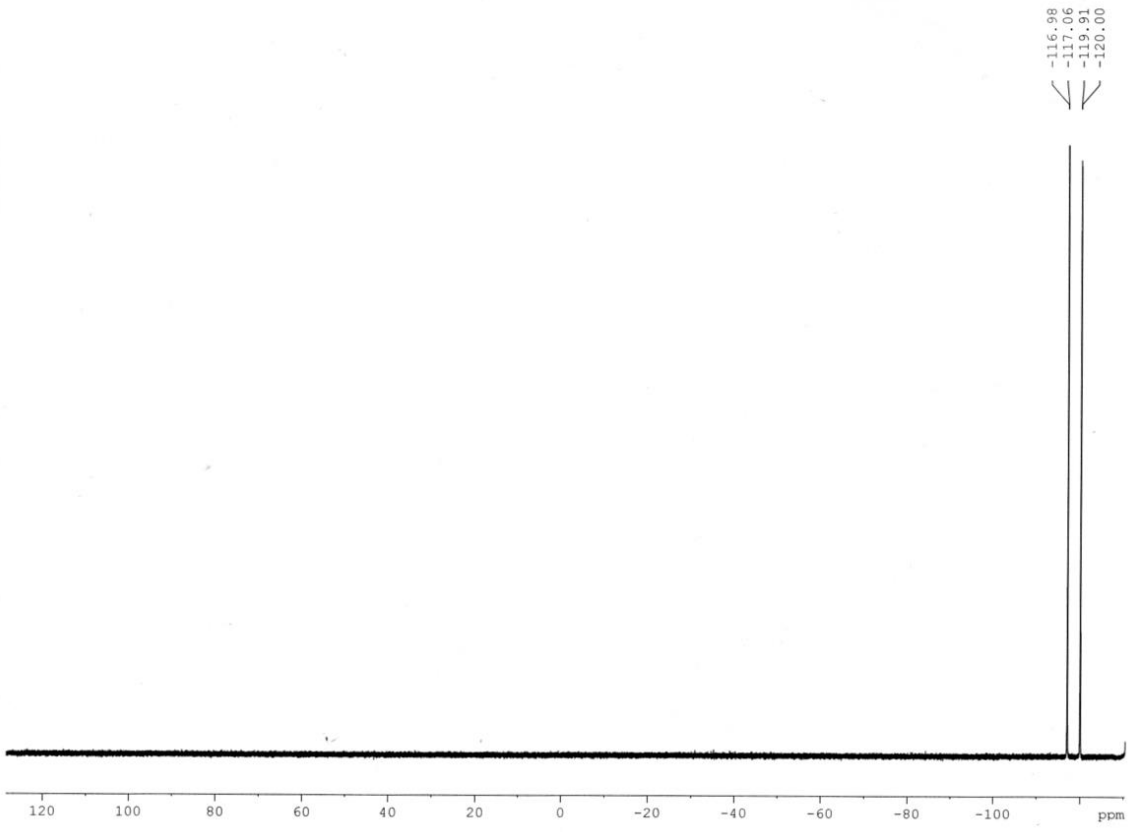


Figure S4: ^{19}F NMR Spectrum of **3a** in $CDCl_3$ at 282.4 MHz.

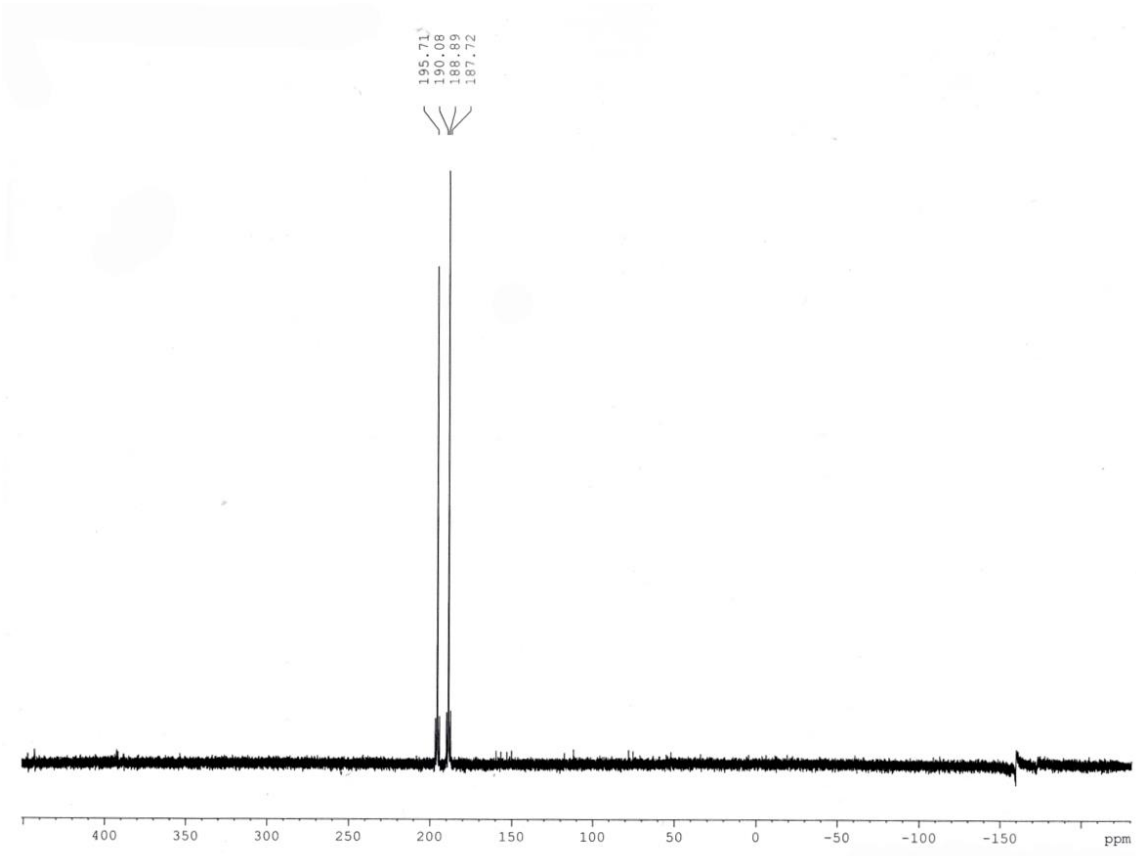


Figure S5: $^{31}P\{^{1}H\}$ NMR Spectrum of **3a** in $CDCl_3$ at 121.5 MHz.

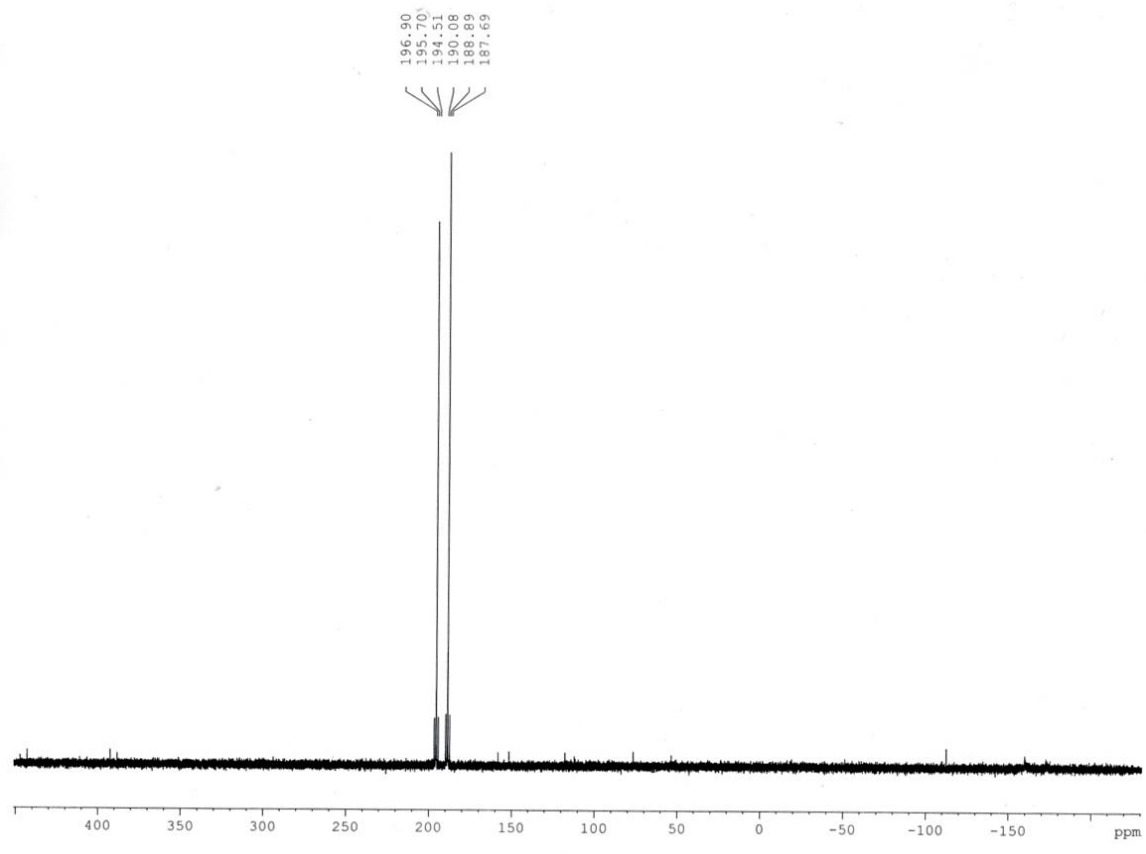


Figure S6: ^{31}P NMR Spectrum of **3a** in $CDCl_3$ at 121.5 MHz.

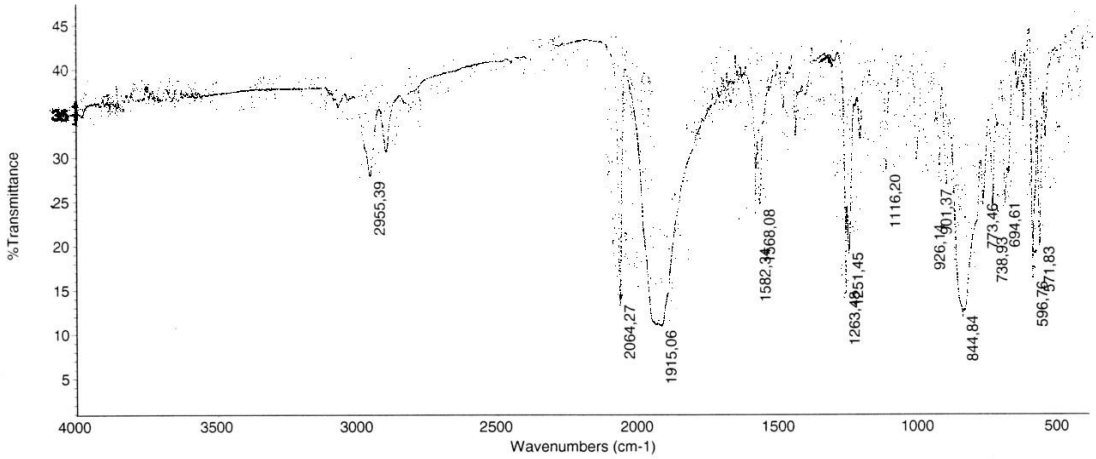


Figure S7: IR Spectrum of **3a**.

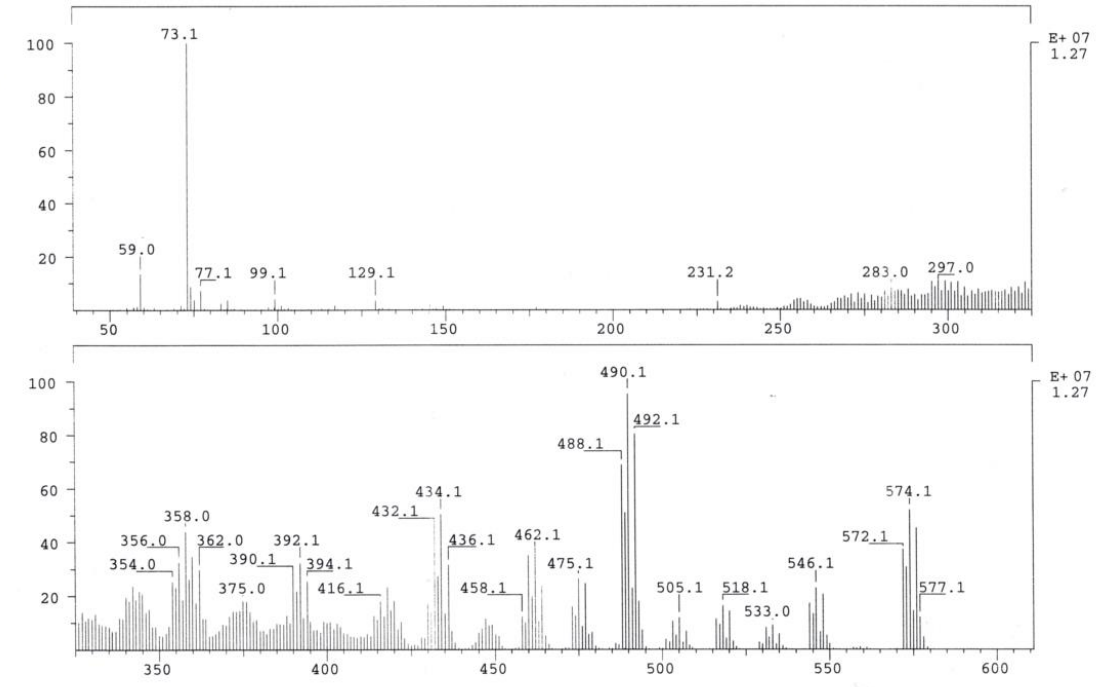


Figure S8: MS Spectrum (EI, 70 eV, ^{184}W) of **3a**.

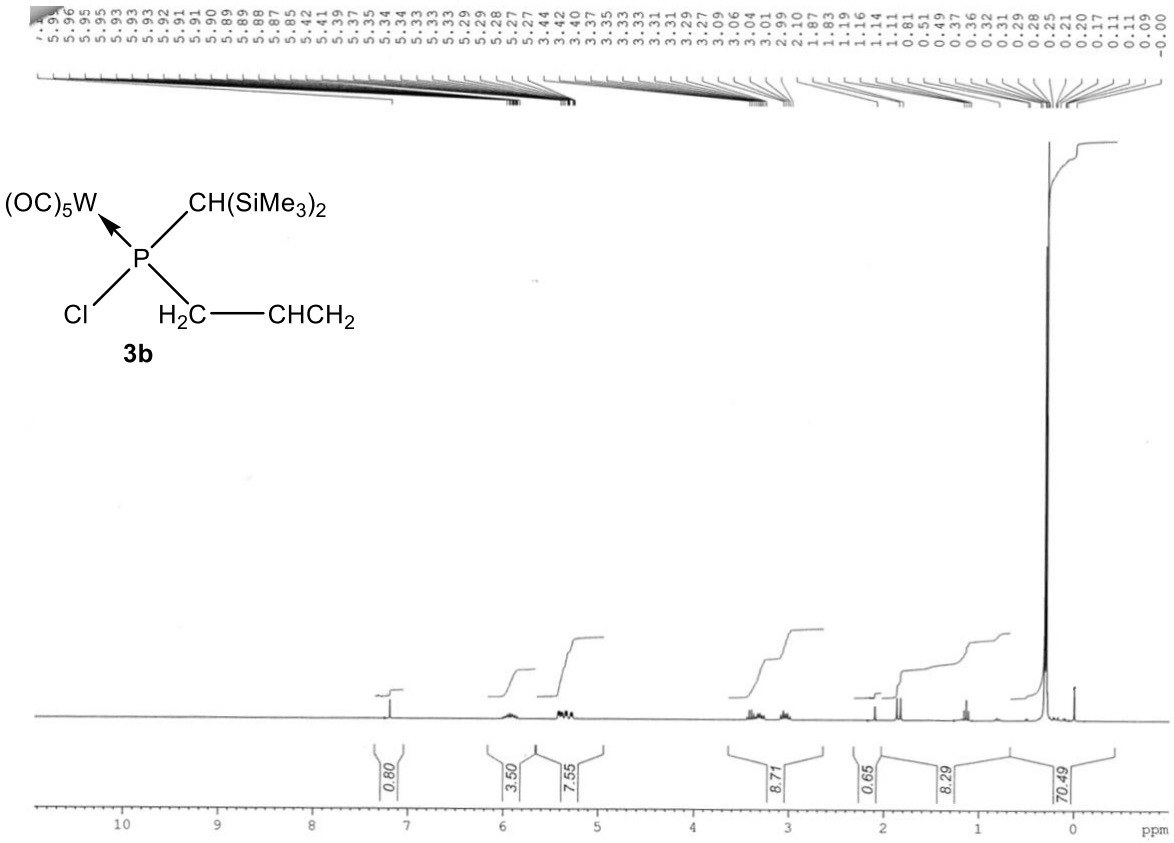


Figure S9: ^{1}H NMR Spectrum of **3b** in $CDCl_3$ at 300.1 MHz.

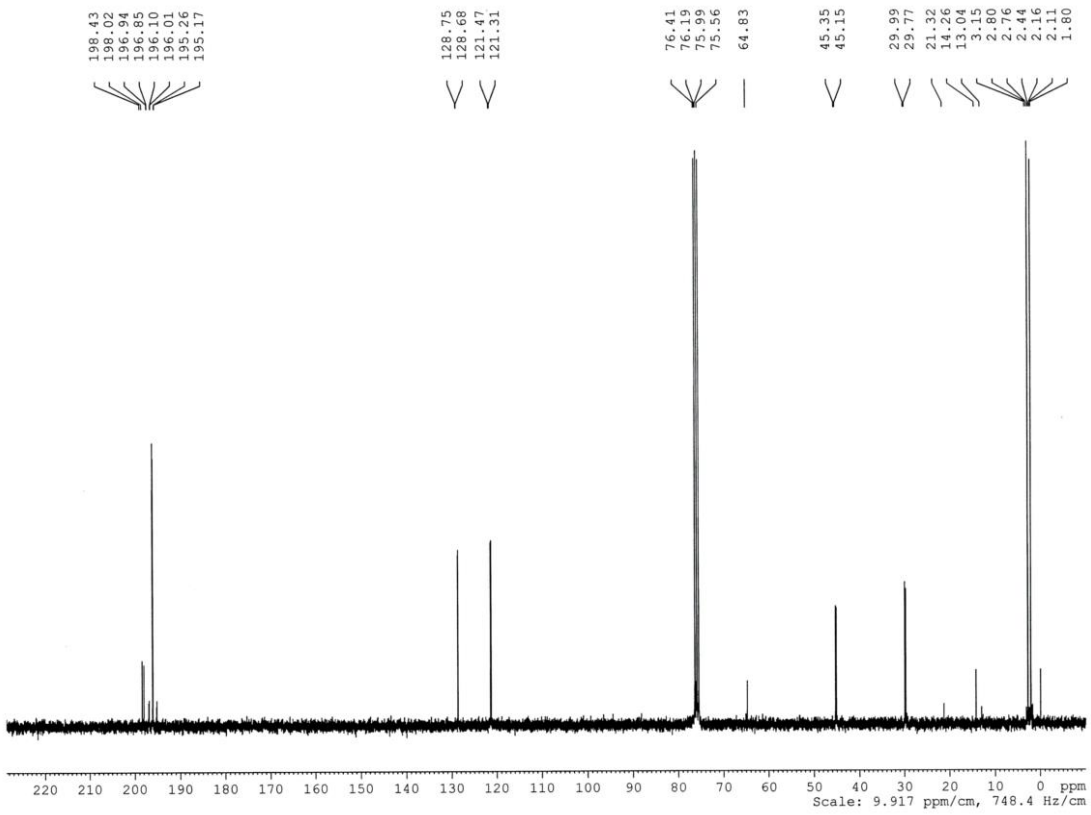


Figure S10: $^{13}C\{^{1}H\}$ NMR Spectrum of **3b** in $CDCl_3$ at 75.5 MHz.

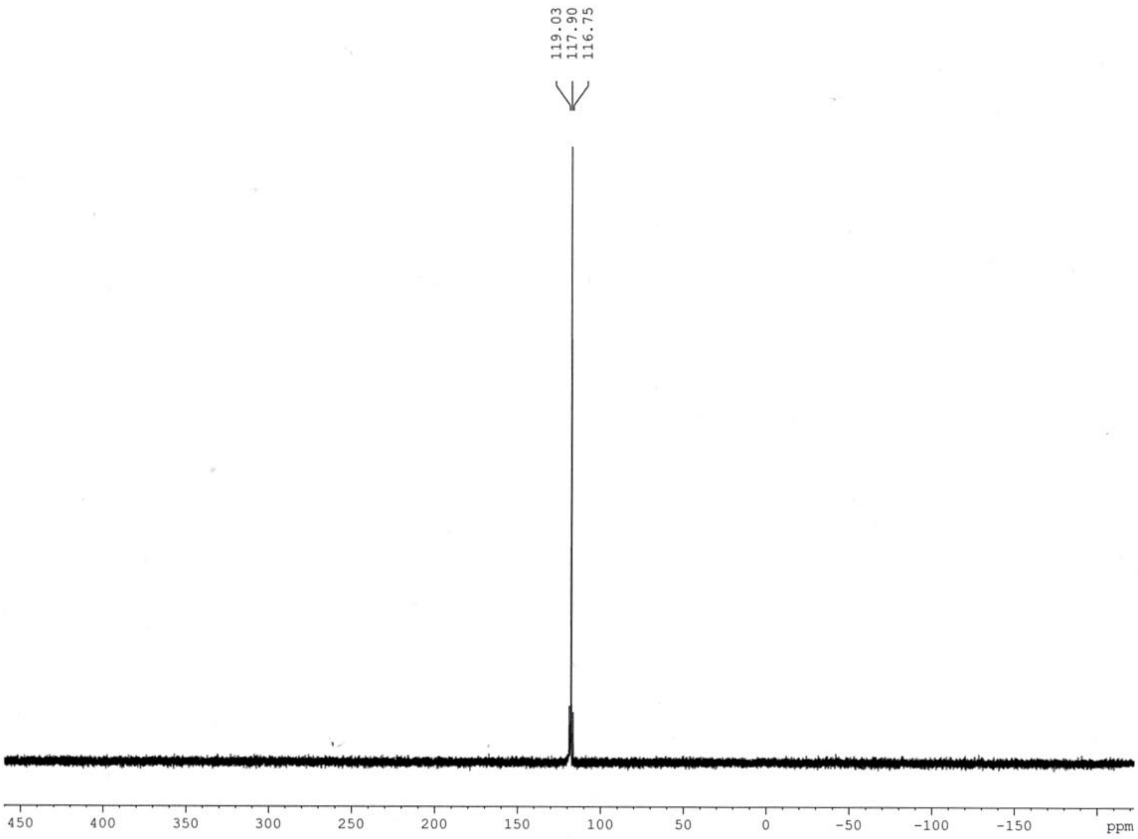


Figure S11: $^{31}P\{^{1}H\}$ NMR Spectrum of **3b** in $CDCl_3$ at 121.5 MHz.

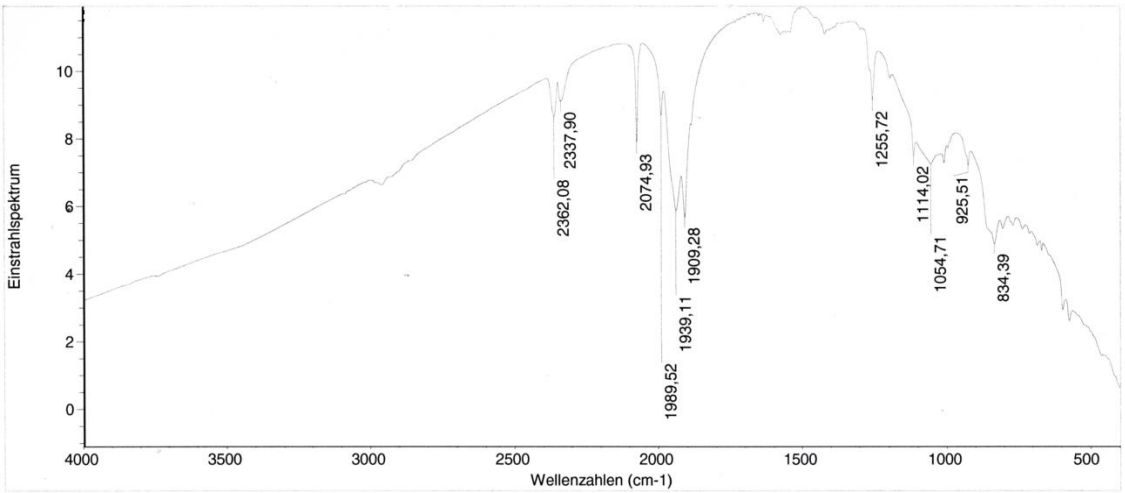


Figure S12: IR Spectrum of **3b**.

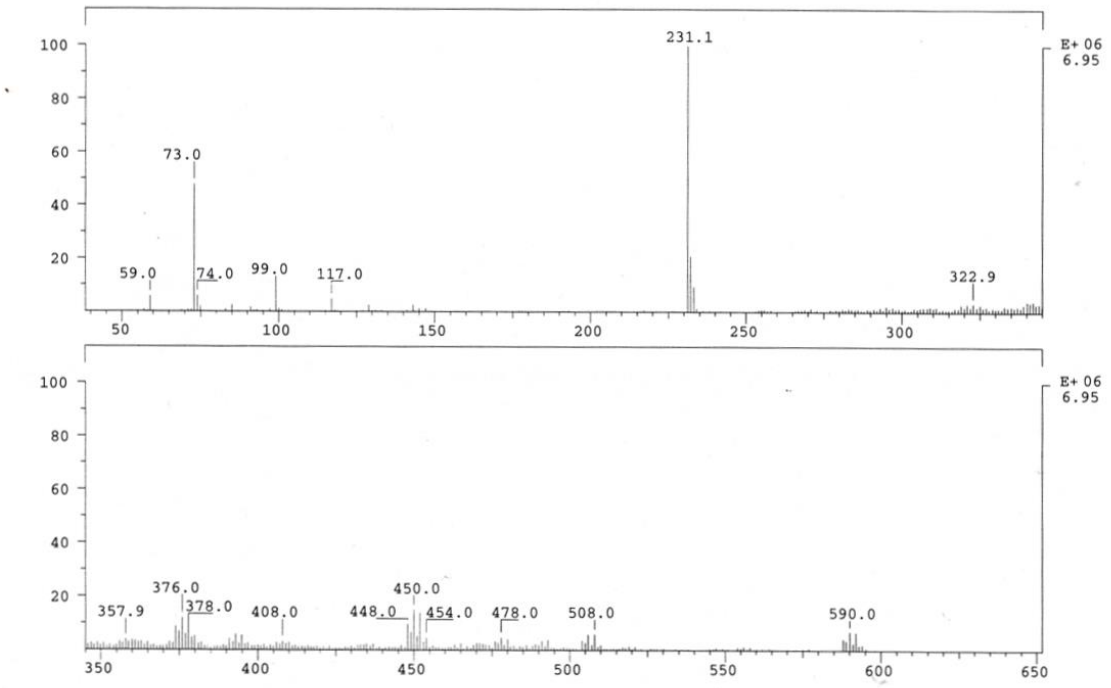


Figure S13: MS Spectrum (EI, 70 eV, ^{184}W) of **3b**.

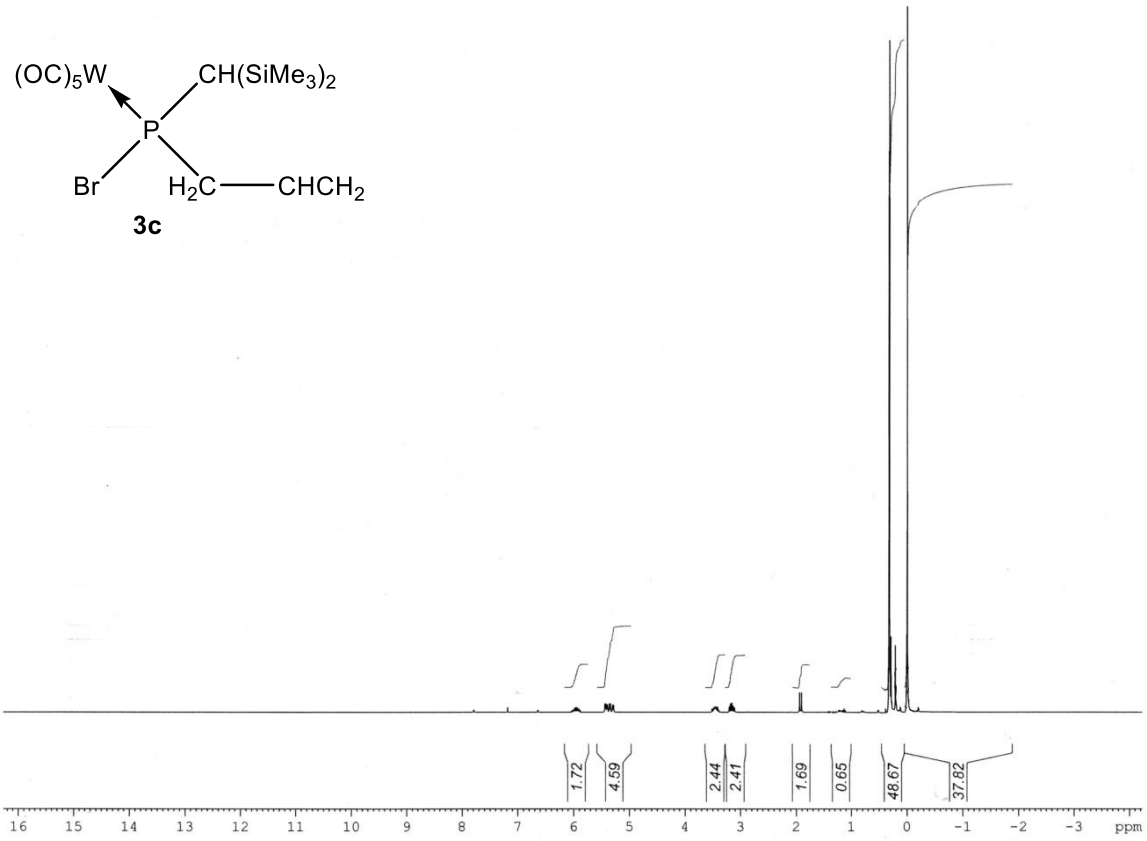


Figure S14: ^{1}H NMR Spectrum of **3c** in $CDCl_3$ at 300.1 MHz.

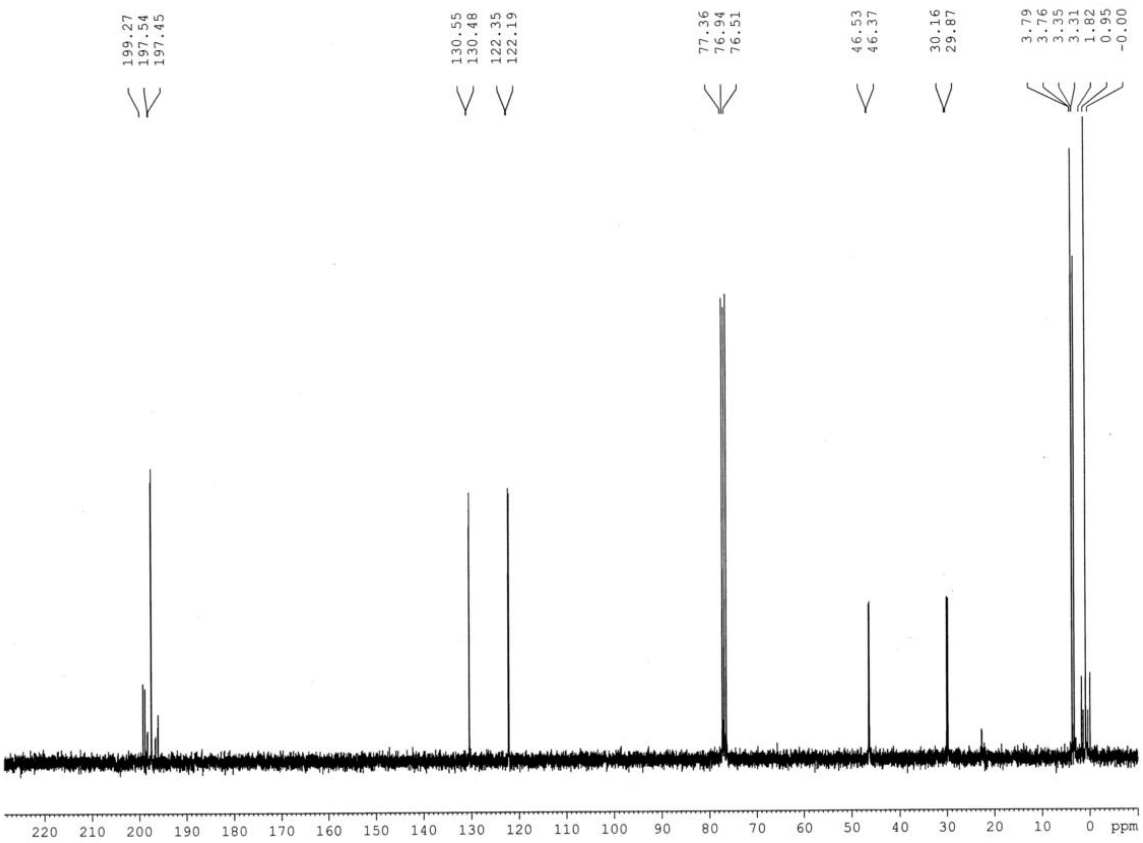


Figure S15: $^{13}C\{^{1}H\}$ NMR of **3c** in $CDCl_3$ at 75.5 MHz.

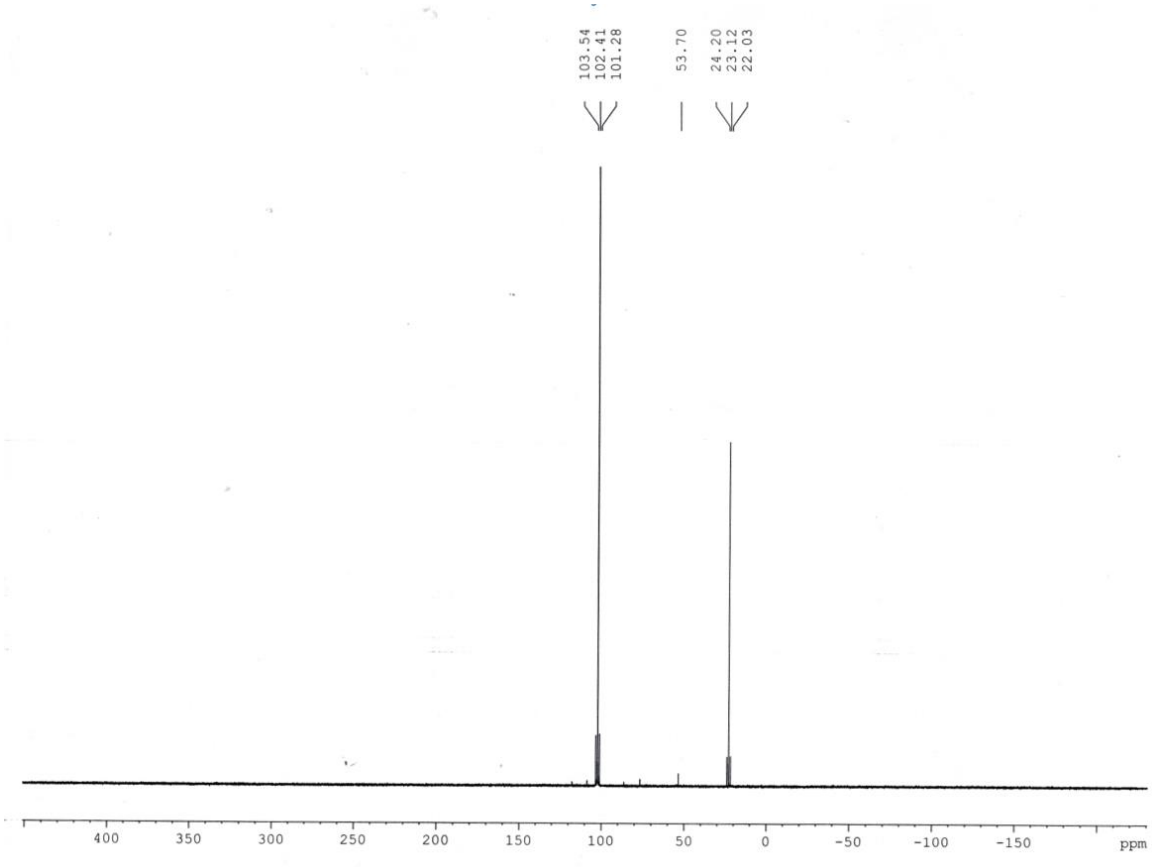


Figure S16: $^{31}P\{^{1}H\}$ NMR Spectrum of **3c** (81 %) and **6** (19 %) in $CDCl_3$ at 121.5 MHz.

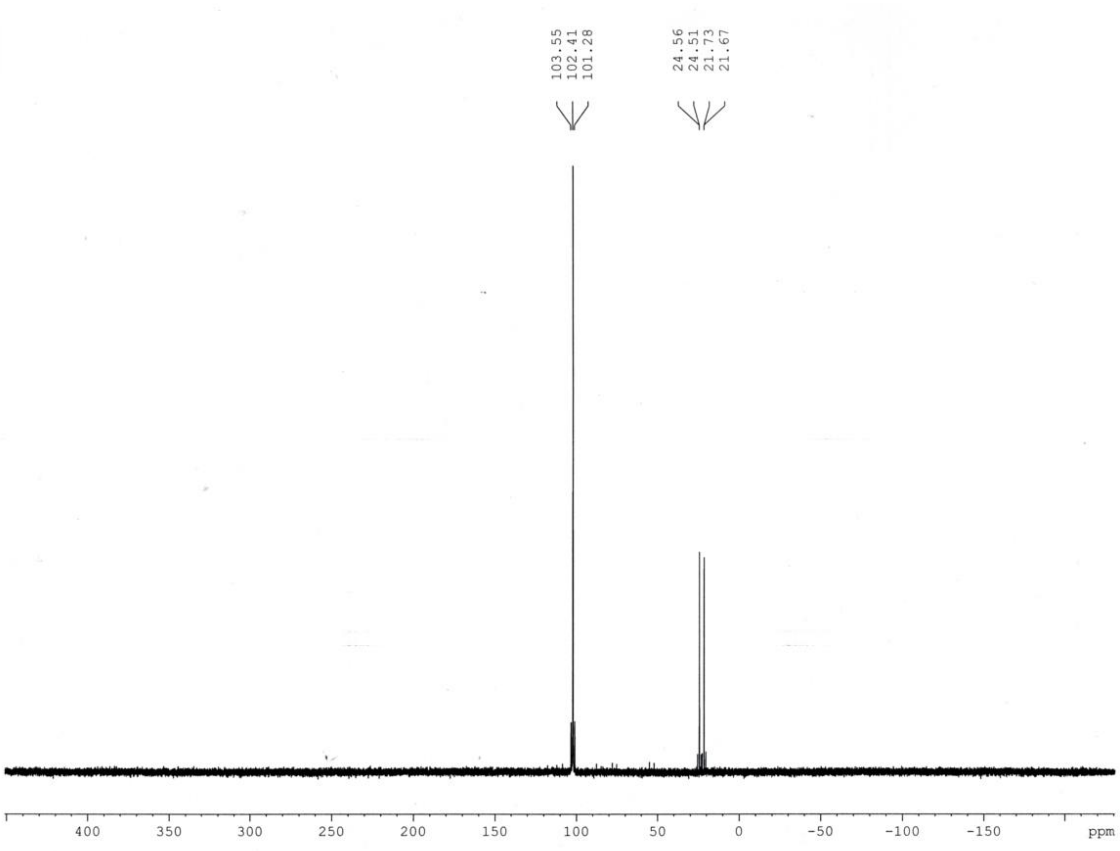


Figure S17: ^{31}P NMR Spectrum of **3c** (81 %) and **6** (19 %) in $CDCl_3$ at 121.5 MHz.

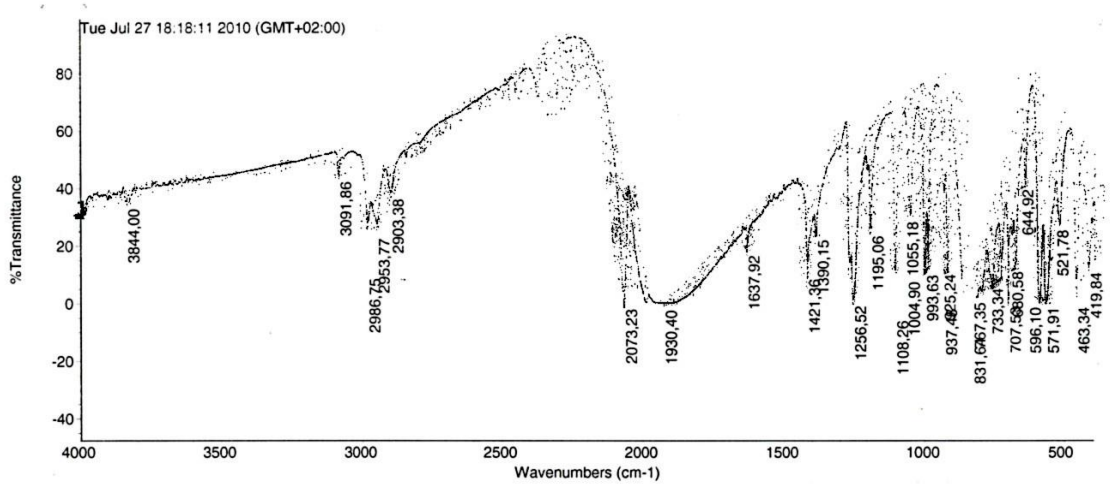


Figure S18: IR Spectrum of **3c**.

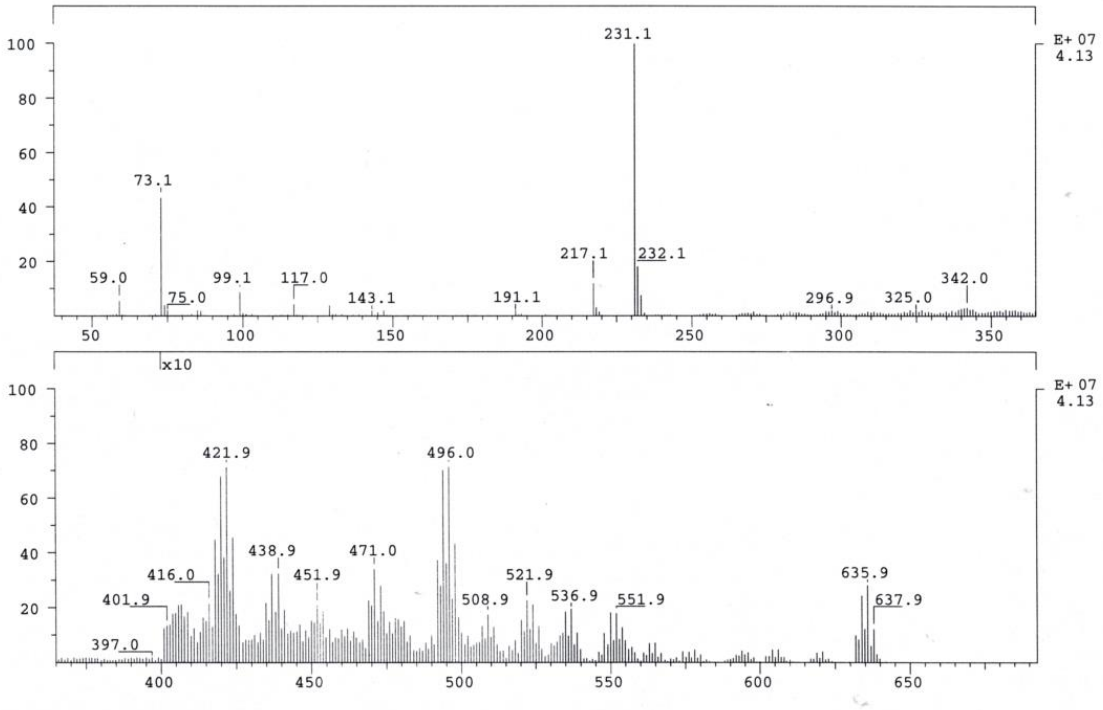
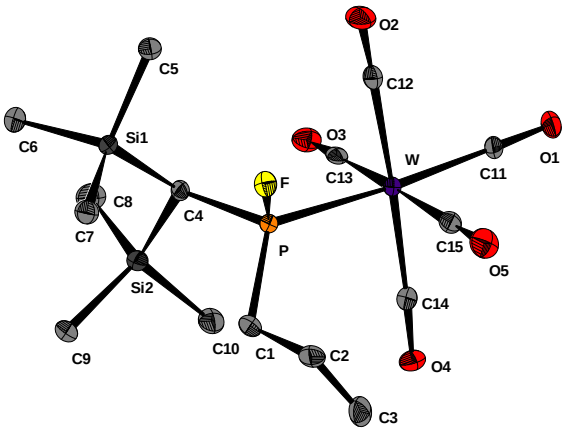
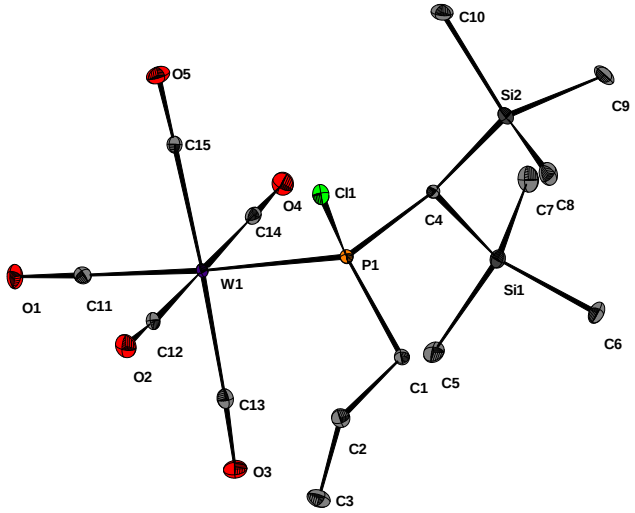


Figure S19: MS Spectrum (EI, 70 eV, ^{184}W) of **3c**.

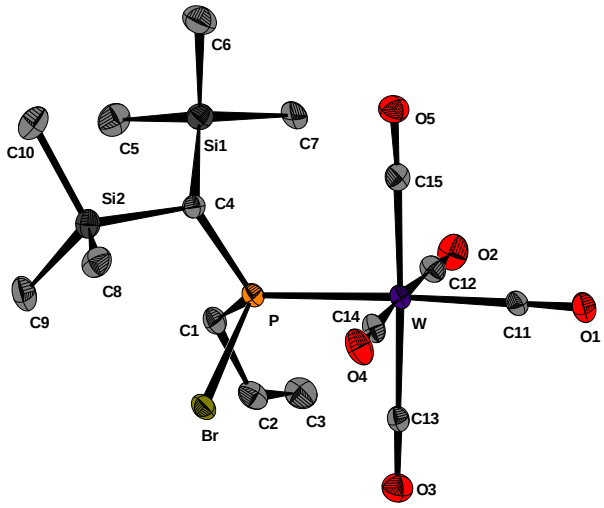
Crystallographic Data



*Crystal Data for **3a**:* Suitable single crystals of **3a** were obtained from a concentrated diethylether solution at 4 °C. Data were collected with a Nonius KappaCCD diffractometer equipped with a low-temperature device at 100.2 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97):$C_{15}H_{24}FO_5PSi_2W$, M_r = 574.34, crystal dimensions 0.40 × 0.40 × 0.30 mm^3, monoclinic, space group $P2_1/n$, Z = 4, a = 9.4372(3) Å, b = 18.8621(6) Å, c = 12.3957(4) Å, α = 90°, β = 94.0074(18)°, γ = 90°, V = 2201.11(12) Å^3, ρ_{calc} = 1.733 g cm^{-3}, μ = 5.458 mm^{-1}, transmission factors (min/max) 0.124/0.190, semi-empirical absorption correction, $2\theta_{max}$ = 25.25°, no. of unique data 3926, R_{int} = 0.1526, R_1 (for I >2σ(I)) = 0.0567, wR_2 (for all data) = 0.1527, final R_1 = 0.619, goodness of fit 1.029, ΔF(max/min) = 2.866 /−3.098 e Å^{-3}. CCDC 1917785.



*Crystal Data for **3b**:* Suitable single crystals of **3b** were obtained from a concentrated diethylether solution at 4 °C. Data were collected with a X8-KappaApexII diffractometer equipped with a low-temperature device at 100.2 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97):$C_{15}H_{24}ClO_5PSi_2W$, M_r = 590.79, crystal dimensions 0.60 × 0.60 × 0.60 mm^3, orthorhombic, space group Pbca, Z = 8, a = 18.1955(6) Å, b = 13.3383(5) Å, c = 18.5737(7) Å, α = 90°, β = 90°, γ = 90°, V = 4507.8(3) Å^3, ρ_{calc} = 1.741 g cm^{-3}, μ = 5.441 mm^{-1}, transmission factors (min/max) 0.04/0.05, integrational absorption correction, $2\theta_{max}$ = 28.00°, no. of unique data 5426, R_{int} = 0.0390, R_1 (for I >2σ(I)) = 0.0217, wR_2 (for all data) = 0.0492, final R_1 = 0.0239, goodness of fit 1.171, ΔF (max/min) = 1.340 /−0.949 e Å^{-3}. CCDC 1917784.



*Crystal Data for **3c**:* Suitable single crystals of **3c** were obtained from a concentrated diethylether solution at 4 °C. Data were collected with a Nonius KappaCCD diffractometer equipped with a low-temperature device at 123.2 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97):$C_{15}H_{24}BrO_5PSi_2W$, M_r = 635.25, crystal dimensions 0.60 × 0.30 × 0.04 mm³, orthorhombic, space group Pbca, Z = 8, a = 18.0162(4) Å, b = 13.6552(3) Å, c = 18.5562(6) Å, α = 90°, β = 90°, γ = 90°, V = 4565.1(2) Å³, ρ_{calc} = 1.849 g cm^{-3}, μ = 7.006 mm^{-1}, transmission factors (min/max) 0.1019/0.7669, semi-empirical absorption correction, $2\theta_{max}$ = 27.99°, no. of unique data 5494, R_{int} = 0.0923, R_1 (for I >2σ(I)) = 0.0393, wR_2 (for all data) = 0.0973, final R_1 = 0.0633, goodness of fit 0.957, ΔF (max/min) = 2.023 /−2.310 e Å^{-3}. CCDC 1917786.

Table S2: Crystal data comparison for complexes **3-c** (bond angles in [°]).

	C(4)-P-X	X-P-W
3a (X = F)	102.9(3)	107.88(17)
3b (X = Cl)	106.34(9)	106.06(3)
3c (X = Br)	107.20(17)	105.22(6)

Computational part.

Validation of *P*-methyl substitution in model derivatives.

In order to assess the validity of using a methyl group as P-substituent instead of the Tms_2CH- (bisyl) group which is present in the experimentally used and obtained compounds, the structures for the latter were computed at the working level of theory for the case of X = F (i.e., **3a**, **4a**^{ap} and **5**+HF), including the key intermediate **8** (**8**^{bis}·HF) that is the most sensitive with regard to the nature of the *P*-substituent, and compared with model (*P*-Me substituted) compounds (**3a**^{Me}, **4a**$^{ap\text{-}Me}$, **5**^{Me}·HF and **8**·HF). Their energies, as well as those for the initial reagents are collected in Table S3.

Table S3: Computed (CCSD(T)/def2-TZVPPecp//B3LYP-D3/def2-TZVPecp) zero-point energy-corrected energies (kcal/mol) relative to the most stable isomer.

7bis+**2a**	**3a**^{ap}	**4a**	**5**+HF	**8**^{bis}·HF
68.80	0.00	33.25	46.33	43.83
7+**2a**	**3a**^{Me}	**4a**$^{ap\text{-}Me}$	**5**^{Me}·HF	**8**·HF
75.54	0.00	32.72	45.30	42.88

The relative energies of all four products and intermediate (**3**, **4**, **5** and **8**) are very similar in both the P-methyl and P-bisyl series (differences below 1.03 kcal/mol), which validates the use of P-methyl model derivatives for the computational study. The most significant difference is the relative instability of the P-methyl model phosphinidene **7** compared to **7**^{bis} (by 6.74 kcal/mol).

Calculated structures.

Cartesian coordinates (in Å) and ZPE-correction (hartrees) for all computed species at the optimization level. Imaginary frequency (cm^{-1}) for transition states. Electronic energies (hartrees) at the DLPNO-CCSD(T)/def2-TZVPPecp level.

2a E = -216.813464594068 au

ZPE = 0.0727911 au

C	-0.068069	0.184876	-0.025901	C	-1.242037	-0.071805	-2.197978
H	-0.016973	0.072423	1.049461	H	-1.410121	-1.049084	-2.660032
H	0.801099	0.609527	-0.515952	H	-0.347320	0.382260	-2.628551
C	-1.140145	-0.180222	-0.715591	F	-2.338603	0.730996	-2.546765
H	-2.007081	-0.594817	-0.210082				

2b E = -576.808546937639 au

ZPE = 0.07135484 au

C	-0.056101	0.229801	-0.006283	C	-1.185574	-0.142539	-2.181733
H	-0.013193	0.136478	1.071107	H	-1.342325	-1.119207	-2.635824
H	0.786441	0.709281	-0.491732	H	-0.310745	0.329557	-2.621673
C	-1.091903	-0.222790	-0.700658	Cl	-2.624274	0.852000	-2.689482
H	-1.931577	-0.688426	-0.195112				

7 E = -1013.2882925228 au

ZPE = 0.07775263 au

P	-1.284747	1.079864	0.277127	C	-3.066926	-1.358971	-0.617762
C	-1.007794	-0.101120	1.673095	O	-3.703662	-2.037188	0.044012
H	-1.971071	-0.165786	2.196951	C	-3.420434	1.254362	-2.027821
H	-0.292985	0.310534	2.387598	O	-4.265372	2.005073	-2.178869
H	-0.716119	-1.110789	1.386654	C	-0.634178	1.202872	-2.799164
W	-1.866963	-0.101535	-1.746637	O	0.039949	1.925539	-3.368107
C	-2.383001	-1.074536	-3.531556	C	-0.313170	-1.428296	-1.401777
O	-2.659305	-1.627484	-4.490050	O	0.534614	-2.154614	-1.163896

7bis E = -1829.34484869038 au

ZPE = 0.28198258 au

P	-0.045388	0.275046	0.171346	H	-1.147789	-2.654305	1.641225
C	-0.939970	0.661528	1.692392	C	1.069564	-0.254585	3.953553
H	-2.026338	0.578226	1.579604	H	1.308287	-1.078063	4.631621
Si	-0.605143	2.463899	2.241987	H	1.915834	-0.124992	3.276698
C	1.224671	2.865477	2.292808	H	0.972063	0.650095	4.554543
H	1.713016	2.608480	1.351576	C	-1.968057	-0.792114	4.169543
H	1.350726	3.939360	2.454640	H	-1.786570	-1.570177	4.915967
H	1.747947	2.343561	3.093300	H	-2.163458	0.141256	4.697212
C	-1.431495	3.575757	0.975460	H	-2.869428	-1.065832	3.616896
H	-1.343188	4.625042	1.267847	W	-1.476157	-0.490184	-1.648274
H	-0.969364	3.466348	-0.008406	C	-2.572460	-1.114348	-3.304279
H	-2.493611	3.348207	0.867620	O	-3.185042	-1.445786	-4.209955
C	-1.388201	2.783153	3.918989	C	-2.829747	-1.206568	-0.274105
H	-1.301639	3.845545	4.162081	O	-3.550071	-1.576429	0.535429
H	-2.450366	2.529744	3.918226	C	-2.564347	1.276413	-1.652809
H	-0.906368	2.221327	4.720239	O	-3.195003	2.227953	-1.639573
Si	-0.497373	-0.668901	3.012546	C	0.000123	0.287474	-2.880369
C	-0.257734	-2.340692	2.188079	O	0.831873	0.718377	-3.533137
H	0.585074	-2.340985	1.492927	C	-0.481357	-2.319913	-1.629020
H	-0.053683	-3.098435	2.949332	O	0.055217	-3.326481	-1.609069

4a^{ap} E = -2046.22011919196 au

ZPE = 0.35992659 au

P	-0.043642	0.368945	-0.054311	H	-1.405520	3.855440	4.067255
C	1.761697	0.063643	-0.178608	H	-2.470433	2.538703	3.578404
C	1.305908	1.442245	-0.636612	H	-1.083250	2.215714	4.622467
H	2.015747	-0.632606	-0.970705	Si	-0.431666	-0.638428	2.926190
C	2.666997	-0.016876	1.006739	C	-0.022234	-2.275098	2.102652
H	2.809995	-1.046224	1.336815	H	0.913814	-2.255444	1.545270
H	2.300124	0.582226	1.837483	H	0.071192	-3.043078	2.875027
F	3.934800	0.485482	0.675096	H	-0.807753	-2.594532	1.418895
H	1.335441	1.655864	-1.696919	C	0.874819	-0.292419	4.233162
H	1.623850	2.271497	-0.022063	H	0.854121	-1.109181	4.959841
C	-0.604438	0.773818	1.639700	H	1.887638	-0.240999	3.833869
H	-1.690500	0.770653	1.475881	H	0.678582	0.631353	4.778760
Si	-0.360993	2.563846	2.243762	C	-2.090975	-0.793654	3.785631
C	1.407832	2.998735	2.706864	H	-2.059024	-1.600160	4.522438
H	2.103327	3.002525	1.867819	H	-2.364705	0.122942	4.309475
H	1.409980	4.008022	3.127998	H	-2.884037	-1.029155	3.073801
H	1.808711	2.330262	3.469584	W	-1.683255	-0.643629	-1.693439
C	-0.984847	3.729869	0.912714	C	-2.990416	-1.426860	-3.040718
H	-0.921348	4.764114	1.260061	O	-3.726295	-1.864482	-3.803415
H	-0.414479	3.655734	-0.013771	C	-2.754476	-1.529551	-0.177960
H	-2.030413	3.524407	0.672577	O	-3.368608	-2.019679	0.657071
C	-1.428786	2.803541	3.771166	C	-2.827204	1.056371	-1.468238

O	-3.448048	2.005464	-1.308327	C	-0.426098	-2.279425	-1.791675
C	-0.648159	0.259722	-3.237465	O	0.314339	-3.151389	-1.806552
O	-0.077705	0.770463	-4.087778				

4a^{ap}-Me E = -1230.17515153232 au

ZPE = 0.15569366 au

P	0.029812	0.257044	-0.071993	H	-1.170826	-0.251224	1.968606
C	1.754031	-0.323878	0.153955	W	-1.496674	-0.376049	-1.961587
C	1.609194	1.155382	-0.178792	C	-2.776653	-0.876709	-3.461926
H	2.084499	-0.943527	-0.673290	O	-3.505375	-1.163006	-4.298524
C	2.321036	-0.750181	1.470463	C	-2.289978	-1.855904	-0.762182
H	2.157331	-1.815182	1.644216	O	-2.716883	-2.673904	-0.084720
H	1.908731	-0.181092	2.304049	C	-2.879326	0.972255	-1.232532
F	3.706453	-0.536785	1.480898	O	-3.641287	1.721588	-0.822175
H	1.934051	1.481929	-1.158115	C	-0.628050	1.120510	-3.092878
H	1.838589	1.856381	0.614891	O	-0.117645	1.953153	-3.687874
C	-0.682521	0.638940	1.571023	C	-0.093352	-1.716730	-2.672953
H	-1.442906	1.408051	1.430977	O	0.691449	-2.456085	-3.055192
H	0.056386	1.000508	2.282581				

4a^{sc}-Me E = -1230.17545561617 au

ZPE = 0.15562738 au

P	0.006232	-0.004574	-0.010268	H	-0.732637	-1.175446	1.963764
C	1.833076	-0.069693	0.013187	W	-1.467900	-0.745031	-1.901631
C	1.241533	1.335328	-0.056742	C	-2.716669	-1.357587	-3.385566
H	2.247279	-0.441403	-0.917901	O	-3.433885	-1.706882	-4.208452
C	2.619934	-0.469303	1.223064	C	-1.539247	-2.632391	-1.059790
H	2.268788	0.038351	2.122916	O	-1.578225	-3.676292	-0.594723
H	3.682086	-0.248526	1.088129	C	-3.094110	-0.167636	-0.772195
F	2.509601	-1.843453	1.445564	O	-3.984532	0.158534	-0.130570
H	1.353188	1.881656	-0.984088	C	-1.343889	1.147880	-2.718584
H	1.341712	1.952523	0.828547	O	-1.251149	2.199846	-3.158811
C	-0.586042	-0.124006	1.715947	C	0.206056	-1.288312	-2.985230
H	-1.548165	0.384373	1.781589	O	1.149744	-1.571785	-3.567001
H	0.100082	0.322892	2.431898				

4b^{ap}-Me E = -1590.17024403476 au

ZPE = 0.15404305 au

P	-0.028800	0.195119	-0.007927	H	-0.970926	-0.852169	1.962570
C	1.794148	-0.042448	0.040278	W	-1.515490	-0.395983	-1.941815
C	1.334018	1.404640	-0.024718	C	-2.729515	-0.844306	-3.511983
H	2.171360	-0.437786	-0.896739	O	-3.412231	-1.094520	-4.397527
C	2.530164	-0.551698	1.235814	C	-2.670773	-1.570540	-0.697384
H	2.606070	-1.635754	1.231130	O	-3.307366	-2.220946	-0.003139
H	2.090789	-0.225160	2.173334	C	-2.683502	1.242456	-1.472032
Cl	4.239734	0.070622	1.256927	O	-3.327456	2.148008	-1.199045
H	1.514957	1.947183	-0.943294	C	-0.328628	0.787596	-3.150299
H	1.482892	1.997370	0.870160	O	0.341981	1.449547	-3.799387
C	-0.670525	0.163957	1.706199	C	-0.322948	-2.032295	-2.357300
H	-1.556910	0.798677	1.739591	O	0.345130	-2.935908	-2.569886
H	0.049183	0.527954	2.436382				

4b$^{sc\text{-}Me}$

E = -1590.17030002774 au

ZPE = 0.15400116 au

P	0.027927	0.017723	-0.046926	H	-0.836430	-1.025660	1.947426
C	1.844544	-0.136397	0.042467	W	-1.441958	-0.701019	-1.944981
C	1.331971	1.294788	-0.100064	C	-2.694610	-1.269466	-3.443981
H	2.265226	-0.564190	-0.860984	O	-3.410323	-1.595130	-4.277686
C	2.572480	-0.533568	1.288767	C	-2.219759	-2.173567	-0.723517
H	2.216070	0.002193	2.163963	O	-2.640572	-2.986204	-0.036927
H	3.644502	-0.371005	1.192100	C	-2.854371	0.635988	-1.255634
Cl	2.360316	-2.294877	1.645804	O	-3.629810	1.380555	-0.861806
H	1.507628	1.799088	-1.041522	C	-0.586460	0.786782	-3.091617
H	1.430070	1.938969	0.765826	O	-0.079437	1.622198	-3.687856
C	-0.623119	0.004231	1.661757	C	-0.003166	-2.032020	-2.609764
H	-1.556196	0.568172	1.671730	O	0.795642	-2.764614	-2.973166
H	0.063227	0.443249	2.382536				

TS(**4a**$^{sc\text{-}Me}$→**3a**^{Me})

E = -1230.09971915625 au

ZPE = 0.15256401 au

$\bar{\upsilon}$ = -519.38 cm^{-1}

P	0.010533	-0.087578	0.178940	H	-0.629089	-1.619885	1.931527
C	1.894604	0.750666	-0.211649	W	-1.307856	-0.818801	-1.778073
C	0.732860	1.558769	0.339722	C	-2.457445	-1.412368	-3.359086
H	2.045593	0.780528	-1.281950	O	-3.111729	-1.738418	-4.240163
C	2.658264	-0.126769	0.539139	C	-1.848107	-2.507545	-0.708390
H	2.680789	-0.065265	1.618100	O	-2.145727	-3.427926	-0.100828
H	3.493664	-0.634118	0.081669	C	-2.923443	0.200159	-1.001351
F	1.566594	-1.666710	0.563078	O	-3.813627	0.770726	-0.562991
H	0.382102	2.320966	-0.346490	C	-0.729982	0.890249	-2.770510
H	0.852423	1.934556	1.352113	O	-0.391938	1.854254	-3.288777
C	-0.411053	-0.556881	1.889164	C	0.356872	-1.828985	-2.514790
H	-1.296907	0.025521	2.157899	O	1.281949	-2.365686	-2.907880
H	0.393521	-0.330396	2.584632				

3a

E = -2046.27165469112 au

ZPE = 0.3584766 au

P	0.022659	-0.012491	-0.005793	H	0.896388	-0.469022	-2.112710
C	-0.148544	0.446157	2.720856	Si	2.864895	-1.058463	-0.852189
C	0.846171	0.290504	1.614135	C	4.160389	-0.082686	0.095985
H	-0.590823	-0.468130	3.100806	H	3.793556	0.238252	1.072397
C	-0.525179	1.613882	3.223606	H	5.033404	-0.717463	0.268190
H	-1.265326	1.676159	4.010227	H	4.498262	0.803183	-0.441895
H	-0.110960	2.547891	2.861753	C	2.466747	-2.600477	0.149404
F	-0.669370	1.445356	-0.140699	H	3.413738	-3.115163	0.337282
H	1.508513	-0.552882	1.806798	H	2.003405	-2.424016	1.118330
H	1.458447	1.185961	1.504043	H	1.831437	-3.289582	-0.404681
W	-1.747785	-1.759009	-0.226779	C	3.547655	-1.676936	-2.485283
C	-3.269595	-3.108720	-0.446404	H	4.366156	-2.376160	-2.296351
O	-4.128732	-3.855655	-0.572366	H	2.775419	-2.218972	-3.036369
C	-0.954611	-2.793100	1.368384	H	3.928074	-0.882213	-3.124173
O	-0.479609	-3.339634	2.256531	Si	1.732220	1.792603	-1.918814
C	-2.941889	-0.644460	1.053873	C	0.265731	2.382183	-2.926966
O	-3.619440	-0.040634	1.747105	H	-0.627670	2.513424	-2.318452
C	-2.425909	-0.642053	-1.828968	H	0.499900	3.339263	-3.400543
O	-2.764031	-0.010386	-2.720254	H	0.028619	1.672217	-3.723220
C	-0.595880	-2.841795	-1.534815	C	2.110619	2.996014	-0.529176
O	0.044444	-3.429267	-2.283880	H	2.409636	3.956783	-0.956176
C	1.340777	0.036708	-1.247301	H	1.236419	3.171119	0.098017

H	2.929516	2.652491	0.104992	H	4.135483	1.441055	-2.618142
C	3.202089	1.745547	-3.091005	H	3.019556	1.085164	-3.940565
H	3.348384	2.754092	-3.487899				

3a^{Me} E = -1230.22585938924 au

ZPE = 0.15426054 au

P	0.010533	-0.087578	0.178940	H	-0.629089	-1.619885	1.931527
C	1.894604	0.750666	-0.211649	W	-1.307856	-0.818801	-1.778073
C	0.732860	1.558769	0.339722	C	-2.457445	-1.412368	-3.359086
H	2.045593	0.780528	-1.281950	O	-3.111729	-1.738418	-4.240163
C	2.658264	-0.126769	0.539139	C	-1.848107	-2.507545	-0.708390
H	2.680789	-0.065265	1.618100	O	-2.145727	-3.427926	-0.100828
H	3.493664	-0.634118	0.081669	C	-2.923443	0.200159	-1.001351
F	1.566594	-1.666710	0.563078	O	-3.813627	0.770726	-0.562991
H	0.382102	2.320966	-0.346490	C	-0.729982	0.890249	-2.770510
H	0.852423	1.934556	1.352113	O	-0.391938	1.854254	-3.288777
C	-0.411053	-0.556881	1.889164	C	0.356872	-1.828985	-2.514790
H	-1.296907	0.025521	2.157899	O	1.281949	-2.365686	-2.907880
H	0.393521	-0.330396	2.584632				

TS(**4b^{sc}→3b^{Me}**) E = -1590.10284285638 au

ZPE = 0.15134951 au

$\tilde{\upsilon}$ = -324.90 cm^{-1}

P	-0.069225	0.123762	0.081117	H	-1.174580	-0.833765	1.983747
C	2.093910	0.315221	-0.162796	W	-1.297406	-0.745289	-1.813897
C	1.128454	1.469187	0.034012	C	-2.444341	-1.401508	-3.389980
H	2.312408	0.053313	-1.189690	O	-3.092719	-1.749014	-4.263633
C	2.623346	-0.453057	0.833115	C	-2.127816	-2.171656	-0.540909
H	2.474544	-0.224178	1.877625	O	-2.589376	-2.938140	0.161711
H	3.346278	-1.220402	0.611419	C	-2.817021	0.572167	-1.352572
Cl	1.038075	-2.512613	1.100170	O	-3.659603	1.302848	-1.101048
H	1.077532	2.125810	-0.827619	C	-0.400557	0.682367	-2.985768
H	1.249145	2.017795	0.963829	O	0.123555	1.495086	-3.599471
C	-0.596827	0.069710	1.816551	C	0.213274	-2.116765	-2.308405
H	-1.204464	0.965391	1.984446	O	1.028102	-2.849332	-2.605014
H	0.248703	0.069282	2.499005				

3b^{Me} E = -1590.20589538021 au

ZPE = 0.15301611 au

P	-0.234350	-0.305210	0.493042	H	-2.140381	-0.182863	1.964615
C	2.339096	0.303972	-0.392078	W	-1.298055	-0.876712	-1.690085
C	1.249717	0.794893	0.505489	C	-2.192306	-1.359929	-3.463010
H	2.195058	0.461751	-1.454349	O	-2.693430	-1.632045	-4.455771
C	3.424867	-0.326679	0.035111	C	-2.270609	-2.443046	-0.739609
H	3.599357	-0.511437	1.088566	O	-2.812230	-3.296044	-0.207105
H	4.174368	-0.685412	-0.657678	C	-2.852539	0.382999	-1.207920
Cl	0.500078	-1.938565	1.546873	O	-3.695491	1.101777	-0.916975
H	0.876896	1.770437	0.176567	C	-0.341493	0.696560	-2.609619
H	1.589967	0.886222	1.538269	O	0.190376	1.576722	-3.114793
C	-1.283367	0.461470	1.773978	C	0.318020	-2.101670	-2.127714
H	-1.645870	1.418334	1.394084	O	1.214203	-2.765075	-2.372727
H	-0.728490	0.615770	2.698785				

TS(**4a**$^{sc\text{-}Me}$→**5**^{Me}·HF) E = -1230.06267687134 au

ZPE = 0.14709186 au

$\bar{\upsilon}$ = -1860.40 cm^{-1}

P	-0.137671	0.231677	0.107810	H	-1.170955	-0.871056	2.000039
C	1.632448	0.148512	0.348510	W	-1.467083	-0.417753	-1.909039
C	1.144187	1.559639	0.220638	C	-2.577375	-0.928288	-3.539114
H	2.469128	-0.393307	-0.518411	O	-3.204856	-1.212507	-4.454430
C	2.563628	-0.476437	1.177734	C	-2.706771	-1.541122	-0.702589
H	2.420291	-1.493572	1.516580	O	-3.384051	-2.166468	-0.023405
H	3.371490	0.078146	1.640773	C	-2.641622	1.248276	-1.589639
F	3.578289	-1.025906	-0.376843	O	-3.282993	2.176761	-1.397756
H	1.360607	2.091932	-0.698673	C	-0.198590	0.718308	-3.084074
H	1.138475	2.188531	1.105380	O	0.503198	1.360593	-3.718560
C	-0.894215	0.159252	1.775062	C	-0.257037	-2.079242	-2.177277
H	-1.803595	0.761581	1.773860	O	0.406784	-2.998765	-2.310481
H	-0.211626	0.526699	2.540832				

5^{Me}·HF E = -1230.14947996159 au

ZPE = 0.15008096 au

P	-0.220165	0.330242	0.278486	H	-1.651047	-0.405832	2.080235
C	1.461697	0.047745	0.799671	W	-1.337926	-0.455817	-1.814532
C	1.234255	1.467709	0.431864	C	-2.309205	-1.091685	-3.487517
H	2.666104	-0.614161	-1.009034	O	-2.863924	-1.446276	-4.424994
C	2.394648	-0.786196	1.227017	C	-2.556030	-1.641156	-0.649458
H	2.177590	-1.833028	1.402612	O	-3.224893	-2.296210	0.010781
H	3.404915	-0.445463	1.432904	C	-2.647021	1.124104	-1.607345
F	2.932777	-0.361402	-1.868267	O	-3.358544	2.010819	-1.471293
H	1.664820	1.820962	-0.500161	C	-0.093491	0.742730	-2.965388
H	1.235896	2.205991	1.228157	O	0.581713	1.413918	-3.594427
C	-1.180590	0.543526	1.824003	C	0.038368	-1.996547	-1.941462
H	-1.965527	1.280004	1.647185	O	0.812181	-2.836729	-1.969618
H	-0.546519	0.868235	2.647507				

5^{Me} E = -1129.79883847875 au

ZPE = 0.13883527 au

P	-0.202995	0.320716	0.281706	W	-1.330449	-0.460041	-1.819557
C	1.482847	0.057028	0.782077	C	-2.291513	-1.081209	-3.502110
C	1.242207	1.472982	0.407621	O	-2.837682	-1.426818	-4.448746
C	2.420756	-0.777652	1.181962	C	-2.539121	-1.666326	-0.658423
H	2.208093	-1.825944	1.351613	O	-3.201681	-2.328352	0.000153
H	3.439511	-0.443881	1.350891	C	-2.651728	1.107938	-1.594783
H	1.655960	1.832086	-0.529858	O	-3.368745	1.988945	-1.451153
H	1.234092	2.218476	1.197497	C	-0.089056	0.758411	-2.934489
C	-1.168845	0.559021	1.820303	O	0.608123	1.437949	-3.535300
H	-1.953649	1.293621	1.635564	C	0.060846	-1.984316	-1.976148
H	-0.532209	0.892920	2.638193	O	0.846685	-2.811613	-2.043294
H	-1.639015	-0.386569	2.091335				

5 E = -1945.84648791552 au

ZPE = 0.34223717 au

P	-0.202995	0.320716	0.281706	C	2.420756	-0.777652	1.181962
C	1.482847	0.057028	0.782077	H	2.208093	-1.825944	1.351613
C	1.242207	1.472982	0.407621	H	3.439511	-0.443881	1.350891

H	1.655960	1.832086	-0.529858
H	1.234092	2.218476	1.197497
C	-1.168845	0.559021	1.820303
H	-1.953649	1.293621	1.635564
H	-0.532209	0.892920	2.638193
H	-1.639015	-0.386569	2.091335
W	-1.330449	-0.460041	-1.819557
C	-2.291513	-1.081209	-3.502110
O	-2.837682	-1.426818	-4.448746
C	-2.539121	-1.666326	-0.658423
O	-3.201681	-2.328352	0.000153
C	-2.651728	1.107938	-1.594783
O	-3.368745	1.988945	-1.451153
C	-0.089056	0.758411	-2.934489
O	0.608123	1.437949	-3.535300
C	0.060846	-1.984316	-1.976148
O	0.846685	-2.811613	-2.043294

TS(**4a**$^{ap\text{-}Me}$→**8**·HF) E = -1230.06654733482 au

ZPE = 0.15117635 au

$\tilde{\upsilon}$ = -405.57 cm^{-1}

P	0.095672	0.400334	-0.204389
C	1.718927	-0.811804	0.167271
C	1.855860	0.635646	-0.307037
H	1.868496	-1.578710	-0.581322
C	1.738157	-1.156031	1.499692
H	2.000540	-2.176662	1.761816
H	1.494354	-0.467488	2.291622
F	2.710592	0.788729	2.356348
H	2.271556	0.708582	-1.304431
H	2.320046	1.228714	0.485416
C	-0.389294	1.091376	1.405956
H	-0.895437	2.034865	1.183864
H	0.491007	1.285501	2.023509
H	-1.099304	0.435863	1.908680
W	-1.477384	-0.308415	-1.947041
C	-2.836939	-0.867895	-3.379202
O	-3.598240	-1.185120	-4.169293
C	-1.933037	-1.999095	-0.835969
O	-2.168438	-2.926125	-0.213500
C	-2.964394	0.731592	-0.952151
O	-3.777092	1.307645	-0.394136
C	-0.996740	1.374339	-3.063804
O	-0.724697	2.293213	-3.682662
C	0.043123	-1.322716	-2.913020
O	0.902749	-1.870855	-3.429290

8·HF E = -1230.15394049703 au

ZPE = 0.15067609 au

P	0.124305	0.913658	-0.320285
C	2.099733	-1.039258	-0.129254
C	1.908891	0.452450	-0.170899
H	2.304228	-1.524065	-1.076263
C	2.009728	-1.767307	0.976579
H	2.149060	-2.840068	0.947268
H	1.783421	-1.324102	1.939511
F	0.112873	0.194681	3.069540
H	2.423073	0.885641	-1.031895
H	2.295979	0.930593	0.729166
C	-0.147090	2.138039	0.762117
H	0.644376	2.592996	1.344412
H	-0.139546	0.688553	2.311216
H	-1.134018	2.574153	0.846540
W	-1.482669	-0.253500	-1.770446
C	-2.844929	-1.239066	-2.937737
O	-3.606141	-1.789110	-3.590009
C	-1.533579	-1.813418	-0.398574
O	-1.568719	-2.669622	0.353219
C	-2.999622	0.712234	-0.747043
O	-3.825189	1.259246	-0.177235
C	-1.445412	1.292892	-3.148674
O	-1.430229	2.138133	-3.916140
C	0.051601	-1.180671	-2.790946
O	0.899959	-1.687597	-3.367242

8bis E = -2046.19958553053 au

ZPE = 0.35625764 au

P	-0.118589	-0.082847	-0.090931
C	2.595395	0.766261	0.098540
C	1.265212	1.051941	-0.540268
H	3.439771	1.218403	-0.413620
C	2.819213	0.037354	1.182784
H	3.825332	-0.099445	1.556863
H	2.031213	-0.448449	1.744483
F	0.204665	-0.909845	3.256015
H	1.361780	0.934517	-1.623889
H	0.975015	2.086653	-0.374074
C	-1.157647	0.577374	1.037285
H	-0.187817	-0.514594	2.495274
W	0.055142	-2.222960	-1.398835
C	0.379792	-3.889796	-2.523665
O	0.576488	-4.821641	-3.159177
C	0.604404	-3.238023	0.330261
O	0.915335	-3.788296	1.279156
C	-1.891596	-2.894261	-1.223055

O	-2.939064	-3.351472	-1.206300	H	-2.441338	1.969534	3.925655
C	-0.485958	-1.138247	-3.072027	H	-0.816831	1.316925	4.150508
O	-0.777284	-0.519353	-3.988751	Si	-2.821764	-0.350807	1.242393
C	2.036928	-1.793165	-1.786315	C	-3.994764	0.422468	2.491743
O	3.128758	-1.626114	-2.081187	H	-3.662338	0.275649	3.518571
Si	-1.027614	2.285892	1.862259	H	-4.190214	1.482427	2.336807
C	0.644215	3.149322	1.787369	H	-4.948096	-0.103265	2.380454
H	0.838746	3.652285	0.839709	C	-3.694524	-0.233348	-0.418149
H	0.626531	3.923851	2.558796	H	-4.020755	0.798343	-0.572923
H	1.481772	2.487928	2.007407	H	-3.057608	-0.504679	-1.257730
C	-2.275866	3.401863	1.005149	H	-4.579296	-0.873340	-0.440854
H	-2.272648	4.393184	1.465717	C	-2.559179	-2.096834	1.876117
H	-2.014921	3.522314	-0.049015	H	-3.498715	-2.651561	1.818387
H	-3.293715	3.015245	1.052480	H	-1.804429	-2.661504	1.337884
C	-1.390312	2.129544	3.700461	H	-2.253065	-2.057341	2.923230
H	-1.084963	3.058492	4.188685				

TS(**4b**$^{ap\text{-}Me}$→**8'**·HCl) E = -1590.09041913536 au

ZPE = 0.1510507 au

$\bar{\upsilon}$ = -158.88 cm^{-1}

P	0.081395	0.412607	-0.234974	H	-1.024761	0.382745	1.923079
C	1.809776	-0.816764	0.135561	W	-1.499806	-0.310950	-1.929719
C	1.851171	0.610533	-0.369829	C	-2.882671	-0.872941	-3.351652
H	1.942073	-1.593182	-0.607039	O	-3.651612	-1.186572	-4.133589
C	1.780211	-1.156398	1.458866	C	-1.960752	-1.996440	-0.804838
H	1.963773	-2.186579	1.740807	O	-2.201259	-2.917279	-0.177383
H	1.571560	-0.453135	2.246954	C	-2.965021	0.741280	-0.914357
Cl	3.138349	1.124651	2.605232	O	-3.757756	1.326227	-0.338525
H	2.223258	0.685726	-1.385120	C	-1.029760	1.359629	-3.073472
H	2.324729	1.272688	0.361464	O	-0.764316	2.270310	-3.705389
C	-0.382772	1.082779	1.389717	C	0.012296	-1.334034	-2.902980
H	-0.966613	1.983918	1.182200	O	0.869916	-1.883423	-3.419345
H	0.493950	1.348218	1.984240				

8'·HCl E = -1590.13578091014 au

ZPE = 0.1495461 au

P	-0.286910	1.429169	0.117983	H	-0.683826	-0.527689	1.623570
C	1.851859	-0.552419	-0.366352	W	-1.362059	-0.197813	-1.857983
C	0.967958	0.559566	-0.700589	C	-2.746781	-1.043505	-3.053566
H	2.509296	-0.848730	-1.179169	O	-3.540991	-1.519786	-3.729253
C	1.977303	-1.218929	0.788635	C	-1.214844	-1.902598	-0.705084
H	2.699540	-2.019637	0.874007	O	-1.119798	-2.846979	-0.067622
H	1.380541	-1.011281	1.662394	C	-2.966947	0.420272	-0.701826
Cl	3.068513	1.888623	2.145973	O	-3.868553	0.724551	-0.070026
H	1.317705	1.126203	-1.558097	C	-1.413497	1.558781	-2.964624
H	2.961134	0.820097	1.426282	O	-1.434767	2.523573	-3.573746
C	-0.636635	0.555555	1.708498	C	0.115993	-0.961567	-3.102860
H	-1.597729	0.919548	2.073266	O	0.914312	-1.405313	-3.788511
H	0.127089	0.832776	2.438506				

8' E = -1129.80079320121 au

ZPE = 0.14107465 au

P	-0.272313	1.382803	0.116261	C	0.971230	0.502845	-0.705006
C	1.801681	-0.644874	-0.347008	H	2.229433	-1.178497	-1.191315

C	2.125758	-1.059226	0.878962	O	-3.556991	-1.443102	-3.793484
H	2.776622	-1.912656	1.014429	C	-1.288936	-1.906849	-0.744492
H	1.788522	-0.556593	1.773124	O	-1.232102	-2.868227	-0.128616
H	1.330739	1.042590	-1.576330	C	-2.992106	0.445734	-0.714379
C	-0.635255	0.462685	1.679020	O	-3.891093	0.754622	-0.080642
H	-1.667530	0.676911	1.957913	C	-1.411506	1.595531	-2.946908
H	0.007358	0.840842	2.477219	O	-1.418020	2.571765	-3.538762
H	-0.501807	-0.613946	1.593858	C	0.088702	-0.942474	-3.106017
W	-1.389902	-0.177798	-1.870306	O	0.893335	-1.390257	-3.782914
C	-2.767559	-0.988081	-3.097056				

TS(**8'→8''**) E = -1129.78581205553 au

ZPE = 0.13912654 au

$\bar{\upsilon}$ = -118.90 cm^{-1}

P	-0.073110	1.129666	-0.194223	W	-1.561317	-0.141897	-2.004483
C	2.239186	-0.618350	0.052331	C	-2.951074	-1.114142	-3.064823
C	1.348376	0.298746	-0.616248	O	-3.760507	-1.674364	-3.658512
H	3.225752	-0.713366	-0.391841	C	-1.126469	-1.854941	-0.949928
C	1.950775	-1.389031	1.109733	O	-0.869224	-2.793249	-0.345478
H	2.690629	-2.067340	1.513228	C	-3.056202	0.345550	-0.667776
H	0.977269	-1.400266	1.573904	O	-3.890156	0.607734	0.070160
H	1.678126	0.595452	-1.607468	C	-1.908545	1.626815	-3.027059
C	-0.510058	0.734587	1.551886	O	-2.104552	2.595533	-3.599584
H	-1.291322	1.429451	1.859903	C	-0.121922	-0.646461	-3.405655
H	0.352767	0.861065	2.207193	O	0.650603	-0.940113	-4.196455
H	-0.900766	-0.277333	1.658753				

8''·HCl E = -1590.14565549824 au

ZPE = 0.14745618 au

P	-0.195743	-0.287037	-0.009646	H	0.004515	0.275494	2.356411
C	2.080933	-1.473626	1.232244	W	-1.652973	-0.049779	-1.987487
C	1.121775	-1.303195	0.158296	C	-2.840648	0.169831	-3.637810
H	2.453250	-2.488133	1.348396	O	-3.499186	0.291127	-4.565722
C	2.575644	-0.529233	2.040314	C	-2.250503	-2.026227	-1.812966
H	3.295725	-0.782736	2.806405	O	-2.573447	-3.117408	-1.717139
H	2.321563	0.516366	1.938003	C	-3.171244	0.557701	-0.729716
Cl	2.614495	1.799772	-1.134043	O	-3.985397	0.905893	-0.005079
H	1.206459	-2.011300	-0.661611	C	-1.073262	1.932571	-2.188134
H	2.165219	0.619288	-0.856554	O	-0.778491	3.028195	-2.309736
C	-0.371900	0.773736	1.463418	C	-0.059897	-0.647141	-3.162831
H	-1.426768	1.016914	1.584492	O	0.837189	-0.982476	-3.785872
H	0.178046	1.705016	1.316279				

TS(**8''**·HCl→**3b^{Me}**) E = -1590.11109050425 au

ZPE = 0.14631814 au

$\bar{\upsilon}$ = -507.93 cm^{-1}

P	-0.198243	-0.208155	-0.084620	H	1.438277	-1.731315	-0.828656
C	2.050303	-1.358826	1.228832	H	1.883767	0.047850	-0.482788
C	1.364791	-0.987539	-0.036843	C	-0.374602	0.741040	1.442654
H	2.001116	-2.409448	1.500501	H	-1.402354	1.080219	1.551813
C	2.714817	-0.508610	2.004326	H	0.288861	1.605213	1.348514
H	3.194229	-0.846368	2.913856	H	-0.058118	0.156634	2.306657
H	2.821857	0.535500	1.735827	W	-1.639191	-0.048830	-1.968166
Cl	2.229083	1.731872	-0.968292	C	-2.865972	0.142677	-3.639001

O	-3.534124	0.247092	-4.555196	C	-1.083998	1.961990	-2.213994
C	-2.206933	-2.040548	-1.813443	O	-0.814659	3.053826	-2.355407
O	-2.510456	-3.136946	-1.738923	C	-0.043543	-0.641214	-3.165691
C	-3.150895	0.567596	-0.708991	O	0.828432	-0.980544	-3.812696
O	-3.957090	0.920448	0.019640				

TS(**8''**·HCl→**3b'**^{Me}) E = -1590.11190485742 au

ZPE = 0.14618818 au

$\bar{\upsilon}$ = -1273.00 cm^{-1}

P	-0.050003	-0.463748	-0.204367	H	-0.762645	0.288914	1.993669
C	2.620909	-0.613464	0.558222	W	-1.535827	-0.015438	-2.065764
C	1.589904	-0.889667	-0.346984	C	-2.774971	0.428507	-3.652028
H	3.624228	-0.724363	0.155476	O	-3.456994	0.677218	-4.533719
C	2.516369	0.028127	1.789895	C	-3.046607	-1.051071	-1.117457
H	3.432212	0.242443	2.326155	O	-3.869549	-1.623963	-0.567284
H	1.651878	-0.120642	2.423089	C	-2.181940	1.720234	-1.110946
Cl	0.865945	2.228310	0.681448	O	-2.565920	2.659025	-0.593612
H	1.884492	-1.107394	-1.367171	C	0.036271	1.014682	-2.952157
H	1.915912	1.224152	1.265047	O	0.914203	1.561780	-3.430116
C	-0.672819	-0.677010	1.499729	C	-0.908921	-1.741155	-3.022907
H	-0.031712	-1.339309	2.077398	O	-0.553270	-2.692757	-3.544201
H	-1.665789	-1.119799	1.418495				

8''·HCl E = -1590.20012309791 au

ZPE = 0.15300061 au

P	0.330243	0.014246	-0.496748	H	1.715349	1.623116	0.736780
C	1.024878	-1.244153	1.975201	W	-1.573866	-0.048747	-2.120056
C	0.147773	-0.978282	1.005133	C	-3.096460	-0.081351	-3.480298
H	0.662236	-1.866129	2.790913	O	-3.941466	-0.098030	-4.253072
C	2.450077	-0.825723	2.104299	C	-0.937763	-1.922286	-2.738298
H	3.084478	-1.710952	2.204746	O	-0.584638	-2.954912	-3.074004
H	2.584740	-0.242771	3.020466	C	-2.785947	-0.923195	-0.703350
Cl	2.125448	-0.657963	-1.335643	O	-3.448181	-1.403174	0.098624
H	-0.843898	-1.407029	1.088600	C	-2.182213	1.805635	-1.459348
H	2.813288	-0.249295	1.259854	O	-2.514488	2.831482	-1.073656
C	0.846618	1.667014	0.084185	C	-0.329974	0.840605	-3.515130
H	0.005221	2.101919	0.625821	O	0.358166	1.335464	-4.281570
H	1.065733	2.288124	-0.783539				

HF E = -100.344372577033 au

ZPE = 0.0092737 au

H	0.912362	0.000000	0.000000	F	-0.012362	0.000000	0.000000