Supporting Information for

Indium promoted C(sp^3)-P bond formation by Domino A^3-coupling method - A combined experimental and computational study

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1. X-ray crystallographic analyses:

Single crystals of complexes **2a, 2b** and **3a** were grown from a concentrated solution of toluene or toluene/THF (3:1) in an argon-filled atmosphere at -35 °C and for **6b** and **6c** crystals grown from DCM at room temperature. A crystal of suitable dimensions of complexes **2a, 2b, 3a, 4m, 6b,** and **6d** was mounted on a CryoLoop (Hampton Research Corp.) with a layer of light mineral oil. All the three crystals **2a**, **2b** and **3a** were measured at 293 K. All measurements were made on an Rigaku Supernova X-calibur Eos CCD detector with graphite monochromatic Mo-Kα (0.71073 Å) radiation. Crystal data and structure refinement parameters of complexes **2a, 2b, 3a, 4m, 6b** and **6d** are summarized in Table TS1. The structures were solved by direct methods (SIR2004)[1] and refined on F^2 by full-matrix least-squares methods, using SHELXL-2016/6.[2] Non-hydrogen atoms were anisotropically refined. H-atoms were included in the refinement on calculated positions riding on their carrier atoms. The function minimized was $[\sum w(Fo^2 - Fc^2)^2]$ ($w = 1 / [\sigma^2 (Fo^2) + (aP)^2 + bP]$), where $P = (\mathrm{Max}(Fo^2,0) + 2Fc^2) / 3$ with $\sigma^2(Fo^2)$ from counting statistics. The function $R1$ and $wR2$ were $(\Sigma||Fo| - |Fc||) / \Sigma|Fo|$ and $[\Sigma w(Fo^2 - Fc^2)^2 / \Sigma(wFo^4)]^{1/2}$, respectively. The ORTEP-3 program was used to draw the molecules of **2a, 2b, 3a, 4m, 6b** and **6d**. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2035016 (**2a**), 2035015 (**2b**), 2035020 (**3a**), 2035017 (**4m**), 2035019 (**6b**), 2035018 (**6d**). Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: + (44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table TS1. Crystallography table of metal complexes **2a, 2b, 3a, 4m**, **6b** and **6d.**

Crystal Parameters	**2a**	**2b**	**3a**	**4m**	**6b**	**6d**
Identification code	6916	6194	8467	10056	9907	SN3
CCDC No.	2035015	2035016	2035020	2035017	2035019	2035018
Empirical formula	$C_{34}H_{48}ClInN_2O_2$	$C_{56}H_{72}Cl_2In_2N_4O_4$	$C_{39}H_{56}F_3InN_2O_6S$	$C_{26}H_{21}N_2OP$	$C_{26}H_{24}NO_3P$	$C_{28}H_{28}NO_3P$
Formula weight	667.01	1165.71	852.73	408.42	429.43	457.48

T (K)	293(2) K	150(2) K	298(2) K	293(2) K	293(2) K	298 K
λ (Å)	0.71073	1.54184	0.71073	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P 21/c	I 2/a	P -1	P -1	P -1	P -1
a(Å)	10.7513(3)	15.9273(12)	11.6241(14)	9.2668(7)	13.9729(6)	10.7629 (15)
b (Å)	28.9206(8)	13.2281(8)	13.2478(16)	9.9885(6)	13.9884(6)	11.3046 (16)
c(Å)	11.1932(3)	28.269(3)	16.0639(10)	12.8946(7)	14.5287(5)	11.5299 (16)
α (°)	90	90	97.765(9)	102.481(5)	117.057(4)	90.972 (11)
β (°)	102.634(3)	91.925(10)	110.219(9)	93.899(5)	96.593(3)	103.876 (12)
γ (°)	90	90	101.393(10)	112.376(6)	101.316(3)	113.970 (14)
V(Å^3)	3396.08(17)	5952.7(8)	2219.2(4)	1062.56(13)	2411.13(19)	1234.1 (3)
Z	4	4	2	2	4	2
D_{calc} g cm^{-3}	1.305	1.301	1.276	1.277	1.183	1.231
μ (mm^{-1})	0.805	7.356	0.634	0.149	0.140	0.140
F(000)	1392	2400	888	428	904	484
Theta range for data collection	3.054 to 29.018 deg	6.256 to 146.516 deg	3.093 to 29.203 deg.	2.285 to 29.104 deg	2.202 to 29.113 deg.	3.493–24.998 deg.
Limiting indices	-14<=h<=13, -33<=k<=39, -7<=l<=14	-17<=h<=19, -14<=k<=16, -34<=l<=34	-15<=h<=14, -17<=k<=17, -21<=l<=21	-12<=h<=9, -13<=k<=12, -16<=l<=16	-17<=h<=18, -17<=k<=18, -19<=l<=17	-12<=h<=12, -11<=k<=13, -13<=l<=13
Reflections collected / unique	15351 / 7774 [R(int) = 0.0372]	11307 / 5681 [R(int) = 0.0517]	48130 / 10793 [R(int) = 0.1066]	7889 / 4867 [R(int) = 0.0211]	21219 / 11118 [R(int) = 0.0222]	7902 / 4255 [R(int) = 0.031]
Completeness to theta	99.8 %	99.6 %	99.8 %	100.0 %	99.9 %	97.9%
Absorption correction	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan	Multi-scan
Max. and min. transmission	1.00000 and 0.82642	1.00000 and 0.91324	1.00000 and 0.68095	1.00000 and 0.82620	1.00000 and 0.81632	1.00000 and 0.679
Refinement method	Full-matrix least-squares on	Full-matrix least-squares	Full-matrix least-squares on F^2	Full-matrix least-squares	Full-matrix least-squares	Full-matrix least-squares

	F^2	on F^2		on F^2	on F^2	on F^2
Data / restraints / parameters	7774 / 0 / 373	5681 / 0 / 306	10793 / 0 / 481	4867 / 0 / 271	11118 / 0 / 561	4255 / 0 / 300
Goodness-of-fit on F^2	1.047	1.143	1.065	1.050	1.436	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.0771	R1 = 0.0769, wR2 = 0.2133	R1 = 0.0616, wR2 = 0.1333	R1 = 0.0503, wR2 = 0.1257	R1 = 0.1129, wR2 = 0.3640	R1 = 0.0744, wR2 = 0.2040
R indices (all data)	R1 = 0.0732, wR2 = 0.0896	R1 = 0.1039, wR2 = 0.2823	R1 = 0.1106, wR2 = 0.1730	R1 = 0.0689, wR2 = 0.1405	R1 = 0.1431, wR2 = 0.3953	R1 = 0.1014, wR2 = 0.1794
Largest diff. peak and hole	0.651 and -0.389 $e.A^{-3}$	2.59 and -5.78 $e.A^{-3}$	1.308 and -1.004 $e.A^{-3}$	0.486 and -0.331 $e.A^{-3}$	2.367 and -0.377 $e.A^{-3}$	

2. NMR spectrum for metal complexes

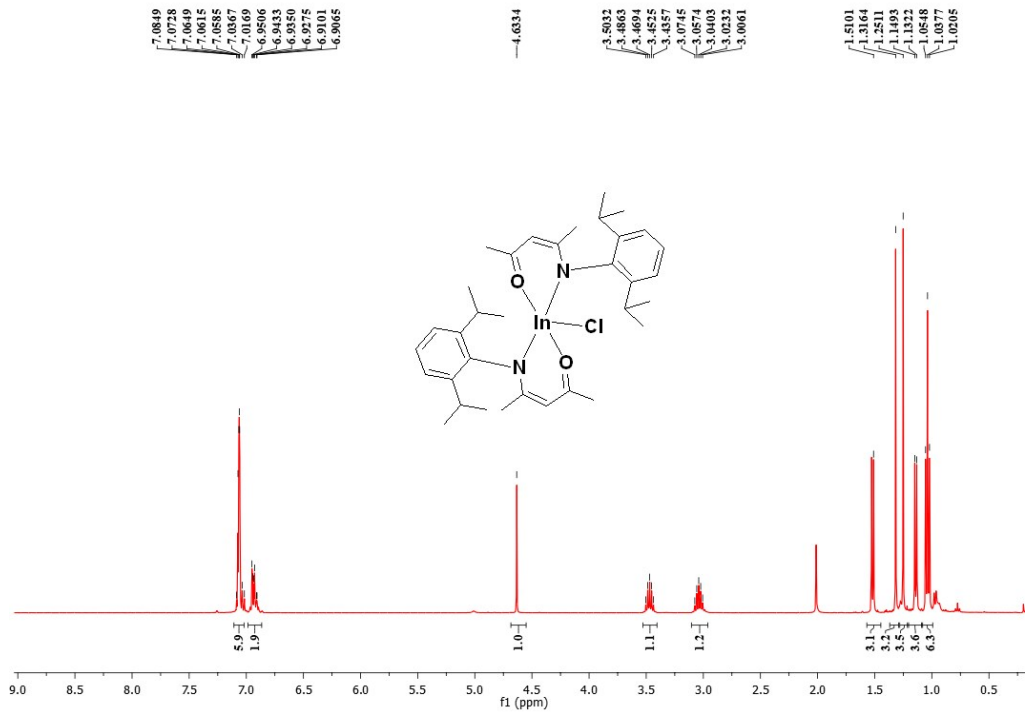


Fig FS1: ^{1}H NMR for complex **2a** in C_6D_6.

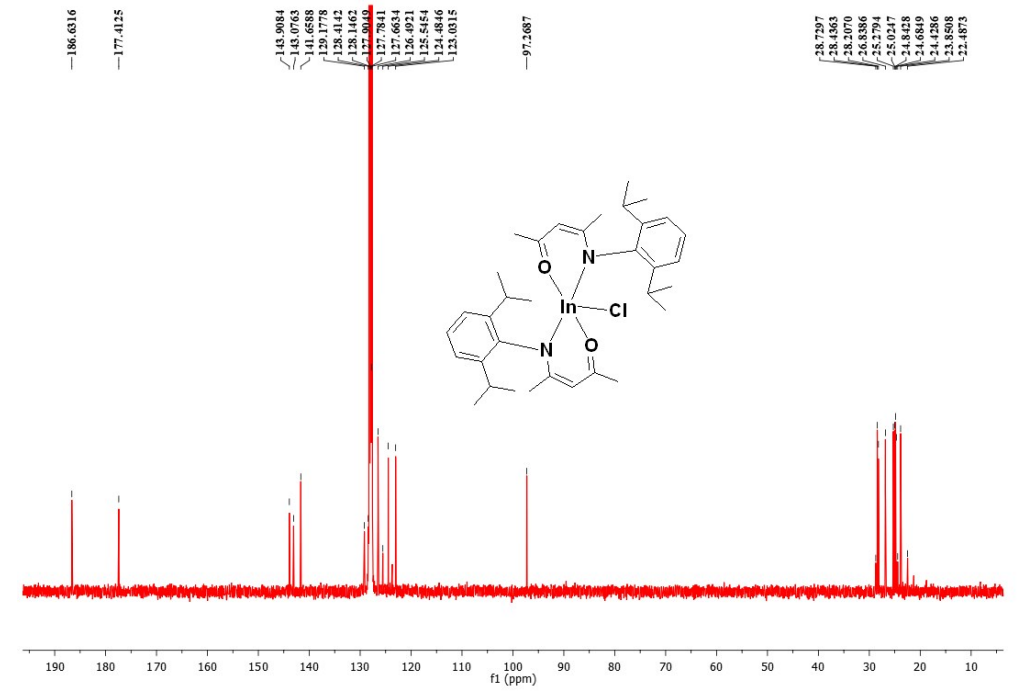


Fig FS2. $^{13}C\{^{1}H\}$ NMR for complex **2a** in C_6D_6.

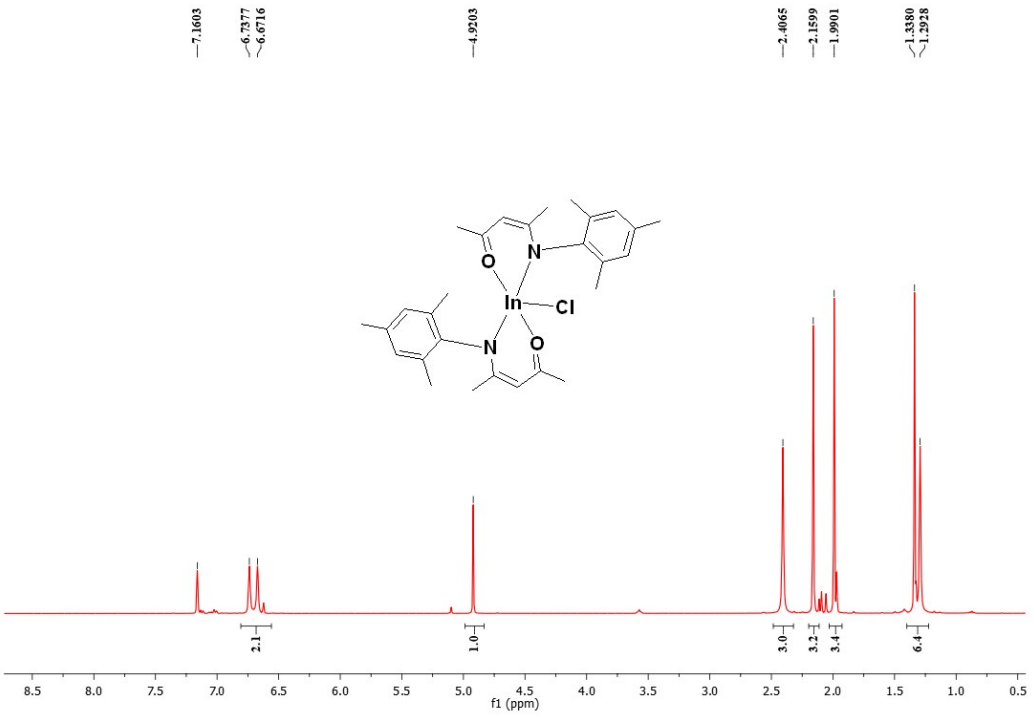


Fig FS3. ^{1}H NMR for complex **2b** in C_6D_6.

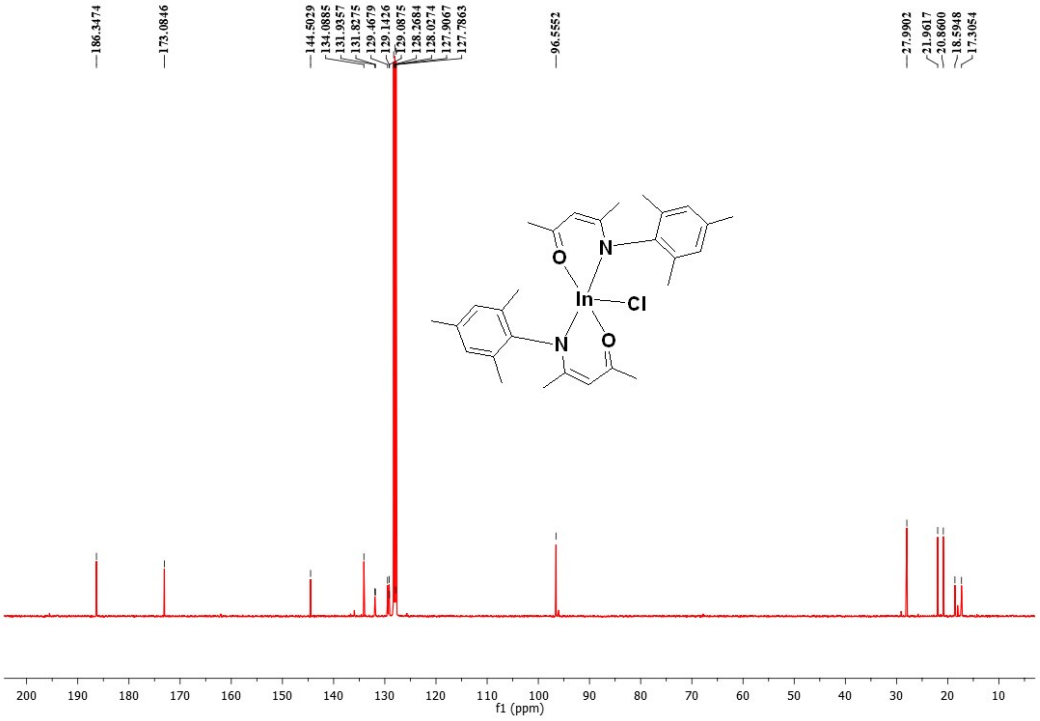


Fig FS4. $^{13}C\{^{1}H\}$NMR for complex **2b** in C_6D_6.

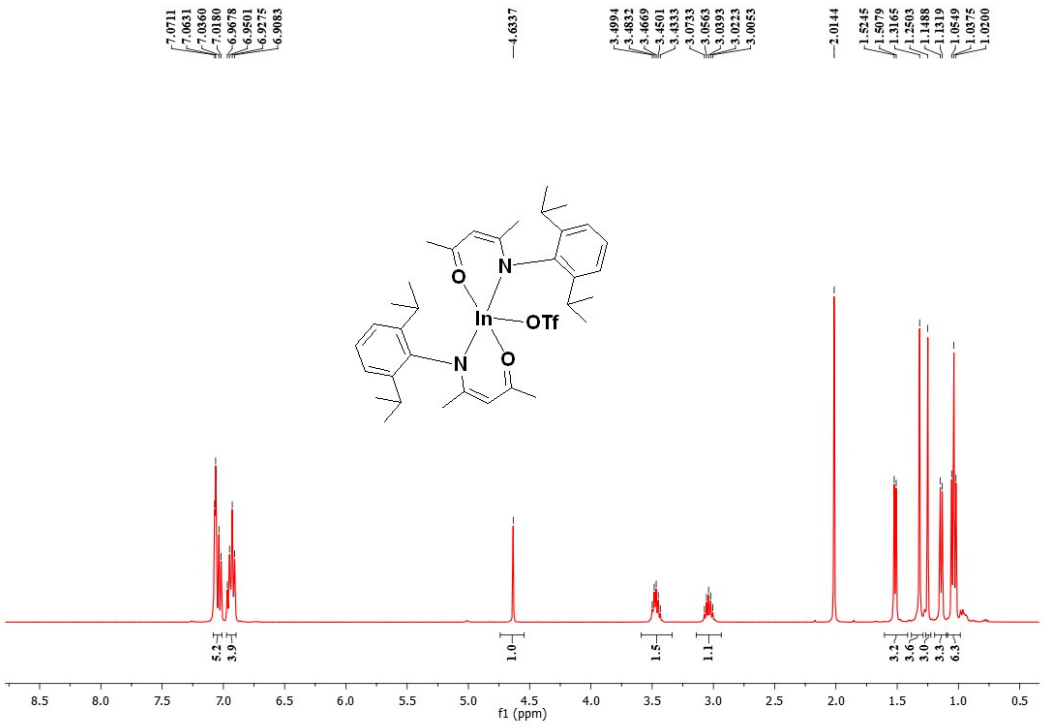


Fig FS5. ^{1}H NMR for complex **3a** in C_6D_6.

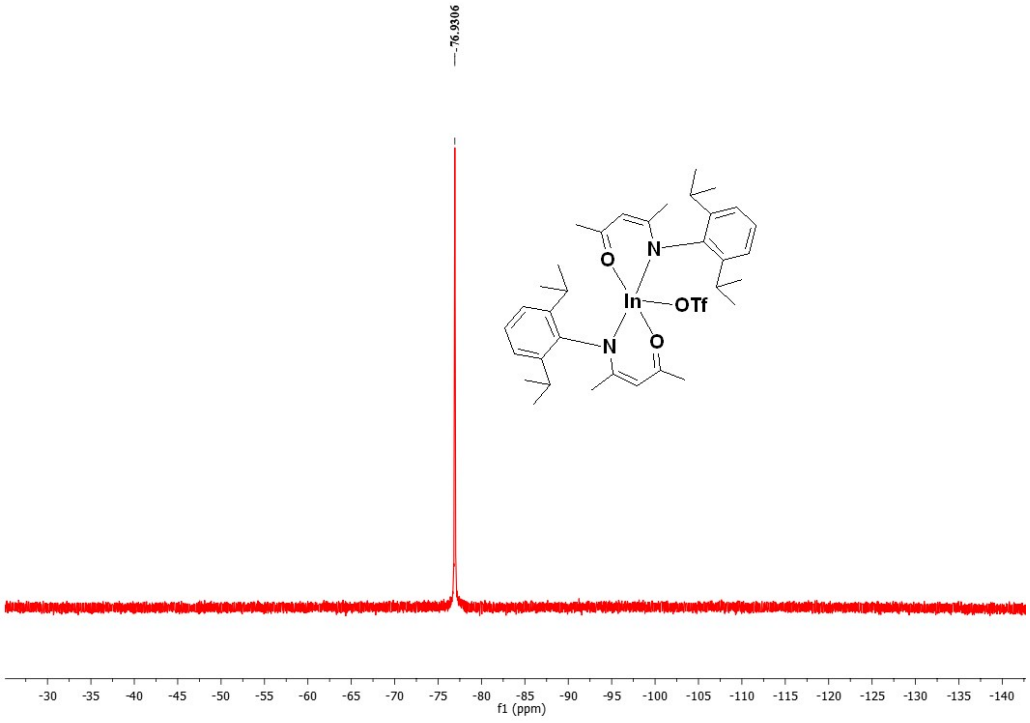


Fig FS6. ^{19}F NMR for complex **3a** in C_6D_6.

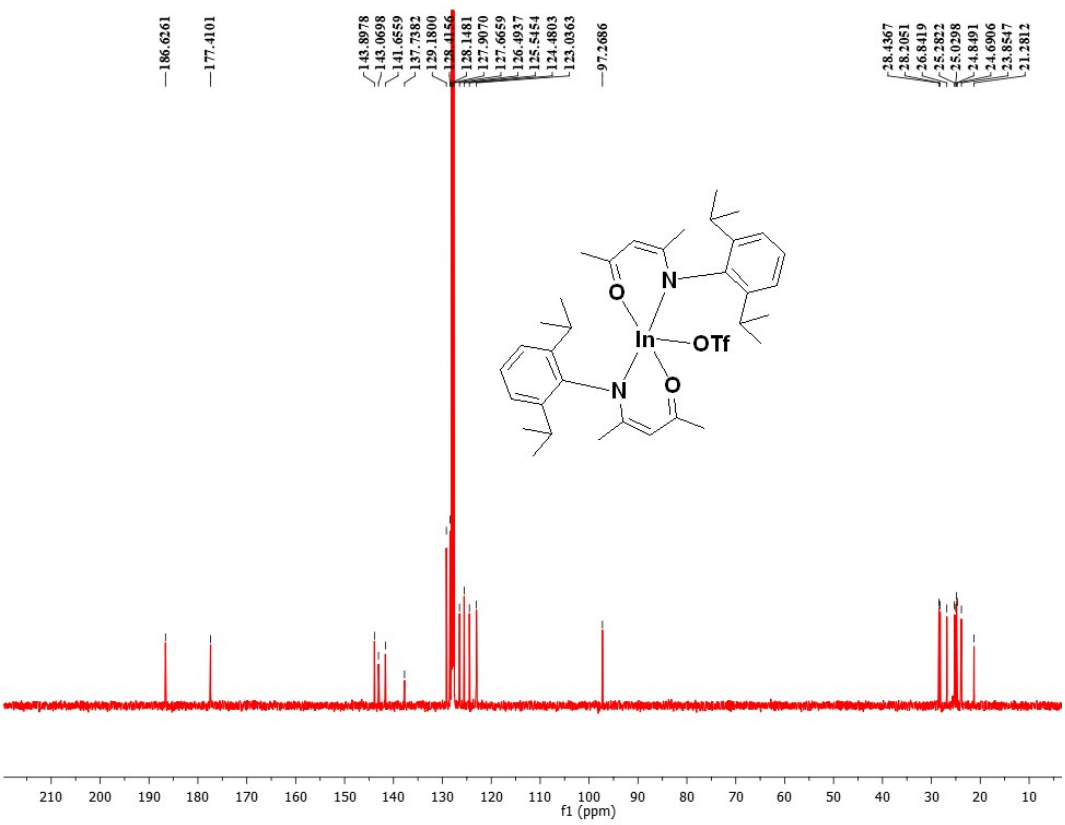
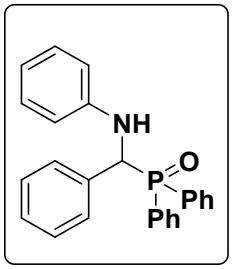


Fig FS7. $^{13}C\{^{1}H\}$ NMR for complex **3a** in C_6D_6.

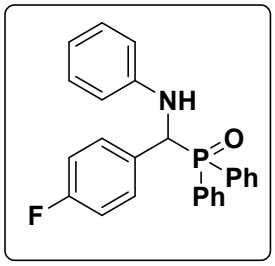
3. General procedure for synthesis of α-aminophosphine oxides using 3a as a catalyst.

Inside the glove box to a 25 mL dry Schlenk flask, the required aldehyde precursor (0.9433 mmol, 1 equiv) was added to the reaction mixture of amine (0.9433 mmol, 1 equiv.) and Diphenyl phosphine oxide (0.9433 mmol, 1 equiv.) and 2 mol% complex **3a** (18 mg, 0.02358 mmol). The colourless reaction mixture was stirred at room temperature. After six hours, the reaction mixture was quenched and workup with water and compound extracted in dichloromethane as an organic layer for 3 times. Then the final product was purified by column chromatography in hexane/EtOAc (100:5). The products were identified according to ^{1}H, ^{31}P ^{13}C, and DEPT NMR spectroscopy (wherever necessary), as well as MS analysis.

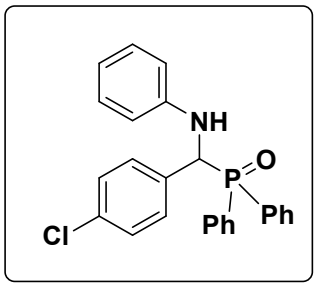
4. Characterization Data of α-aminophosphine oxides



Yield (**4a**): 346 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.88 - 7.84 (m, 3H, Ar), 7.56 - 7.54 (m, 1H, Ar), 7.50 - 7.46 (m, 3H, Ar), 7.40 - 7.35 (m, 4H, Ar), 7.28 - 7.25 (m, 3H, Ar), 7.15 - 7.06 (m, 9H, Ar), 6.68 - 6.58 (m, 3H, Ar), 5.20 - 5.17 (m, 1H, C*H*), ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 160.4, 152.9, 136.2, 131.7, 131.6, 131.3, 129.7, 129.2, 129.1, 128.8, 128.4, 128.3, 128.1, 128.0, 125.9, 120.8, 118.3, 115.1, 113.9, 57.3 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.2 ppm.

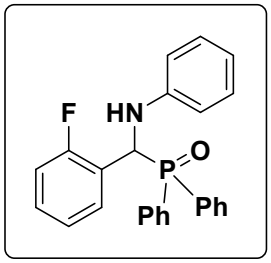


Yield (**4b**): 355 mg, 94%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.86 - 7.83 (m, 2H, Ar), 7.49 - 7.48 (m, 1H, Ar), 7.43 - 7.42 (m, 5H Ar), 7.40 - 7.29 (m, 2H, Ar), 7.12 - 7.07 (m, 4H, Ar), 6.83 - 6.79 (m, 2H, Ar), 6.70 - 6.69 (m, 1H, Ar), 6.58 – 6.56 (m, 2H, Ar), 5.17- 5.16 (m, 1H, C*H*) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 165.9, 163.4, 158.8, 151.8, 146.0,145.8, 131.6, 131.5, 130.7, 129.2, 128.9, 128.3, 128.2, 126.0, 120.8, 118.2, 116.0, 115.8, 115.3, 115.0, 113.9, 57.0, 56.3, ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.13 ppm.

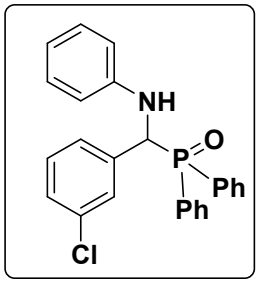


Yield (**4c**): 385 mg, 98%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.90 - 7.85 (m, 2H, Ar), 7.51 - 7.47 (m, 1H, Ar), 7.46 - 7.43 (m, 5H, Ar), 7.34 - 7.28 (m, 2H, Ar), 7.13 - 7.09 (m, 6H, Ar), 6.74 - 6.70 (m, 1H, Ar), 6.60 - 5.58 (m, 2H, Ar), 5.20 - 5.17 (m, 1H, C*H*), ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 145.8, 145.7,

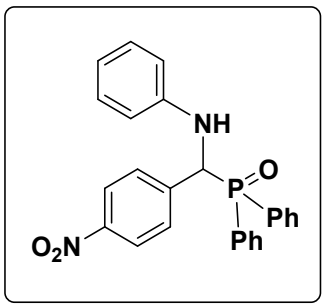
133.8, 133.5,132.4,132.2, 131.6, 131.5, 130.4, 130.0, 129.6, 129.4, 128.9, 128.8, 128.3, 128.2, 118.6, 113.9, 57.2, 56.4 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 33.1 ppm.



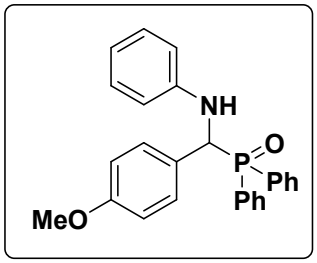
Yield (**4d**): 359 mg, 95%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.89 - 7.84 (m, 2H, Ar), 7.58 - 7.57 (m, 1H, Ar), 7.53 - 7.47 (m, 5H, Ar), 7.34 - 7.28 (m, 2H, Ar), 7.20 - 7.17 (m, 6H, Ar), 6.97 - 6.92 (m, 1H, Ar), 6.85 - 5.83 (m, 1H, Ar), 6.64 – 6.58 (m, 2H, Ar), 5.26 - 5.20 (m, 2H, C*H*) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 150.8, 134.6, 134.5, 132.0, 131.9, 131.7, 131.6, 131.5, 130.4, 129.0, 128.8, 128.3, 128.2, 127.8, 127.4, 127.3, 124.4, 118.6, 114.8, 114.6, 113.8, 57.2, 56.4 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 32.2 ppm.



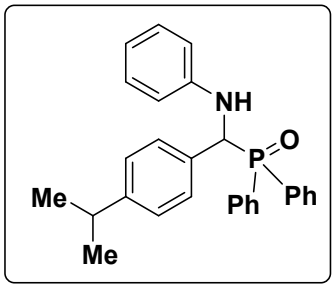
Yield (**4e**): 369 mg, 94%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.78 - 7.76 (m, 2H, Ar), 7.63 - 7.48 (m, 1H, Ar), 7.43 - 7.30 (m, 4H, Ar), 7.26 - 7.12 (m, 2H, Ar), 7.09 - 6.98 (m, 4H, Ar), 6.67 - 6.59 (m, 1H, Ar), 6.51 - 5.49 (m, 1H, Ar), 5.14 - 5.04 (m, 1H, C*H*) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 158.6, 145.8, 145.7, 137.4, 134.1, 132.3, 131.6, 131.5, 131.2, 130.0, 129.4, 129.3, 129.2, 128.9, 128.8, 128.4, 128.2, 127.8, 127.1, 126.3, 120.8, 118.6, 118.5, 115.1, 113.8, 57.5, 56.7 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 33.12 ppm.



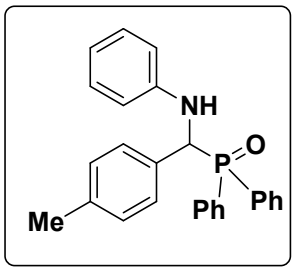
Yield (**4f**): 387 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.98 - 7.89 (m, 1H, Ar), 7.87 - 7.79 (m, 2H, Ar), 7.67 - 7.56 (m, 2H, Ar), 7.50 - 7.39 (m, 5H, Ar), 7.33 - 7.24 (m, 3H, Ar), 7.16 - 7.02 (m, 3H, Ar), 6.75 - 6.68 (m, 2H, Ar), 6.64 - 6.58 (m, 2H, Ar), 5.44 - 5.29 (m, 2H, C*H*) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 158.8, 151.7, 146.3, 134.7, 133.5, 131.6, 131.5, 131.5, 130.9, 130.3, 129.9, 129.6, 129.1, 128.9, 128.8, 128.4, 128.2, 126.2, 120.8, 118.6, 115.1, 113.9, 57.2, 56.4 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.5 ppm.



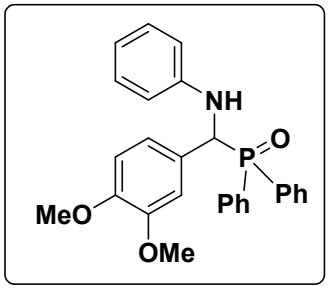
Yield (**4g**): 381 mg, 98%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.87 - 7.83 (m, 2H, Ar), 7.54 - 7.48 (m, 1H, Ar), 7.47 - 7.39 (m, 4H, Ar), 7.29 - 7.25 (m, 2H, Ar), 7.09 - 7.05 (m, 4H, Ar), 6.68 - 6.58 (m, 5H, Ar), 5.13 (s, 2H, C*H*), 3.70 (s, 3H, OCH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 162.2, 159.6, 152.4, 131.9, 131.7. 131.6, 130.5, 129.5, 129.3, 129.2, 129.1, 128.8,128.1, 125.5, 120.8, 118.3, 115.1, 114.3, 114.0, 113. 7, 55.4, 55.1, ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.03 ppm.



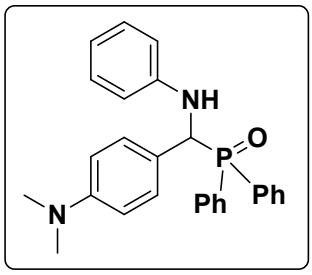
Yield (**4h**): 380 mg, 95%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.92 - 7.87 (m, 2H Ar), 7.54 - 7.50 (m, 3H Ar), 7.42 - 7.35 (m, 2H Ar), 7.28 - 7.26 (m, 3H Ar), 7.13 - 7.06 (m, 4H Ar), 7.00 - 6.96 (m, 2H Ar), 6.71 - 6.63 (m, 2H Ar), 5.21 - 5.18 (m, 1H, C*H*), 2.82 - 2.77 (m, 1H, $(CH_3)_2$C*H*), 1.18 - 1.16 (dd, *J* = 5.5 Hz 6H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 148.4, 148.3, 146.1, 132.2, 131.8, 131.7. 131.6, 130.5, 129.1, 128.8, 128.7, 128.2, 128.0, 127.9, 126.2, 113.9, 57.4, 56.6, 33.9, 23.8, ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.51 ppm.



Yield (**4i**): 359 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.91 - 7.86 (m, 2H, Ar), 7.48 - 7.43 (m, 1H, Ar), 7.31 - 7.28 (m, 5H, Ar), 7.27 - 7.25 (m, 2H, Ar), 7.10 - 7.08 (m, 4H, Ar), 7.05 – 7.04 (m, 2H, Ar), 6.96 - 6.94 (m, 1H, Ar), 6.63 - 6.61 (m, 2H, Ar), 5.22 - 5.13 (m, 2H, C*H*), 2.25 (s, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 146.2,137.3,132.2, 131.7. 131.6, 131.4, 129.1, 128.9, 128.3, 128.2, 118.3, 113.9, 57.4, 56.7, 21.1 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 32.87 ppm.

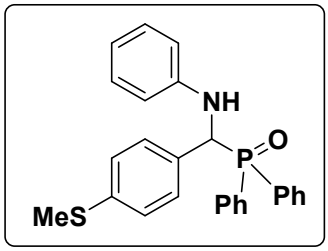


Yield (**4j**): 392 mg, 94%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.92 - 7.87 (m, 2H, Ar), 7.59 - 7.57 (m, 1H, Ar), 7.51 - 7.42 (m, 4H, Ar), 7.34 - 7.28 (m, 2H, Ar), 7.19 - 7.09 (m, 2H, Ar), 6.78 - 6.60 (m, 6H, Ar), 5.18 - 5.13 (m, 2H, C*H*), 3.80 (s, 3H, OCH_3), 3.64 (s, 3H, OCH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 148.6, 148.4, 146.2, 146.1, 132.3, 131.8, 131.7. 131.6, 129.2, 129.1, 128.8, 128.7, 128.2,128.1, 127.1, 120.8, 118.4, 115.1, 114.0, 11.3, 110.7, 57.4, 56.7, 55.7 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 32.28 ppm.

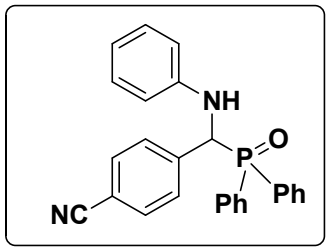


Yield (**4k**): 358 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.39 - 7.36 (m, 2H, Ar), 7.27 - 7.17 (m, 5H, Ar), 7.14 - 7.11 (m, 5H, Ar), 6.89 - 6.87 (m, 2H, Ar), 6.71 - 6.64 (m, 5H, Ar), 5.08 - 5.02 (m, 1H, C*H*), 2.89 (s, 6H, N(CH_3)$_2$) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 150.6, 150.5, 150.3, 146.2, 146.1, 129.6,

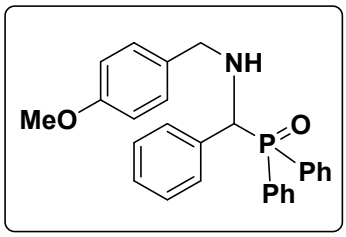
129.5, 129.2, 129.0, 125.2, 125.1, 120.8, 120.7, 118.6, 115.5, 114.1, 113.0, 112.9, 56.2, 54.7, 40.6 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 33.0 ppm.



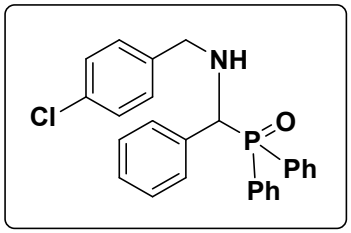
Yield (**4l**): 396 mg, 98%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.87 - 7.79 (m, 2H, Ar), 7.47 - 7.43 (m, 1H, Ar), 7.42 - 7.40 (m, 5H, Ar), 7.31 - 7.25 (m, 3H, Ar), 6.69 - 6.65 (m, 1H, Ar), 5.16 – 5.14 (m, 2H, C*H*), 2.38 (s, 3H, SCH_3) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 159.6, 146.0, 145.9, 137.9, 132.3, 132.0, 131.8,131.7, 131.6, 129.1, 128.8, 128.7, 128.3, 128.1, 125.8, 125.7, 120.9, 125.1, 120.8, 118.4, 113.9, 57.3, 56.5, 15.6, 15.12 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 32.9 ppm.



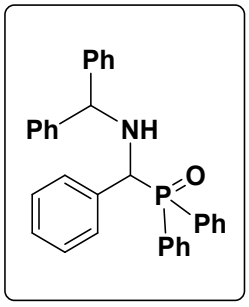
Yield (**4m**): 340 mg, 86%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 8.45 (s, 1H, Ar), 7.97 - 7.95 (m, 3H, Ar), 7.71 - 7.69 (m, 3H Ar), 7.40 - 7.38 (m, 3H, Ar), 7.23 - 7.21 (m, 4H, Ar), 6.66 - 6.64 (m, 1H, C*H*), ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 157.9, 151.0, 139.9, 132.5, 129.3, 129.1, 126.9, 121.0, 118.5, 118.4, 115.8, 115.1, 114.3, ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = -19.89 ppm.



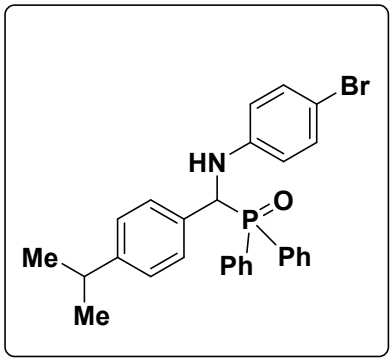
Yield (**4n**): 386 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.81 - 7.77 (m, 2H, Ar), 7.56 - 7.54 (m, 1H, Ar), 7.47 - 7.42 (m, 4H, Ar), 7.26 - 7.20 (m, 6H, Ar), 7.06 - 7.04 (m, 1H, Ar), 6.85 - 6.83 (m, 1H, Ar), 4.40 - 4.37 (m, 1H, Ar), 3.82 (s, 1H, CH_3), 3.47 - 3.44 (m, 1H, C*H*) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 158.7, 135.0, 132.0,131.8, 131.5,131.4, 129.9, 129.2, 128.4, 128.2, 128.0, 127.9, 127.7, 127.6, 61.2, 60.4, 55.1, 50.3, 50.2 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 31.88 ppm.



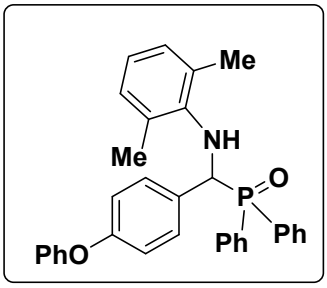
Yield (**4o**): 374 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.81 - 7.75 (m, 2H, Ar), 7.58 - 7.76 (m, 1H, Ar), 7.50 -7.47 (m, 2H, Ar), 7.42 - 7.40 (m, 3H, Ar), 7.25 - 7.20 (m, 6H, Ar), 7.18 - 7.14 (m, 2H, Ar), 7.04 - 7.02 (m, 1H, Ar), 4.30 - 4.27 (m, 1H, C*H*), 3.79 - 3.76 (m, 1H, C*H*), 3.47 - 3.44 (m, 1H, C*H*) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 137.6, 134.9, 132.8, 132.5, 132.4, 132.1, 132.0, 131.6,131.4, 131.3, 129.2, 129.0,128.6, 128.4, 128.4, 128.2, 128.1, 127.9, 127.8, 127.5, 127.4, 61.3, 60.5, 50.1,50.0 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 31.85 ppm.



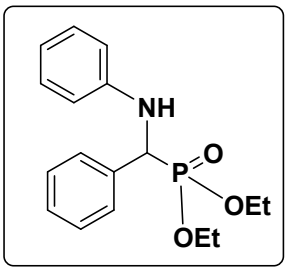
Yield (**4p**): 423 mg, 95%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.86 - 7.81 (m, 2H, Ar), 7.59 (m, 1H, Ar), 7.53 - 7.49 (m, 2H, Ar), 7.40 - 7.28 (m, 6H, Ar), 7.21 - 7.13 (m, 11H, Ar), 7.04 - 7.02 (m, 1H, Ar), 5.59 - 5.48 (m, 1H, Ar), 4.61 (s, 1H, C*H*), 4.24 - 4.21 (m, 1H, C*H*), ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 160.9, 143.9, 143.6, 141.9, 136.3, 134.5, 132.4, 132.1, 132.0, 131.9,131.4, 129.7, 129.2, 129.0,128.6, 128.4, 128.2, 128.1, 127.9, 127.7, 127.4, 127.0, 64.1, 64.0, 60.4, 59.6, ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 32.5 ppm.



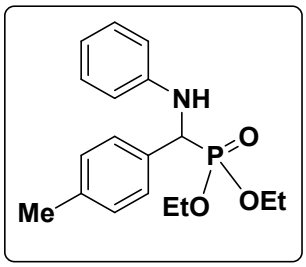
Yield (**4q**): 460 mg, 97%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.87 - 7.84 (m, 2H, Ar), 7.59 - 7.57 (m, 2H, Ar), 7.44 - 7.40 (m, 1H, Ar), 7.35 - 7.25 (m, 3H, Ar), 7.18 - 7.06 (m, 2H, Ar), 7.04 - 6.97 (m, 3H, Ar), 6.51 - 6.49 (m, 2H, Ar), 5.12 - 5.07 (m, 1H, C*H*), 2.85 - 2.77 (m, 1H, $(CH_3)_2CH$), 1.22 - 1.16 (m, 6H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 148.6, 145.2, 131.9, 131.7. 131.6, 128.8, 128.7, 128.2, 128.0, 127.9, 126.2, 115.5, 110.0, 57.4, 56.6, 33.7, 23.9 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.44 ppm.



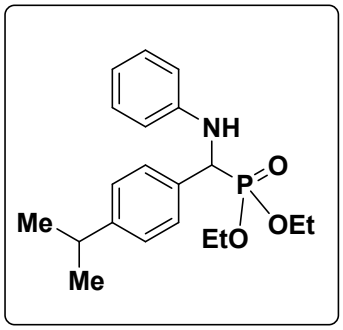
Yield (**4r**): 455 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.92 - 7.87 (m, 3H, Ar), 7.53 -7.51 (m, 3H, Ar), 7.45 - 7.34 (m, 3H, Ar), 7.34 - 7.26 (m, 4H, Ar), 7.14 - 7.06 (m, 3H, Ar), 6.83 - 6.79 (m, 4H, Ar), 6.72 - 6.89 (m, 3H, Ar), 5.08 (s, 1H, C*H*), 2.09 (s, 6H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 150.6, 150.5, 150.3, 146.2, 146.1, 129.6, 129.5, 129.2, 129.0, 125.2, 125.1, 120.8, 120.7, 118.6, 115.5, 114.1, 113.0, 112.9, 56.2, 54.7, 40.6 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 33.59 ppm.



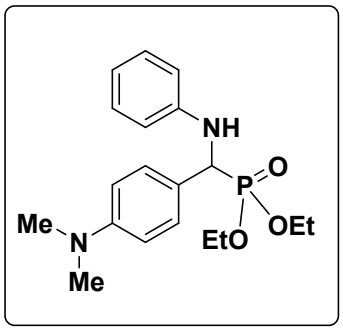
Yield (**5a**): 285 mg, 95%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.52 - 7.50 (m, 2H, Ar), 7.38 - 7.34 (m, 2H Ar), 7.31 - 7.28 (m, 1H, Ar), 7.15 - 7.11 (m, 2H, Ar), 6.73 - 6.70 (m, 1H, Ar), 6.64 - 6.62 (m, 2H, Ar), 4.83 - 4.77 (m, 1H, C*H*), 4.17 - 4.11 (m, 2H, CH_2), 3.98 - 3.93 (m, 1H, CH_2), 3.73 - 3.67 (m, 1H, CH_2), 1.33 - 1.29 (m, 3H, CH_3), 1.16 - 1.12 (m, 3H, CH_3), ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 146.4, 146.2, 135.9, 129.1,128.6, 128.5, 127.9, 127.8, 118.4, 113.8, 63.3, 62.2, 56.8, 55.3, ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 22.7 ppm.



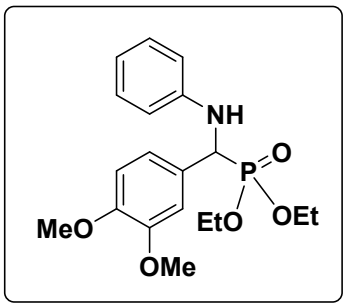
Yield (**5b**): 292 mg, 93%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.26 - 7.24 (m, 2H Ar), 6.98 - 6.92 (m, 4H Ar), 6.51 - 6.47 (m, 3H Ar), 4.67 - 4.61 (m, 1H C*H*), 4.01 - 3.95 (m, 2H, CH_2), 3.93 - 3.78 (m, 1H, CH_2), 3.78 - 3.54 (m, 1H, CH_2), 2.13 (s, 3H, CH_3), 1.13 – 1.10 (m, 3H, CH_3), 0.98 – 0.94 (m, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 146.4, 146.3, 136.4,136.3, 134.3,134.2, 130.5,129.2,128.6, 128.9, 127.7, 127.2, 127.1, 126.5, 118.2, 113.8, 113.5, 63.3, 63.1, 52.8, 51.3, 19.7, 16.5, 14.2 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 22.9 ppm.



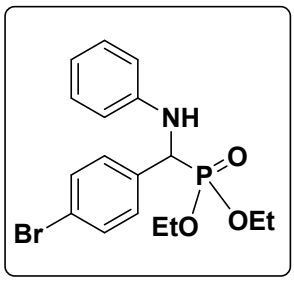
Yield (**5c**): 326 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.30 - 7.28 (m, 2H Ar), 7.04 - 7.02 (m, 2H, Ar), 6.95 - 6.91 (m, 2H, Ar), 6.52 - 6.49 (m, 3H, Ar), 4.69 - 4.62 (m, 1H, C*H*), 4.01 - 3.93 (m, 2H, CH_2), 3.79 - 3.77 (m, 1H, CH_2), 3.56 - 3.50 (m, 1H, CH_2), 2.74 - 2.68 (s, 1H, $(CH_3)_2$C*H*), 1.17 - 1.08 (m, 3H, CH_3), 1.07 - 1.05 (dd, *J* = 6.9 Hz, 6H, $(CH_3)_2$), 0.94 – 0.91 (m, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 148.4, 146.7, 146.7, 146.5, 133.2, 129.0,128.6, 128.9, 127.7, 127.2, 127.1, 126.5, 118.2, 113.8, 113.5, 63.3, 63.1, 56.3, 54.8, 33.7, 23.9, 16.4, 16.3, 16.1 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 23.0 ppm.



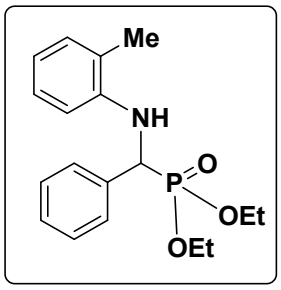
Yield (**5d**): 334 mg, 98%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.36 - 7.33 (m, 2H, Ar), 7.14 - 7.10 (m, 2H, Ar), 6.72 - 6.70 (m, 3H, Ar), 6.65 - 6.63 (m, 2H, Ar), 4.73 - 4.68 (m, 1H, C*H*), 4.17 - 4.13 (m, 2H, CH_2), 4.12 - 3.94 (m, 1H, CH_2), 2.93 (s, 6H, N(CH_3)$_2$), 1.33 – 1.29 (m, 3H, CH_3), 1.18 – 1.15 (m, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 150.1, 146.7, 146.5, 129.1,128.6, 123.7, 118.1, 113.9, 112.6, 63.2, 63.1, 56.1, 54.6, 40.5, 16.5, 16.3 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 23.4 ppm.



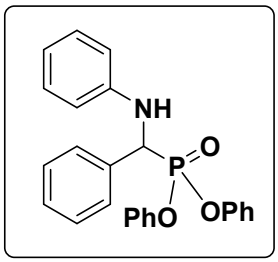
Yield (**5e**): 343 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.06 - 7.01 (m, 3H, Ar), 6.74 - 6.72 (m, 1H, Ar), 6.65 - 6.56 (m, 3H, Ar), 4.74 - 4.68 (m, 1H, C*H*), 4.09 - 4.01 (m, 2H, CH_2), 3.92 - 3.78 (m, 1H, CH_2), 3.75 (s, 3H, OCH_3), 3.71 (s, 3H, OCH_3), 1.94 (s, 3H, CH_3), 1.27 – 1.21 (m, 3H, CH_3), 1.09 – 1.06 (m, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 170.8, 149.0, 148.7, 146.8, 146.6, 129.0, 128.2, 128.9, 120.3, 120.2, 118.2, 117.9, 117.0, 114.9, 113.8, 112.7, 111.1, 111.0, 63.1, 61.6, 60.2, 56.3, 55.7, 55.6, 54.8, 20.8, 16.4, 16.2, 14.6 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 22.8 ppm.



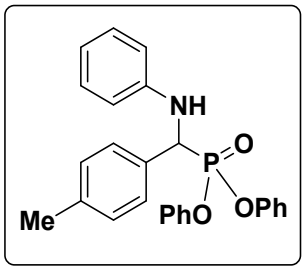
Yield (**5f**): 352 mg, 94%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.81 - 7.79 (m, 1H, Ar), 7.53 - 7.35 (m, 3H, Ar), 7.30 - 7.21 (m, 2H, Ar), 6.96 - 6.92 (m, 1H, Ar), 6.51 - 6.43 (m, 1H, Ar), 4.85 - 4.79 (m, 1H, C*H*), 4.13 - 3.94 (m, 1H, CH_2), 3.79 - 3.73 (m, 1H, CH_2), 1.30 - 1.20 (m, 3H, CH_3), 1.13 – 1.10 (m, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 143.3, 143.1, 132.3, 128.9, 128.6, 128.3, 127.7, 127.6, 119.0, 112.7, 110.4, 63.5, 63.4, 63.3, 56.7, 55.2, 16.4, 16.3, 16.2, 16.1 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 21.7 ppm.



Yield (**5g**): 285 mg, 93%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.43 - 7.42 (m, 1H, Ar), 7.03 - 7.02 (m, 2H, Ar), 6.98 - 6.94 (m, 3H, Ar), 6.56 - 6.52 (m, 1H, Ar), 6.44 - 6.42 (m, 2H, Ar), 4.93 - 4.86 (m, 2H, C*H*), 4.07 - 3.98 (m, 2H, CH_2), 3.79 - 3.73 (m, 1H, CH_2), 3.44 - 3.39 (m, 1H, CH_2), 2.41 (s, 3H, CH_3), 1.19 – 1.15 (m, 3H, CH_3), 0.94 – 0.90 (m, 3H, CH_3), ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 146.6, 146.5, 137.4, 132.9, 129.2, 129.1, 127.9, 127.8, 118.2, 113.8, 63.2, 63.1, 60.3, 56.4, 54.9, 21.1, 20.9, 16.4, 16.2, 14.2 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 23.5 ppm.

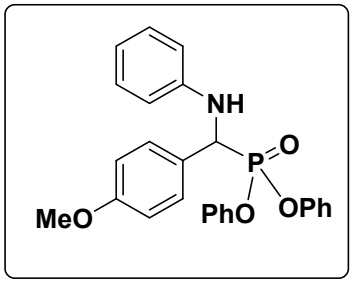


Yield(**6a**): 375 mg, 96%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.33 - 7.22 (m, 8H, Ar), 7.18 – 7.14 (m, 4H, Ar), 7.10 - 7.07 (m, 2H, Ar), 6.56 - 6.87 (m, 4H, Ar), 6.79 - 6.75 (m, 1H, Ar), 6.65 - 6.63 (m, 1H, Ar), 5.15 - 5.09 (m, 1H, C*H*) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 157.5, 156.9, 150.3,150.2, 145.8, 145.6 136.9, 130.2, 129.3, 125.4, 125.3, 123.3,123.0, 122.9, 120.6, 120.3,120.2, 119.0, 119.3, 118.7, 118.6, 114.1, 56.7, 55.1 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 14.8 ppm.

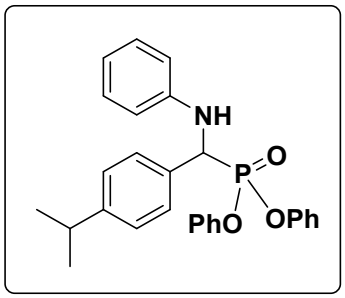


Yield (**6b**): 368 mg, 91%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.43 - 7.41 (m, 2H, Ar), 7.25 - 7.18 (m, 3H, Ar), 7.12 - 7.18 (m, 7H, Ar), 6.87 - 6.85 (m, 2H, Ar), 6.72 - 6.69 (m, 1H, Ar), 6.64 - 6.62 (m, 2H, Ar), 5.14 - 5.08 (m, 1H, C*H*), 2.28 (s, 1H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 150.4, 150.3, 150.2,

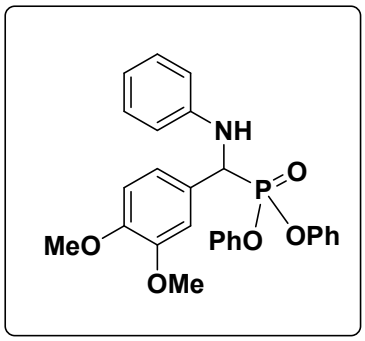
146.1, 145.9, 136.6, 133.3, 130.8, 129.8, 129.6, 129.3, 128.2, 127.7, 127.6, 126.8, 125.5, 125.2, 120.8, 120.2, 118.8, 113.8, 52.7, 51.2, 19.8 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 15.6 ppm.



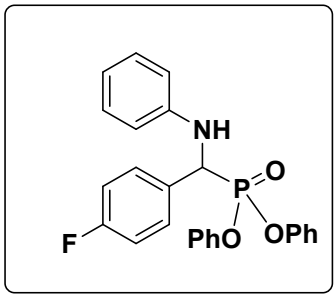
Yield (**6c**): 398 mg, 95%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.55 - 7.53 (m, 2H Ar), 7.34 - 7.27 (m, 6H, Ar), 7.25 - 7.15 (m, 6H, Ar), 7.06 - 7.02 (m, 1H, Ar), 6.97 - 6.91 (m, 4H, Ar), 6.82 - 6.27 (m, 1H, Ar), 5.22 - 5.16 (m, 1H, C*H*), 3.80 (s, 3H, OCH_3) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 159.7, 156.6, 151.2, 150.4, 150.2, 146.0, 145.9, 132.0, 129.8, 129.6, 129.4, 129.3, 126.5, 125.3, 125.3, 122.3, 120.8, 120.7, 120.5, 120.4, 119.7, 118.8, 115.5, 114.3, 114.1, 113.8, 56.8, 55.2, 54.6 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 15.68 ppm.



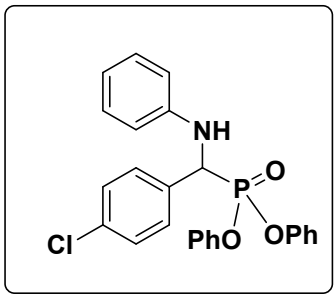
Yield (**6d**): 387 mg, 90%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.46 - 7.43 (m, 2H Ar), 7.25 - 7.15 (m, 2H, Ar), 7.12 - 7.10 (m, 5H, Ar), 7.10 - 7.06 (m, 3H, Ar), 6.78 - 6.70 (m, 2H, Ar), 6.66 - 6.64 (m, 2H, Ar), 5.15 - 5.09 (s, 1H, C*H*), 2.89 - 2.82 (m, 1H, $(CH_3)_2$C*H*), 1.21 - 1.19 (m, 6H, CH_3), ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 150.4, 150.4, 150.3, 149.2,149.1, 146.1, 145.9, 131.9, 129.7, 129.5, 129.2, 128.2, 128.1, 126.9, 125.3, 125.1, 120.7, 120.3, 118.7, 114.3, 56.8, 54.6, 33.8, 23.9 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 15.63 ppm.



Yield (**6e**): 398 mg, 89%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.33 - 7.23 (m, 7H Ar), 7.20 - 7.11 (m, 2H, Ar), 7.03 - 6.98 (m, 2H, Ar), 6.94 - 6.92 (m, 2H, Ar), 6.77 - 6.85 (m, 1H, Ar), 6.81 - 6.79 (m, 1H, Ar), 6.72 - 6.70 (m, 1H, Ar), 5.17 - 5.11 (m, 1H, C*H*), 3.87 (s, 3H, OCH_3), 3.82 (s, 3H, OCH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 151.3,150.4, 150.3, 149.2, 149.1, 146.1, 145.9, 133.1, 129.7, 129.6, 129.5, 129.4, 129.3,127.1, 127.0, 128.2, 125.4, 125.3, 125.2, 123.8, 122.5, 120.8, 120.6, 120.3, 118.9, 115.4, 114.1, 111.3, 111.1, 111.0, 56.6, 55.9, 55.0 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 15.46 ppm.

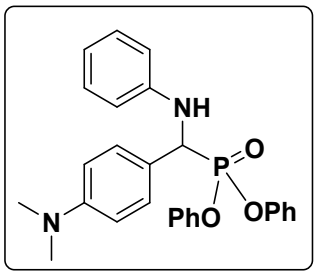


Yield (**6f**): 379 mg, 93%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.58 (s, 1H, Ar), 7.34 - 7.26 (m, 4H, Ar), 7.22 - 7.12 (m, 5H, Ar), 7.04 - 7.05 (m, 1H Ar), 6.95 - 6.93 (m, 1H, Ar), 6.82 - 6.78 (m, 1H, Ar), 6.68 - 6.60 (m, 1H, Ar), 5.22 – 5.15 (m, 1H, C*H*) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 150.3, 150.2, 145.8, 145.6, 130.6, 129.9, 129.7, 129.3,125.4, 120.8, 120.6, 120.3, 120.2, 120.8, 120.6, 120.3, 119.0, 115.9, 115.7, 114.0, 56.0, 54.5, ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 15.02 ppm.

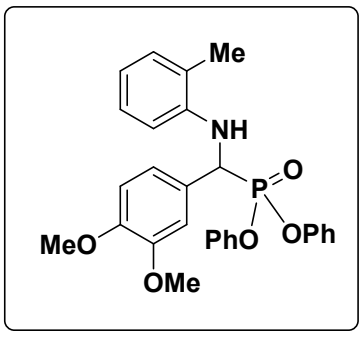


Yield (**6g**): 410 mg, 97%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.54 - 7.52 (m, 1H, Ar), 7.36 - 7.30 (m, 6H, Ar), 7.28 - 7.13 (m, 6H, Ar), 6.96 - 6.94 (m, 2H, Ar), 6.82 - 6.78 (m, 1H, Ar), 6.66 - 6.64 (m, 1H, Ar),

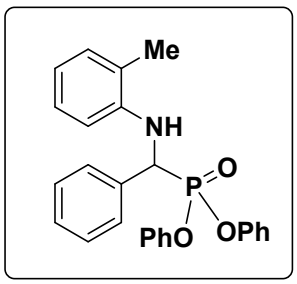
5.19 - 5.13 (m, 1H, C*H*) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 150.3, 150.2, 150.1, 145.7, 145.6, 130.6, 129.9, 129.8, 129.7, 125.5, 120.6, 120.4, 120.3, 120.2, 119.0, 115.4, 114.0, 56.0, 54.6, ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 15.02 ppm.



Yield (**6h**): 397 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.43 - 7.37 (m, 2H, Ar), 7.28 - 7.10 (m, 11H, Ar), 6.92 - 6.90 (m, 1H, Ar), 6.73 – 6.67 (m, 4H, Ar), 5.13 – 5.03 (m, 1H, C*H*), 2.90 (m, 6H, $N(CH_3)_2$), ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 150.4, 150.4, 150.3, 146.1, 145.9, 131.9, 129.7, 129.5, 129.2, 128.2, 126.9, 125.3, 125.1, 120.7, 120.3, 118.7, 114.3, 114.1, 113.8, 56.8, 54.6, 33.8, 23.9 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 16.04 ppm.



Yield (**6i**): 433 mg, 94%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.26 - 7.20 (m, 4H, Ar), 7.14 - 7.04 (m, 8H, Ar), 7.01 - 6.99 (m, 1H, Ar), 6.93 - 6.90 (m, 2H, Ar), 6.83 - 6.81 (m, 1H, Ar), 6.71 - 6.69 (m, 1H, Ar), 5.14 - 5.08 (m, 1H, C*H*), 3.84 (s, 3H, OCH_3), 3.79 (s, 3H, OCH_3), 2.20 (s, 3H, CH_3) ppm. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$): δ_C 150.5, 149.2, 149.1, 144.1, 143.9, 130.3, 129.7, 129.6, 127.0, 120.5, 120.2, 118.6, 111.5, 111.3, 111.0, 56.7, 55.9, 55.2, 17.5 ppm. $^{31}P\{^{1}H\}$ NMR (161.9 MHz, $CDCl_3$): δ_P = 15.46 ppm.



Yield (**6j**): 372 mg, 92%. ^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC): δ_H 7.61 - 7.59 (m, 2H, Ar), 7.15 - 7.14 (m, 3H, Ar), 7.11 - 7.09 (m, 7H, Ar), 6.74 - 6.67 (m, 2H, Ar), 6.58 - 6.56 (m, 1H, Ar), 5.42 - 5.36 (m, 1H, C*H*), 2.51 (s, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ_C 150.4, 150.3, 150.2, 146.1, 145.9, 136.6, 133.3, 130.8, 129.8, 129.6, 129.3, 128.2, 127.7, 127.6, 126.8, 125.5, 125.2, 120.8, 120.2, 118.8, 113.8, 52.8, 51.2, 19.8 ppm. ^{31}P{^{1}H} NMR (161.9 MHz, $CDCl_3$): δ_P = 16.25 ppm.

5. NMR data of α-aminophosphine oxides

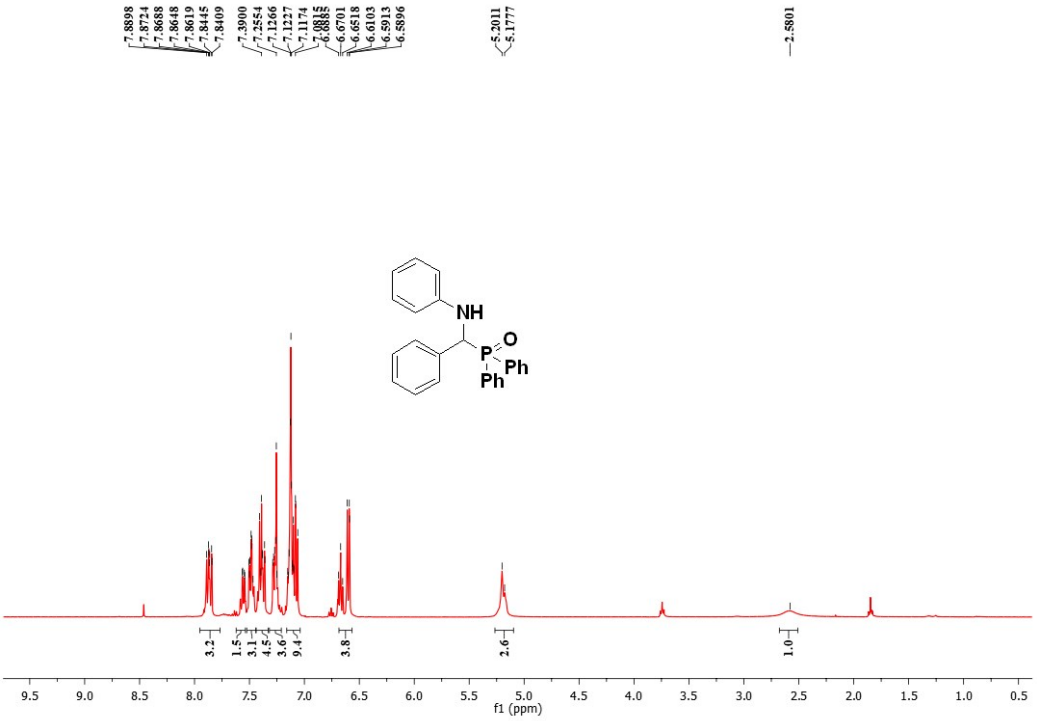


Fig FS8. ^{1}H NMR for compound **4a** in $CDCl_3$.

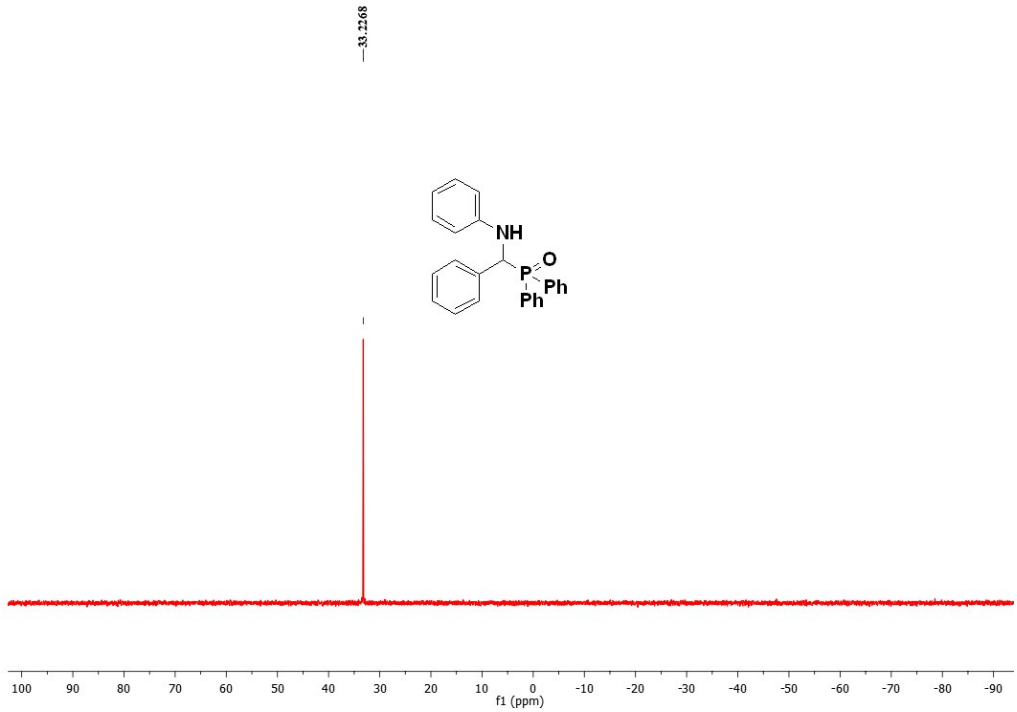


Fig FS9. $^{31}P\{^{1}H\}$ NMR for compound **4a** in $CDCl_3$.

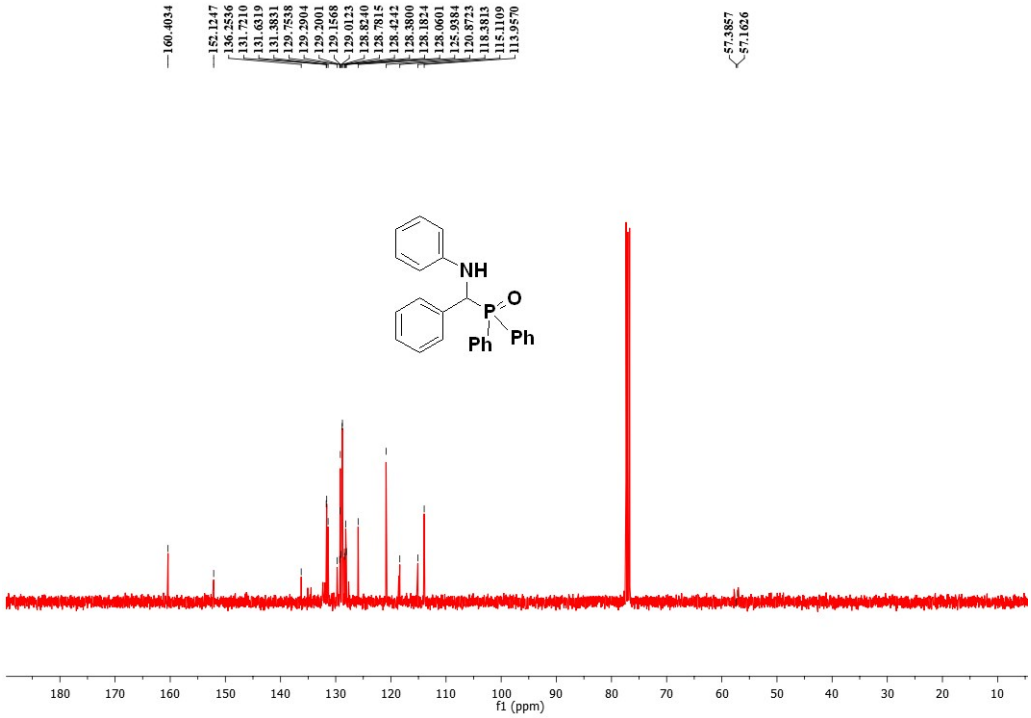


Fig FS10: $^{13}C\{^{1}H\}$ NMR for compound **4a** in $CDCl_3$.

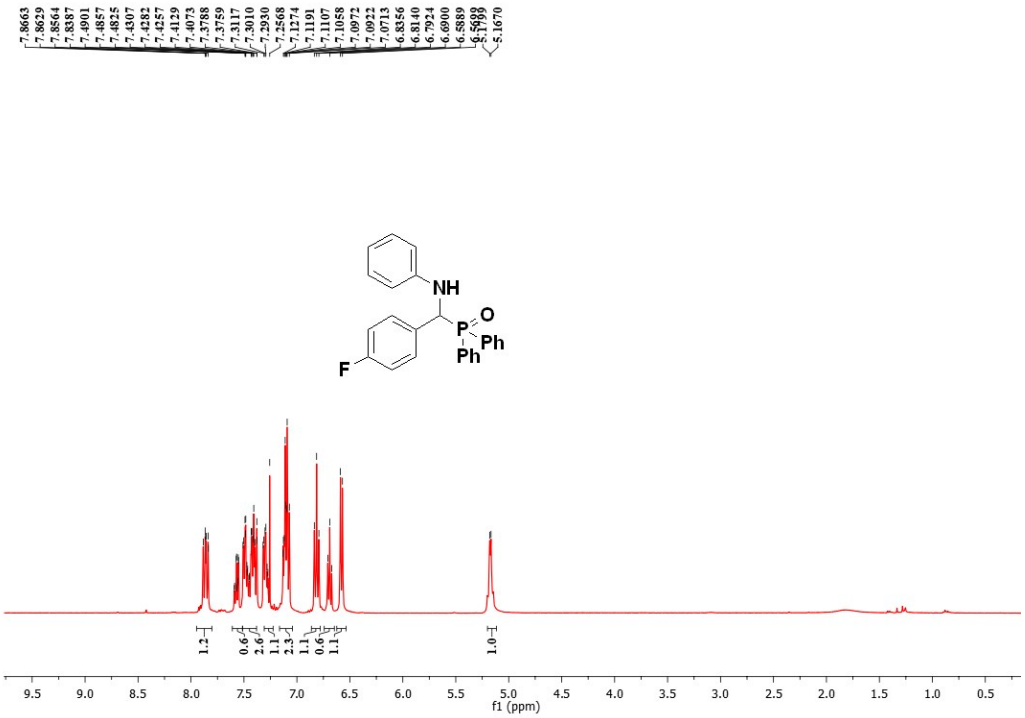


Fig FS11. ^{1}H NMR for compound **4b** in $CDCl_3$.

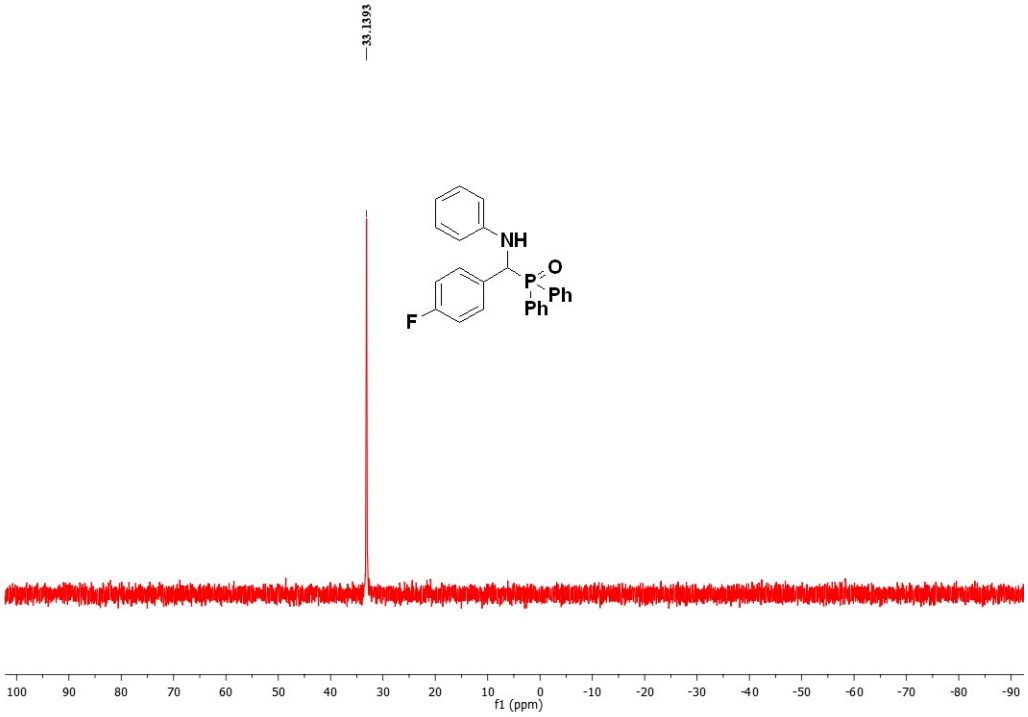


Fig FS12. $^{31}P\{^{1}H\}$ NMR for compound **4b** in $CDCl_3$.

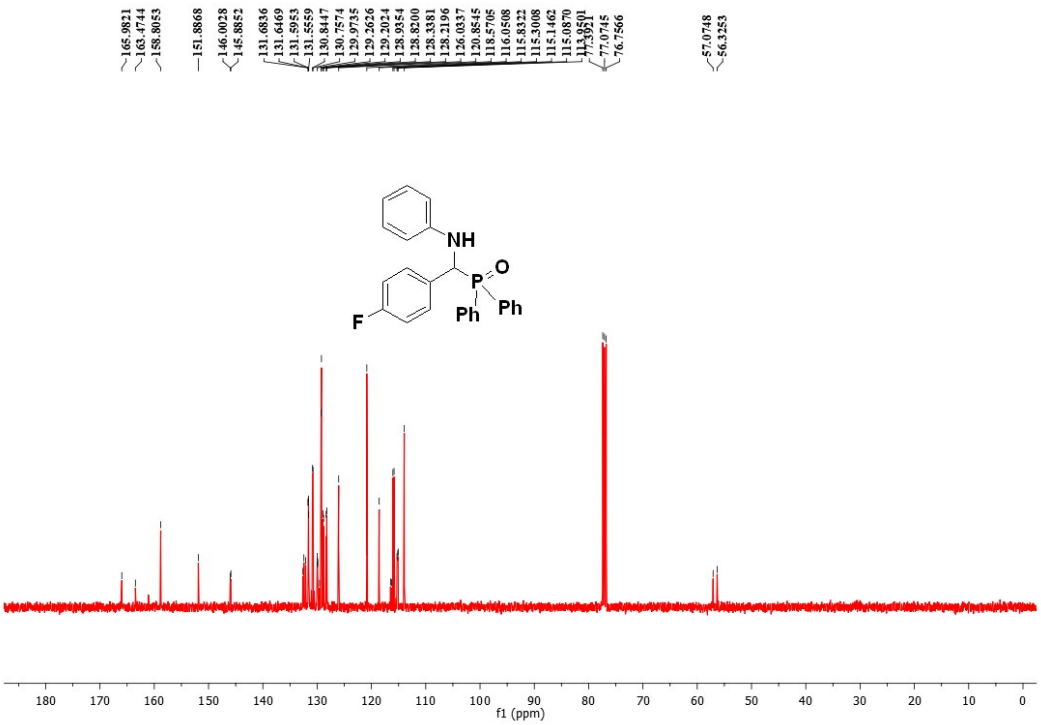


Fig FS13. $^{13}C\{^{1}H\}$ NMR for compound **4b** in $CDCl_3$.

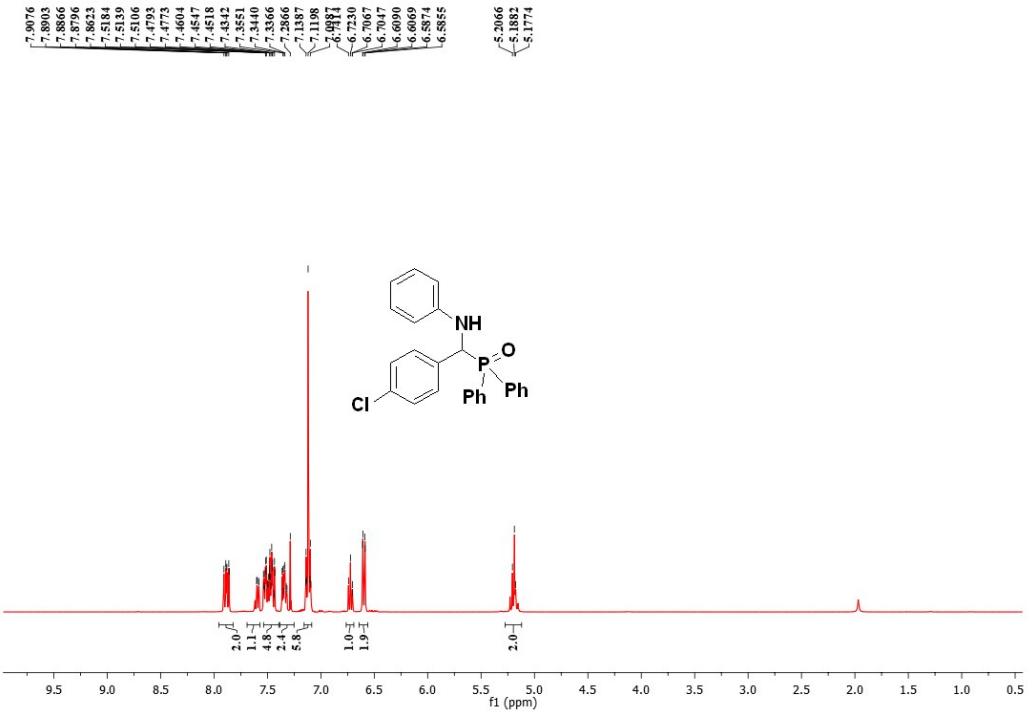


Fig FS14. ^{1}H NMR for compound **4c** in $CDCl_3$.

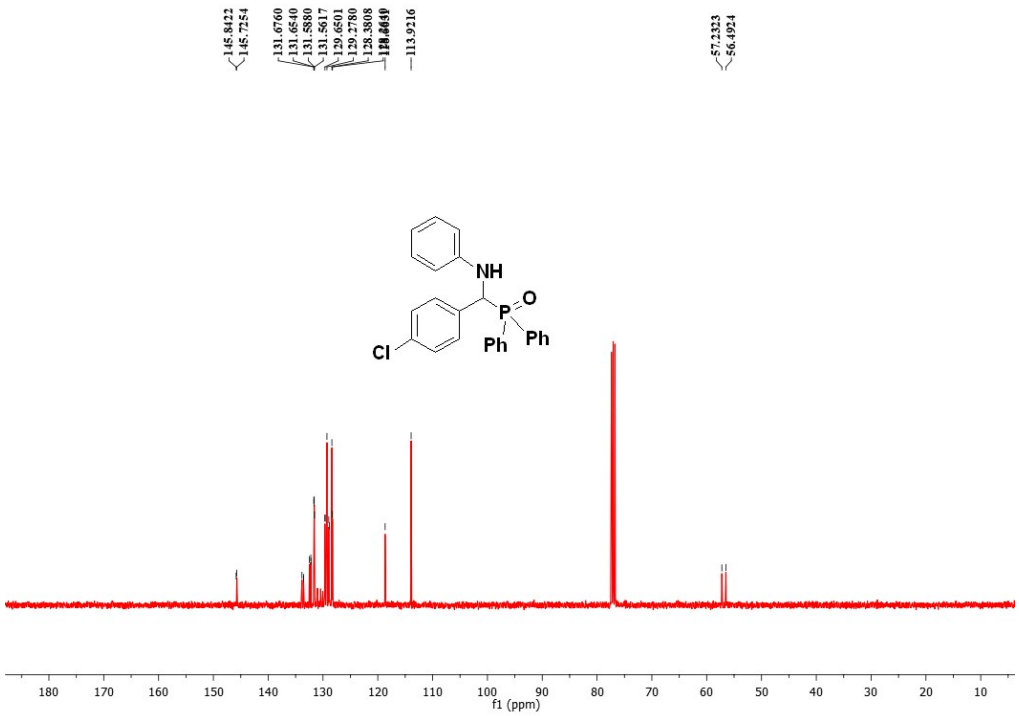


Fig FS15. $^{13}C\{^{1}H\}$ NMR for compound **4c** in $CDCl_3$.

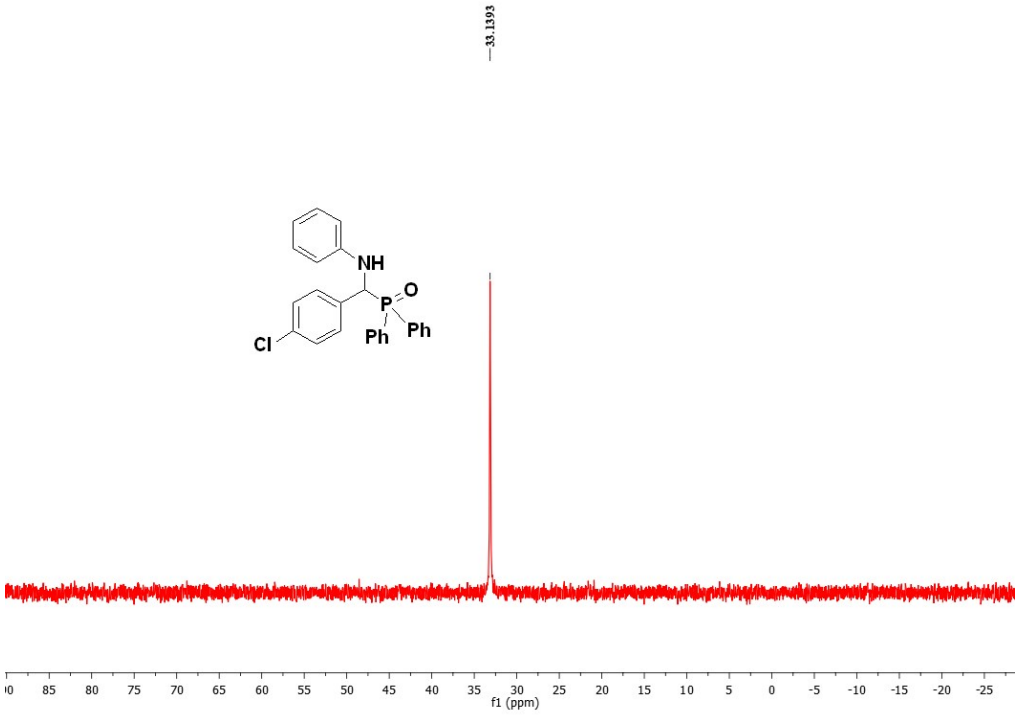


Fig FS16. $^{31}P\{^{1}H\}$ NMR for compound **4c** in $CDCl_3$.

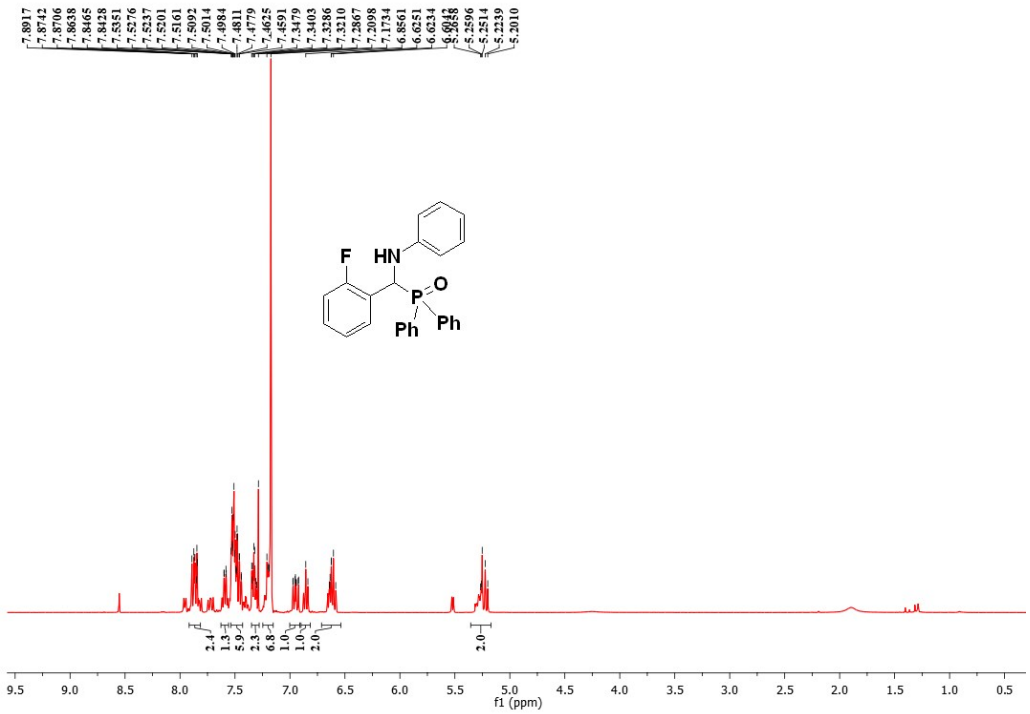


Fig FS17. ^{1}H NMR for compound **4d** in $CDCl_3$.

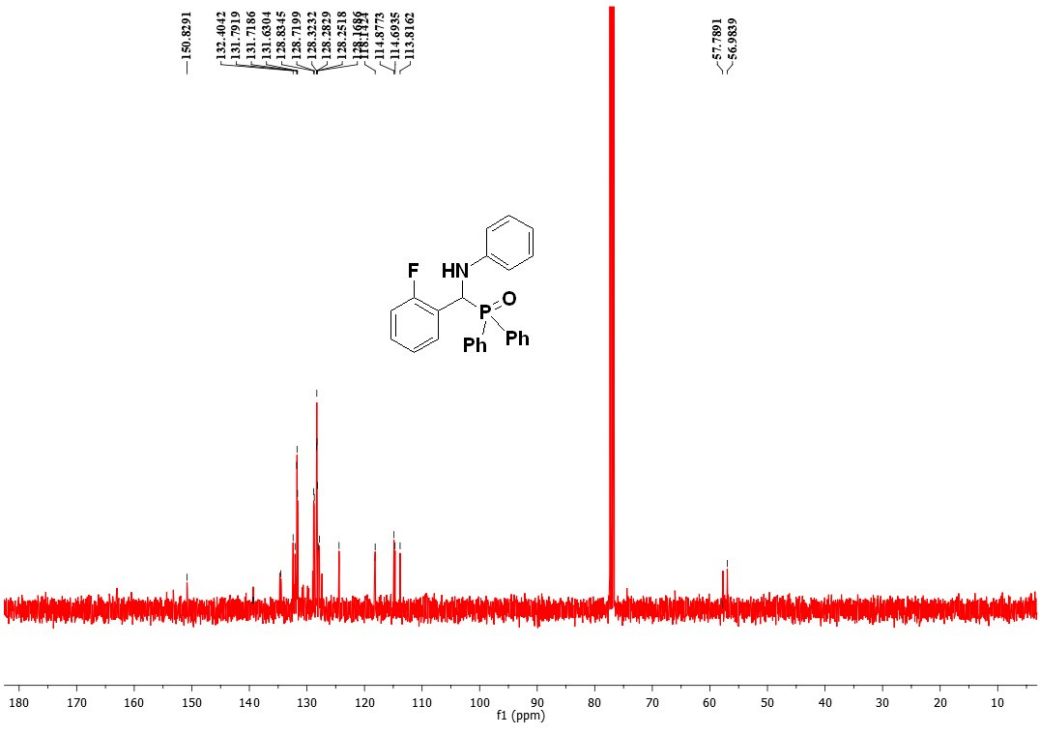


Fig FS18. $^{13}C\{^{1}H\}$ NMR for compound **4d** in $CDCl_3$.

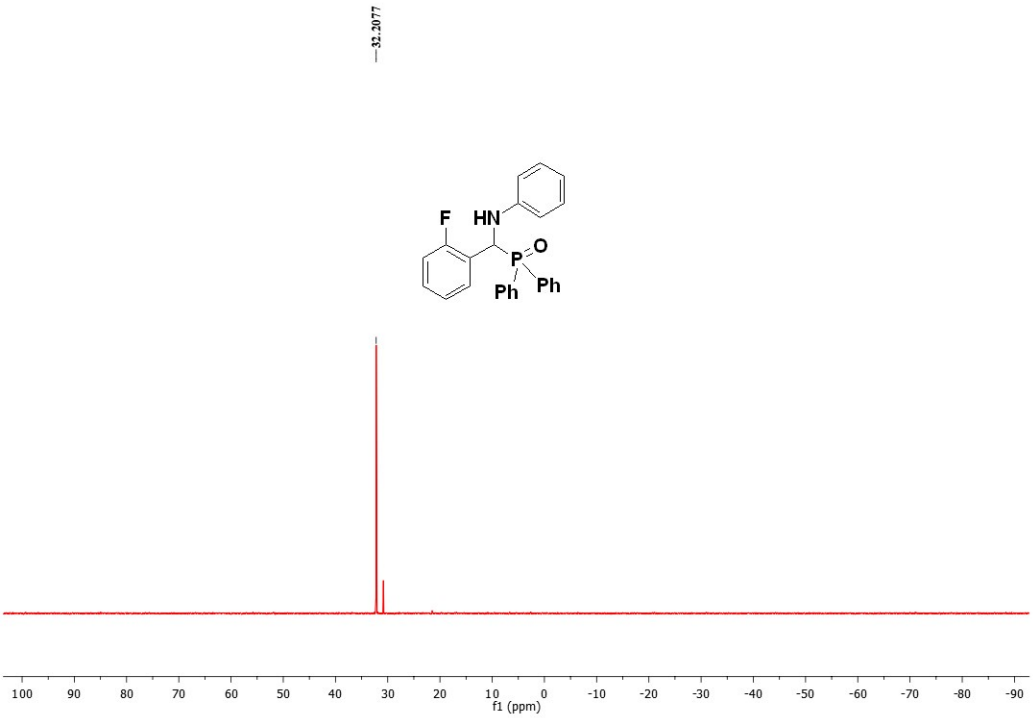


Fig FS19. $^{31}P\{^{1}H\}$ NMR for compound **4d** in $CDCl_3$.

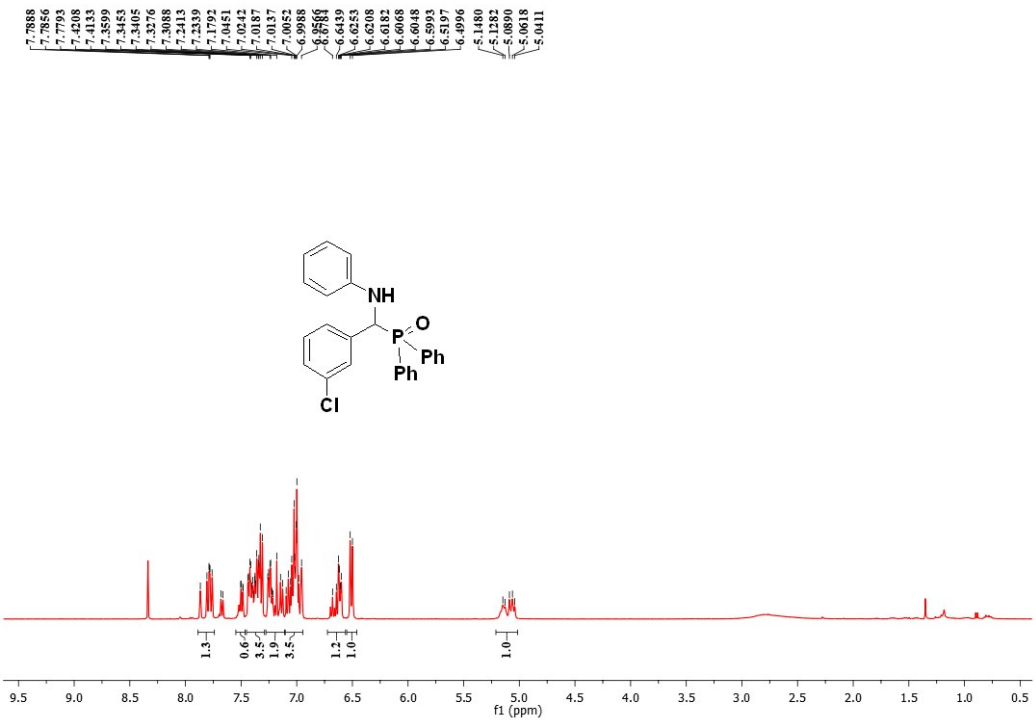


Fig FS20. ^{1}H NMR for compound **4e** in $CDCl_3$.

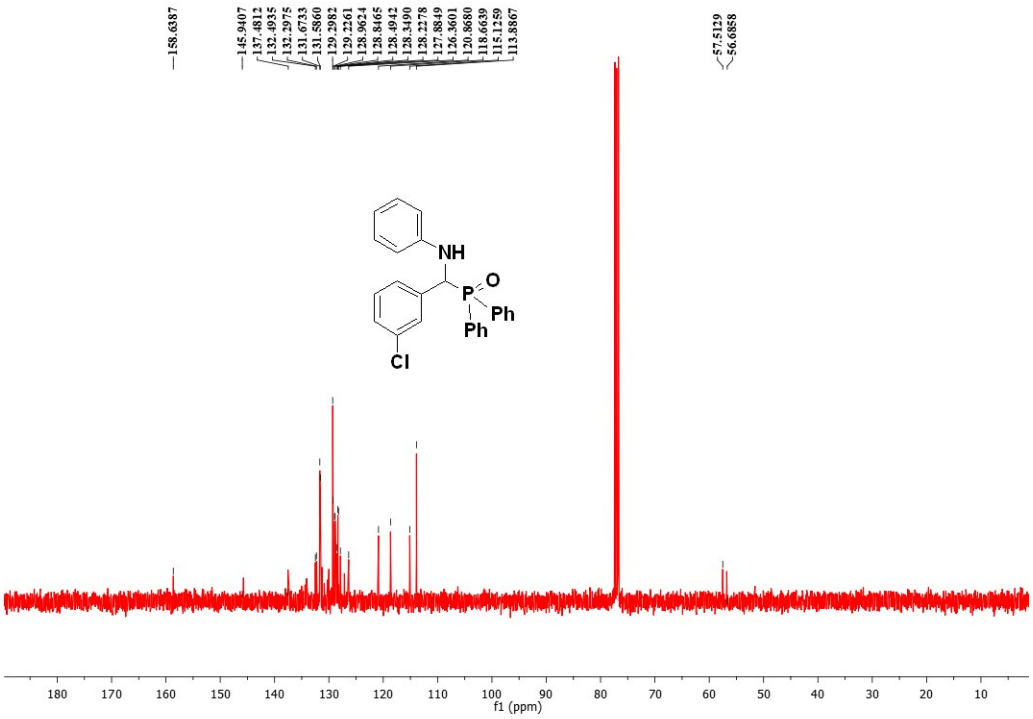


Fig FS21. $^{13}C\{^{1}H\}$ NMR for compound **4e** in $CDCl_3$.

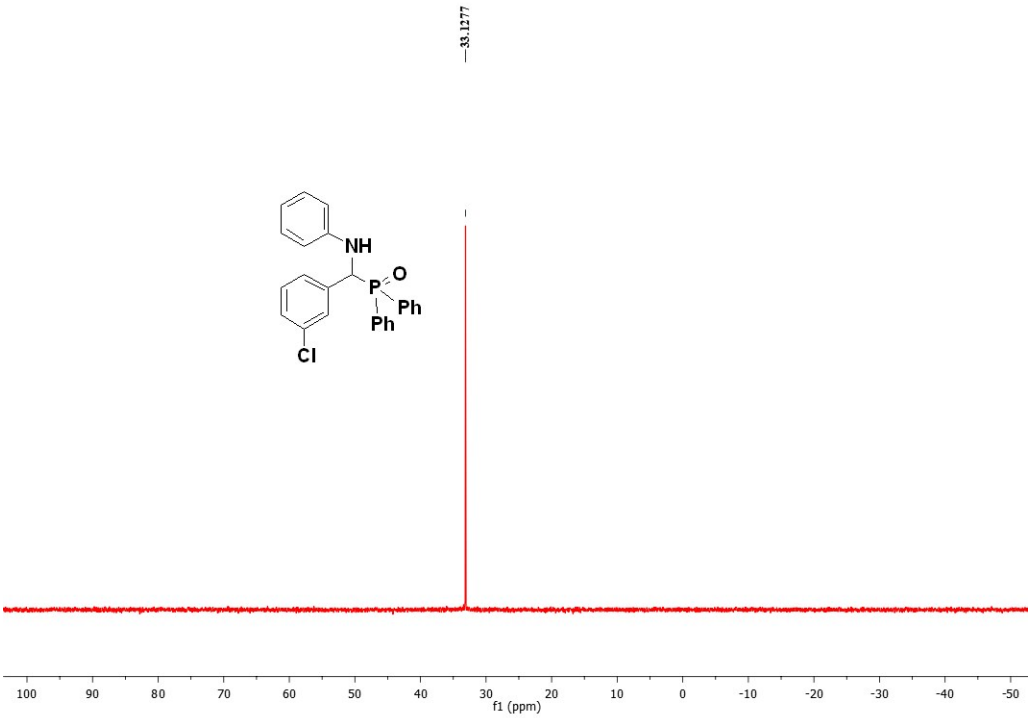


Fig FS22. $^{31}P\{^{1}H\}$ NMR for compound **4e** in $CDCl_3$.

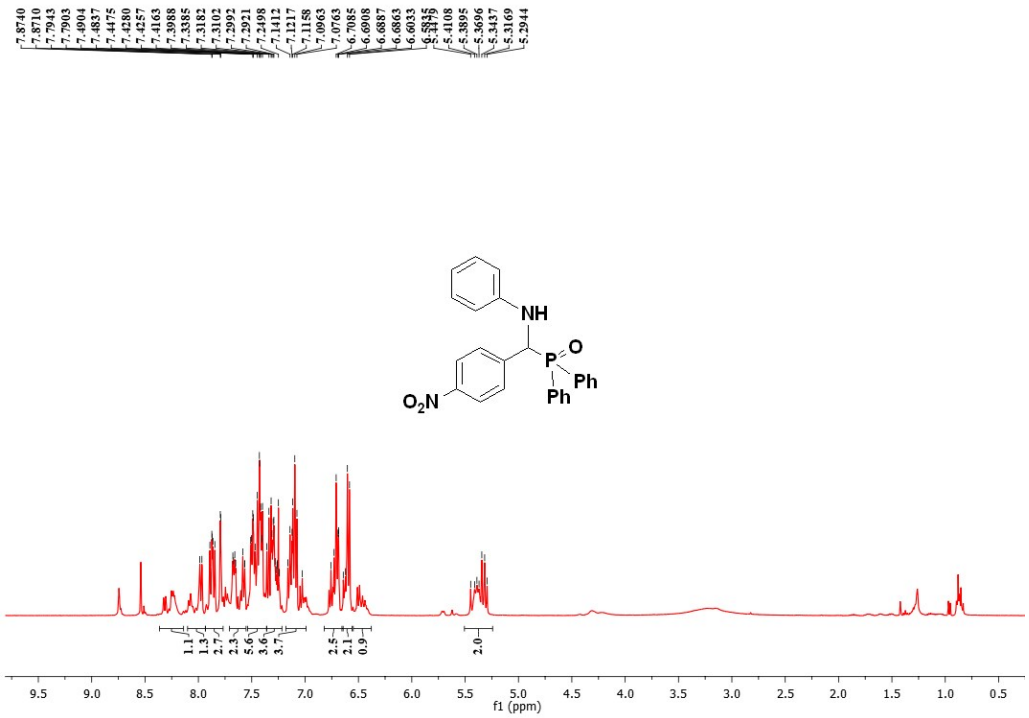


Fig FS23. ^{1}H NMR for compound **4f** in $CDCl_3$.

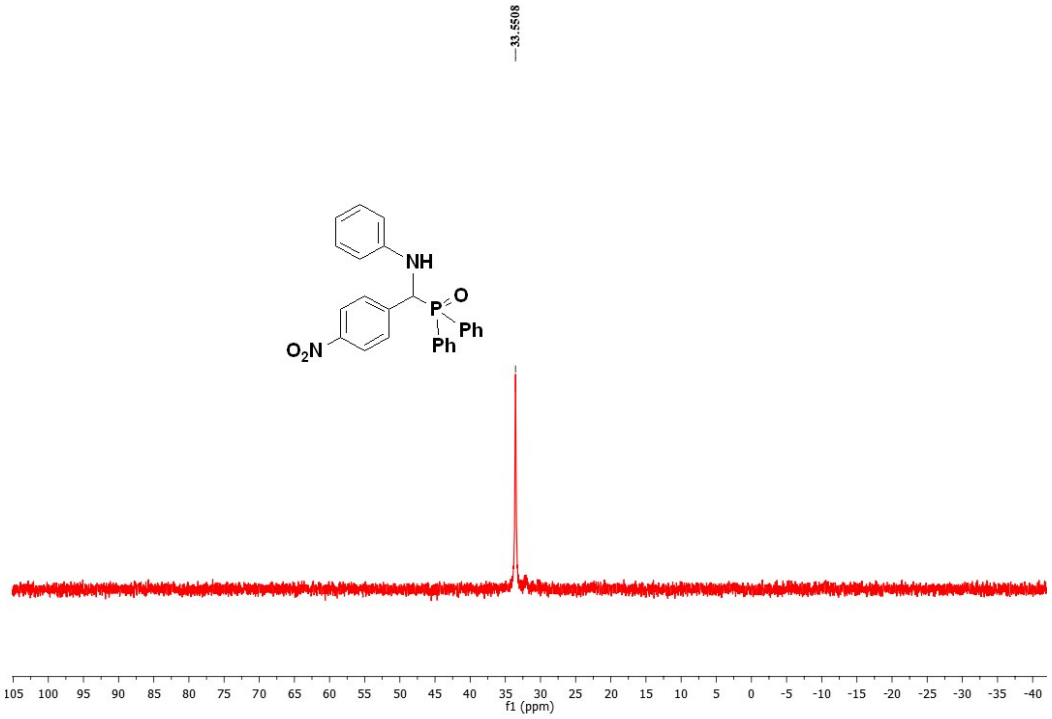


Fig FS24: $^{31}P\{^{1}H\}$ NMR for compound **4f** in $CDCl_3$.

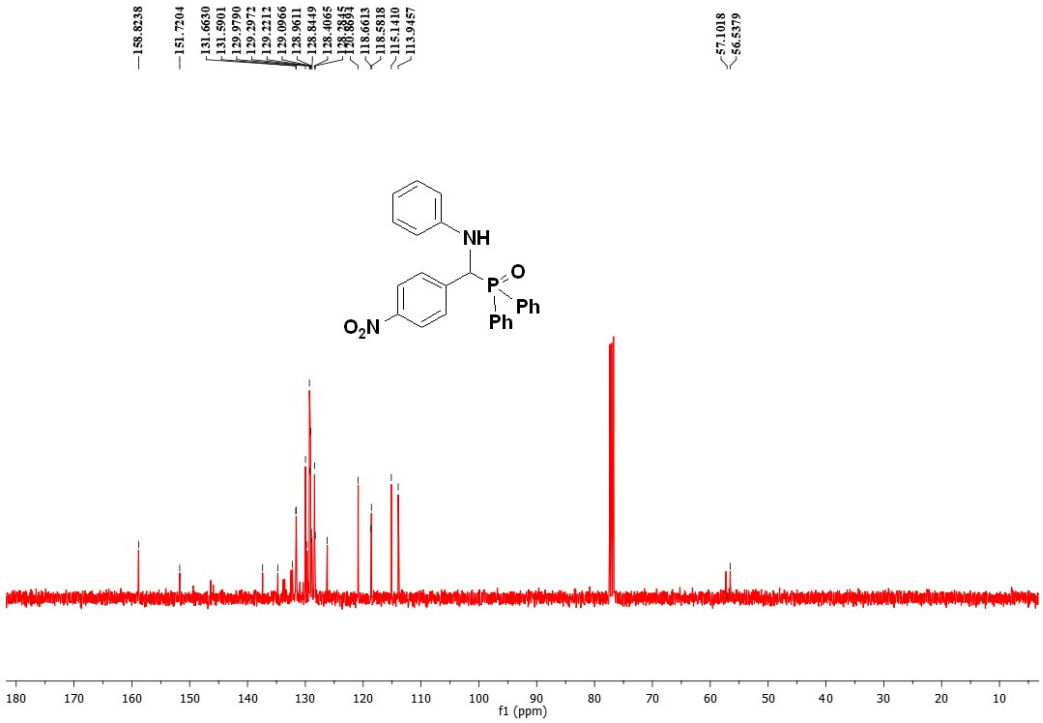


Fig FS25. $^{13}C\{^{1}H\}$ NMR for compound **4f** in $CDCl_3$.

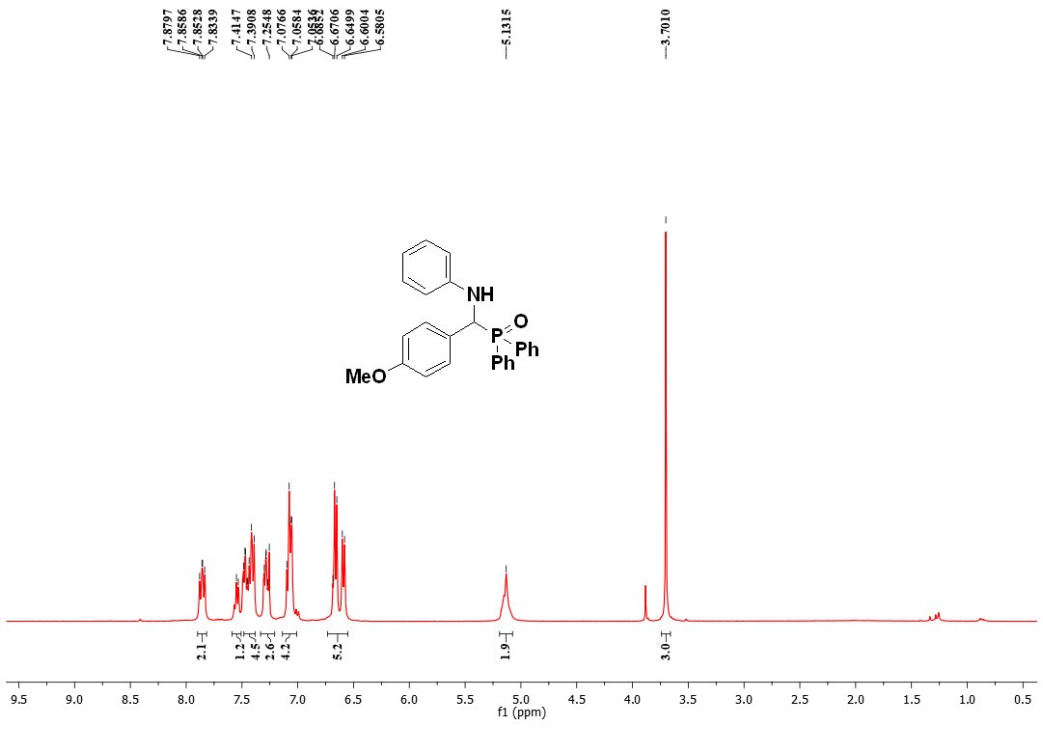


Fig FS26. ^{1}H NMR for compound **4g** in $CDCl_3$.

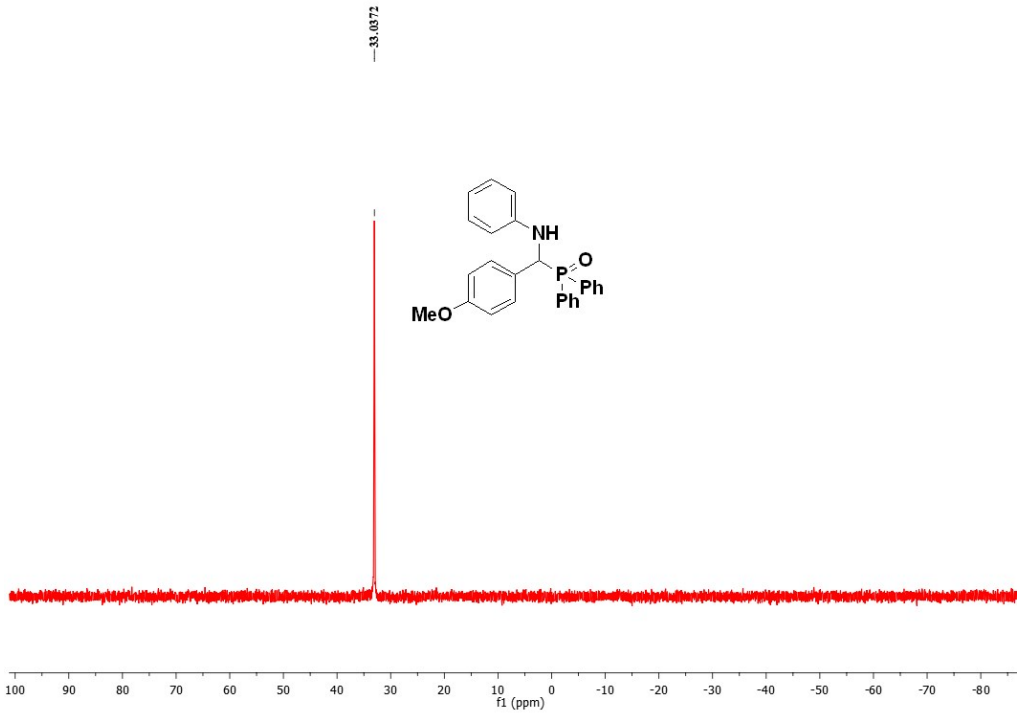


Fig FS27. $^{31}P\{^{1}H\}$ NMR for compound **4g** in $CDCl_3$.

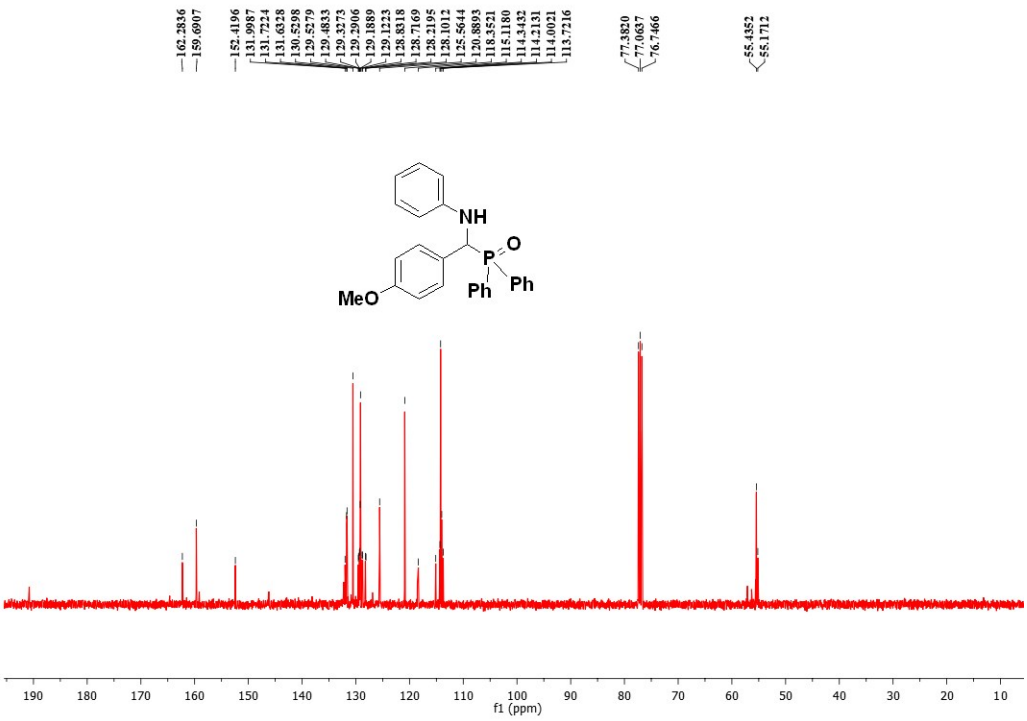


Fig FS28. $^{13}C\{^{1}H\}$ NMR for compound **4g** in $CDCl_3$.

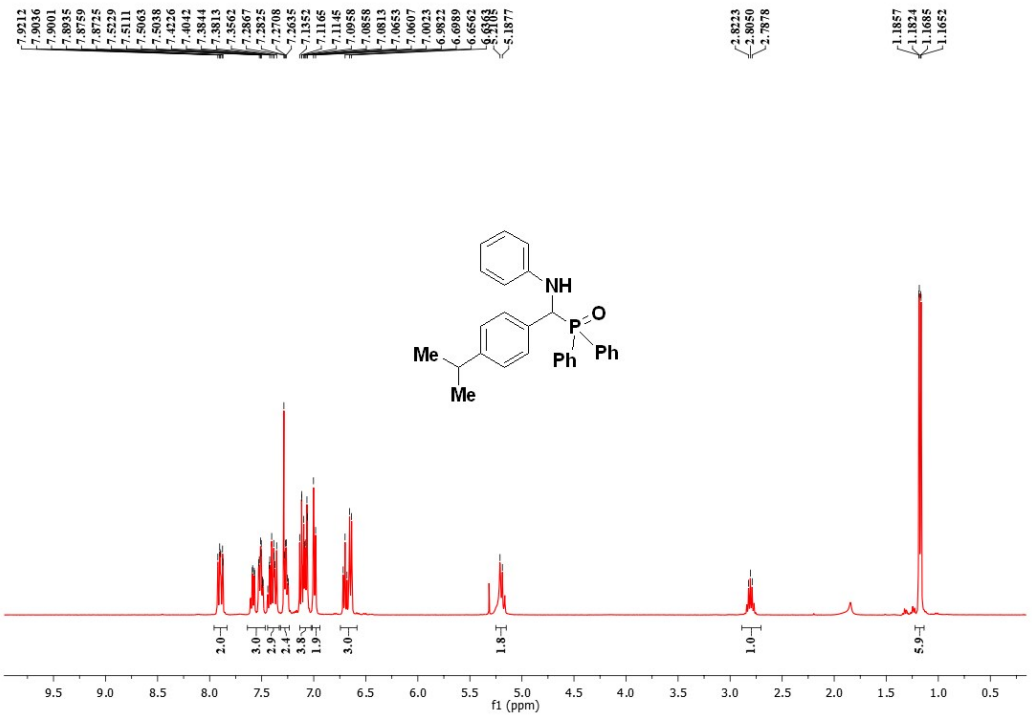


Fig FS29. ^{1}H NMR for compound **4h** in $CDCl_3$.

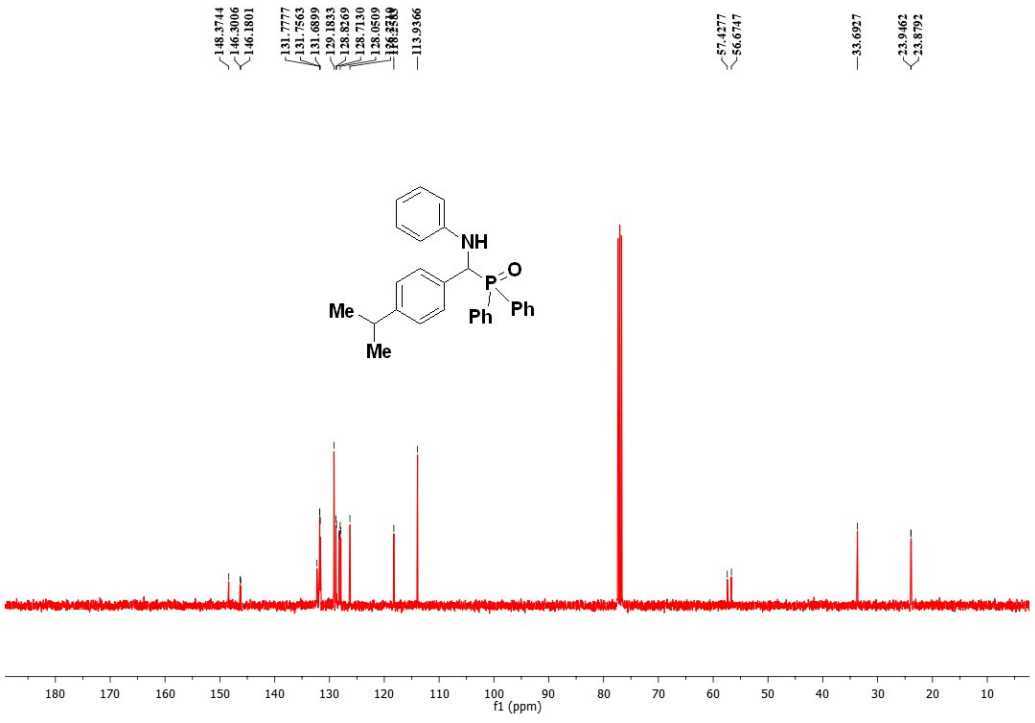


Fig FS30. $^{13}C\{^{1}H\}$ NMR for compound **4h** in $CDCl_3$.

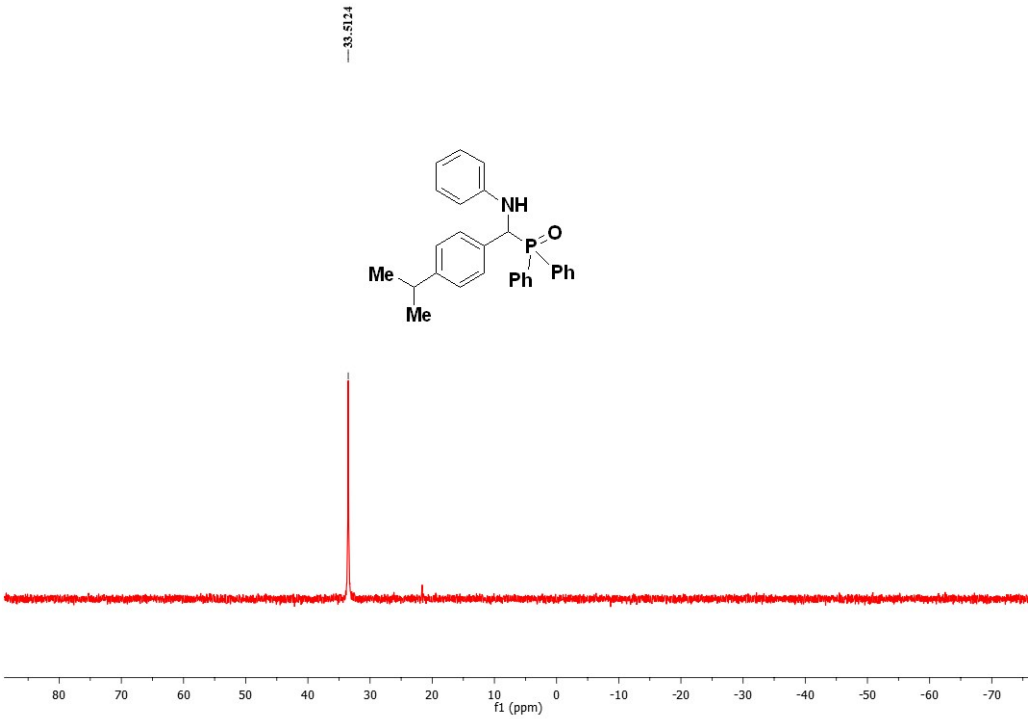


Fig FS31. $^{31}P\{^{1}H\}$ NMR for compound **4h** in $CDCl_3$.

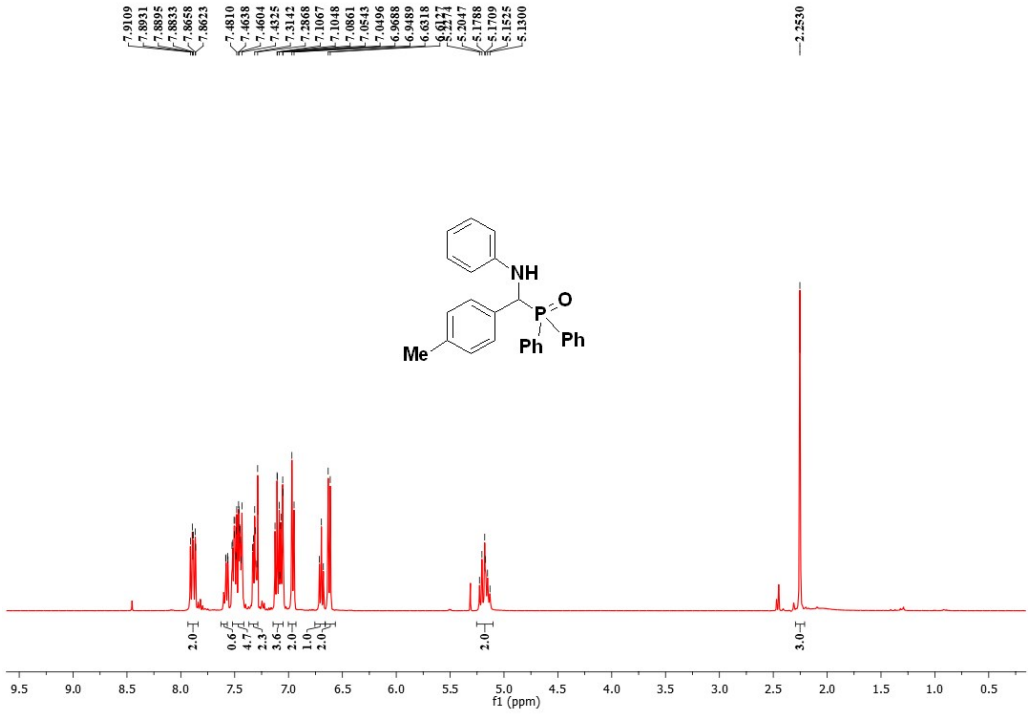


Fig FS32. ^{1}H NMR for compound **4i** in $CDCl_3$.

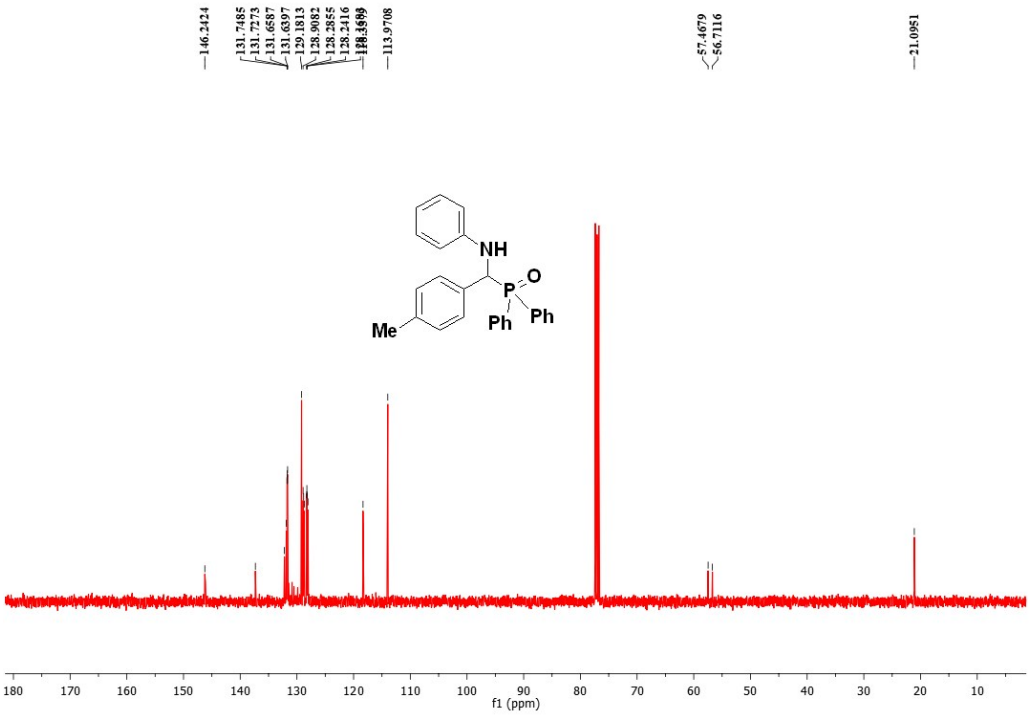


Fig FS33. $^{13}C\{^{1}H\}$ NMR for compound **4i** in $CDCl_3$.

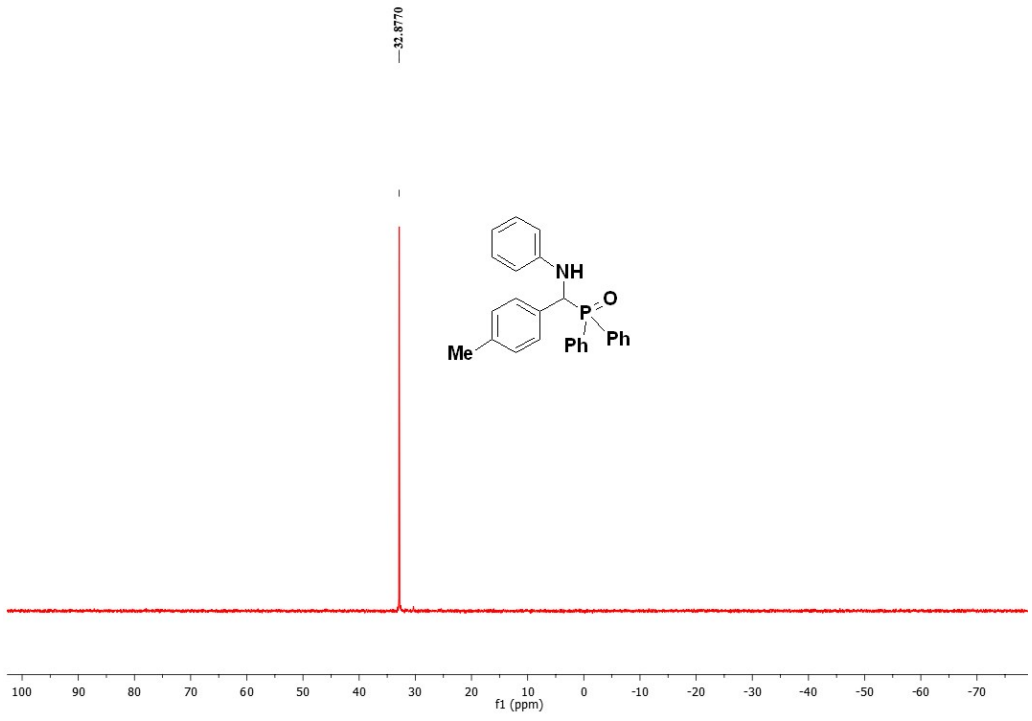


Fig FS34. $^{31}P\{^{1}H\}$ NMR for compound **4i** in $CDCl_3$.

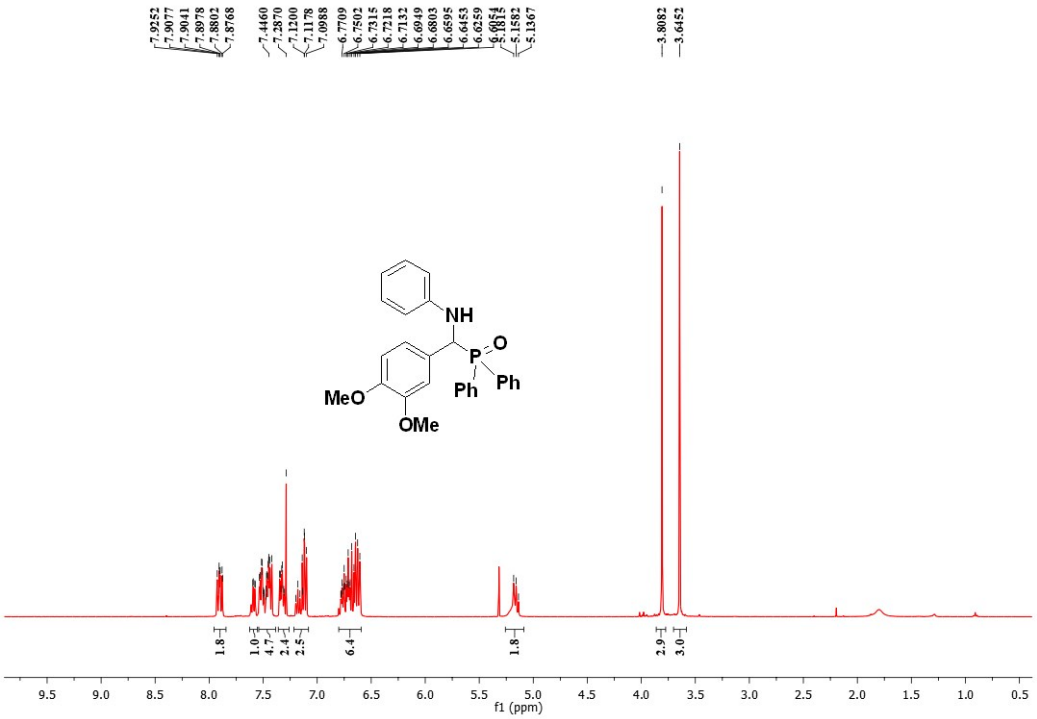


Fig FS35. ^{1}H NMR for compound **4j** in $CDCl_3$.

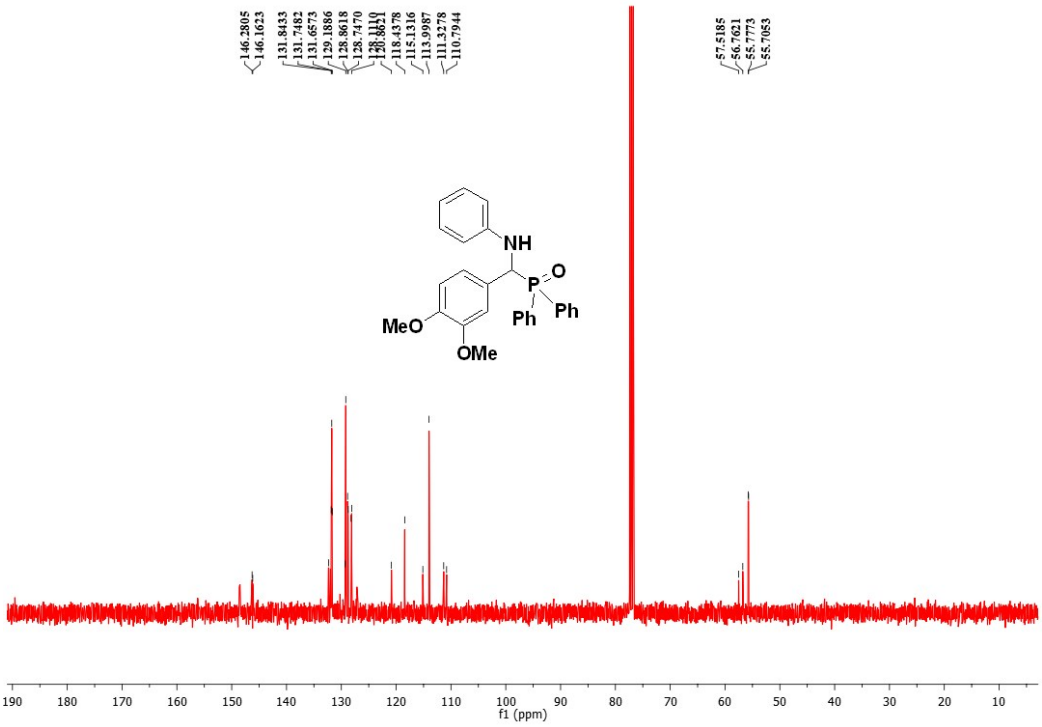


Fig FS36. $^{13}C\{^{1}H\}$ NMR for compound **4j** in $CDCl_3$.

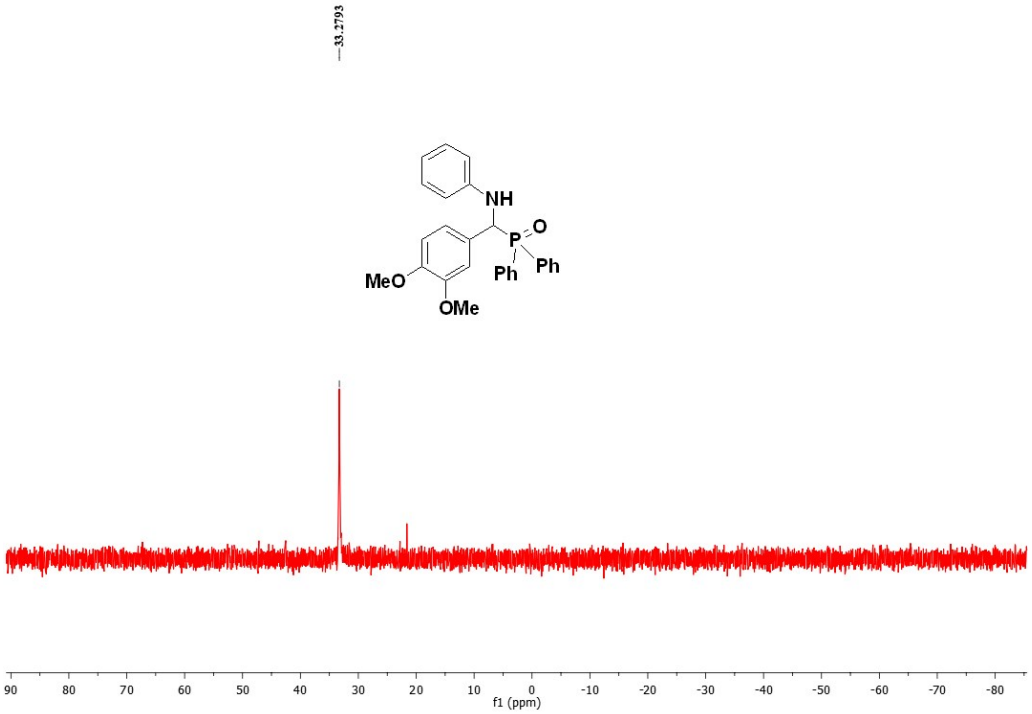


Fig FS37. $^{31}P\{^{1}H\}$ NMR for compound **4j** in $CDCl_3$.

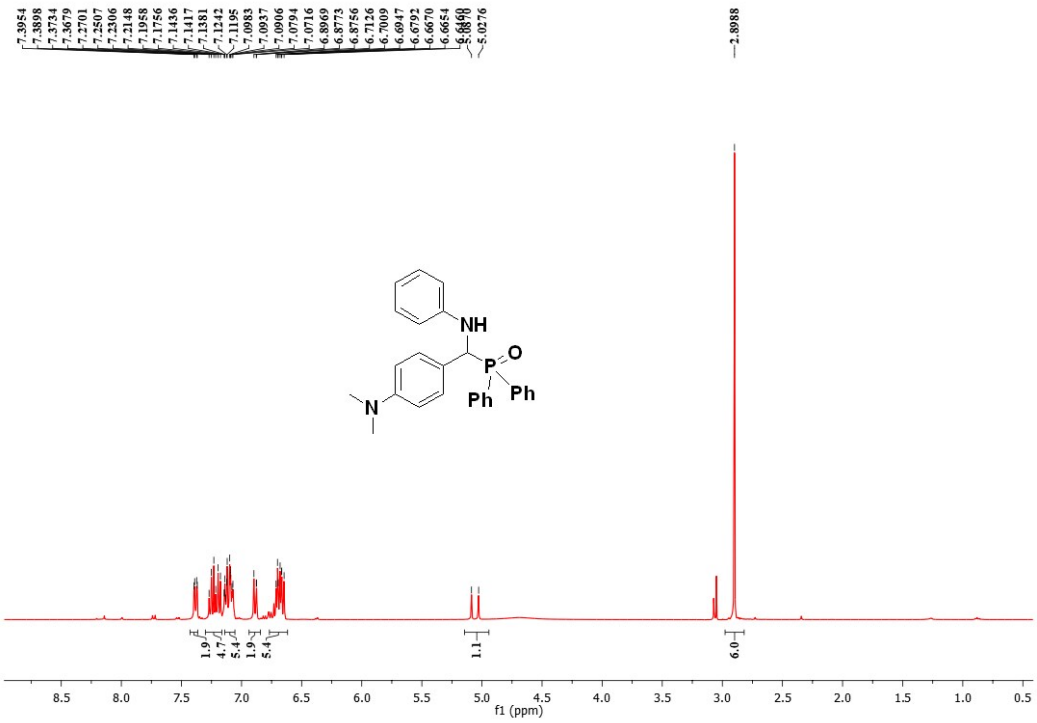


Fig FS38. ^{1}H NMR for compound **4k** in $CDCl_3$.

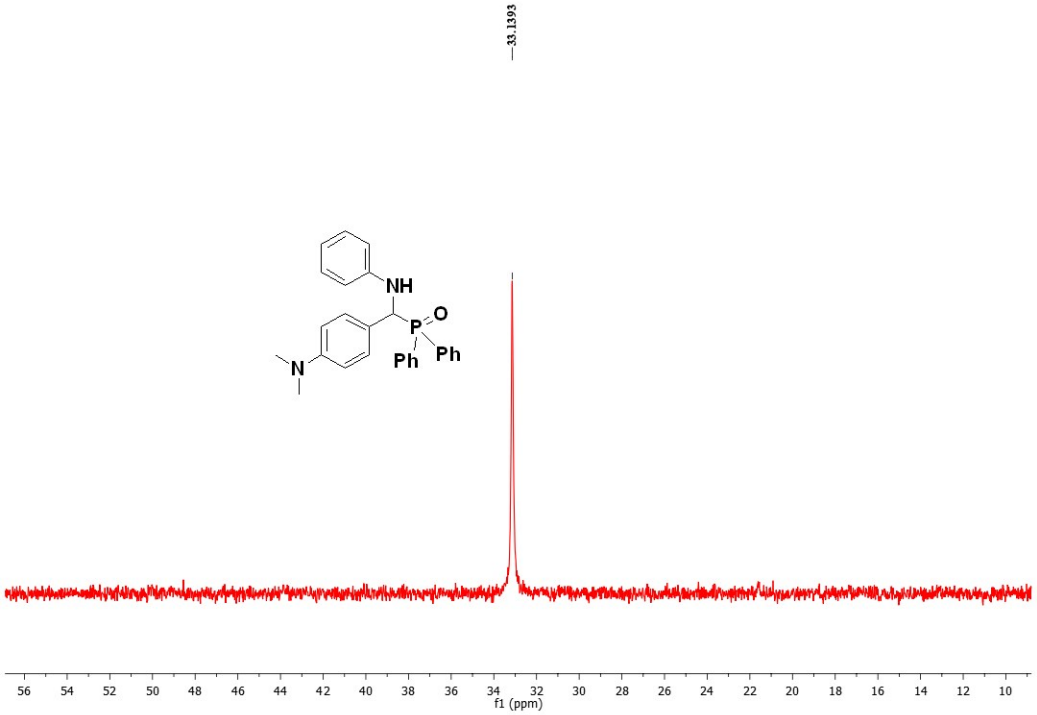


Fig FS39. $^{31}P\{^{1}H\}$ NMR for compound **4k** in $CDCl_3$.

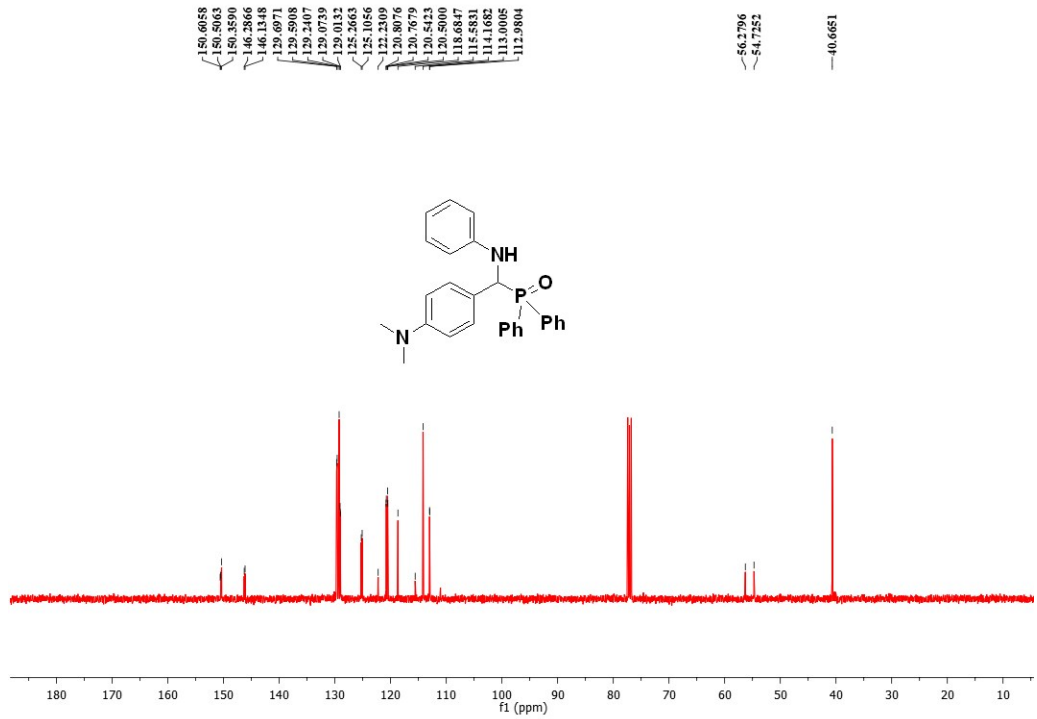


Fig FS40. $^{13}C\{^{1}H\}$ NMR for compound **4k** in $CDCl_3$.

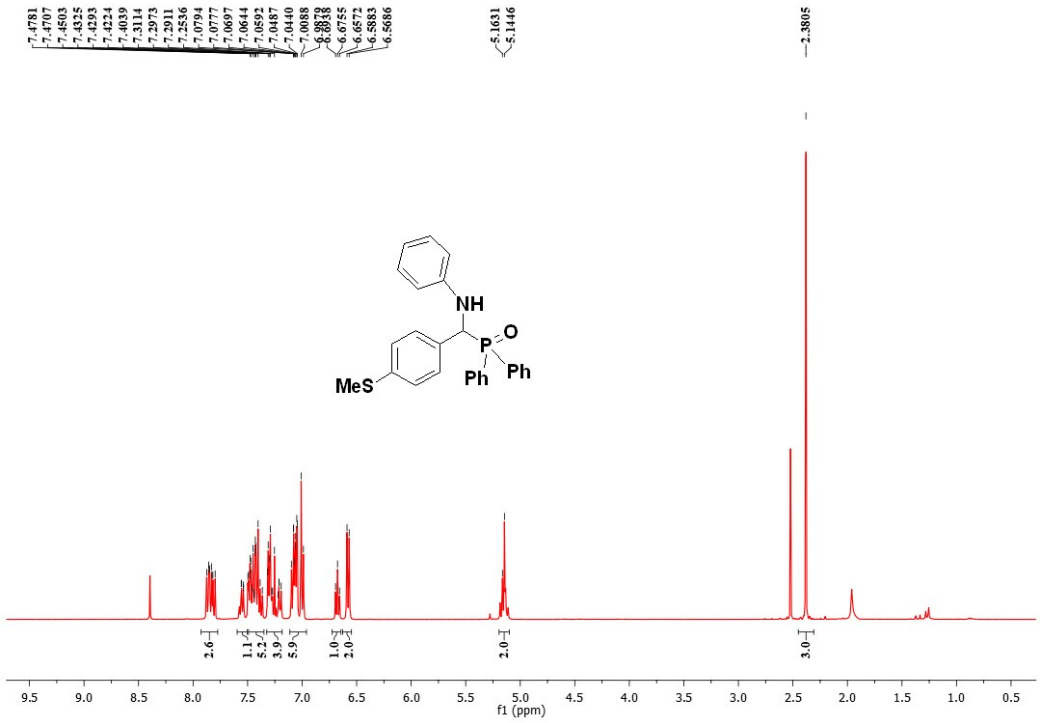


Fig FS41. ^{1}H NMR for compound **4l** in $CDCl_3$.

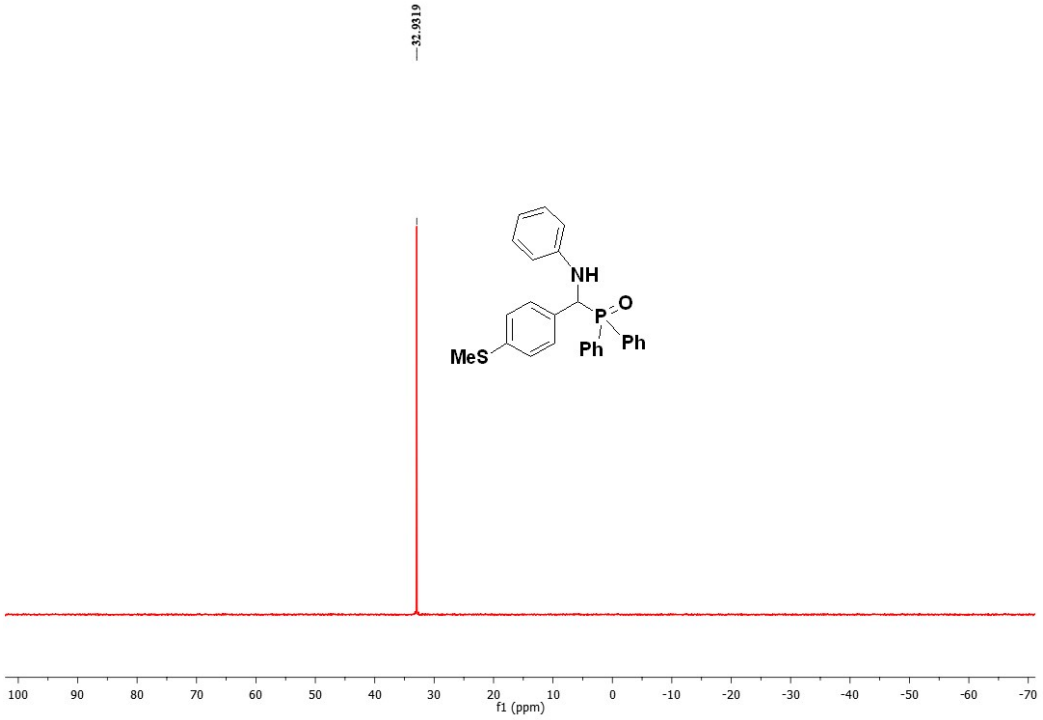


Fig FS42. $^{31}P\{^{1}H\}$ NMR for compound **4l** in $CDCl_3$.

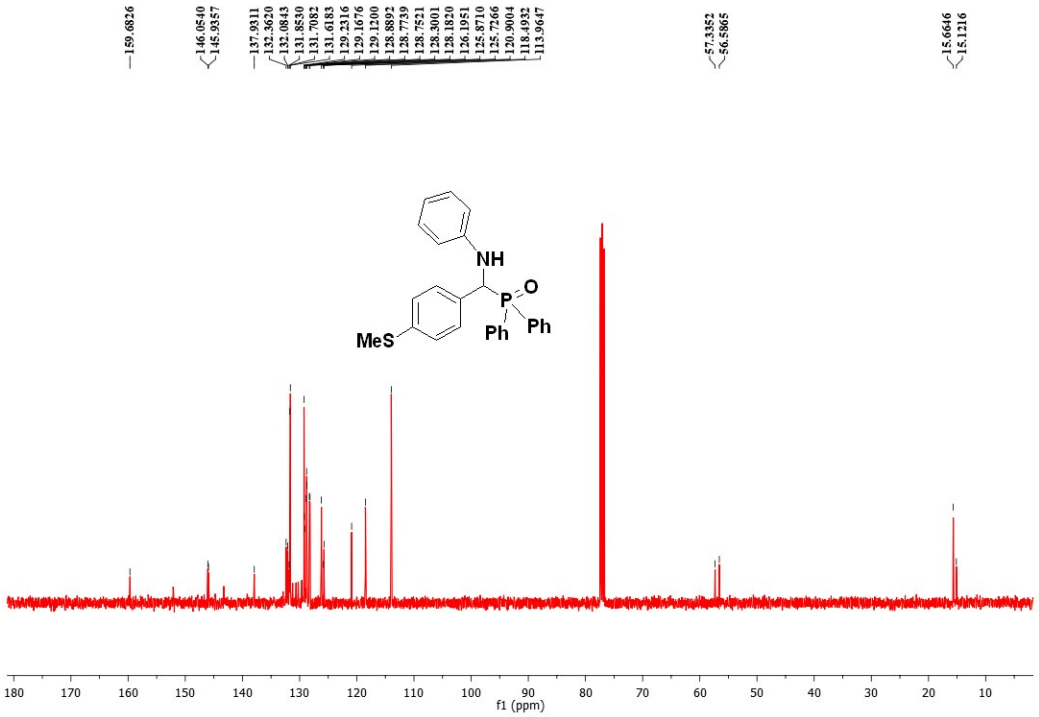


Fig FS43: $^{13}C\{^{1}H\}$ NMR for compound **4l** in $CDCl_3$.

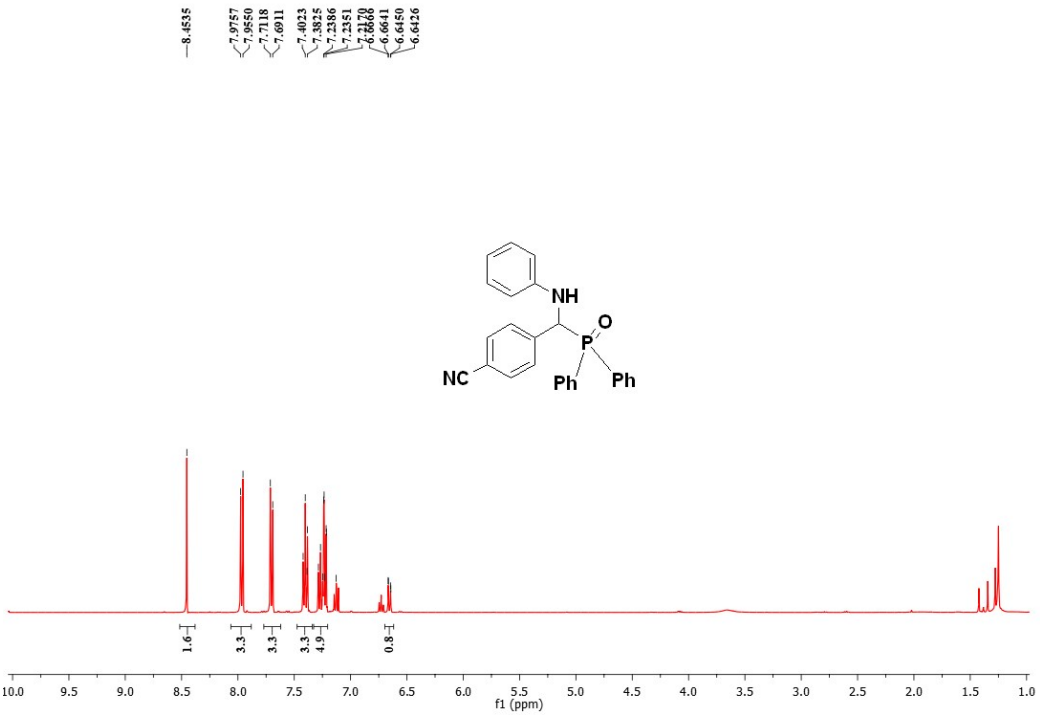


Fig FS44. ^{1}H NMR for compound **4m** in $CDCl_3$.

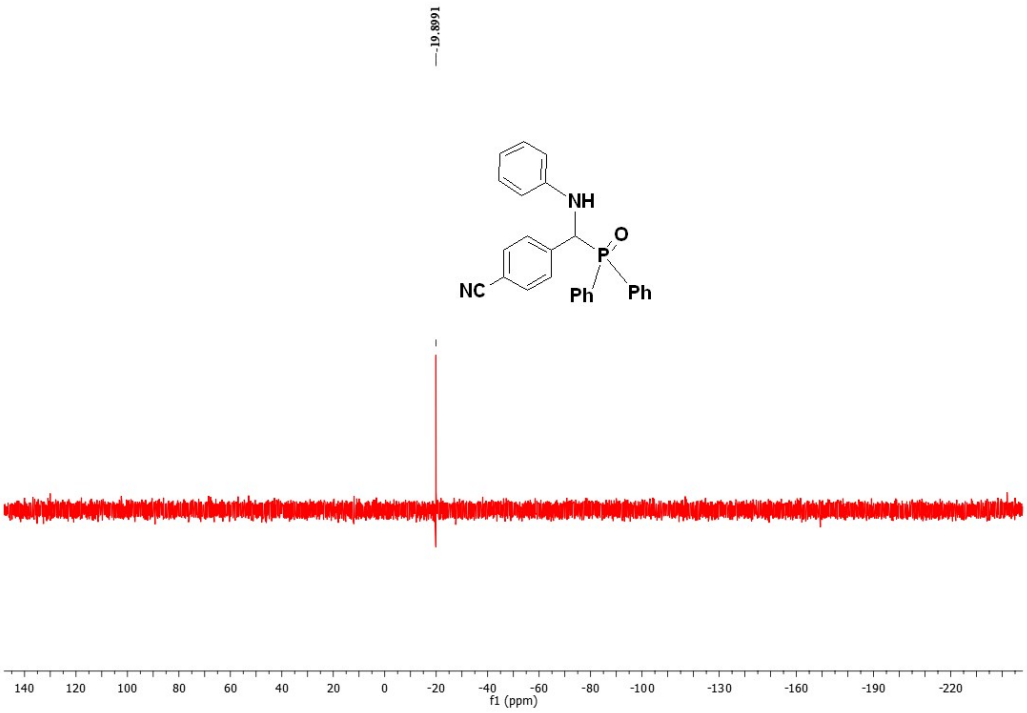


Fig FS45. $^{31}P\{^{1}H\}$ NMR for compound **4m** in $CDCl_3$.

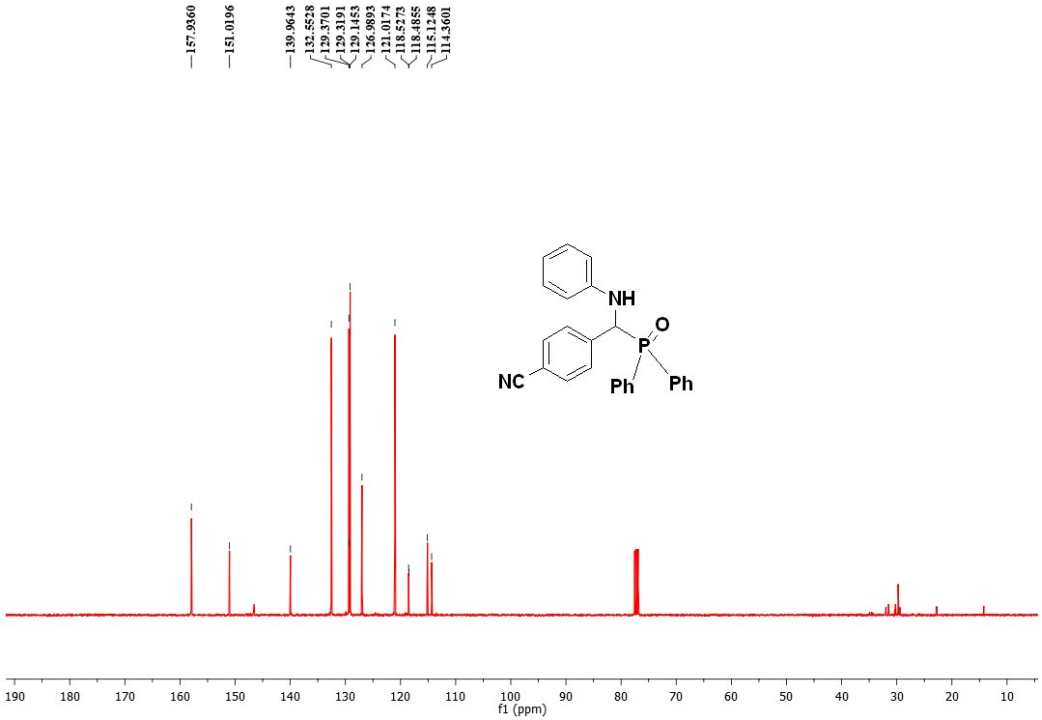


Fig FS46: $^{13}C\{^{1}H\}$ NMR for compound **4m** in $CDCl_3$.

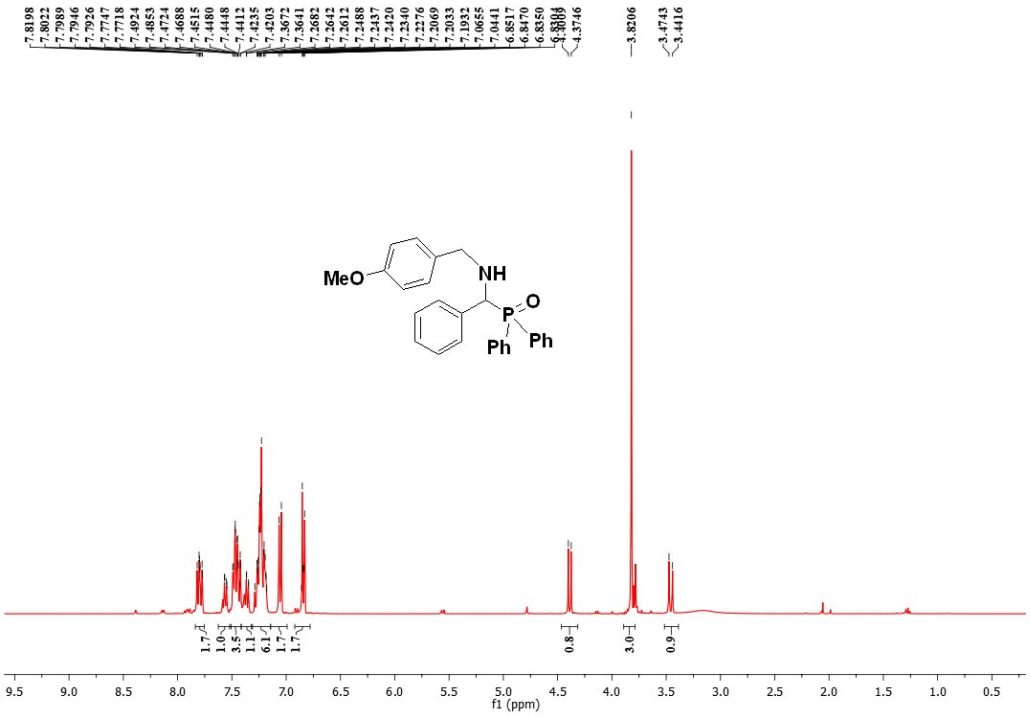


Fig FS47. ^{1}H NMR for compound **4n** in $CDCl_3$.

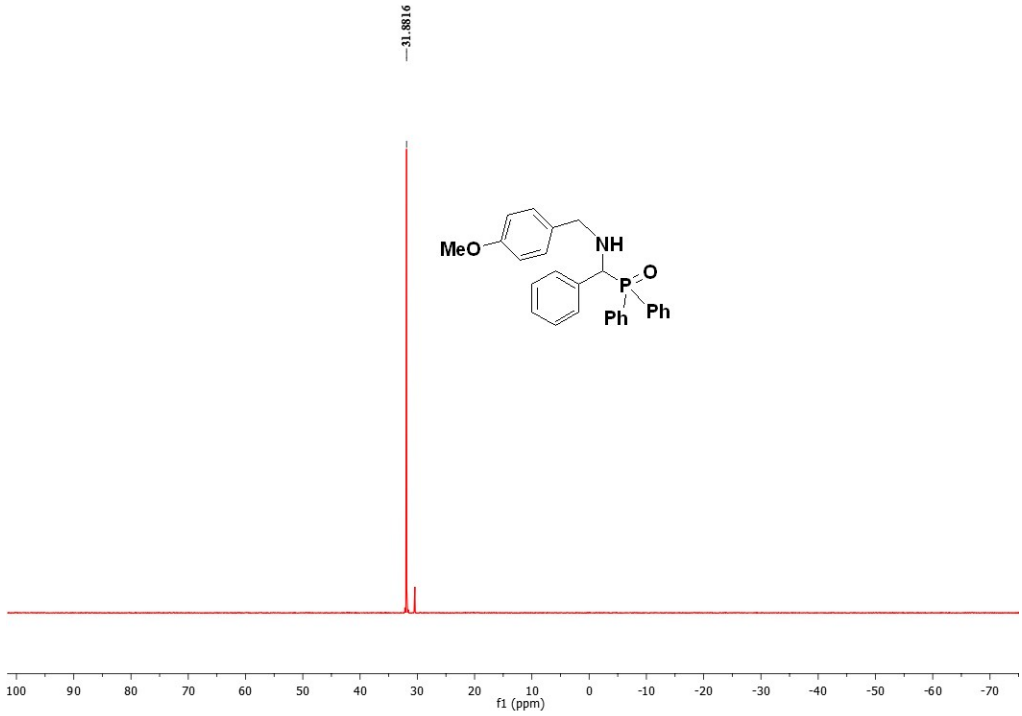


Fig FS48. $^{31}P\{^{1}H\}$ NMR for compound **4n** in $CDCl_3$.

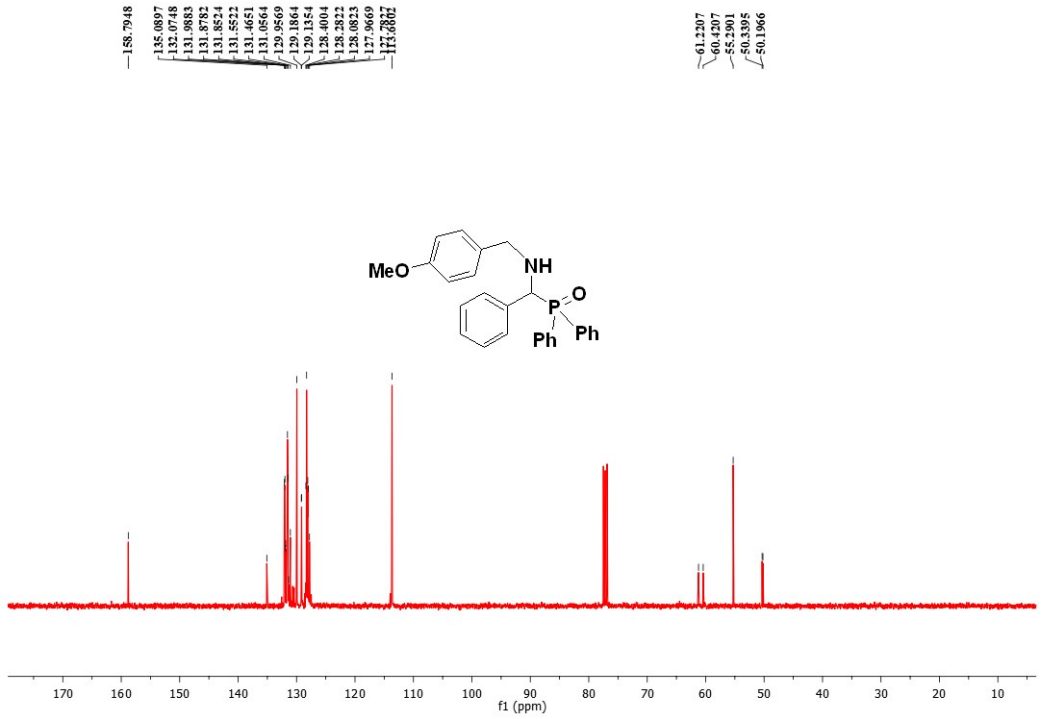


Fig FS49. $^{13}C\{^{1}H\}$ NMR for compound **4n** in $CDCl_3$.

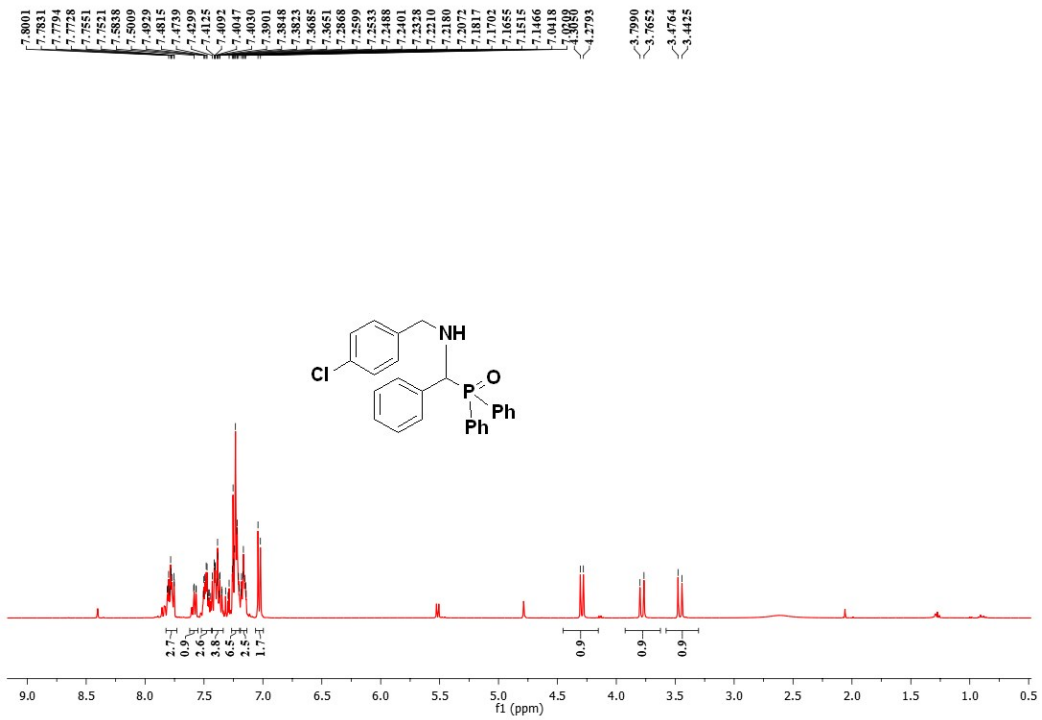


Fig FS50. ^{1}H NMR for compound **4o** in $CDCl_3$.

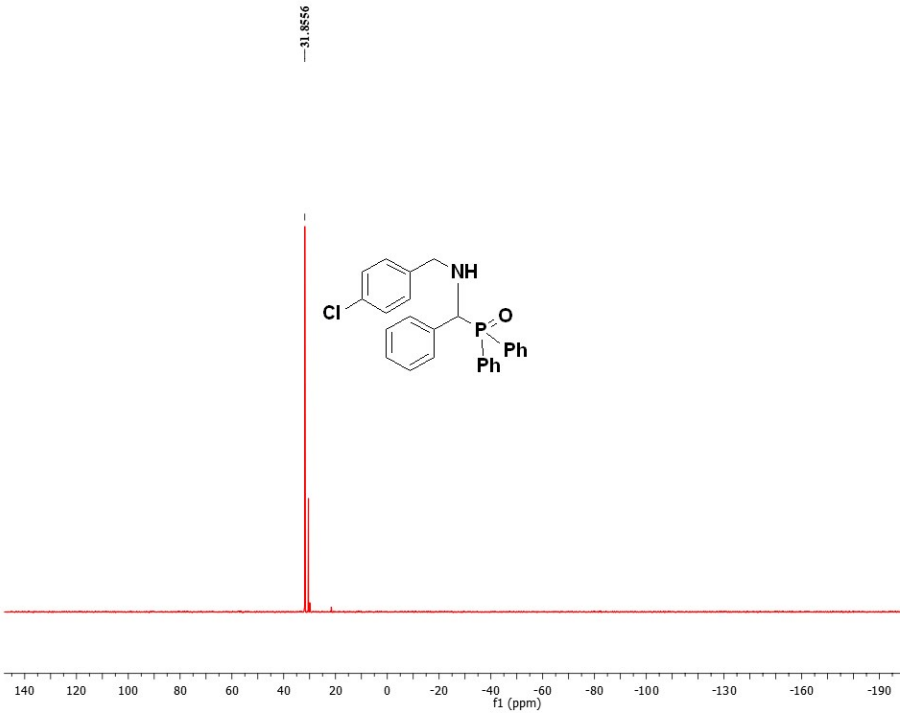


Fig FS51. $^{31}P\{^{1}H\}$ NMR for compound **4o** in $CDCl_3$.

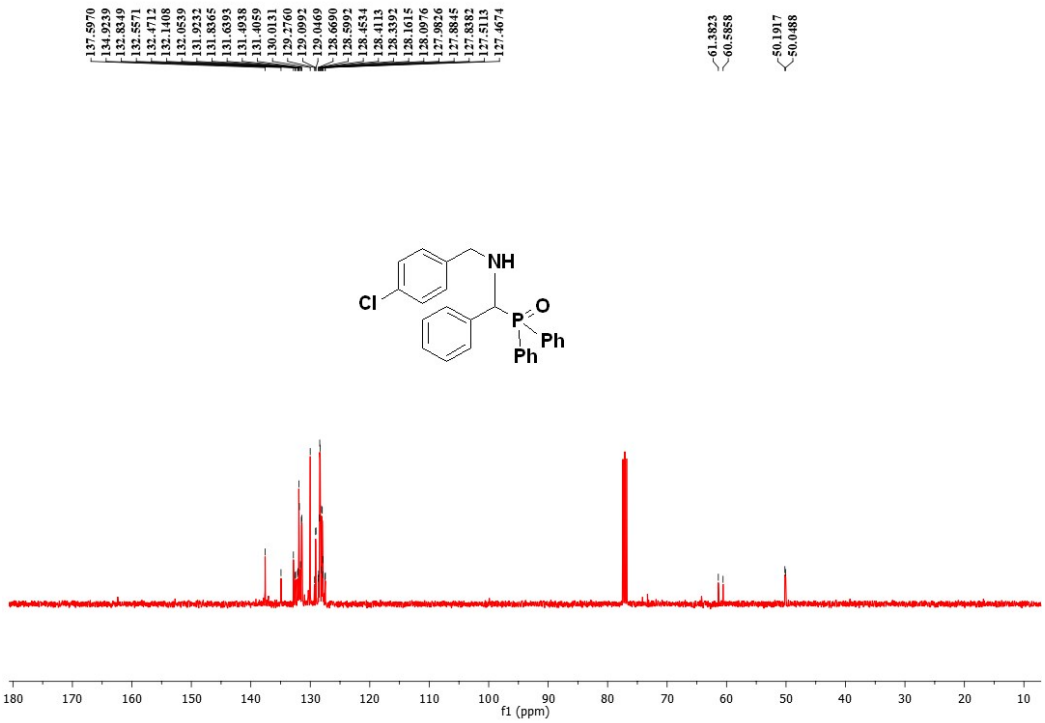


Fig FS52. $^{13}C\{^{1}H\}$ NMR for compound **4o** in $CDCl_3$.

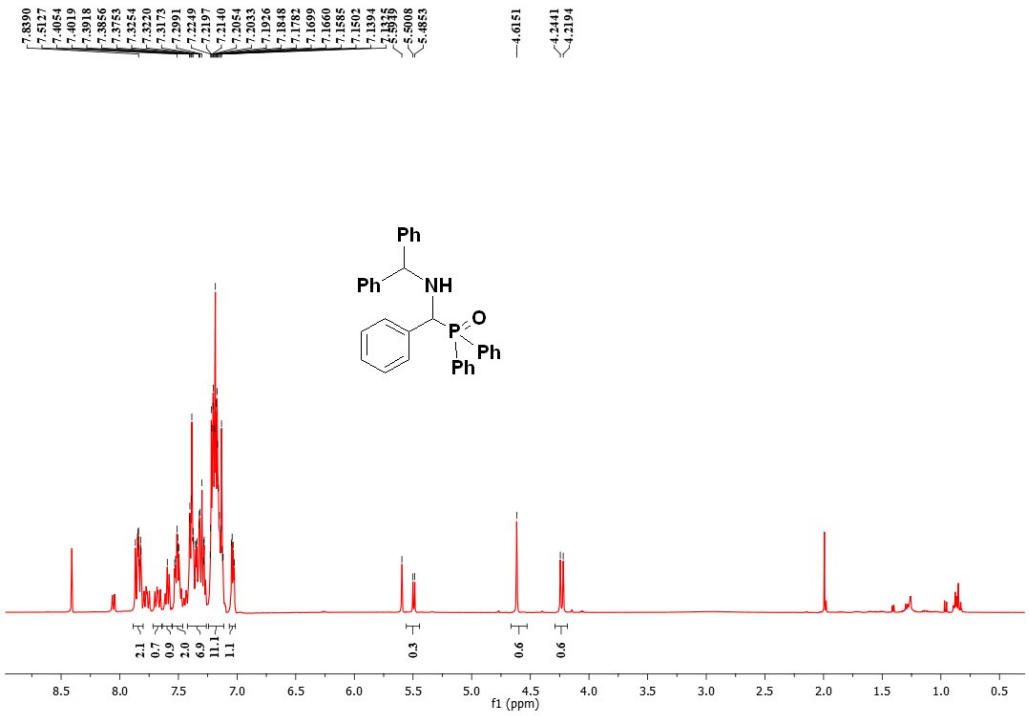


Fig FS53. ^{1}H NMR for compound **4p** in $CDCl_3$.

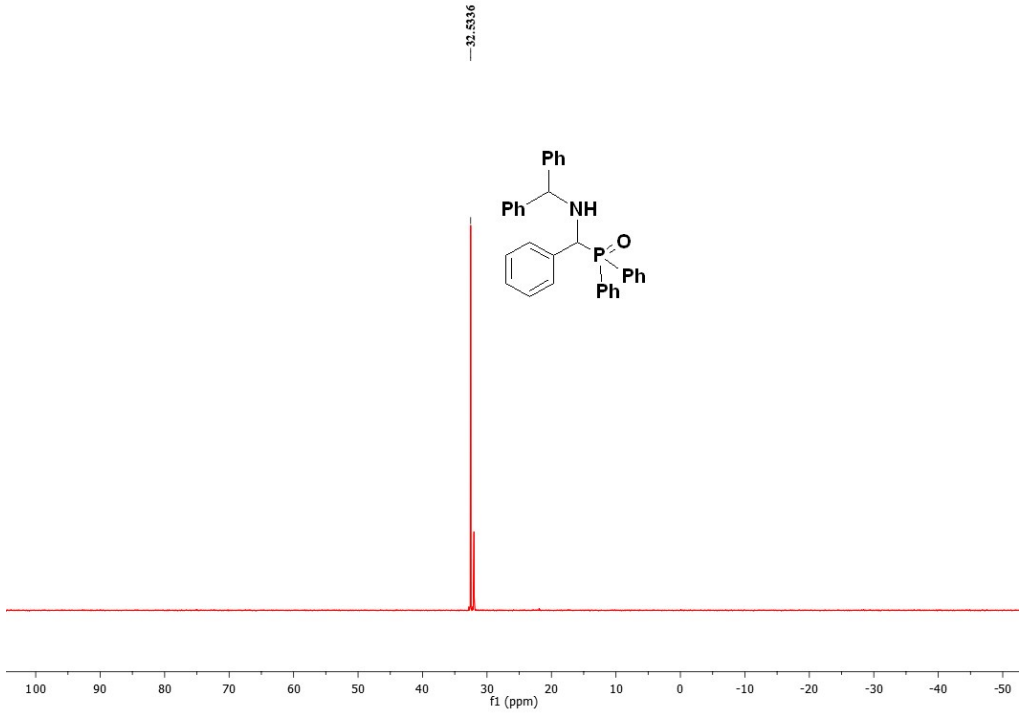


Fig FS54. $^{31}P\{^{1}H\}$ NMR for compound **4p** in $CDCl_3$.

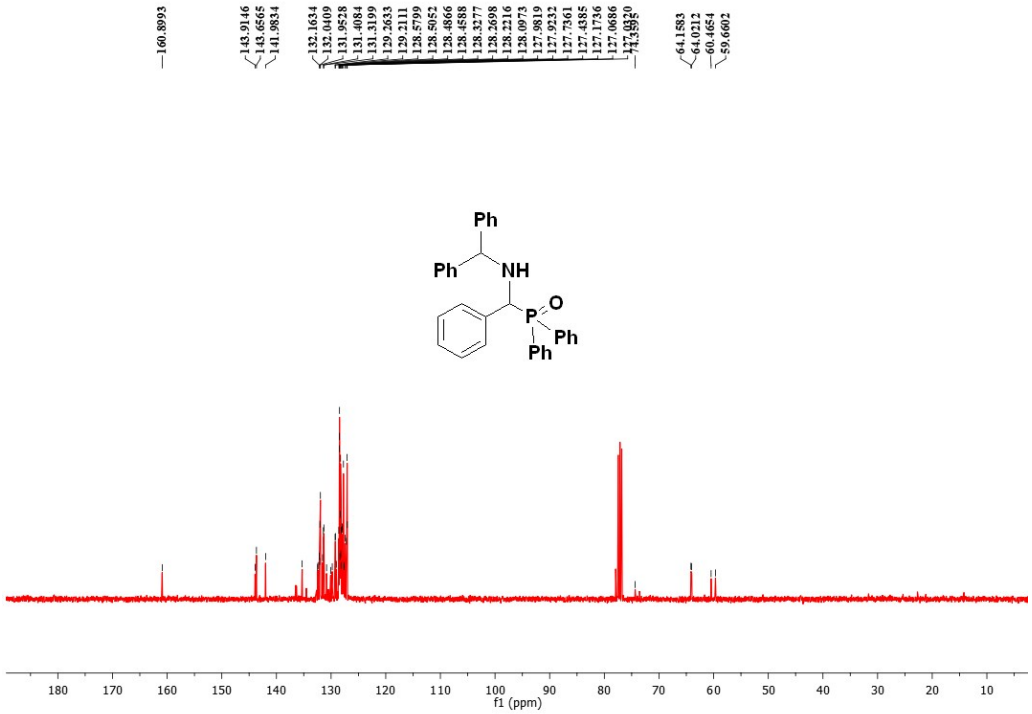


Fig FS55. $^{13}C\{^{1}H\}$ NMR for compound **4p** in $CDCl_3$.

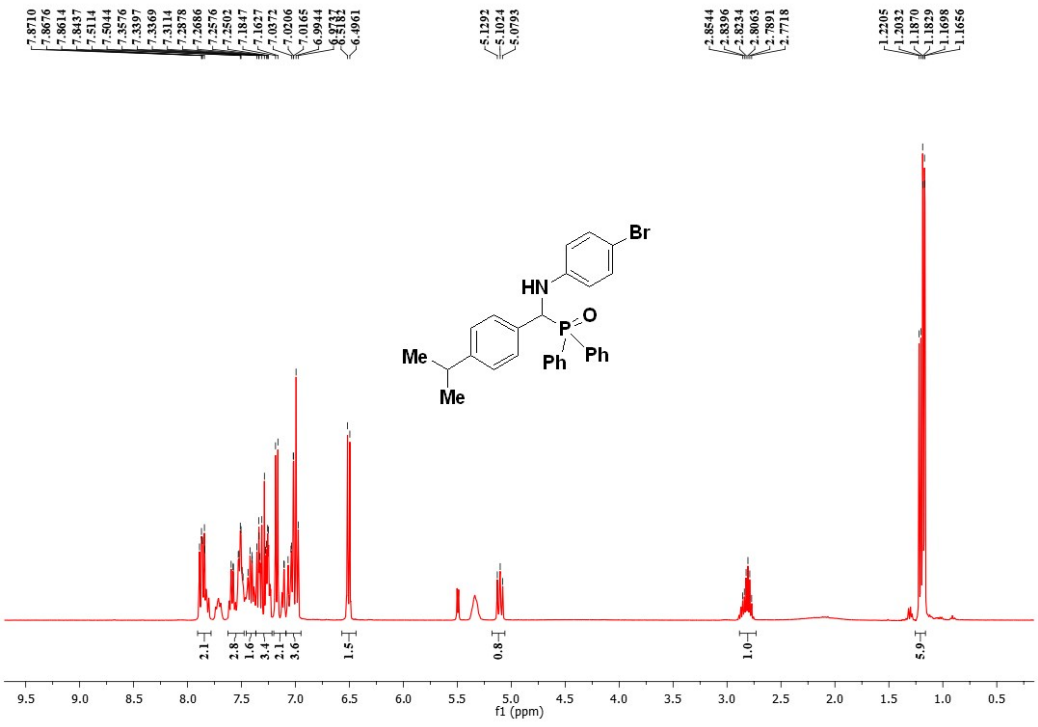


Fig FS56. ^{1}H NMR for compound **4q** in $CDCl_3$.

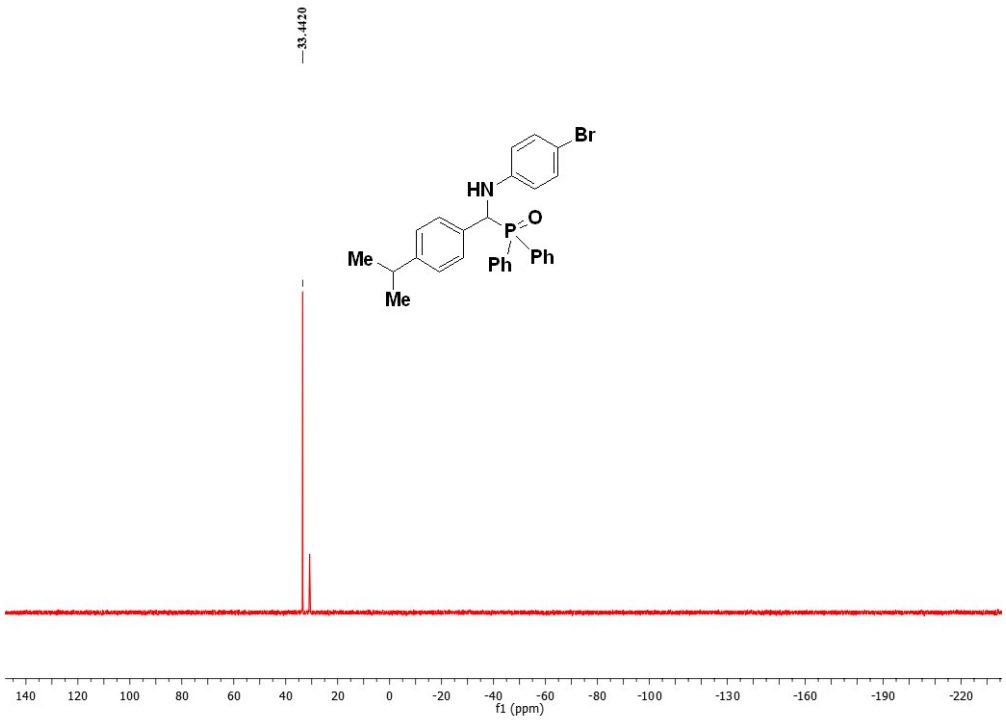


Fig FS57. $^{31}P\{^{1}H\}$ NMR for compound **4q** in $CDCl_3$.

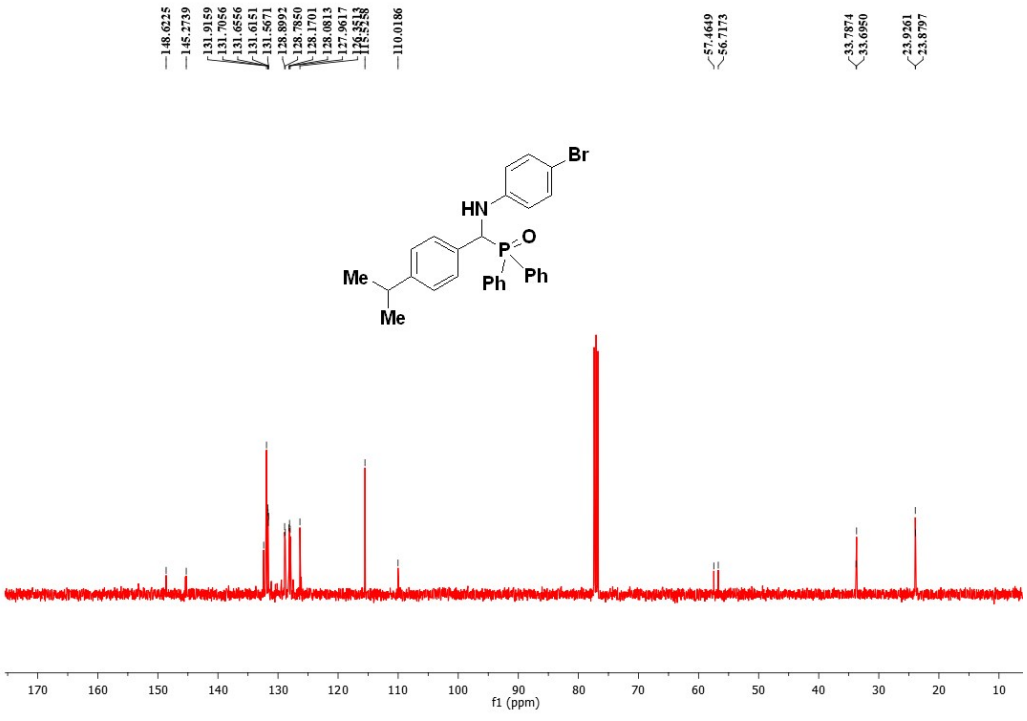


Fig FS58. $^{13}C\{^{1}H\}$ NMR for compound **4q** in $CDCl_3$.

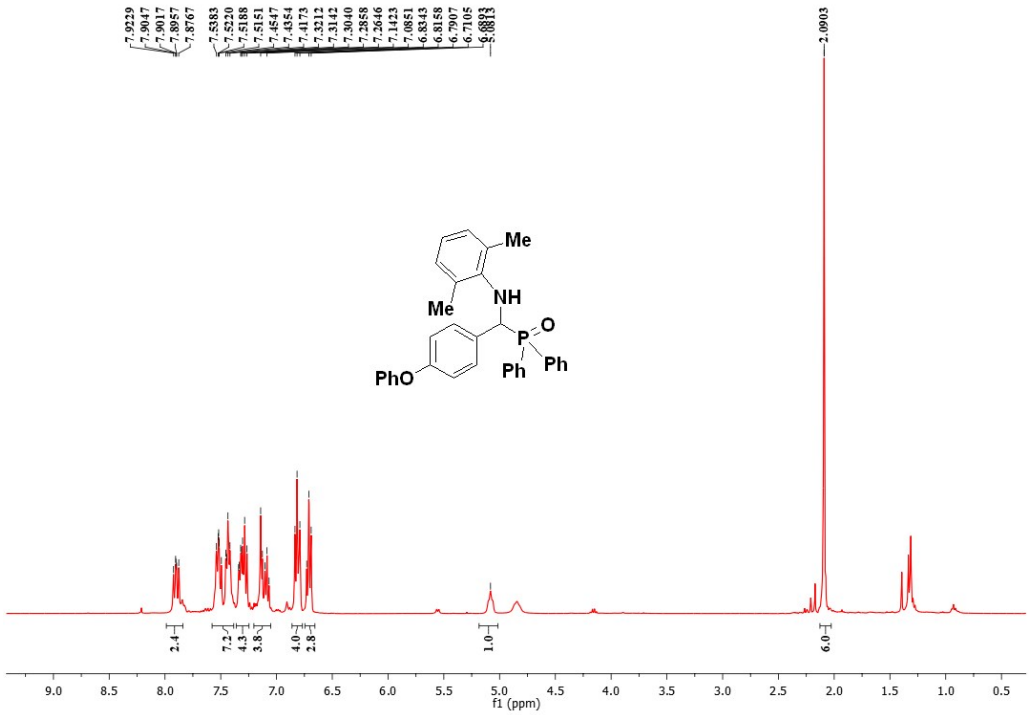


Fig FS59. ^{1}H NMR for compound **4r** in $CDCl_3$.

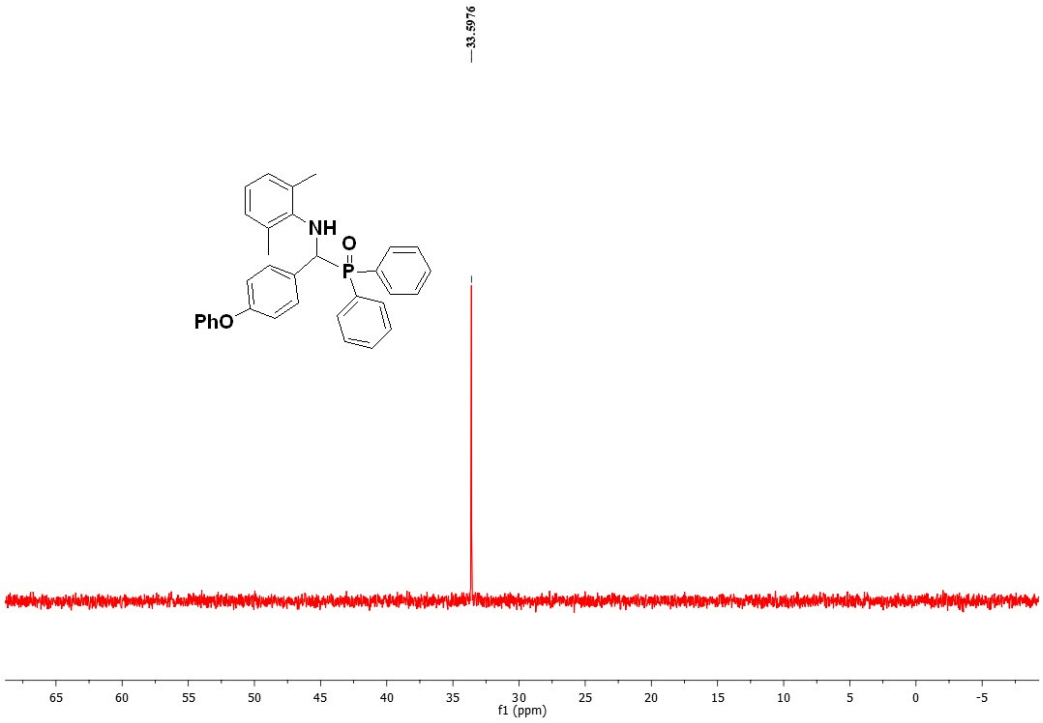


Fig FS60. $^{31}P\{^{1}H\}$ NMR for compound **4r** in $CDCl_3$.

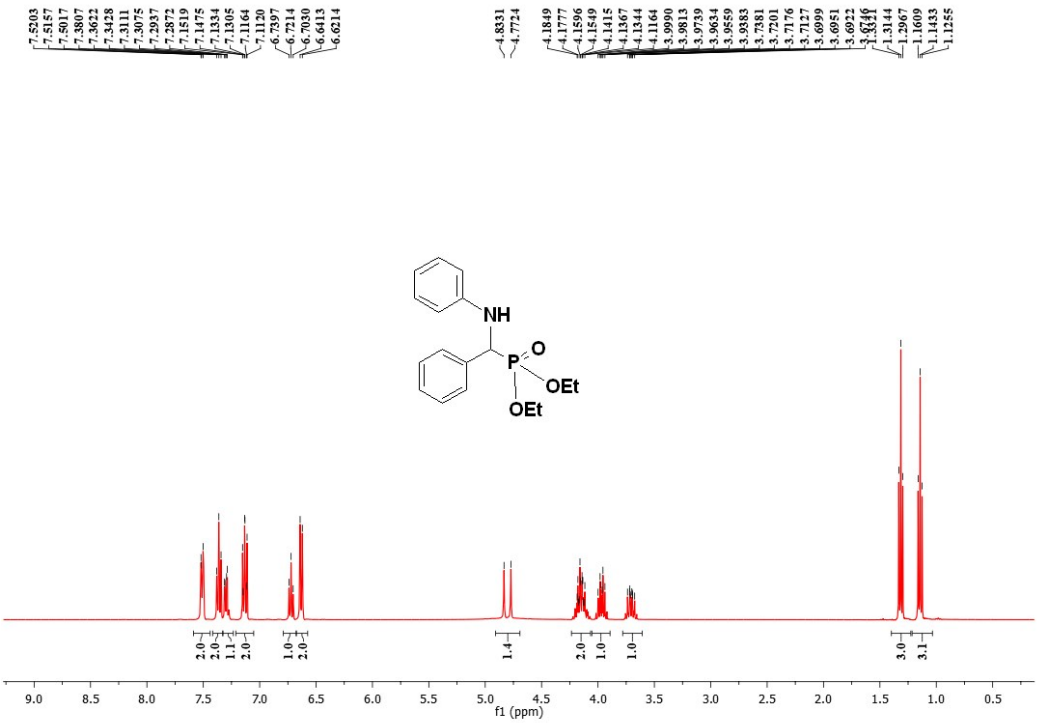


Fig FS61. ^{1}H NMR for compound **5a** in $CDCl_3$.

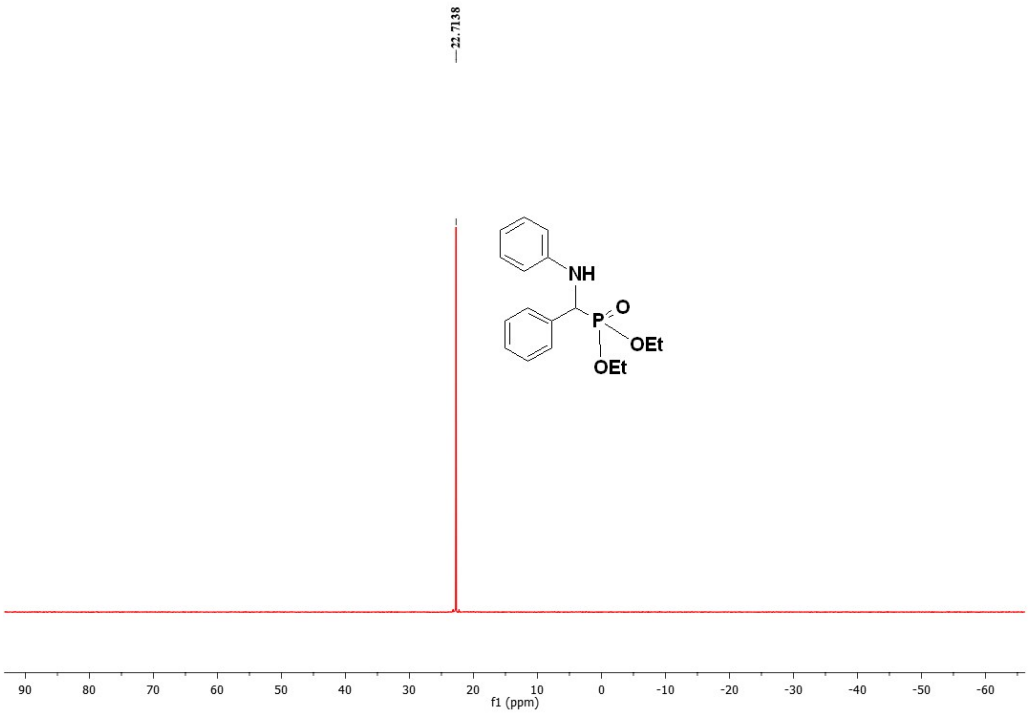


Fig FS62. $^{31}P\{^{1}H\}$ NMR for compound **5a** in $CDCl_3$.

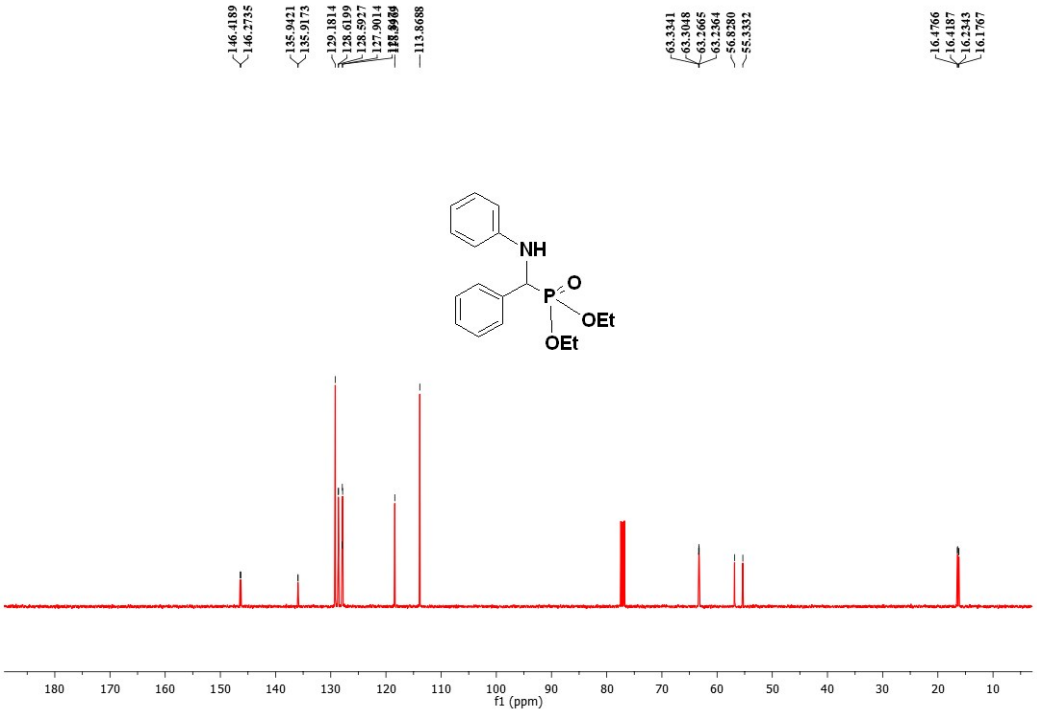


Fig FS63. $^{13}C\{^{1}H\}$ NMR for compound **5a** in $CDCl_3$.

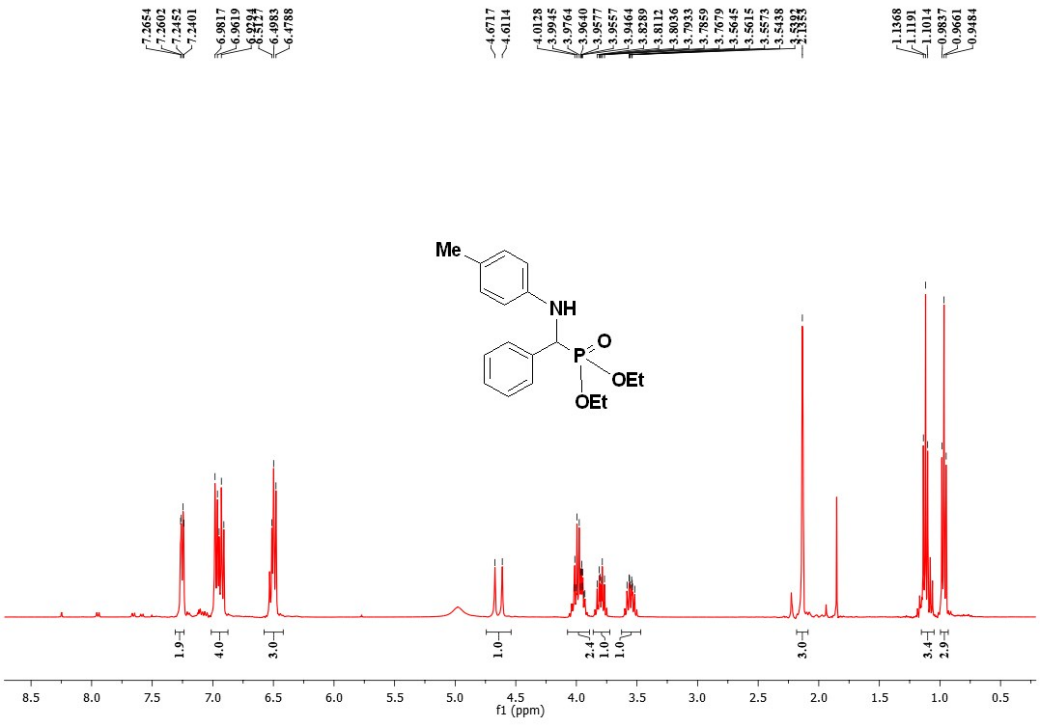


Fig FS64. ^{1}H NMR for compound **5b** in $CDCl_3$.

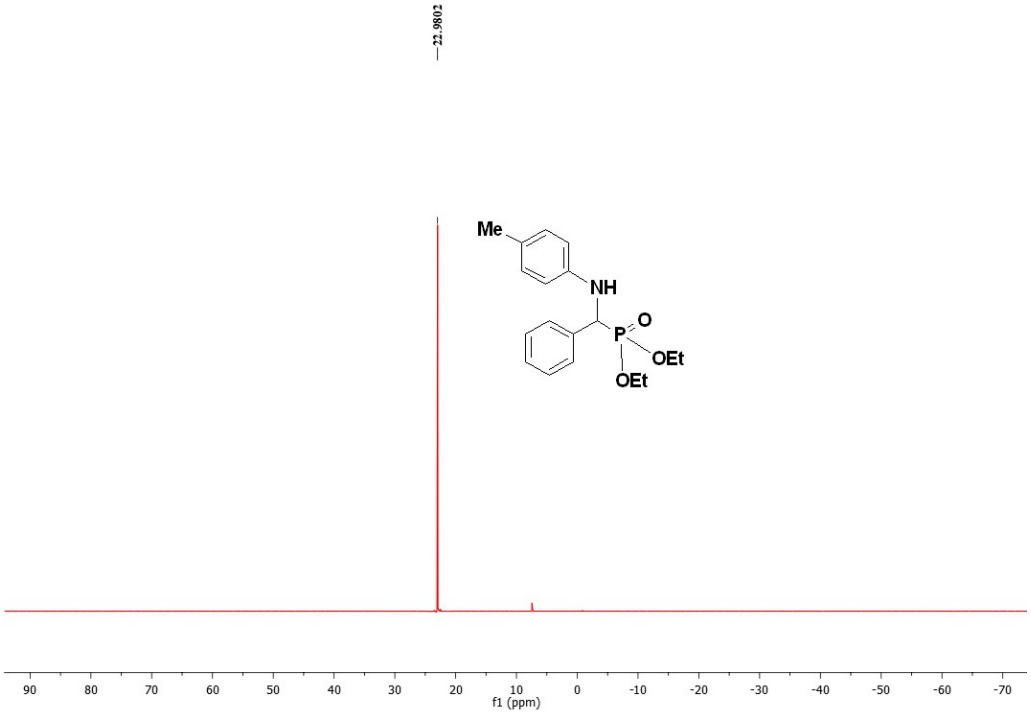


Fig FS65. $^{31}P\{^{1}H\}$ NMR for compound **5b** in $CDCl_3$.

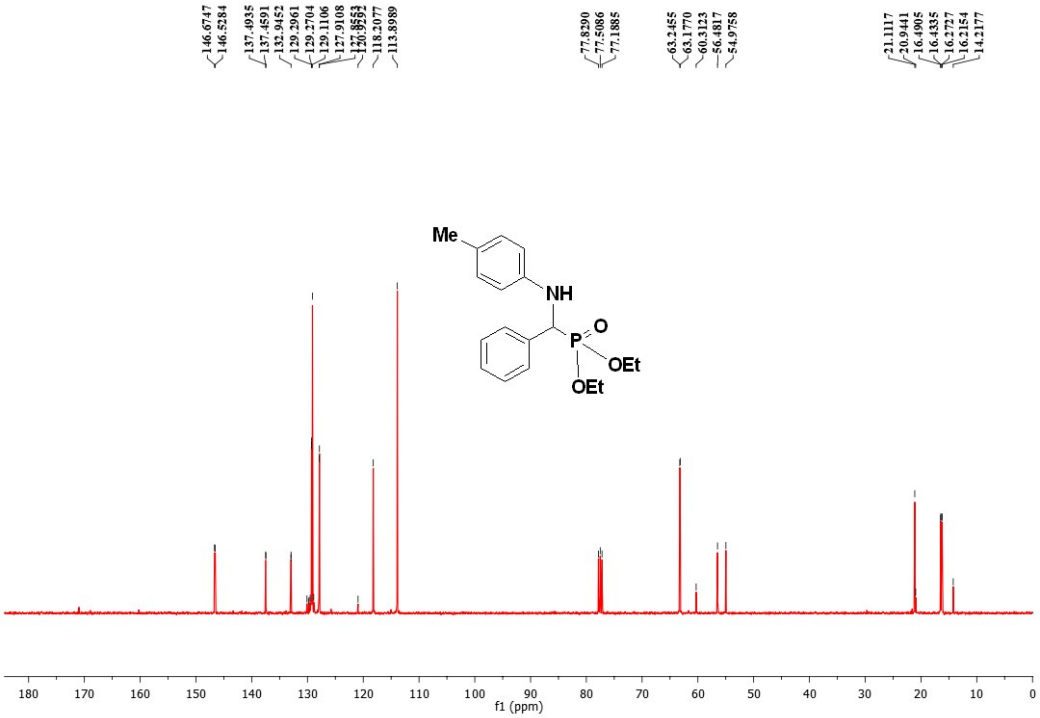


Fig FS66. $^{13}C\{^{1}H\}$ NMR for compound **5b** in $CDCl_3$.

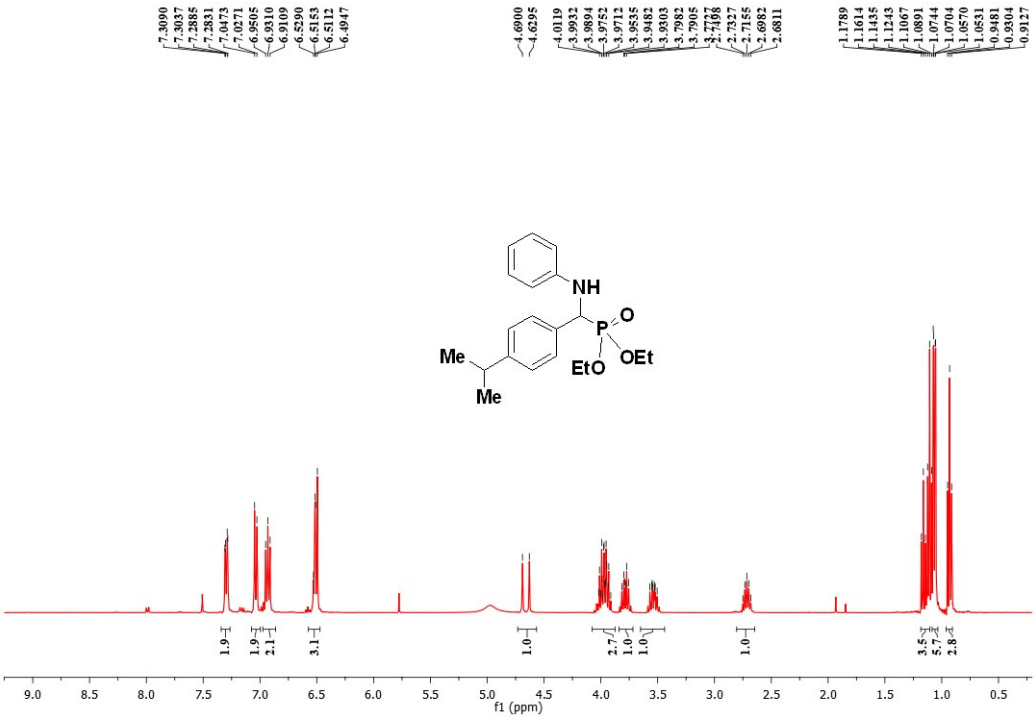


Fig FS67. ^{1}H NMR for compound **5c** in $CDCl_3$.

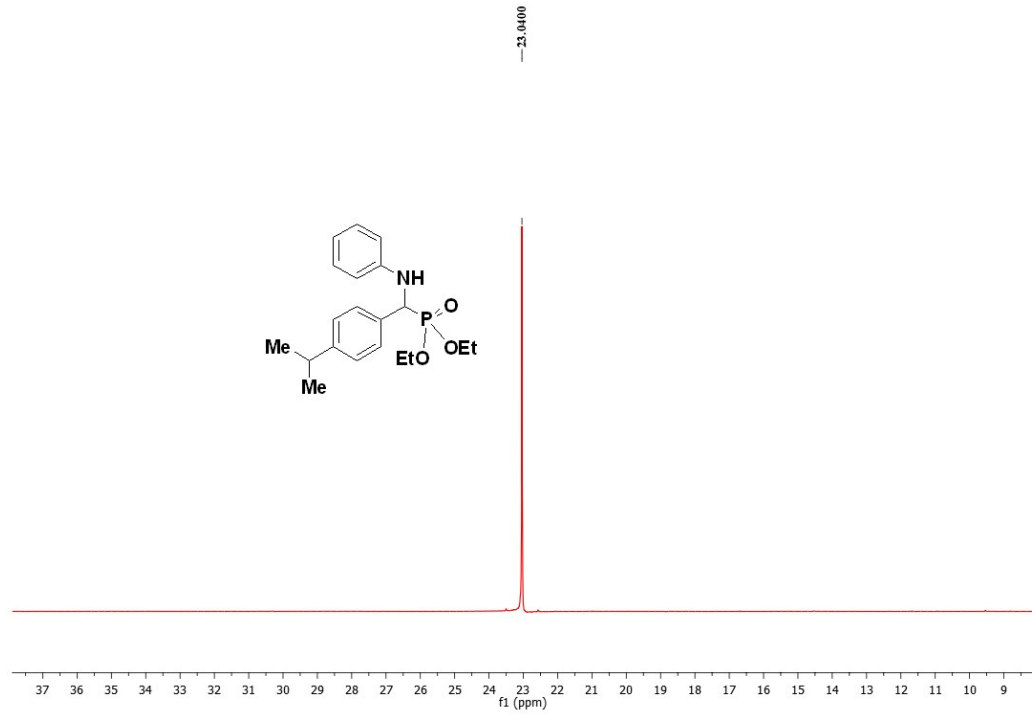


Fig FS68. $^{31}P\{^{1}H\}$ NMR for compound **5c** in $CDCl_3$.

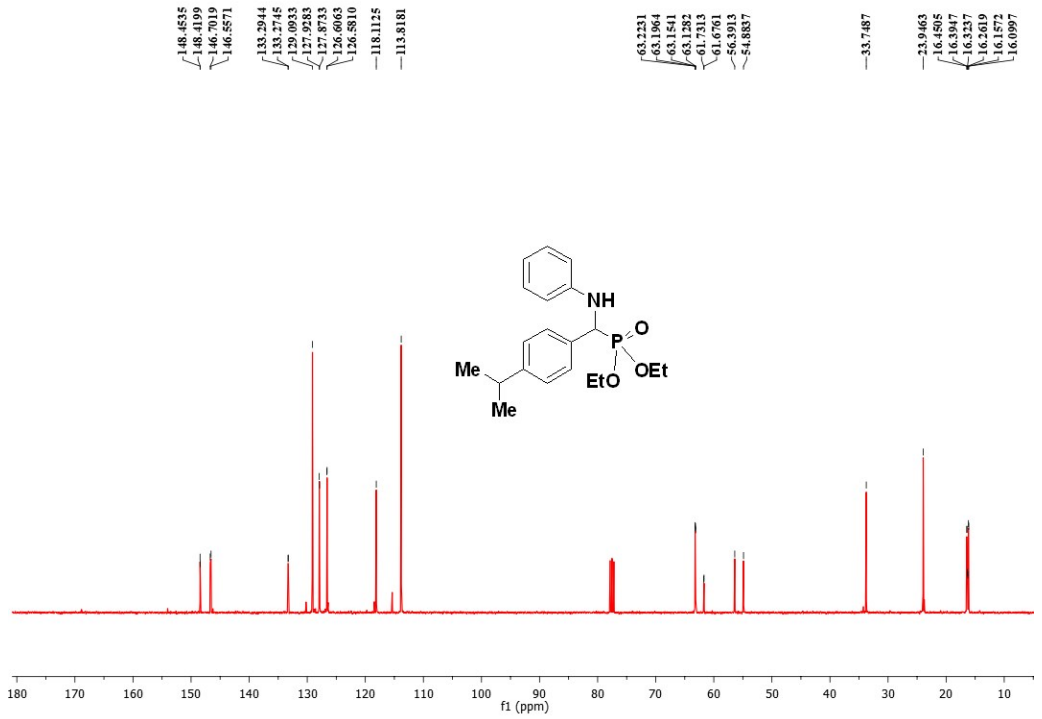


Fig FS69. $^{13}C\{^{1}H\}$ NMR for compound **5c** in $CDCl_3$.

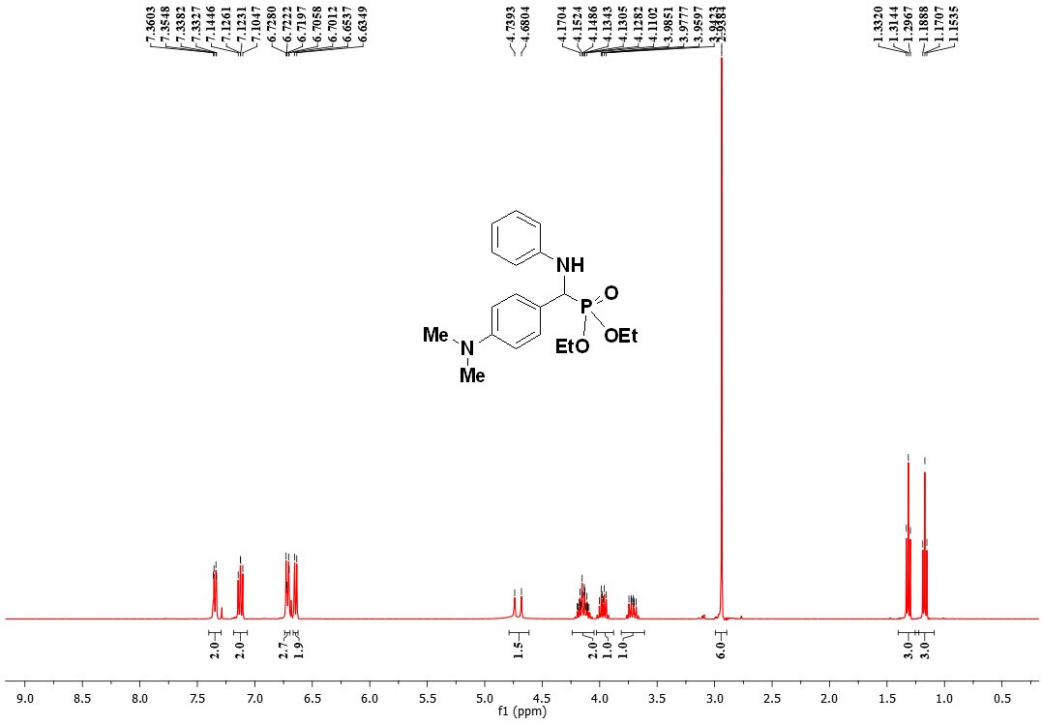


Fig FS70. ^{1}H NMR for compound **5d** in $CDCl_3$.

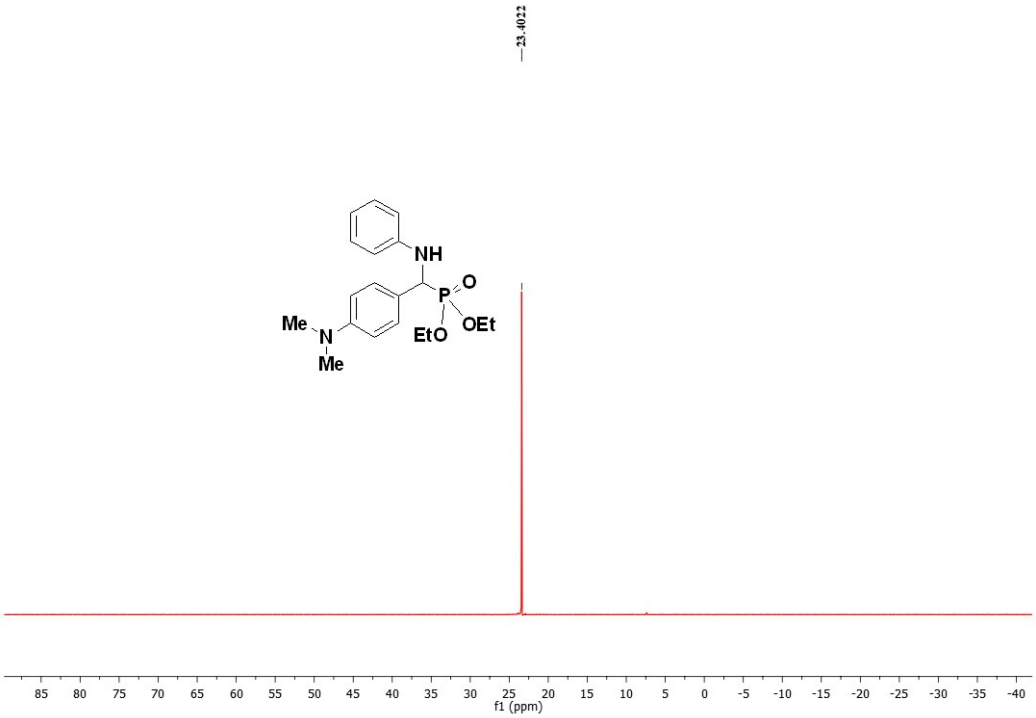


Fig FS71: $^{31}P\{^{1}H\}$ NMR for compound **5d** in $CDCl_3$.

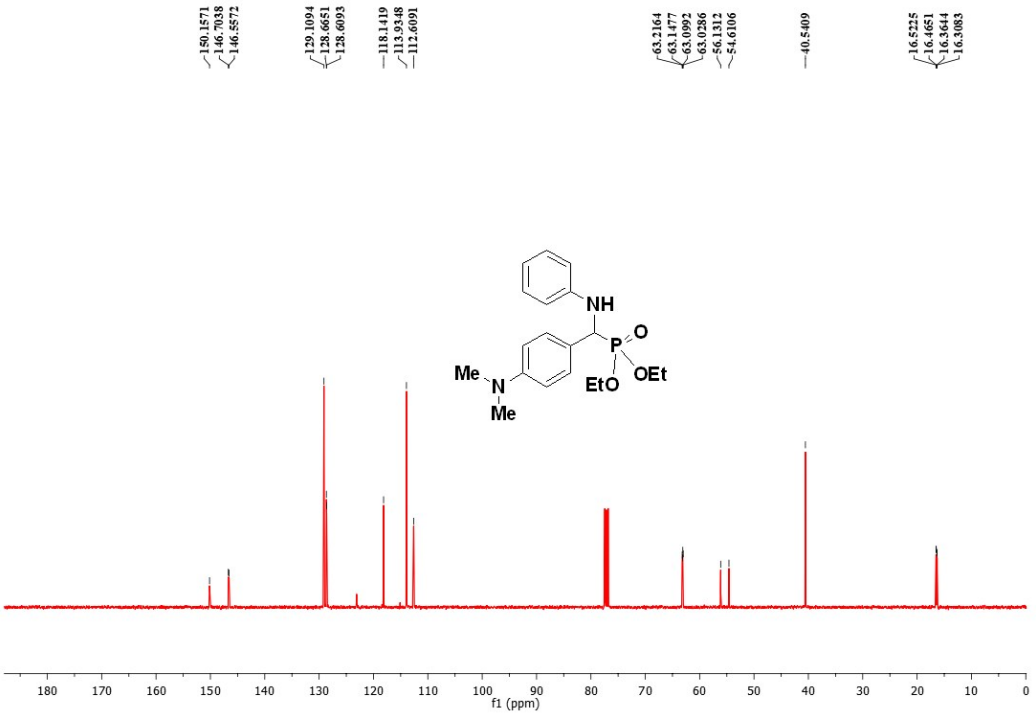


Fig FS72. $^{13}C\{^{1}H\}$ NMR for compound **5d** in $CDCl_3$.

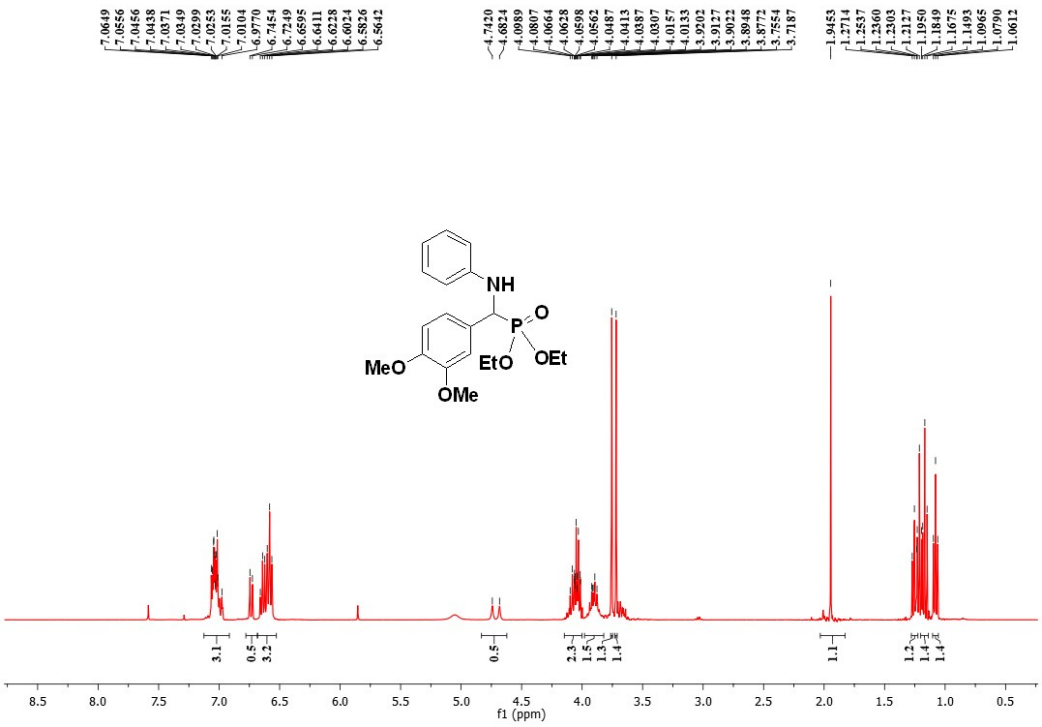


Fig FS73. ^{1}H NMR for compound **5e** in $CDCl_3$.

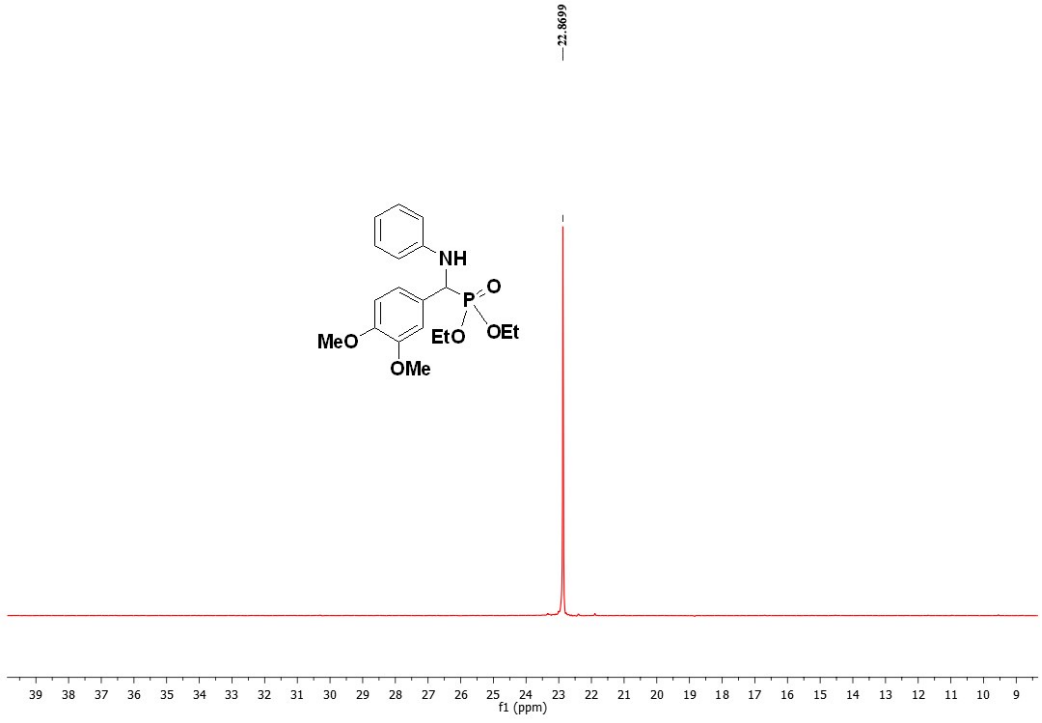


Fig FS74. $^{31}P\{^{1}H\}$ NMR for compound **5e** in $CDCl_3$.

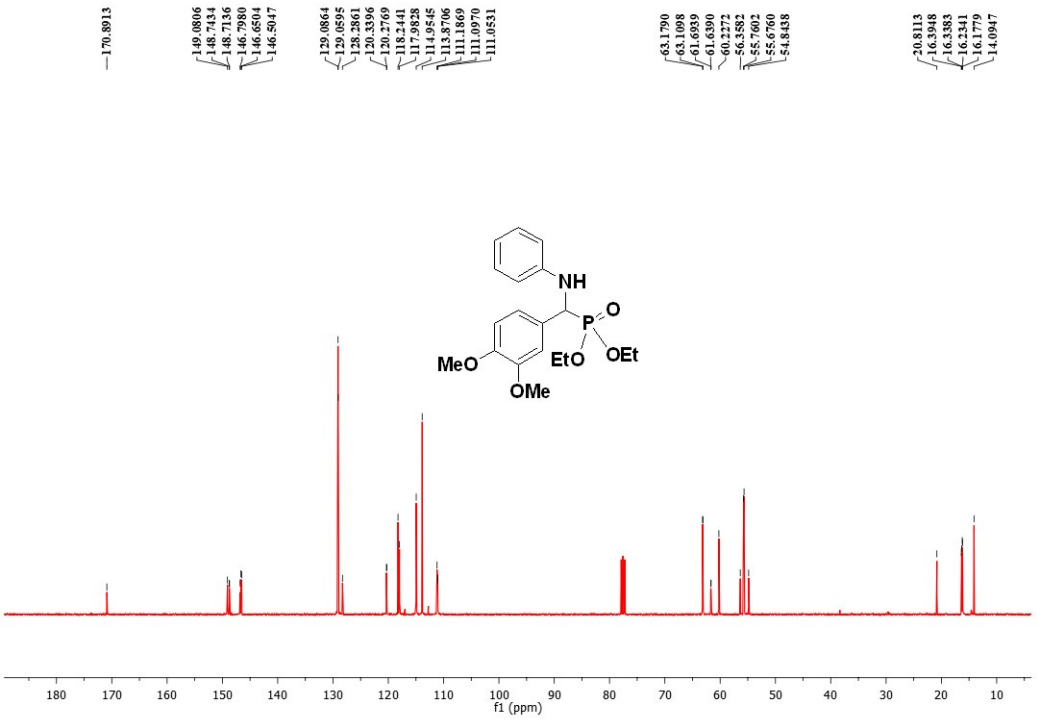


Fig FS75. $^{13}C\{^{1}H\}$ NMR for compound **5e** in $CDCl_3$.

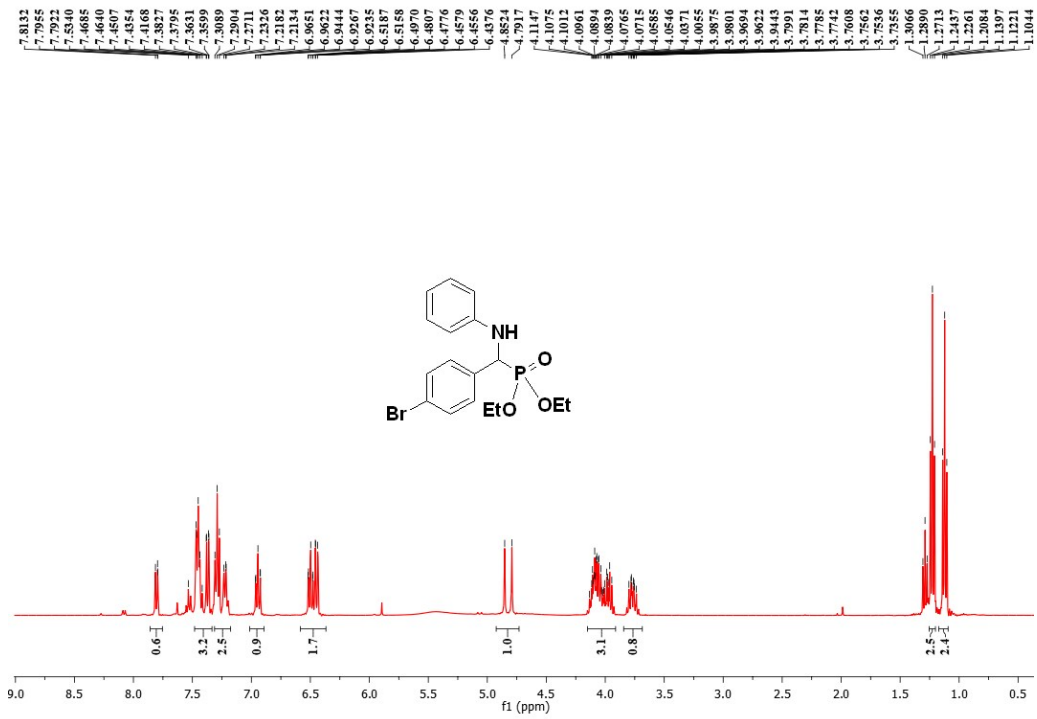


Fig FS76. ^{1}H NMR for compound **5f** in $CDCl_3$.

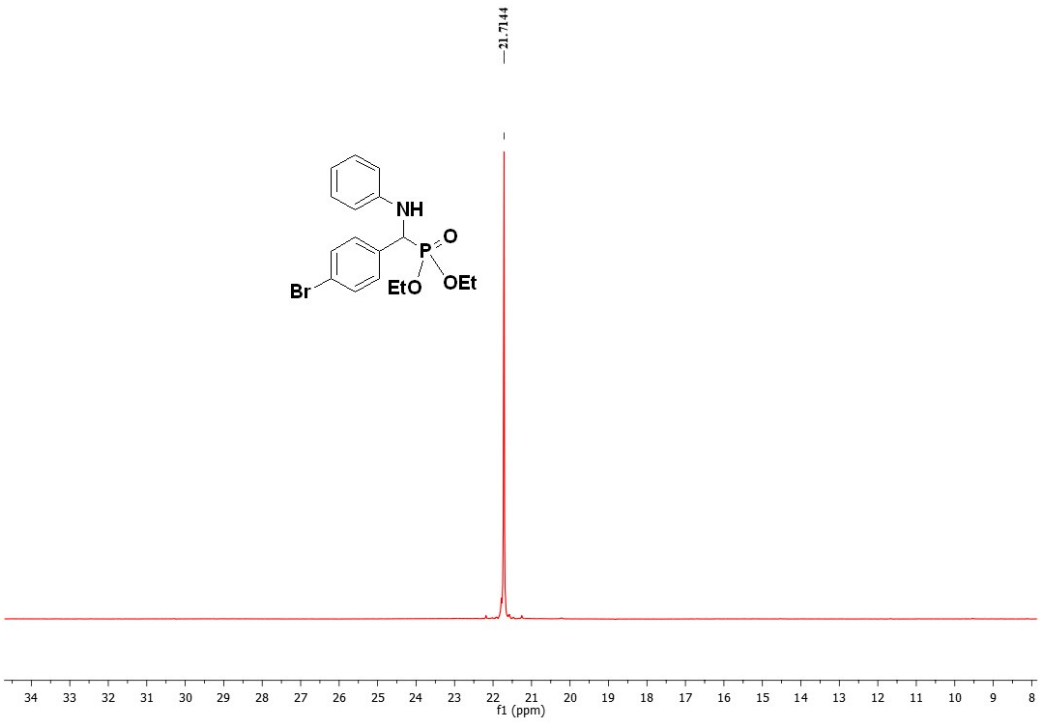


Fig FS77. $^{31}P\{^{1}H\}$ NMR for compound **5f** in $CDCl_3$.

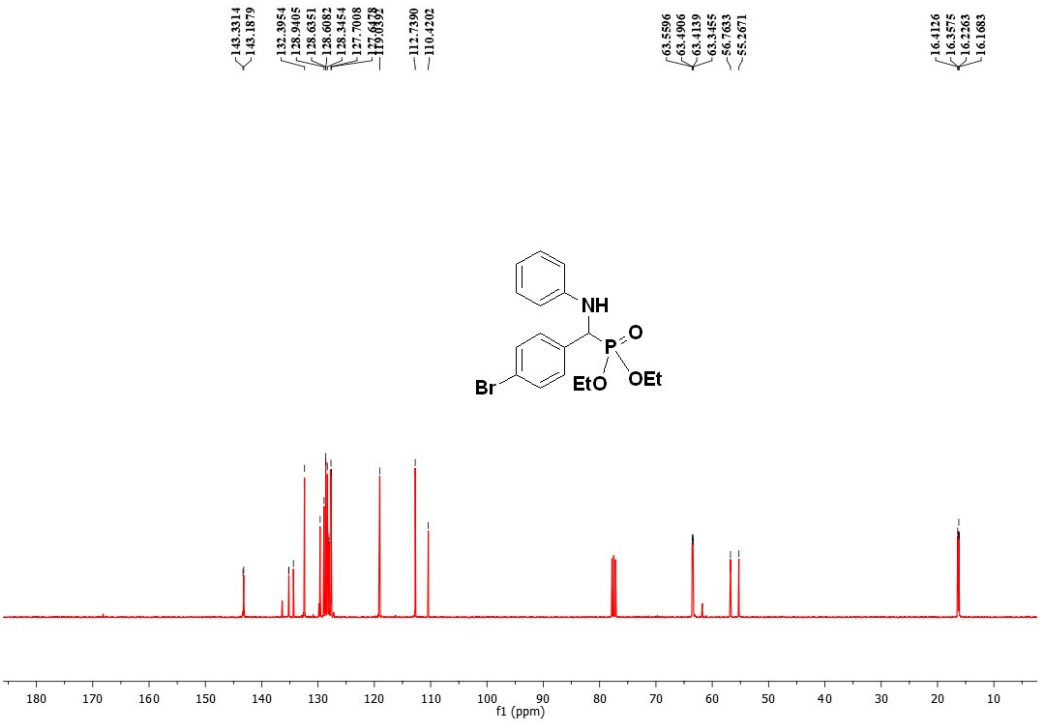


Fig FS78. $^{13}C\{^{1}H\}$ NMR for compound **5f** in $CDCl_3$.

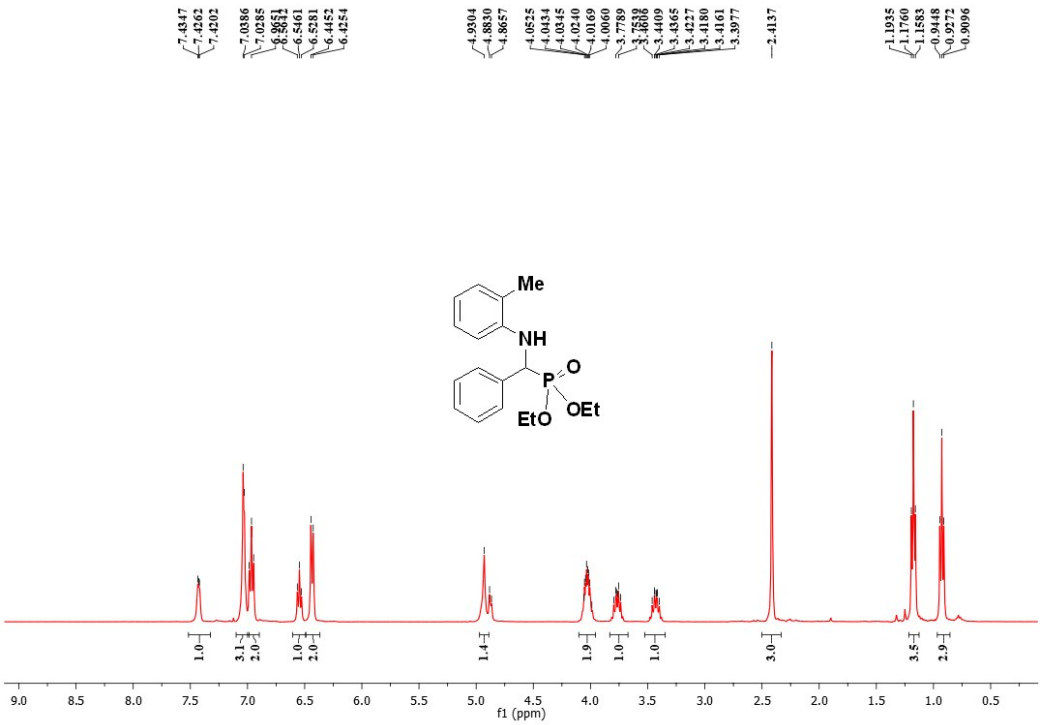


Fig FS79. ^{1}H NMR for compound **5g** in $CDCl_3$.

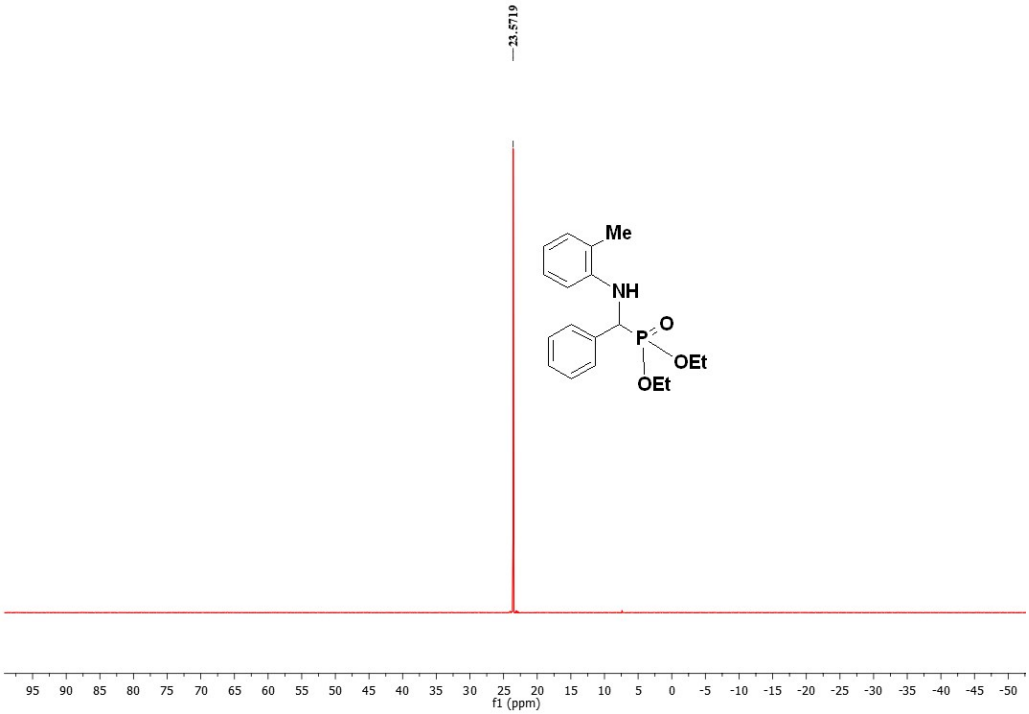


Fig FS80. $^{31}P\{^{1}H\}$ NMR for compound **5g** in $CDCl_3$.

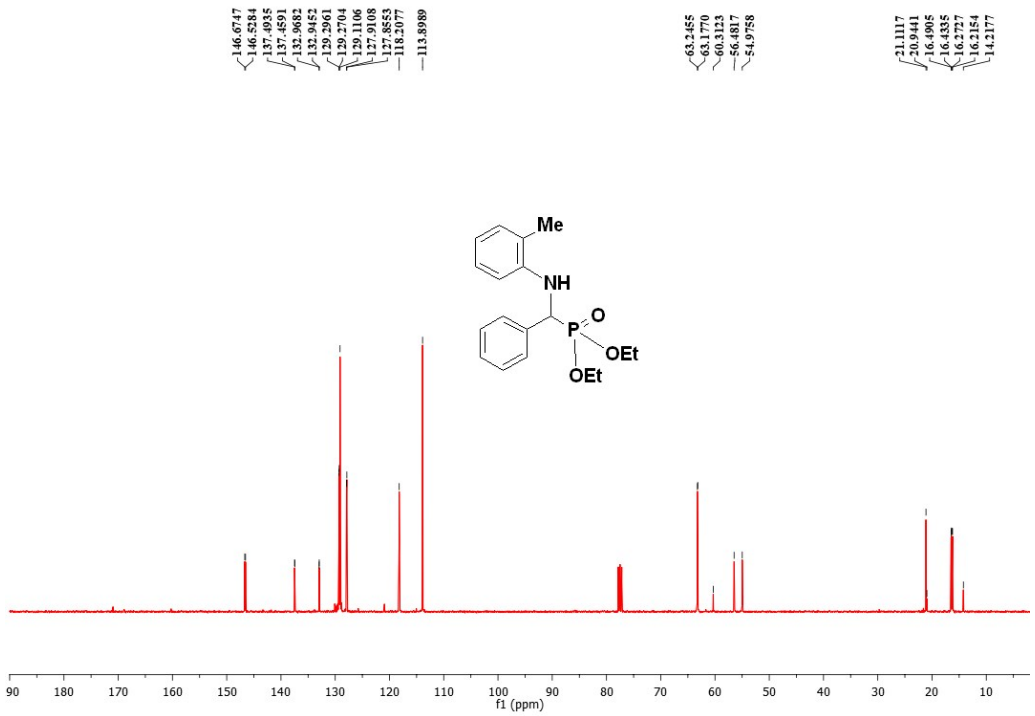


Fig FS81. $^{13}C\{^{1}H\}$ NMR for compound **5g** in $CDCl_3$.

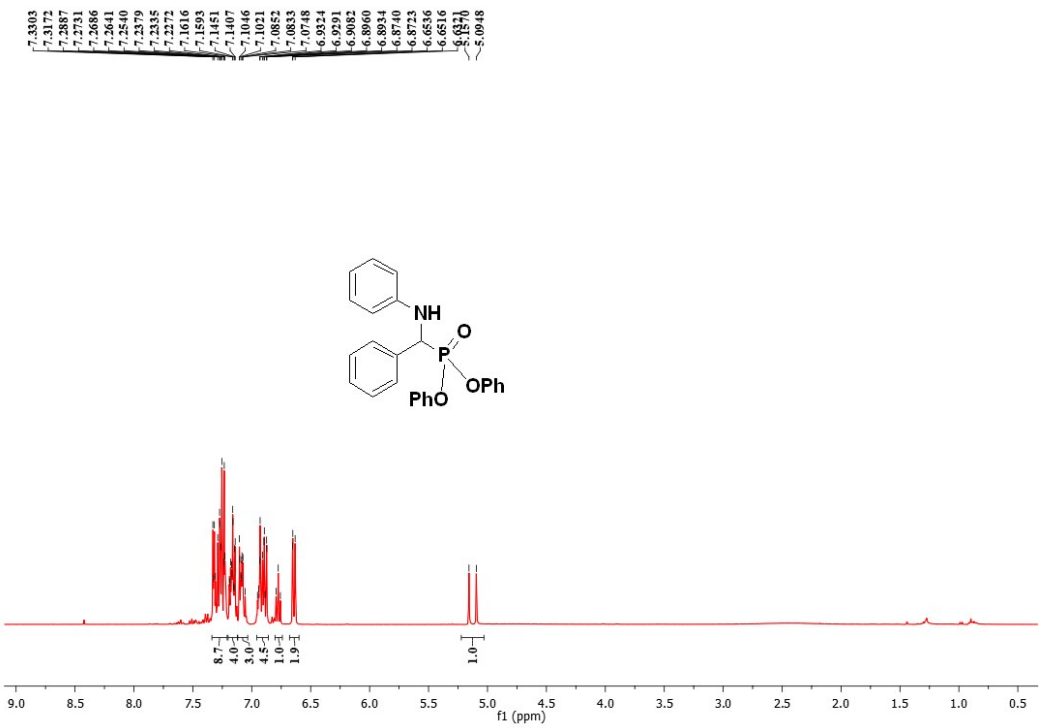


Fig FS82. ^{1}H NMR for compound **6a** in $CDCl_3$.

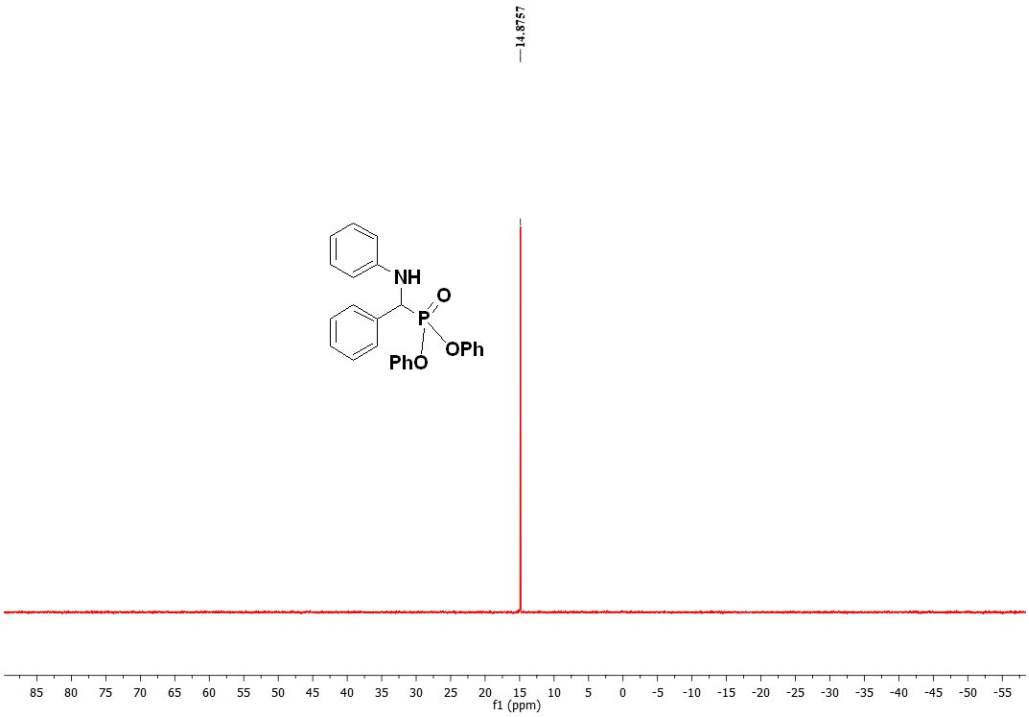


Fig FS83. $^{31}P\{^{1}H\}$ NMR for compound **6a** in $CDCl_3$.

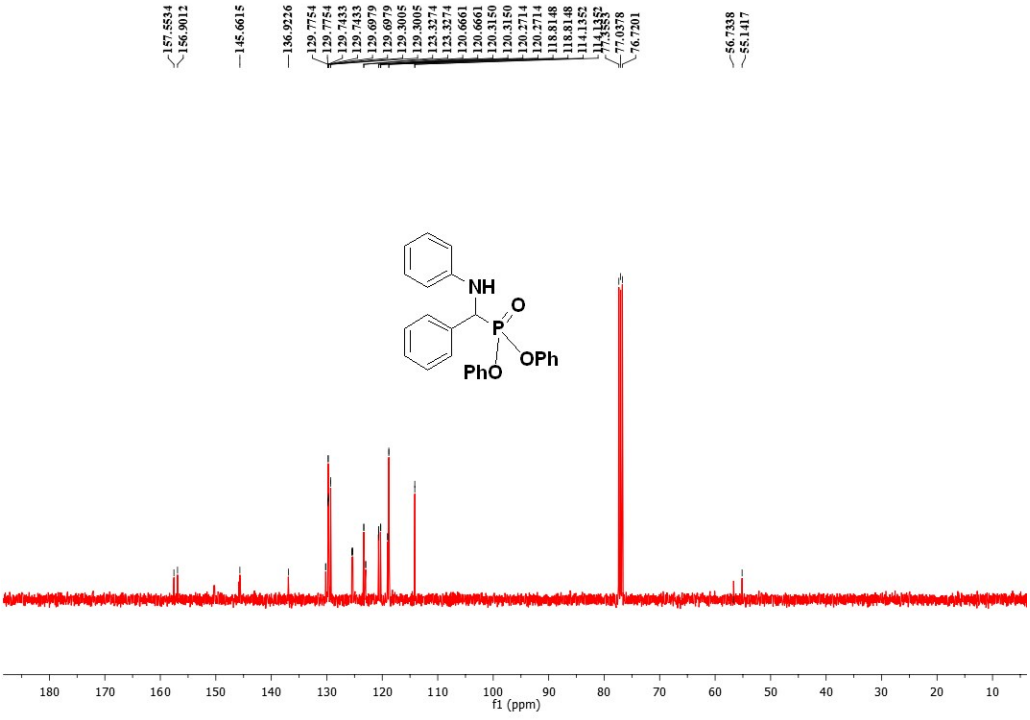


Fig FS84. $^{13}C\{^{1}H\}$ NMR for compound **6a** in $CDCl_3$.

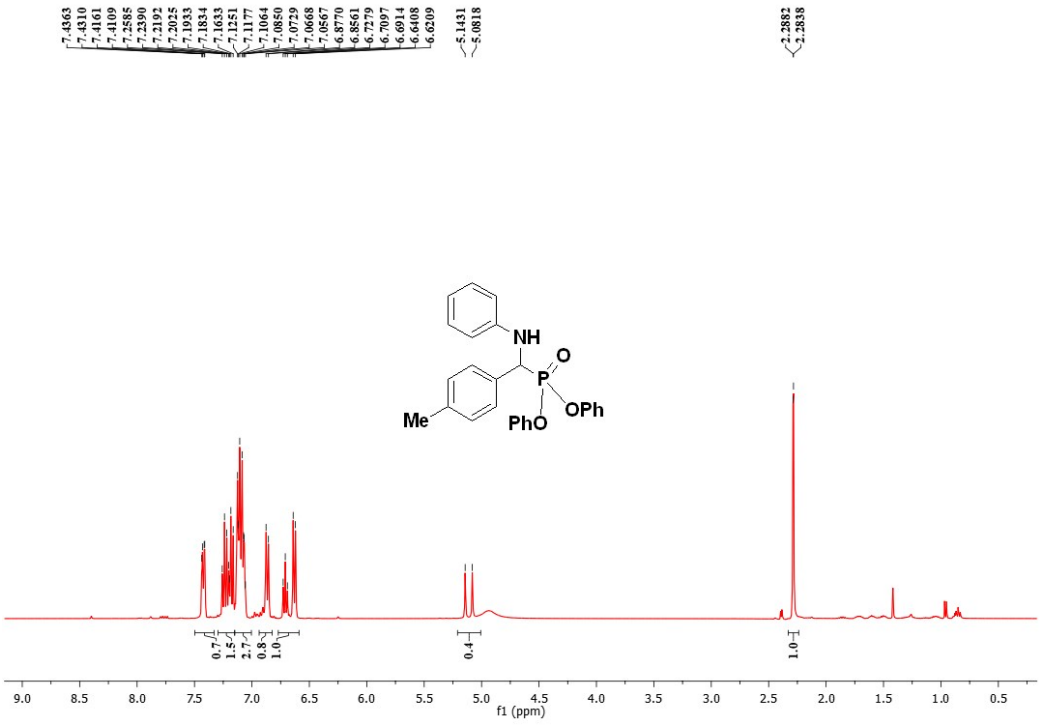


Fig FS85. ^{1}H NMR for compound **6b** in $CDCl_3$.

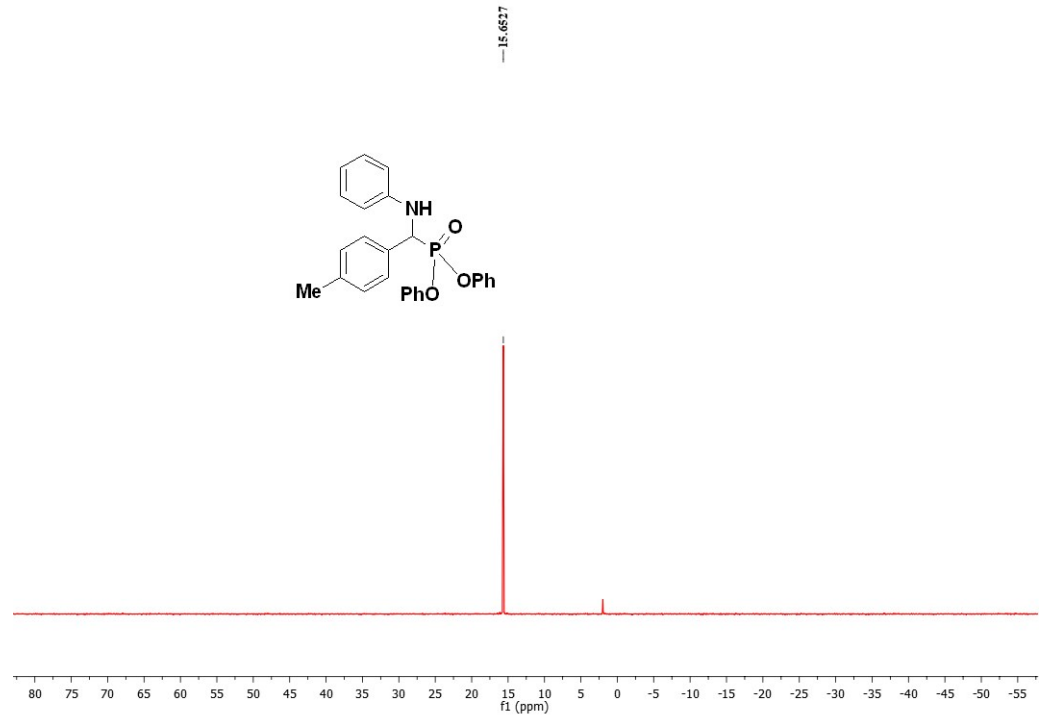


Fig FS86. $^{31}P\{^{1}H\}$ NMR for compound **6b** in $CDCl_3$.

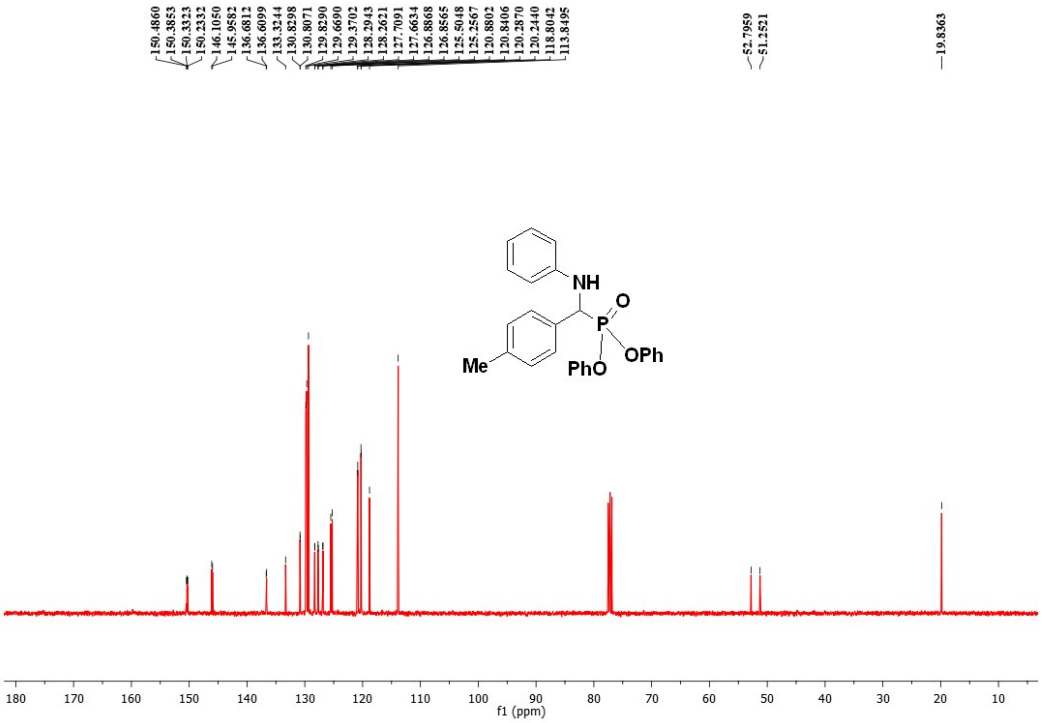


Fig FS87. $^{13}C\{^{1}H\}$ NMR for compound **6b** in $CDCl_3$.

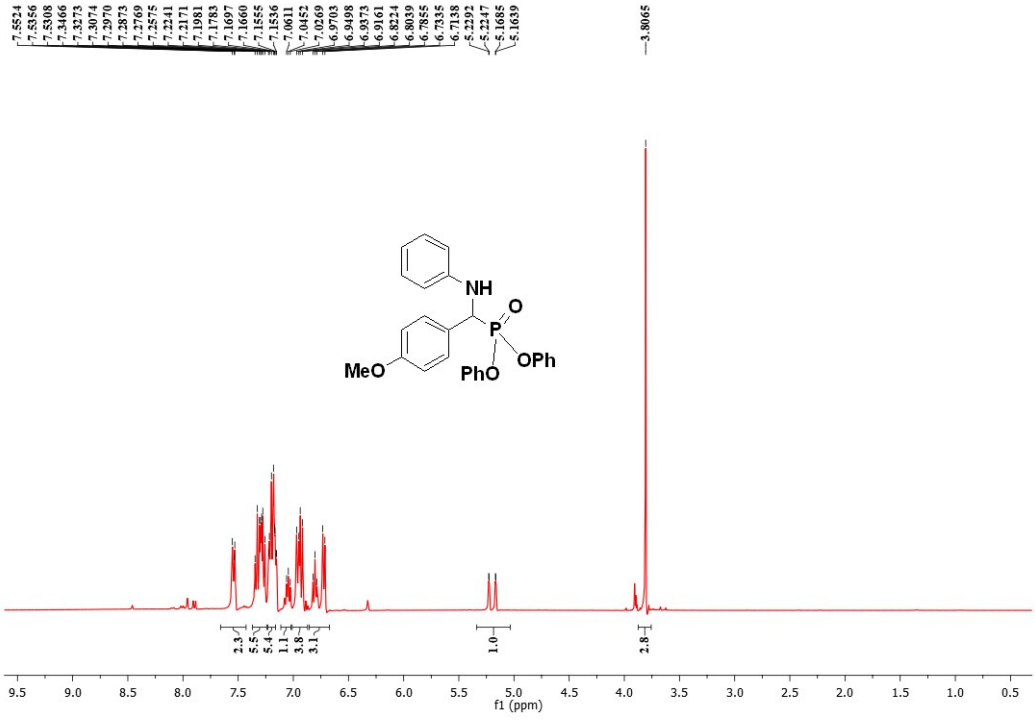


Fig FS88. ^{1}H NMR for compound **6c** in $CDCl_3$.

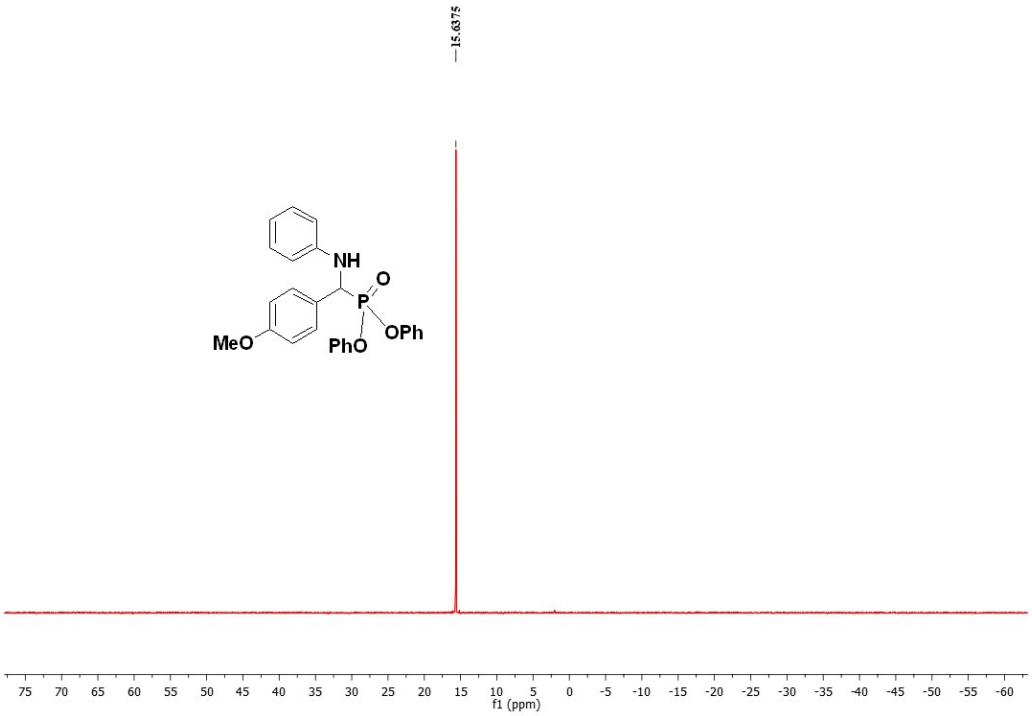


Fig FS89. $^{31}P\{^{1}H\}$ NMR for compound **6c** in $CDCl_3$.

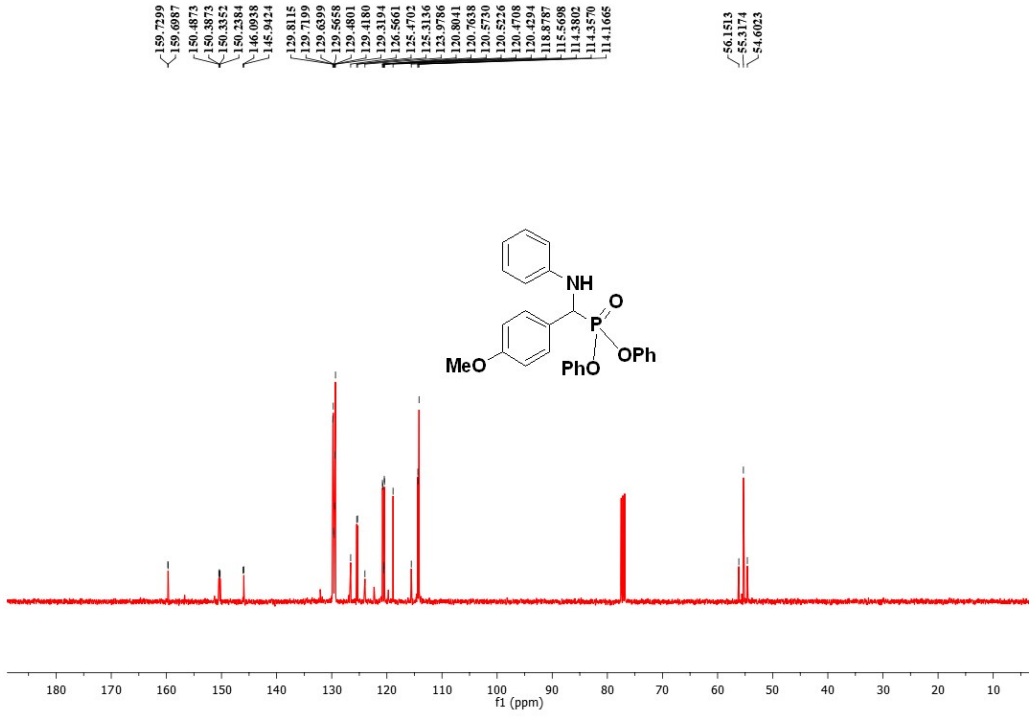


Fig FS90. $^{13}C\{^{1}H\}$ NMR for compound **6c** in $CDCl_3$.

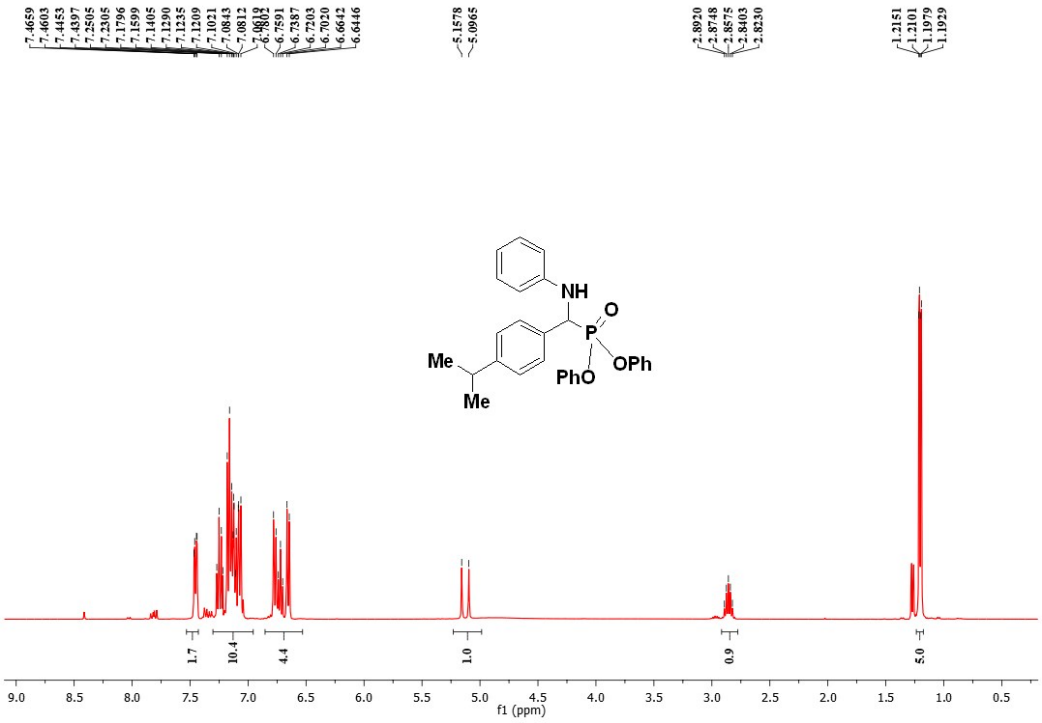


Fig FS91. ^{1}H NMR for compound **6d** in $CDCl_3$.

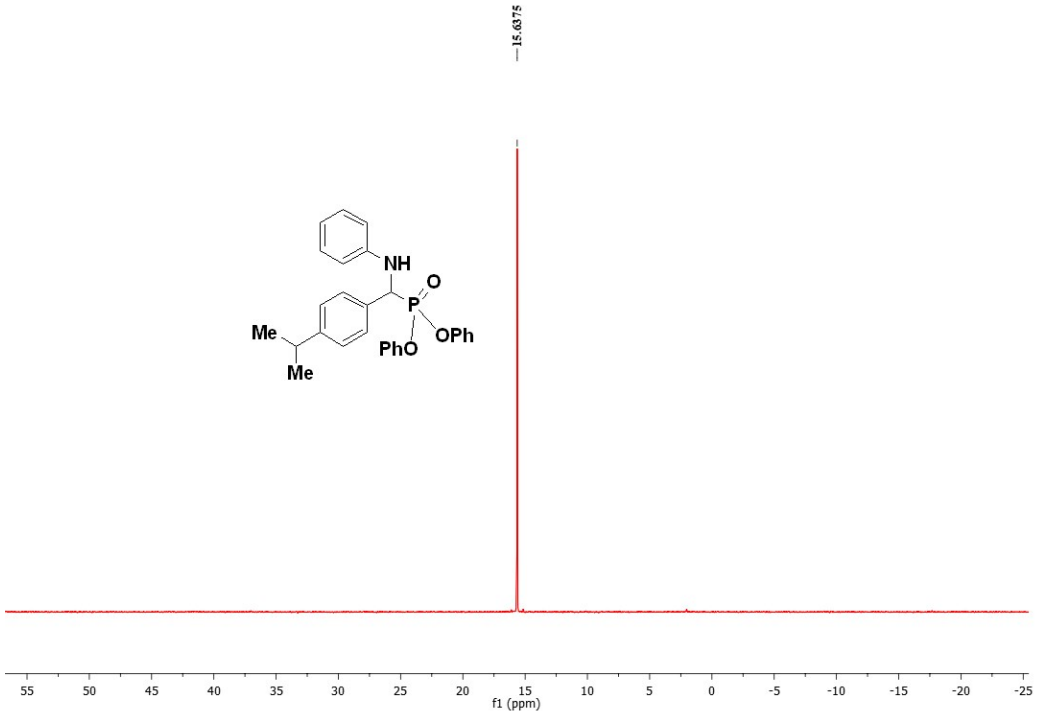


Fig FS92. $^{13}C\{^{1}H\}$ NMR for compound **6d** in $CDCl_3$.

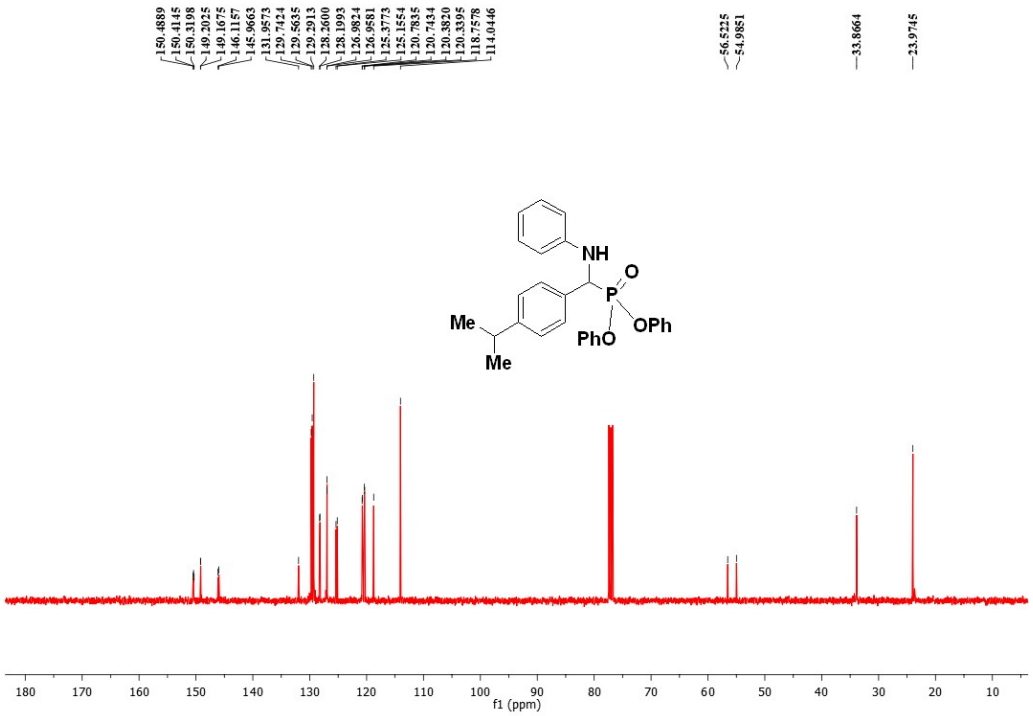


Fig FS93. $^{13}C\{^{1}H\}$ NMR for compound **6d** in $CDCl_3$.

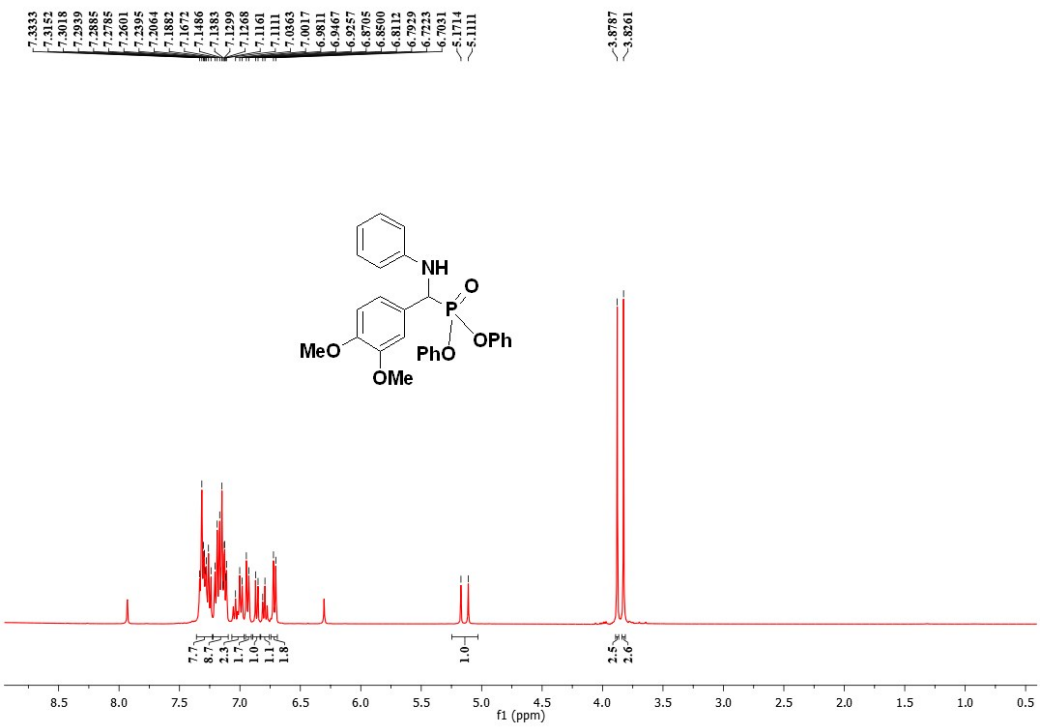


Fig FS94. ^{1}H NMR for compound **6e** in $CDCl_3$.

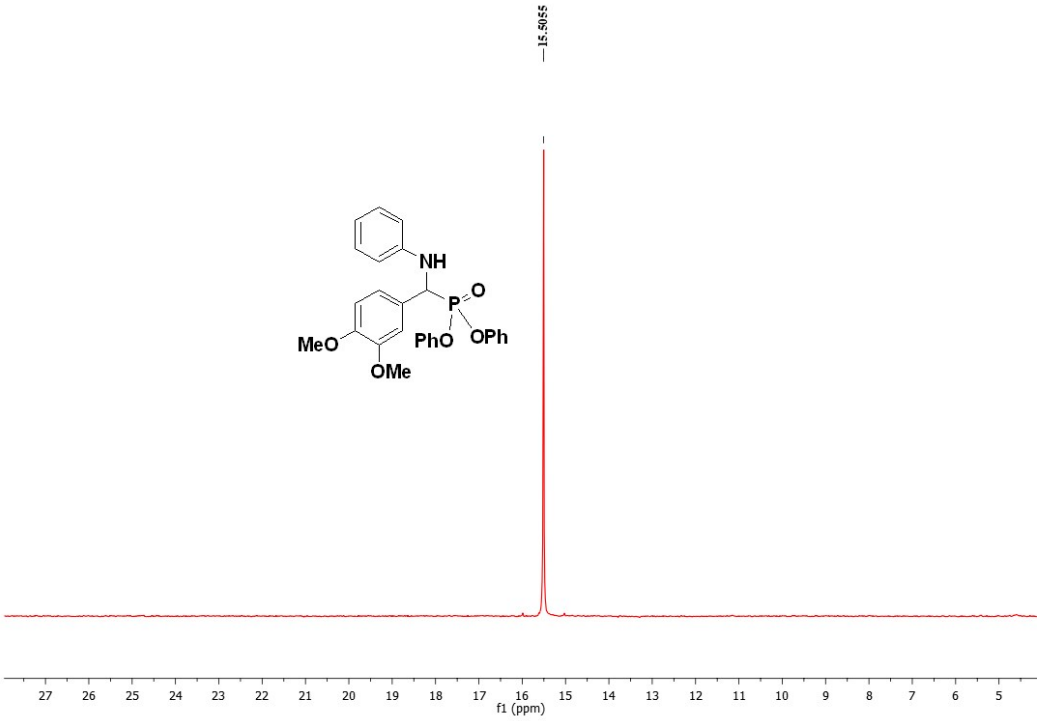


Fig FS95. $^{31}P\{^{1}H\}$ NMR for compound **6e** in $CDCl_3$.

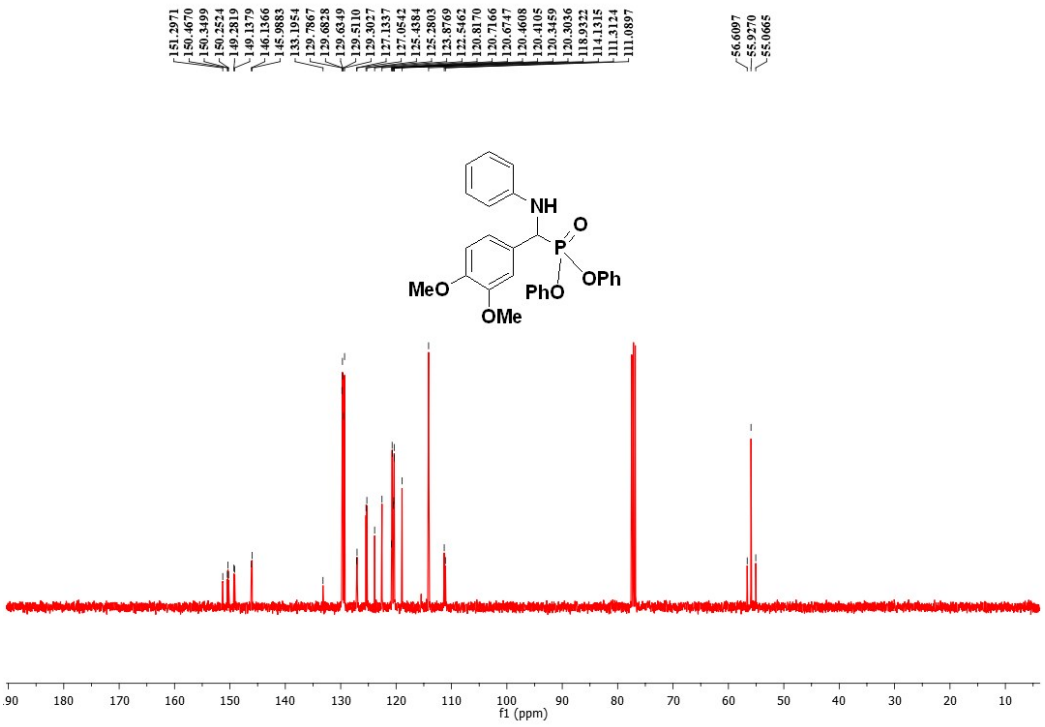


Fig FS96. $^{13}C\{^{1}H\}$ NMR for compound **6e** in $CDCl_3$.

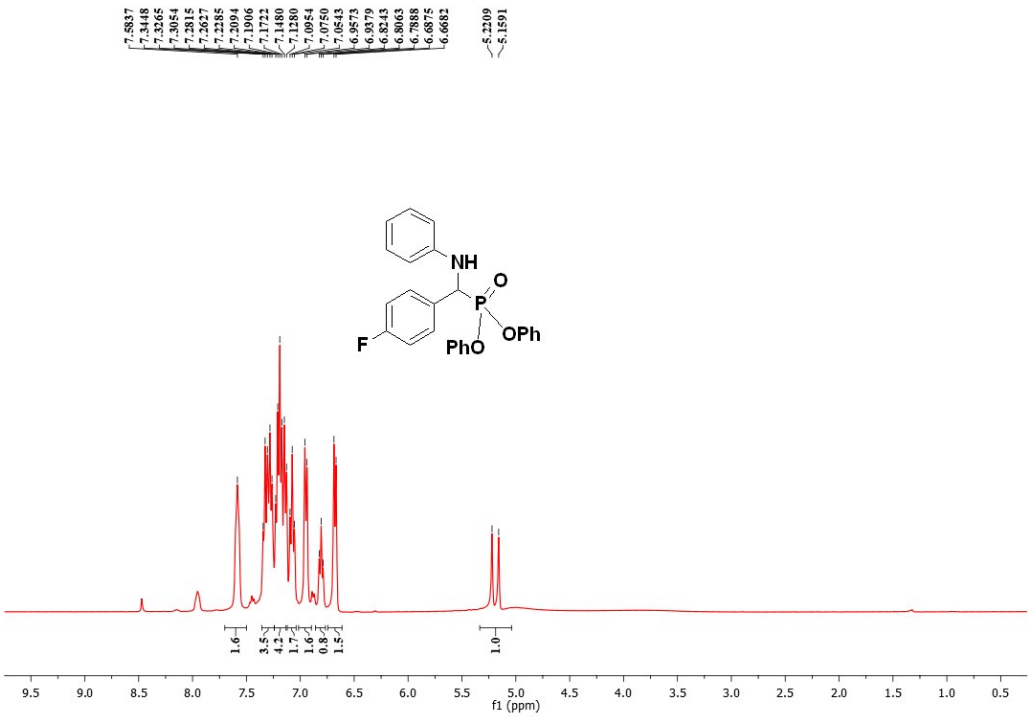


Fig FS97. ^{1}H NMR for compound **6f** in $CDCl_3$.

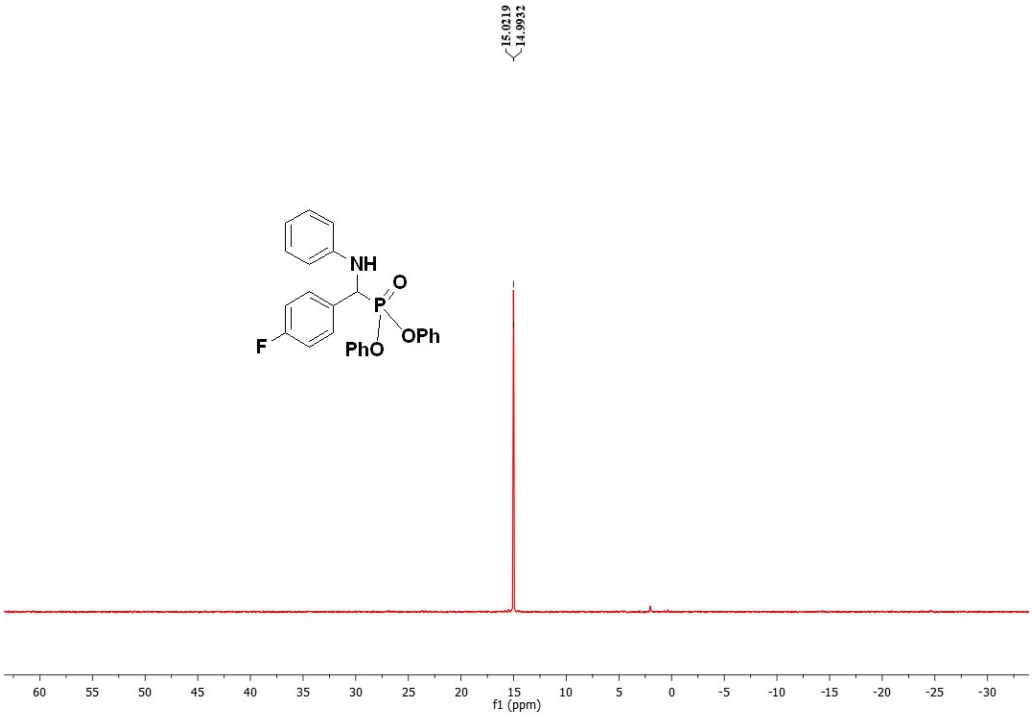


Fig FS98. $^{31}P\{^{1}H\}$ NMR for compound **6f** in $CDCl_3$.

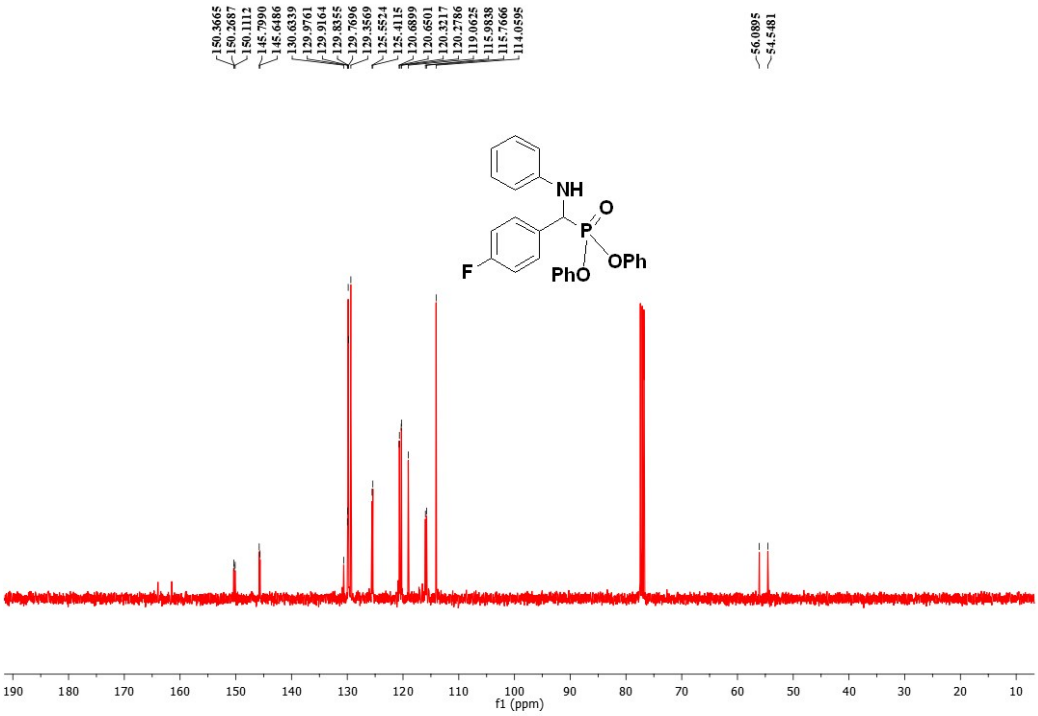


Fig FS99. $^{13}C\{^{1}H\}$ NMR for compound **6f** in $CDCl_3$.

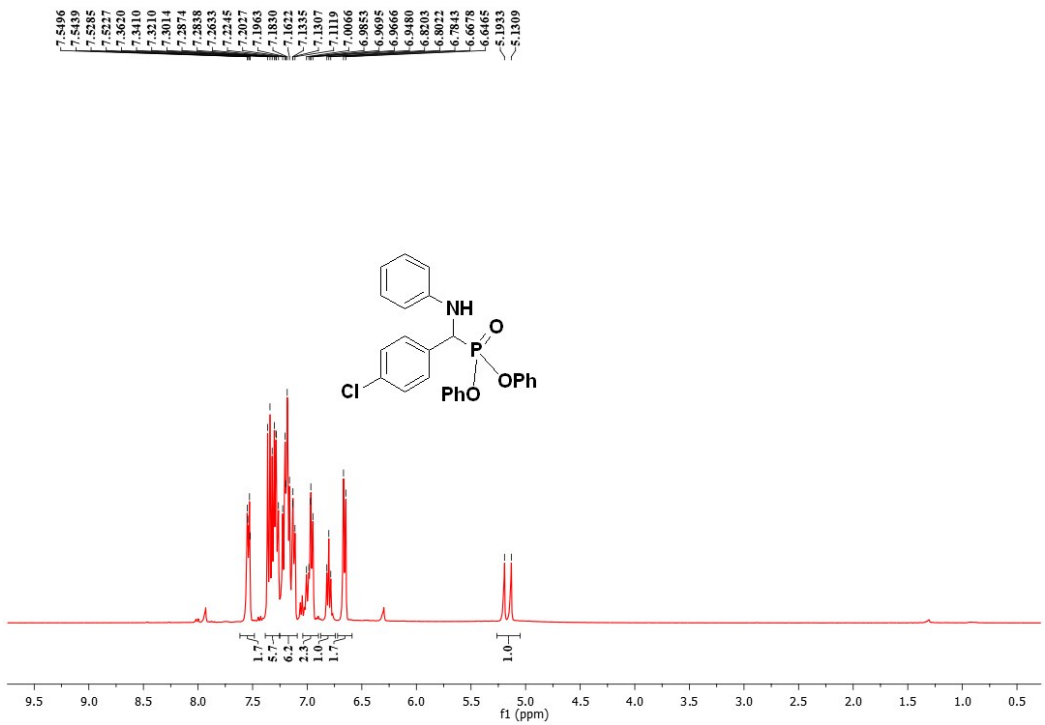


Fig FS100. ^{1}H NMR for compound **6g** in $CDCl_3$.

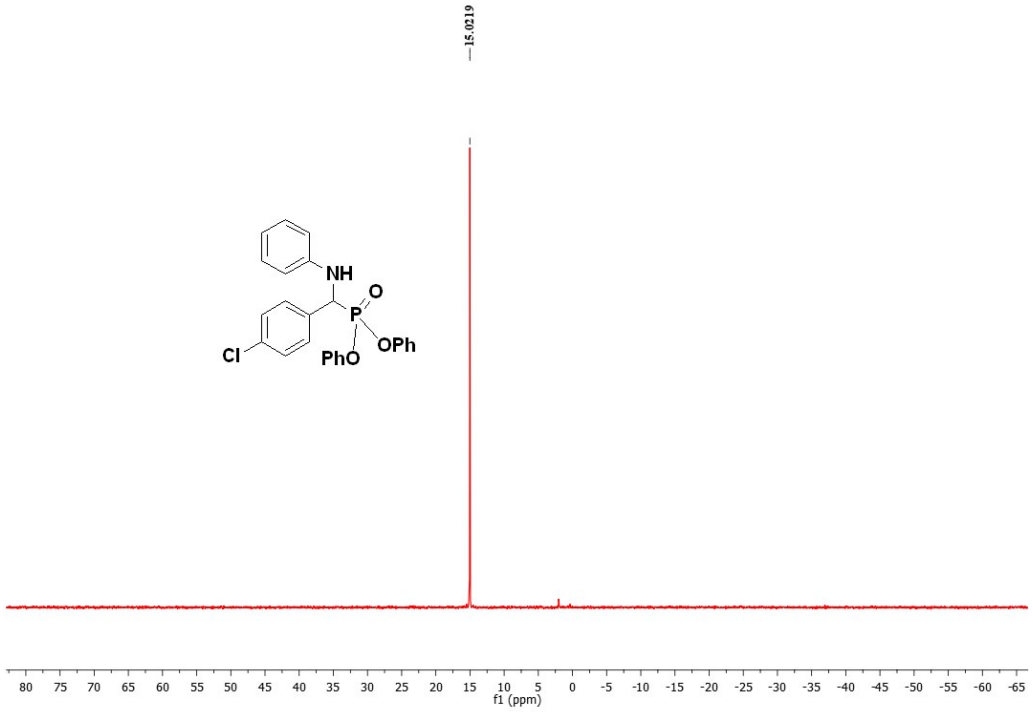


Fig FS101. $^{31}P\{^{1}H\}$ NMR for compound **6g** in $CDCl_3$.

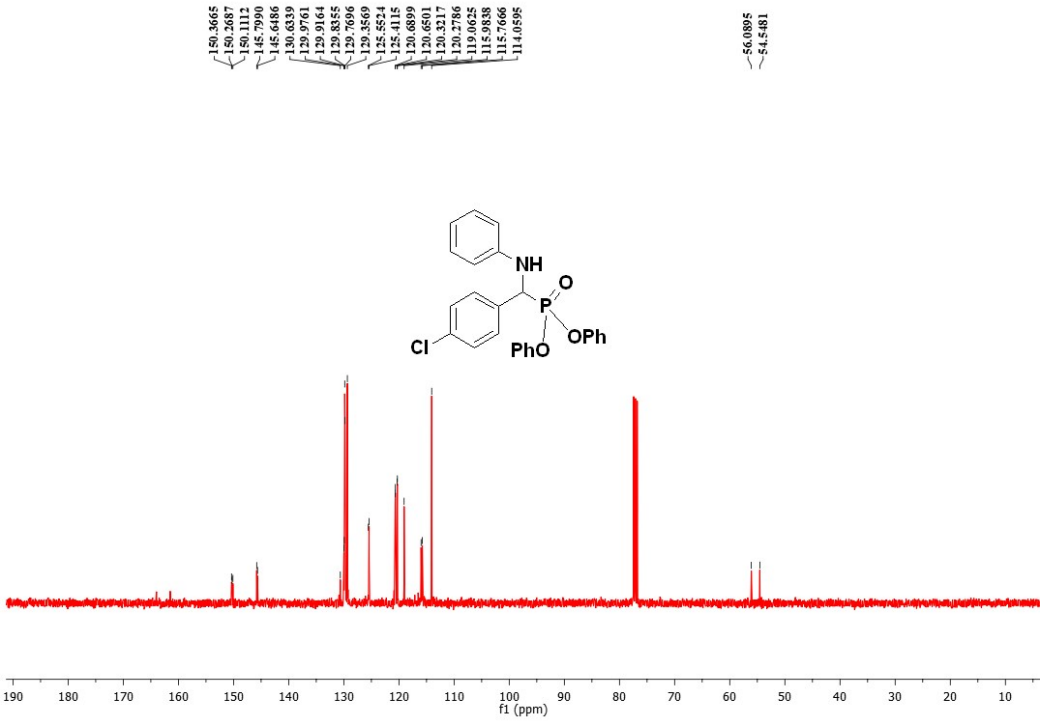


Fig FS102. $^{13}C\{^{1}H\}$ NMR for compound **6g** in $CDCl_3$.

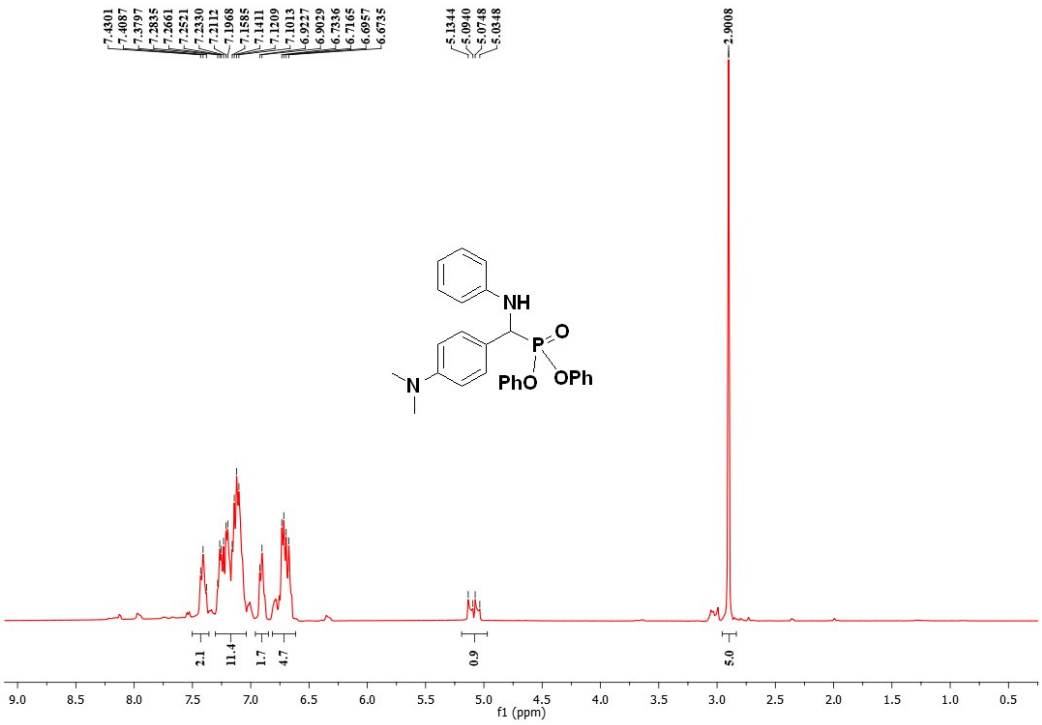


Fig FS103. ^{1}H NMR for compound **6h** in $CDCl_3$.

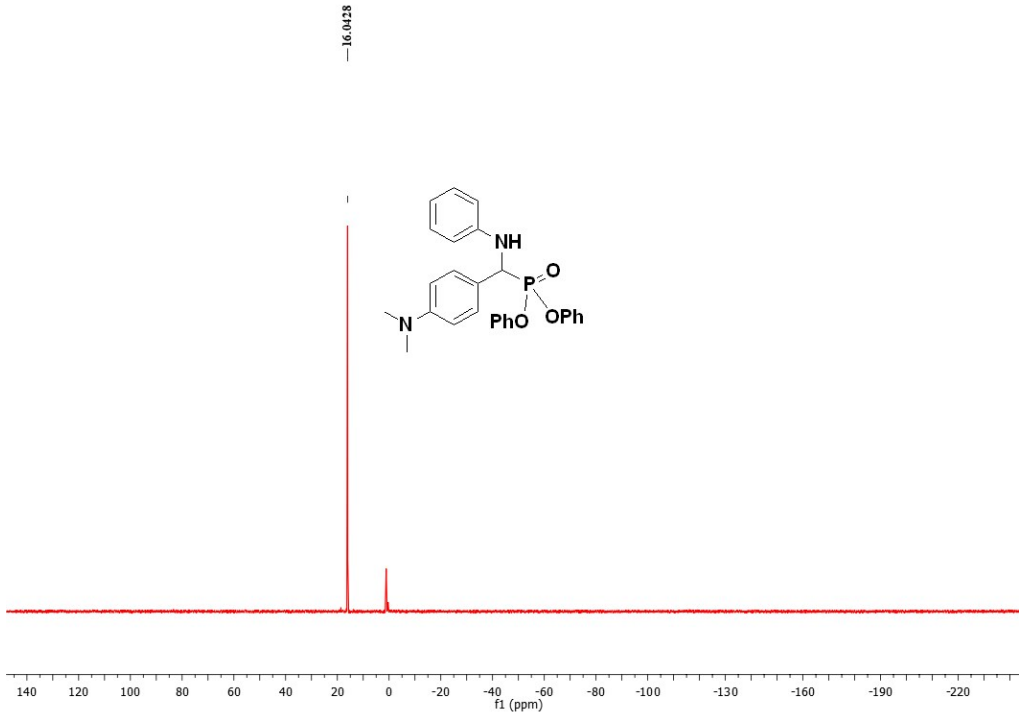


Fig FS104. $^{31}P\{^{1}H\}$ NMR for compound **6h** in $CDCl_3$.

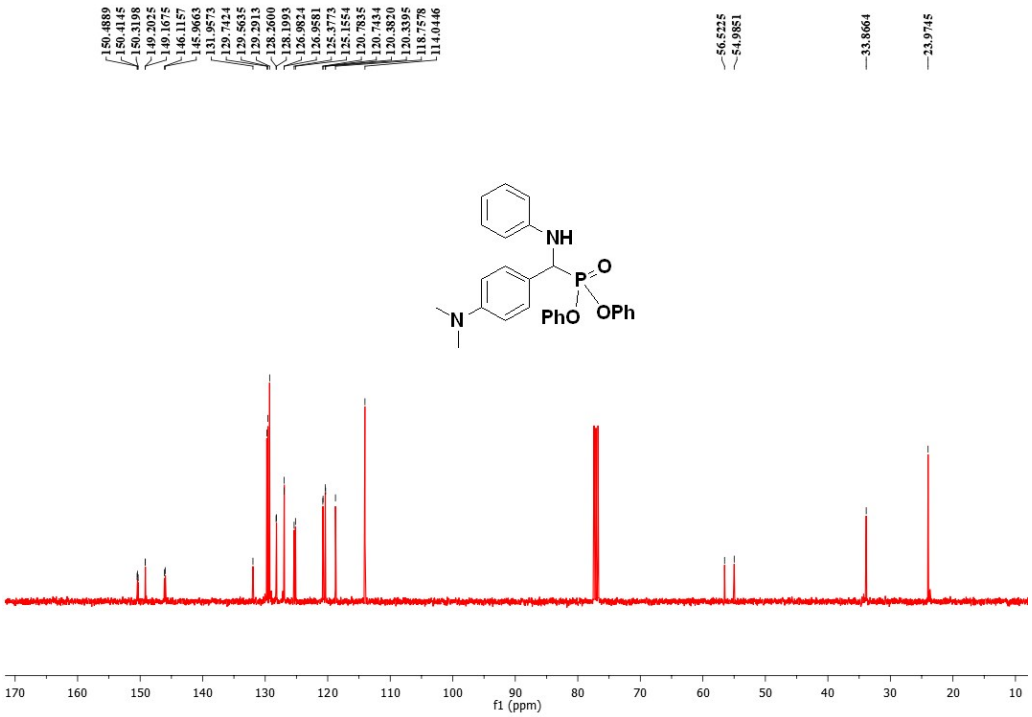


Fig FS105. $^{13}C\{^{1}H\}$ NMR for compound **6h** in $CDCl_3$.

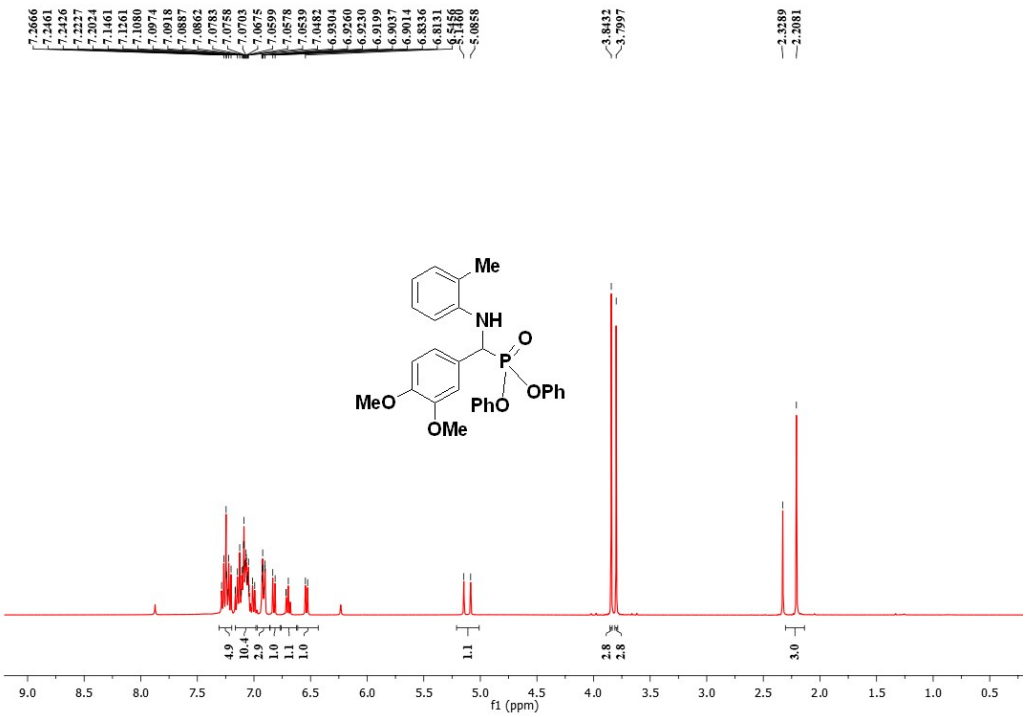


Fig FS106. ^{1}H NMR for compound **6i** in $CDCl_3$.

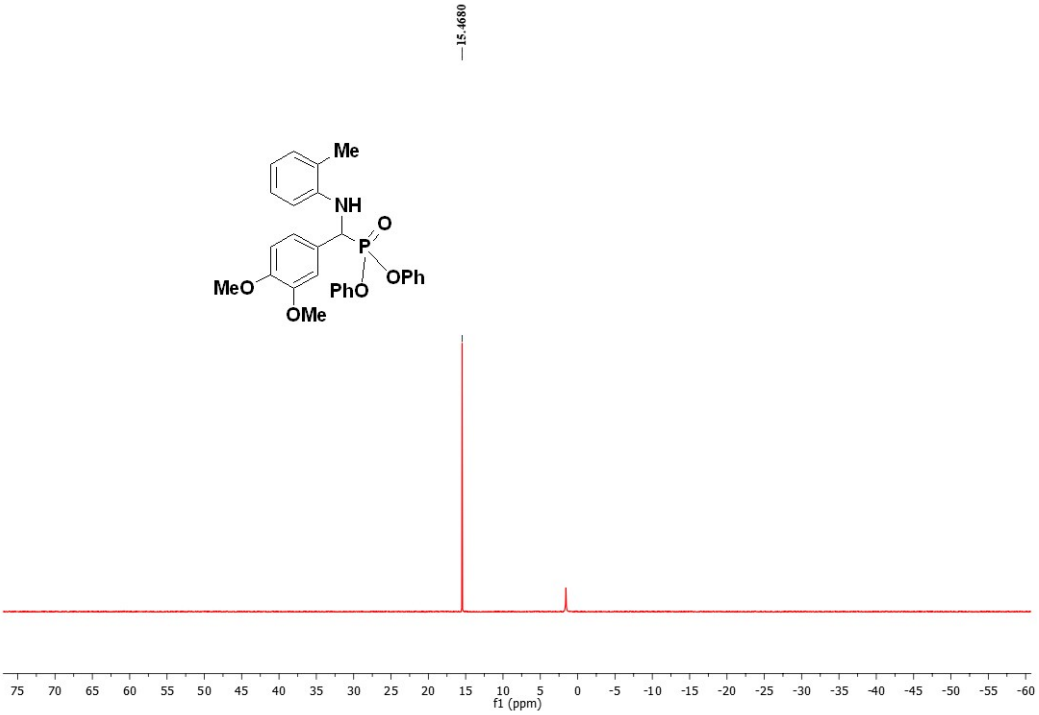


Fig FS107. $^{31}P\{^{1}H\}$ NMR for compound **6i** in $CDCl_3$.

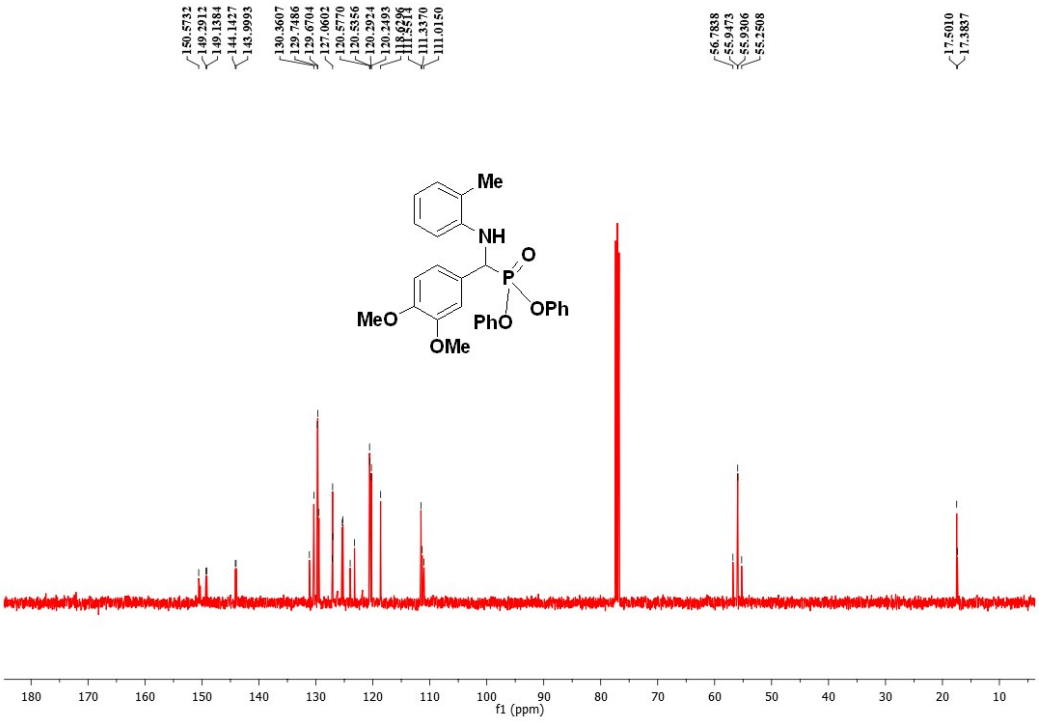


Fig FS108. $^{13}C\{^{1}H\}$ NMR for compound **6i** in $CDCl_3$.

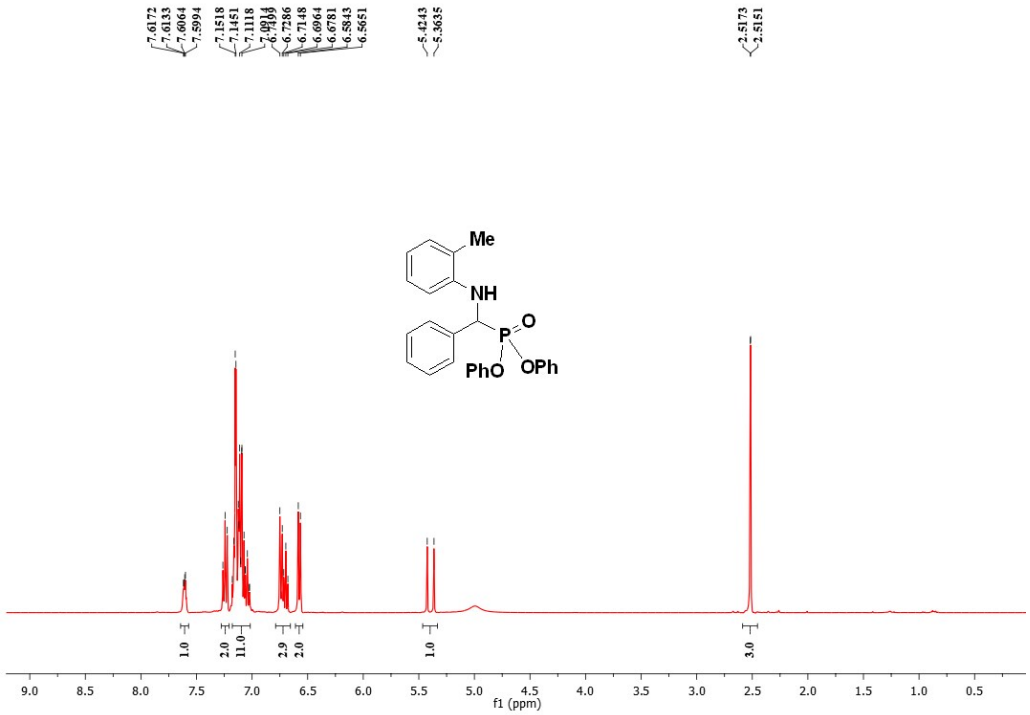


Fig FS109. ^{1}H NMR for compound **6j** in $CDCl_3$.

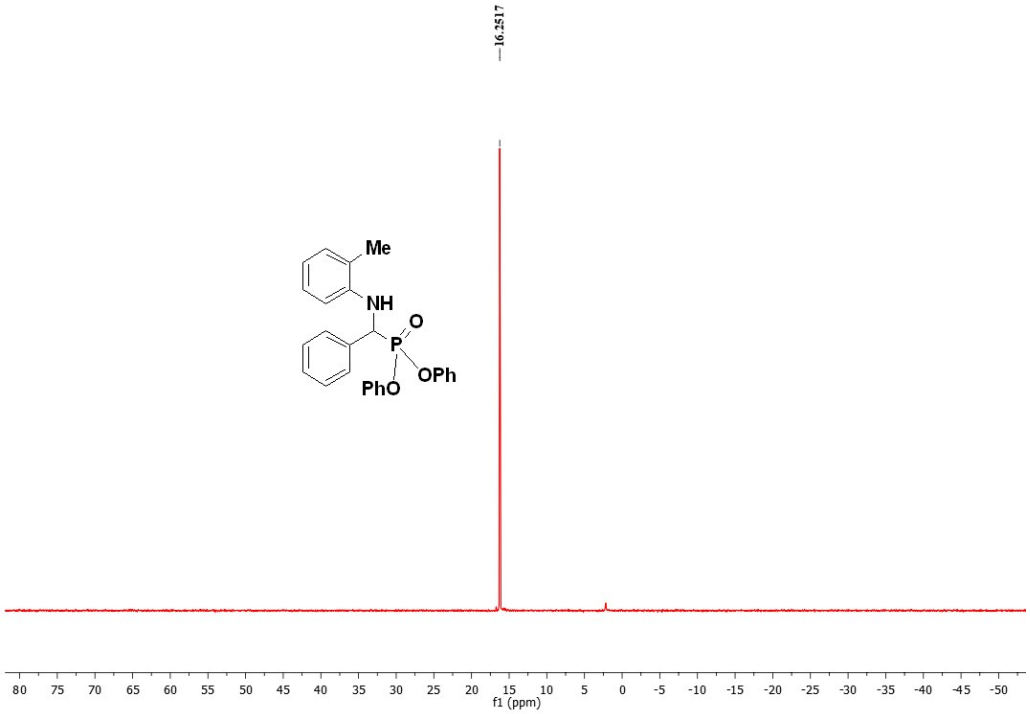


Fig FS110. $^{31}P\{^{1}H\}$ NMR for compound **6j** in $CDCl_3$.

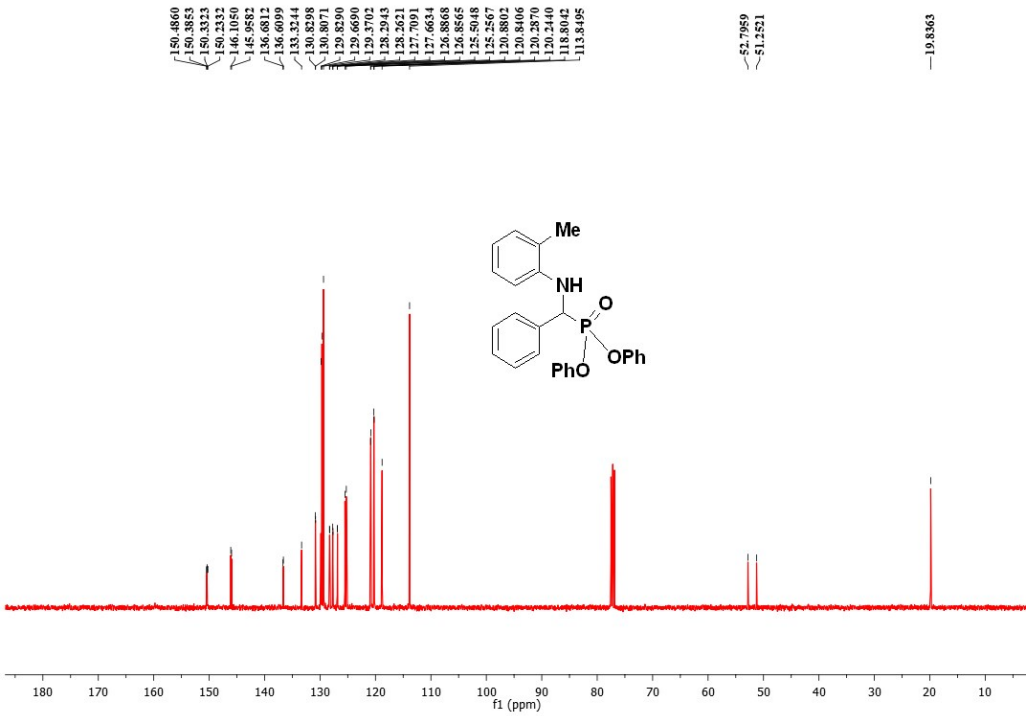


Fig FS111. $^{13}C\{^{1}H\}$ NMR for compound **6j** in $CDCl_3$.

6. Computational Details

All calculations were performed using the ORCA quantum chemical program package[5]. Geometries were optimized with the GGA (generalized gradient approximation) density functional BP86[6-7] in conjunction with def2-SVP[8] basis sets. To accelerate the overall calculations, the RI[9-11] (resolution-of-identity) approximation was applied for the expensive integral calculations. Noncovalent interactions were accounted by using atom-pairwise dispersion corrections with Becke-Johnson (D3BJ) damping.[12] Subsequent numerical frequency calculations were undertaken for the optimized geometries to confirm that they correspond to stationary points featuring no imaginary frequencies. Gibbs free energies were calculated by single point calculations with BP86/def2-TZVP[8] method on the BP86/def2-SVP geometries.

7. $(Ph)_2P(=O)H \rightarrow (Ph)_2P{-}OH$ Tautomerization : A DFT Study

Phosphorylation of the imine complex of indium (**F**) with diphenylphosphine oxide ($(Ph)_2P(=O)H$) was computed to be high in energy for the reaction to take place at room temperature (See MS, Fig. 12). So, we explored the other routes for the phosphorylation reaction. Montchamp and co-workers[13] have earlier reported a tautomerization of phosphine oxide ($H_2P(=O)H$) to phosphinous acid ($H_2P{-}OH$) involving a monomeric pathway. Thus, we studied the tautomerization of $(Ph)_2P(=O)H \rightarrow (Ph)_2P{-}OH$, in which $(Ph)_2P(=O)H$ (**P(V))** tautomerizes via a three membered transition state $^{\mathbf{Monomer}}\mathbf{TS_{P(V)-P(III)}}$ to an unstable $(Ph)_2P{-}OH$ **(P(III))** form (ΔG_{298} = 7.7 kcal mol^{-1}, relative to **P(V)**, Fig. FS112(I)). The activation barrier for this tautomerization is still too high (51.2 kcal mol^{-1}) thus we do not expect this tautomerization to occur at room temperature. The high barrier for **P(V)→P(III)** conversion is attributed to a strained three membered cyclic transition state.[14] In another study, a dimeric route for the tautomerization of phosphine oxide to phosphinous acid was reported.[15] Based on this study, we derived a dimeric pathway, in which firstly the two molecules of **P(V)** form a adduct $^{\mathbf{Dimer}}\mathbf{P(V)}$ (Fig. FS112(II)), which then undergoes via a six-membered cyclic transition state $^{\mathbf{Dimer}}\mathbf{TS_{P(V)-P(III)}}$ to produce $^{\mathbf{Dimer}}\mathbf{P(III)}$. The conversion via dimeric route is energetically affordable but endothermic in nature suggesting that **P(V)** dominates over **P(III)** in the solution. The phosphorylation of imine complex of indium is also studied with **P(III)** as this form is accessible in solution (See MS, Fig. 13).

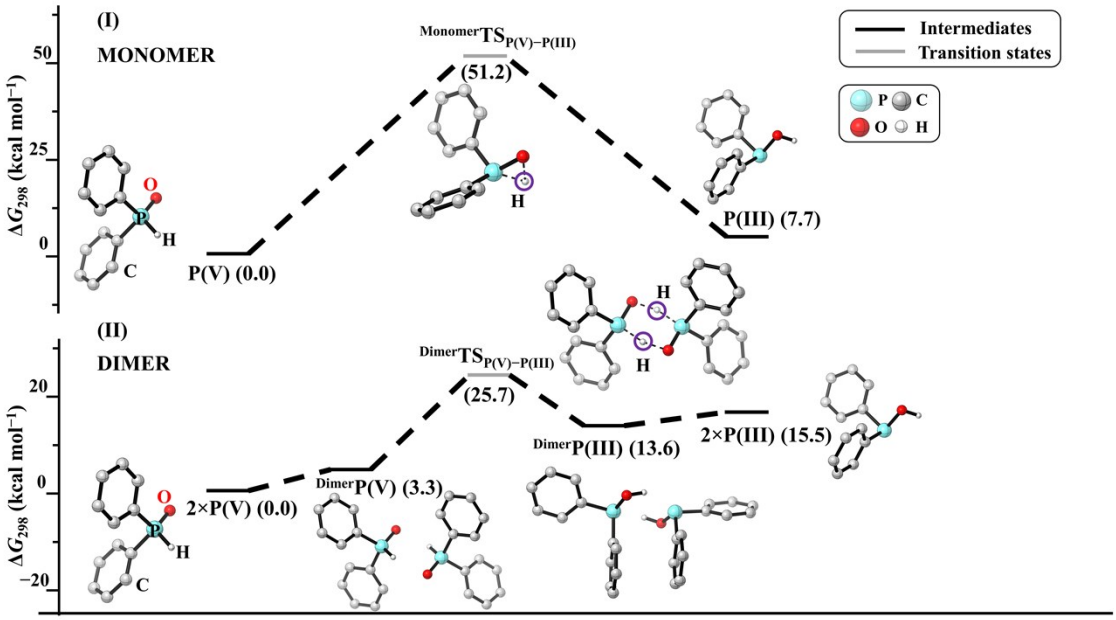


Fig. FS112 Here, **P(V)** is diphenylphosphine oxide, and **P(III)** is diphenylphosphinous acid. DFT derived mechanistic pathway for the conversion of **P(V)→P(III)** is presented in **(I)** monomer and **(II)** dimer pathways. DFT method used in the study is BP86-D3/def2-TZVP // BP86-D3/def2-SVP. Gibbs free energies are in kcal mol^{-1}.

8. Energy Table for Fig. 8

Total electronic energies and Gibbs free energies (298 K) of the molecules in Fig. 8. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

Molecule	E_{tot} [au]	G_{298} [au]	Imaginary Frequency
A	−1553.266589	−1552.804887	
TS_{AB}	−1553.228079	−1552.768911	*i*1368
B	−1553.256589	−1552.793128	
TS_{BC}	−1553.254272	−1552.791489	*i*89
C	−1553.255218	−1552.791923	
TS_{CD}	−1553.253246	−1552.791159	*i*38
D	−1553.258423	−1552.795556	
TS_{DE}	−1553.246379	−1552.786491	*i*66

E	−1553.267767	−1552.808568
F	−1476.784786	−1476.347438
H_2O	−76.464923	−76.461977

9. Energy Table for Fig. 12

Total electronic energies and Gibbs free energies (298 K) of the molecules present in Fig. 12. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

Molecule	E_{tot} [au]	G_{298} [au]	Imaginary Frequency
F	−1476.784786	−1476.347438	
G'	−2357.622829	−2357.004622	
$TS_{G'H'}$	−2357.532884	−2356.918405	*i*1564
H'	−2357.658349	−2357.035017	
$(Ph)_2P(=O)H$	−880.802463	−880.650119	

10. Energy Table for Fig. 13

Total electronic energies and Gibbs free energies (298 K) of the molecules present in Fig. 13. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

Molecule	E_{tot} [au]	G_{298} [au]	Imaginary Frequency
F	−1476.784786	−1476.347438	
G	−2357.616988	−2356.996624	
TS_{GH}	−2357.615327	−2356.994783	*i*103
H	−2357.629563	−2357.008440	
TS_{HI}	−2357.625984	−2357.005790	*i*200
I	−2357.658323	−2357.034499	
$(Ph)_2P-OH$	−880.790757	−880.637806	

11. Energy Table for Fig. FS112

Total electronic energies and Gibbs free energies (298 K) of the molecules in Fig. FS112. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

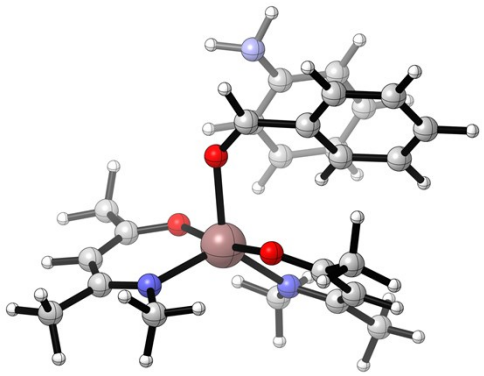
Molecule	E_{tot} [au]	G_{298} [au]	Imaginary Frequency
P(V)	−880.802463	−880.650119	
^{Monomer}**TS**$_{P(V)-P(III)}$	−880.717108	−880.568584	*i*1387
^{Dimer}**P(V)**	−1761.624399	−1761.294981	
^{Dimer}**TS**$_{P(V)-P(III)}$	−1761.583517	−1761.259327	*i*1069
^{Dimer}**P(III)**	−1761.609622	−1761.278529	
P(III)	−880.790757	−880.637806	

12. Cartesian Coordinates of the Optimized Structures

DFT optimization method: BP86-D3/def2-SVP

12.1 XYZ coordinates of the molecules present in Fig. 8

A



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O       -1.670699000     -0.329270000      1.859426000
N       -0.604144000     -1.902791000     -0.662164000
N        0.855809000     -1.684988000      2.903069000
C        2.431252000     -1.450654000     -1.070084000
C        1.499230000     -2.063490000     -1.921721000
H        1.899117000     -2.415689000     -2.880794000
C        0.105368000     -2.282643000     -1.735347000
C        3.852863000     -1.256207000     -1.529542000
H        4.030082000     -0.168569000     -1.670609000
H        4.073779000     -1.779915000     -2.476753000
H        4.555962000     -1.596518000     -0.743060000
C       -0.624011000     -2.987892000     -2.856093000
H       -1.089234000     -3.930141000     -2.499776000
H        0.058944000     -3.230474000     -3.688078000
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H	-1.448626000	-2.356004000	-3.247683000
C	-1.200195000	-1.076689000	4.103525000
H	-1.655040000	-1.124496000	5.101331000
C	-1.992806000	-0.483300000	3.114007000
C	0.104659000	-1.648033000	4.010784000
C	-3.364954000	0.039894000	3.459769000
H	-3.416563000	1.126425000	3.236787000
H	-3.632416000	-0.122955000	4.519235000
H	-4.121650000	-0.451638000	2.814753000
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H	0.893159000	-3.332055000	5.133597000
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H	1.619471000	-1.765951000	5.562073000
C	1.801666000	2.006442000	-0.908521000
C	1.035573000	1.216317000	-1.796203000
C	2.917691000	2.728281000	-1.400541000
C	1.404164000	1.122797000	-3.143485000
C	3.287862000	2.622824000	-2.744908000
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H	0.141828000	0.683064000	-1.440148000
H	3.505018000	3.354980000	-0.710281000
H	0.800962000	0.510034000	-3.828169000
H	4.167775000	3.165765000	-3.120162000
H	2.818359000	1.735568000	-4.676757000
C	1.465169000	2.131926000	0.506837000
O	0.750204000	1.341176000	1.177389000
H	1.998638000	2.932393000	1.068935000
C	-1.210655000	3.241100000	-2.113918000
C	-1.176005000	3.110342000	-0.706554000
C	-2.007720000	2.379418000	-2.880905000
H	-2.032344000	2.500193000	-3.974680000
C	-1.947898000	2.101822000	-0.085842000
C	-2.764418000	1.368066000	-2.264318000
H	-1.921822000	1.978422000	1.005463000
H	-3.394443000	0.699777000	-2.870484000
C	-2.730273000	1.239412000	-0.864073000
H	-3.323600000	0.465885000	-0.356406000
H	-0.602899000	4.016127000	-2.605927000
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C	2.180555000	-2.310972000	2.940911000
H	2.837365000	-1.834402000	3.698730000
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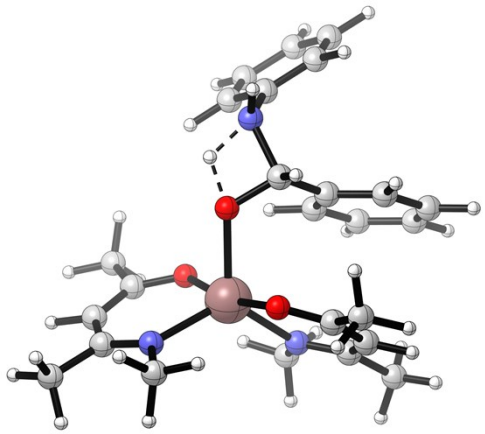

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N	0.981477000	-1.710329000	3.081725000
C	3.317412000	-1.097861000	-0.545908000
C	2.673905000	-1.797600000	-1.575184000
H	3.285379000	-1.997620000	-2.463955000
C	1.349501000	-2.322135000	-1.626986000
C	4.764478000	-0.697511000	-0.703311000
H	4.868188000	0.395583000	-0.543589000
H	5.179391000	-0.966589000	-1.691524000
H	5.370642000	-1.188734000	0.085801000
C	0.978711000	-3.097723000	-2.869575000
H	0.680977000	-4.136975000	-2.619364000
H	1.820768000	-3.139785000	-3.582253000
H	0.111135000	-2.626740000	-3.375528000
C	-1.380827000	-1.513410000	3.731127000
H	-2.047013000	-1.685627000	4.586175000
C	-2.000719000	-0.994941000	2.584956000
C	-0.014405000	-1.854202000	3.964808000
C	-3.481847000	-0.701785000	2.603714000
H	-3.648463000	0.367125000	2.356647000
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H	-3.986840000	-1.292265000	1.811809000
C	0.317488000	-2.413340000	5.329589000
H	0.788397000	-3.414714000	5.245041000
H	-0.586292000	-2.505962000	5.955971000
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C	-0.606056000	0.772728000	-1.526657000
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H	-1.267519000	0.703690000	-0.650599000
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H	-2.047071000	-0.143426000	-2.861802000
H	1.773242000	0.923191000	-4.630341000
H	-0.528288000	-0.042609000	-4.857838000
C	1.127399000	1.946969000	-0.102806000
O	0.728953000	1.246421000	1.067995000
H	2.217612000	2.165416000	-0.119042000
C	-0.628182000	4.332827000	-1.657760000
C	-0.778277000	3.649366000	-0.439614000
C	-1.765860000	4.642230000	-2.416796000
H	-1.654431000	5.174060000	-3.372951000
C	-2.048866000	3.278882000	0.027948000

C	-3.041962000	4.269764000	-1.959601000
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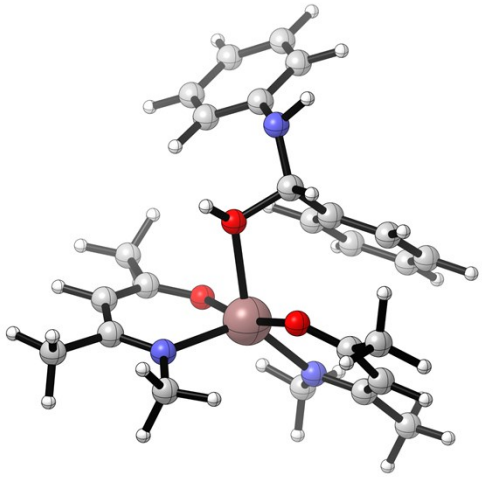

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H	3.668658000	-2.366291000	-2.307169000
C	1.611685000	-2.599917000	-1.792984000
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H	4.855865000	0.374140000	-0.653144000
H	5.400870000	-1.178860000	-1.395402000
H	5.274791000	-0.998230000	0.395196000
C	1.449613000	-3.509867000	-2.987001000
H	1.090458000	-4.513418000	-2.678815000
H	2.400884000	-3.631783000	-3.532738000
H	0.689390000	-3.102637000	-3.685773000
C	-1.557898000	-0.805383000	3.262354000
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C	-0.268082000	-1.305724000	3.617754000
C	-3.590960000	-0.258886000	1.872820000
H	-3.659087000	0.648716000	1.238281000
H	-4.067958000	-0.064731000	2.849735000
H	-4.155763000	-1.055325000	1.345164000
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C	-0.875679000	0.886145000	-1.549194000
C	1.426544000	0.925150000	-2.352107000
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C	-0.311044000	-0.107356000	-3.701501000
H	-1.624490000	1.123048000	-0.783835000
H	2.481901000	1.204216000	-2.210320000
H	-2.317664000	-0.064262000	-2.857099000
H	1.785922000	-0.002185000	-4.280469000
H	-0.622370000	-0.626574000	-4.620794000
C	0.941778000	2.034258000	-0.137767000
O	0.524018000	1.246451000	1.027381000
H	2.050540000	2.082186000	-0.154733000
C	-1.327717000	4.459721000	-1.279164000
C	-0.917521000	3.680681000	-0.178810000
C	-2.686010000	4.757026000	-1.470132000
H	-2.992568000	5.370972000	-2.330501000
C	-1.886829000	3.204666000	0.731451000
C	-3.650984000	4.263106000	-0.577451000
H	-1.566973000	2.618781000	1.603764000
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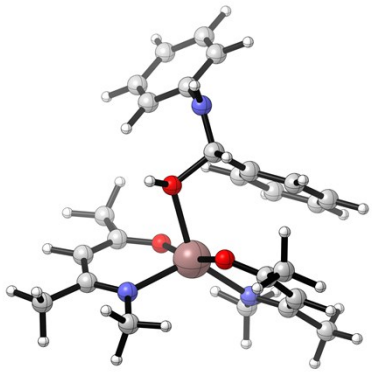

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N	0.710296000	-1.579783000	2.718783000
C	3.384060000	-1.162271000	-0.579454000
C	2.936476000	-2.061361000	-1.554886000
H	3.696890000	-2.388383000	-2.275050000
C	1.637399000	-2.614418000	-1.767040000

C	4.824689000	-0.713631000	-0.577154000
H	4.870586000	0.390437000	-0.686454000
H	5.422540000	-1.181912000	-1.379441000
H	5.285034000	-0.950151000	0.404569000
C	1.485354000	-3.554557000	-2.939005000
H	1.128804000	-4.551644000	-2.607746000
H	2.439814000	-3.686126000	-3.476859000
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C	-1.562965000	-0.829080000	3.245803000
H	-2.223241000	-0.624384000	4.098287000
C	-2.148594000	-0.668836000	1.980079000
C	-0.274743000	-1.338748000	3.592979000
C	-3.591011000	-0.243661000	1.865174000
H	-3.649075000	0.685089000	1.260537000
H	-4.071314000	-0.077094000	2.845569000
H	-4.159000000	-1.017527000	1.308467000
C	-0.029618000	-1.637112000	5.053892000
H	0.177208000	-2.717582000	5.201099000
H	-0.902437000	-1.366115000	5.672869000
H	0.858364000	-1.092253000	5.434845000
C	0.472838000	1.277131000	-1.386824000
C	-0.880474000	0.897023000	-1.556120000
C	1.416354000	0.917531000	-2.372801000
C	-1.270024000	0.175257000	-2.695317000
C	1.021616000	0.196137000	-3.508342000
C	-0.324185000	-0.172686000	-3.673623000
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H	-2.324700000	-0.113176000	-2.815590000
H	1.769471000	-0.078206000	-4.266919000
H	-0.637781000	-0.727139000	-4.571301000
C	0.937456000	2.100646000	-0.199890000
O	0.527089000	1.255042000	1.020241000
H	2.043888000	2.129521000	-0.181938000
C	-1.383549000	4.492523000	-1.348619000
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H	-1.530658000	2.686052000	1.562462000
H	-4.743896000	4.589814000	-0.661967000
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H	-0.645327000	4.825842000	-2.092502000
N	0.443485000	3.406407000	-0.128614000
H	0.996893000	1.584081000	1.814568000
H	1.066326000	4.126322000	0.240705000
C	1.971640000	-2.173215000	3.165087000
H	2.473343000	-1.555407000	3.940215000
H	1.820004000	-3.190429000	3.585471000
H	2.662458000	-2.251769000	2.305613000
C	-0.723740000	-2.995987000	-1.333765000
H	-1.027302000	-2.794630000	-2.381420000
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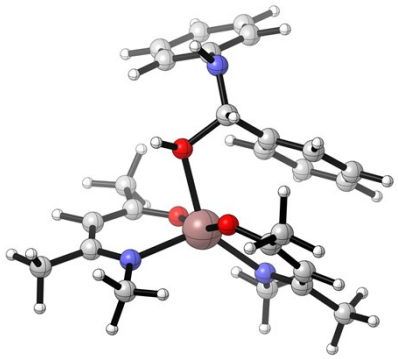
C



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N	0.641810000	-1.600634000	2.700257000
C	3.323482000	-1.154075000	-0.578891000
C	2.870213000	-2.038879000	-1.564834000
H	3.629174000	-2.364465000	-2.287144000
C	1.566556000	-2.576562000	-1.787308000
C	4.767449000	-0.716793000	-0.569769000
H	4.821918000	0.387093000	-0.677346000
H	5.364997000	-1.187966000	-1.370550000
H	5.221694000	-0.958368000	0.413461000
C	1.407861000	-3.501307000	-2.970465000
H	1.040117000	-4.498350000	-2.651465000
H	2.362412000	-3.636562000	-3.507193000
H	0.655574000	-3.099240000	-3.680676000
C	-1.598731000	-0.775202000	3.250318000
H	-2.244053000	-0.549892000	4.109051000
C	-2.185343000	-0.578773000	1.989776000
C	-0.329746000	-1.338756000	3.583720000
C	-3.598477000	-0.064018000	1.887199000
H	-3.584300000	0.919721000	1.371808000
H	-4.089554000	0.047035000	2.870131000
H	-4.195847000	-0.747709000	1.250393000
C	-0.088957000	-1.670808000	5.037981000
H	0.069381000	-2.762029000	5.165936000
H	-0.945178000	-1.371517000	5.667089000
H	0.824926000	-1.172974000	5.421816000
C	0.505699000	1.340983000	-1.362104000
C	-0.840432000	0.935568000	-1.531514000
C	1.453657000	1.017493000	-2.354573000
C	-1.220702000	0.226925000	-2.681758000
C	1.067939000	0.308213000	-3.501320000
C	-0.271274000	-0.082978000	-3.669266000
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H	-2.269987000	-0.079210000	-2.803747000
H	1.817979000	0.060111000	-4.266670000
H	-0.576749000	-0.626217000	-4.576521000
C	0.945996000	2.135746000	-0.149598000
O	0.490267000	1.276580000	1.043664000
H	2.051274000	2.155949000	-0.088945000
C	-1.477160000	4.063056000	-1.466300000
C	-0.962763000	3.692513000	-0.209977000
C	-2.858037000	4.250175000	-1.632200000
H	-3.256321000	4.538848000	-2.616311000
C	-1.834720000	3.527016000	0.884412000
C	-3.728600000	4.080875000	-0.542141000
H	-1.428551000	3.228299000	1.862057000
H	-4.810187000	4.236993000	-0.671536000
C	-3.214949000	3.727119000	0.717895000

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H	-0.780390000	4.191407000	-2.307058000
N	0.448813000	3.449684000	-0.081218000
H	0.981926000	1.553182000	1.844067000
H	0.927702000	4.048607000	0.598140000
C	1.880803000	-2.252395000	3.125960000
H	2.410841000	-1.673363000	3.911994000
H	1.691105000	-3.272352000	3.523501000
H	2.564005000	-2.338929000	2.261095000
C	-0.799694000	-2.941720000	-1.358928000
H	-1.098456000	-2.737336000	-2.407260000
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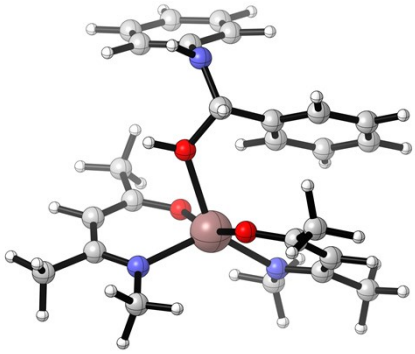

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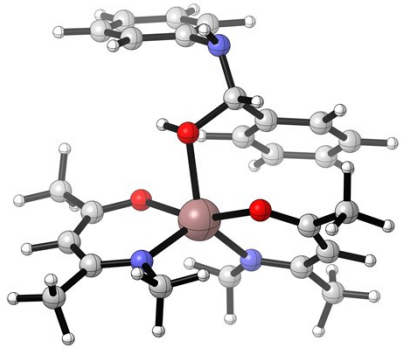
N	0.579726000	-1.603650000	2.780466000
C	3.126778000	-1.265667000	-0.799128000
C	2.569026000	-2.073843000	-1.798134000
H	3.221698000	-2.270624000	-2.657804000
C	1.287171000	-2.693756000	-1.868130000
C	4.533674000	-0.747505000	-0.952168000
H	4.518607000	0.362545000	-0.944474000
H	5.021131000	-1.098428000	-1.879315000
H	5.141924000	-1.062053000	-0.078910000
C	1.007801000	-3.540679000	-3.086321000
H	0.739985000	-4.579191000	-2.802038000
H	1.882259000	-3.578148000	-3.759151000
H	0.144412000	-3.133016000	-3.652717000
C	-1.590143000	-0.557067000	3.235429000
H	-2.207941000	-0.189706000	4.064899000
C	-2.182776000	-0.467342000	1.963017000
C	-0.361757000	-1.172733000	3.629386000
C	-3.544832000	0.154434000	1.806171000
H	-3.437224000	1.112045000	1.252208000
H	-4.042020000	0.354413000	2.771894000
H	-4.183759000	-0.505243000	1.185432000
C	-0.126568000	-1.346347000	5.111639000
H	-0.028806000	-2.421831000	5.367793000
H	-0.957082000	-0.925554000	5.704357000
H	0.818356000	-0.860614000	5.431499000
C	0.836839000	1.414591000	-1.360490000
C	-0.319065000	0.672101000	-1.683710000
C	1.847290000	1.576357000	-2.327946000
C	-0.449932000	0.094988000	-2.958752000
C	1.708866000	1.005556000	-3.601381000
C	0.560129000	0.259218000	-3.918728000
H	-1.136761000	0.564672000	-0.953966000
H	2.746716000	2.161394000	-2.081789000

H	-1.360172000	-0.472956000	-3.203150000
H	2.504335000	1.140134000	-4.349711000
H	0.452681000	-0.188141000	-4.918016000
C	0.998728000	2.085156000	-0.008676000
O	0.460633000	1.098835000	0.978587000
H	2.077287000	2.213100000	0.214722000
C	-1.616899000	3.475227000	-1.323611000
C	-1.042569000	3.491516000	-0.036119000
C	-3.006631000	3.592169000	-1.473123000
H	-3.445966000	3.577863000	-2.482088000
C	-1.872625000	3.665231000	1.089927000
C	-3.833133000	3.761179000	-0.348916000
H	-1.425432000	3.696197000	2.096702000
H	-4.920560000	3.872793000	-0.473765000
C	-3.259993000	3.812994000	0.932801000
H	-3.895434000	3.967482000	1.817720000
H	-0.964734000	3.388884000	-2.202786000
N	0.373244000	3.356154000	0.121763000
H	0.403020000	1.489078000	1.873050000
H	0.747738000	3.906792000	0.900492000
C	1.791197000	-2.262208000	3.271332000
H	2.342022000	-1.632875000	4.002305000
H	1.560133000	-3.231818000	3.761970000
H	2.472527000	-2.456664000	2.422371000
C	-0.968474000	-3.236209000	-1.135693000
H	-1.460889000	-2.909349000	-2.076832000
H	-0.861369000	-4.341034000	-1.170214000
H	-1.642529000	-2.971762000	-0.301469000

D



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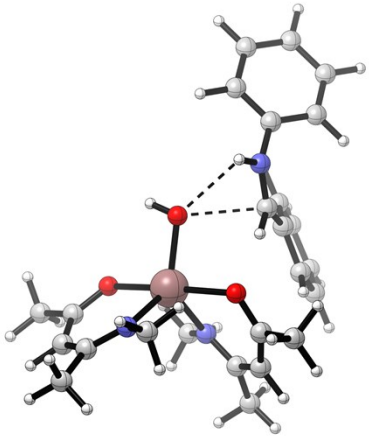
N	0.291487000	-2.366102000	-0.743372000
N	0.597226000	-1.574540000	2.923259000
C	3.122929000	-1.110732000	-0.702581000
C	2.517510000	-1.922042000	-1.670567000
H	3.138144000	-2.140405000	-2.548398000
C	1.222078000	-2.517177000	-1.693869000
C	4.533133000	-0.622250000	-0.909759000
H	4.542888000	0.487932000	-0.907131000
H	4.978348000	-0.987320000	-1.852381000
H	5.167108000	-0.944927000	-0.057980000
C	0.889949000	-3.380112000	-2.887161000
H	0.662267000	-4.421199000	-2.576865000
H	1.725602000	-3.407910000	-3.608109000
H	-0.011483000	-2.995852000	-3.407051000
C	-1.749679000	-1.011813000	3.397977000
H	-2.473052000	-1.006846000	4.223536000
C	-2.238858000	-0.525976000	2.178195000
C	-0.453764000	-1.502665000	3.749650000
C	-3.651242000	-0.010505000	2.075903000

H	-3.627113000	1.030066000	1.689921000
H	-4.190352000	-0.035427000	3.039737000
H	-4.209793000	-0.609274000	1.327066000
C	-0.268480000	-1.960521000	5.177394000
H	0.063554000	-3.018521000	5.212441000
H	-1.204845000	-1.869110000	5.754110000
H	0.517339000	-1.364799000	5.686480000
C	0.870788000	1.418119000	-1.536463000
C	-0.312577000	0.707052000	-1.823203000
C	1.865847000	1.527920000	-2.527356000
C	-0.489861000	0.114345000	-3.084324000
C	1.687275000	0.934083000	-3.784679000
C	0.507920000	0.222163000	-4.065334000
H	-1.120137000	0.625310000	-1.078003000
H	2.785759000	2.092551000	-2.310603000
H	-1.425166000	-0.422702000	-3.303088000
H	2.472761000	1.026195000	-4.549955000
H	0.365463000	-0.241121000	-5.052970000
C	1.090503000	2.116708000	-0.206181000
O	0.494032000	1.304563000	0.899495000
H	2.168437000	2.127355000	0.040567000
C	-1.431204000	3.629915000	-1.556679000
C	-0.835020000	3.595235000	-0.279560000
C	-2.826042000	3.706418000	-1.676530000
H	-3.284072000	3.736969000	-2.676732000
C	-1.651740000	3.662471000	0.871550000
C	-3.638649000	3.770528000	-0.530284000
H	-1.185304000	3.664368000	1.870299000
H	-4.731530000	3.847737000	-0.632794000
C	-3.048684000	3.762083000	0.743742000
H	-3.674340000	3.842513000	1.645424000
H	-0.786900000	3.606823000	-2.446056000
N	0.588260000	3.456120000	-0.159754000
H	-0.476671000	1.499114000	0.908190000
H	0.950276000	3.948084000	0.665036000
C	1.891699000	-2.068505000	3.402554000
H	2.255634000	-1.486459000	4.274661000
H	1.838827000	-3.137230000	3.701355000
H	2.642610000	-1.969453000	2.596219000
C	-1.016281000	-3.005926000	-0.877796000
H	-1.551687000	-2.659312000	-1.788370000
H	-0.930189000	-4.111600000	-0.930168000
H	-1.644578000	-2.745826000	-0.006887000

TS_{DE}



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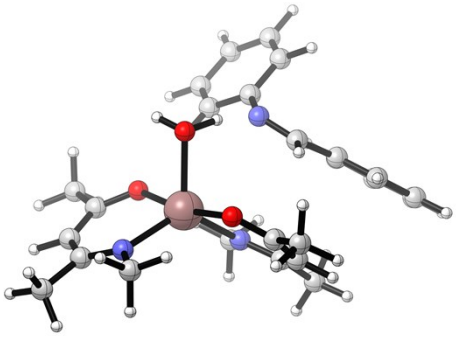
O	-1.827962000	-1.449086000	1.991803000

N	0.083088000	-1.901300000	-0.431158000
N	1.002232000	-1.665472000	3.115311000
C	2.883393000	-0.749821000	0.002605000
C	2.512859000	-1.905433000	-0.701053000
H	3.330009000	-2.462471000	-1.177081000
C	1.195618000	-2.395380000	-0.974560000
C	4.332120000	-0.324387000	0.038081000
H	4.422449000	0.718042000	-0.331519000
H	4.992501000	-0.979606000	-0.558081000
H	4.687816000	-0.311096000	1.089674000
C	1.081310000	-3.520094000	-1.978186000
H	0.561054000	-4.394412000	-1.535521000
H	2.072205000	-3.845380000	-2.338279000
H	0.473995000	-3.208336000	-2.852906000
C	-0.967451000	-3.055542000	3.571901000
H	-1.288379000	-3.911689000	4.179567000
C	-1.973281000	-2.464387000	2.788623000
C	0.387151000	-2.654546000	3.773670000
C	-3.381772000	-3.008002000	2.856693000
H	-4.071990000	-2.197117000	3.169048000
H	-3.484344000	-3.859797000	3.553103000
H	-3.706832000	-3.324413000	1.843632000
C	1.162896000	-3.402217000	4.835946000
H	2.114115000	-3.805874000	4.432342000
H	0.573177000	-4.237945000	5.249890000
H	1.436540000	-2.724945000	5.671907000
C	-0.147228000	1.536952000	-2.090663000
C	-1.398115000	1.852194000	-2.688972000
C	0.623530000	0.464798000	-2.614328000
C	-1.844367000	1.123037000	-3.792422000
C	0.185992000	-0.232251000	-3.745503000
C	-1.047923000	0.092891000	-4.333870000
H	-2.027420000	2.648958000	-2.271822000
H	1.571444000	0.187226000	-2.132396000
H	-2.820000000	1.357432000	-4.242192000
H	0.805956000	-1.038016000	-4.164908000
H	-1.399141000	-0.460985000	-5.217445000
C	0.356775000	2.156262000	-0.884672000
O	-0.510244000	1.299513000	1.432901000
H	1.104564000	1.582821000	-0.306982000
C	-0.470994000	4.881736000	-2.214146000
C	-0.734726000	4.392970000	-0.920006000
C	-1.252288000	5.928985000	-2.718326000
H	-1.048383000	6.321096000	-3.725213000
C	-1.744437000	4.959084000	-0.120121000
C	-2.277282000	6.490863000	-1.935032000
H	-1.928774000	4.567316000	0.891212000
H	-2.881609000	7.318457000	-2.334552000
C	-2.518372000	6.008690000	-0.637589000
H	-3.313688000	6.452556000	-0.020933000
H	0.344750000	4.447857000	-2.810204000
N	0.057312000	3.336178000	-0.378759000
H	-1.425450000	1.282083000	1.776851000
H	0.328577000	3.424737000	0.611804000
C	2.369397000	-1.284171000	3.467380000
H	2.470816000	-1.052900000	4.548258000
H	3.101830000	-2.084082000	3.219454000
H	2.650846000	-0.381803000	2.894278000
C	-1.222400000	-2.383756000	-0.877231000
H	-1.384717000	-2.162097000	-1.954696000
H	-1.338524000	-3.480069000	-0.733909000
H	-2.013638000	-1.887424000	-0.288559000

E



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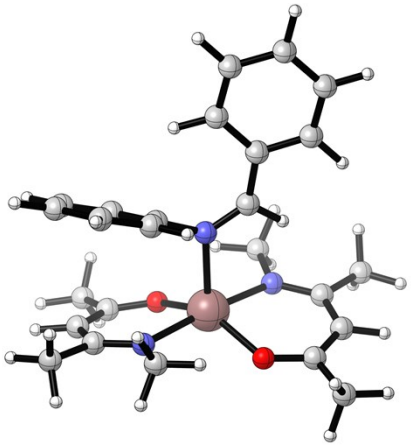
O	-1.356646000	-0.182849000	2.248554000
N	0.079025000	-1.223355000	-0.399561000
N	0.986133000	-1.807262000	3.327418000
C	3.159125000	-1.034717000	-0.182771000
C	2.368994000	-1.533448000	-1.229748000
H	2.920435000	-1.905372000	-2.102957000
C	0.949436000	-1.609663000	-1.342727000
C	4.661779000	-1.024904000	-0.314327000
H	5.044978000	-0.003651000	-0.113044000
H	5.010266000	-1.363016000	-1.306936000
H	5.104378000	-1.682714000	0.462761000
C	0.401132000	-2.153591000	-2.640129000
H	-0.240545000	-3.040443000	-2.456953000
H	1.212488000	-2.442057000	-3.329108000
H	-0.233314000	-1.397330000	-3.147090000
C	-1.349577000	-1.729135000	4.093988000
H	-2.010132000	-2.150129000	4.862764000
C	-1.949562000	-0.802674000	3.233427000
C	0.005835000	-2.175591000	4.162032000
C	-3.401266000	-0.434870000	3.409947000
H	-3.488710000	0.661578000	3.559005000
H	-3.876302000	-0.954459000	4.261138000
H	-3.961387000	-0.675295000	2.481669000
C	0.345213000	-3.127066000	5.285931000
H	0.780759000	-4.068177000	4.892374000
H	-0.546897000	-3.376987000	5.885207000
H	1.107382000	-2.685168000	5.961330000
C	0.606641000	1.380202000	-2.790798000
C	-0.708258000	1.357959000	-3.325820000
C	1.682728000	0.941514000	-3.603569000
C	-0.924206000	0.913433000	-4.635475000
C	1.463221000	0.518420000	-4.919739000
C	0.157092000	0.501960000	-5.438139000
H	-1.560297000	1.684102000	-2.716997000
H	2.700283000	0.931638000	-3.183971000
H	-1.947123000	0.893197000	-5.040146000
H	2.309801000	0.192680000	-5.541579000
H	-0.022556000	0.164615000	-6.469805000
C	0.935209000	1.718238000	-1.402936000
O	0.888410000	1.602031000	1.905556000
H	1.946043000	1.392694000	-1.087513000
C	-1.225328000	3.972530000	-1.478398000
C	-1.051369000	2.856879000	-0.630458000
C	-2.488130000	4.570334000	-1.585779000
H	-2.620022000	5.443965000	-2.241410000
C	-2.132613000	2.369871000	0.135247000
C	-3.579333000	4.064498000	-0.856332000
H	-1.985762000	1.516021000	0.814833000
H	-4.569079000	4.535406000	-0.947465000
C	-3.395851000	2.967712000	0.002589000
H	-4.244113000	2.575001000	0.583108000

H	-0.365821000	4.363123000	-2.042221000
N	0.226470000	2.265993000	-0.463628000
H	0.160596000	1.901745000	2.488229000
H	0.658825000	2.020802000	0.924971000
C	2.352952000	-2.293091000	3.539886000
H	2.723756000	-2.032067000	4.553030000
H	2.422222000	-3.396366000	3.424102000
H	3.022728000	-1.821170000	2.799138000
C	-1.357557000	-1.288217000	-0.672844000
H	-1.628942000	-0.657016000	-1.545789000
H	-1.695534000	-2.325109000	-0.883138000
H	-1.909793000	-0.914520000	0.206418000

F



In	0.157988000	-1.455688000	0.651067000
O	2.262591000	-1.834822000	0.631025000
O	-1.790804000	-2.066018000	1.271553000
N	-0.021524000	-2.732979000	-1.127462000
N	0.365917000	-0.346968000	2.521726000
C	2.932628000	-2.459373000	-0.294424000
C	2.386455000	-3.090507000	-1.420511000
H	3.109939000	-3.570542000	-2.091594000
C	1.018554000	-3.250521000	-1.792736000
C	4.423349000	-2.479824000	-0.067390000
H	4.802277000	-1.440461000	0.018650000
H	4.973851000	-3.004337000	-0.868986000
H	4.637811000	-2.974296000	0.902883000
C	0.745138000	-4.066096000	-3.036233000
H	0.132328000	-4.958920000	-2.794041000
H	1.682289000	-4.406655000	-3.508084000
H	0.164558000	-3.481526000	-3.779634000
C	-1.943392000	-0.712638000	3.259280000
H	-2.643920000	-0.436425000	4.057770000
C	-2.434416000	-1.621920000	2.317599000
C	-0.649013000	-0.117967000	3.359146000
C	-3.829271000	-2.177774000	2.458317000
H	-4.415571000	-1.956460000	1.541982000
H	-4.361887000	-1.775093000	3.338531000
H	-3.776043000	-3.283573000	2.539725000
C	-0.435929000	0.845461000	4.502787000
H	0.400327000	0.522180000	5.156291000
H	-1.345171000	0.943729000	5.121017000
H	-0.166894000	1.848463000	4.110969000
C	0.155857000	1.531623000	-2.833004000
C	-0.576583000	2.740716000	-2.684978000
C	0.834107000	1.282144000	-4.056204000
C	-0.608768000	3.667488000	-3.731013000
C	0.813114000	2.223441000	-5.090651000

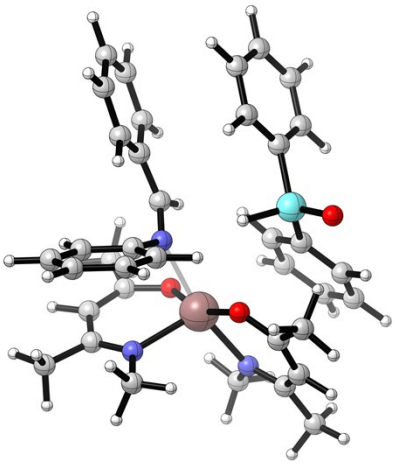
C	0.091223000	3.418656000	-4.927781000
H	-1.130823000	2.945823000	-1.761225000
H	1.385275000	0.336721000	-4.181288000
H	-1.184687000	4.597507000	-3.615770000
H	1.351077000	2.024793000	-6.029016000
H	0.065419000	4.159528000	-5.741617000
C	0.235190000	0.472982000	-1.833730000
H	0.640147000	-0.487898000	-2.205965000
C	0.357726000	2.627254000	0.471881000
C	-0.544445000	1.584990000	0.176479000
C	-0.054868000	3.683938000	1.296908000
H	0.648455000	4.498301000	1.527606000
C	-1.842667000	1.588909000	0.720175000
C	-1.356711000	3.702384000	1.829494000
H	-2.525176000	0.756169000	0.498125000
H	-1.675330000	4.533477000	2.475900000
C	-2.247640000	2.654893000	1.537504000
H	-3.264572000	2.660022000	1.955931000
H	1.374664000	2.598779000	0.054715000
N	-0.109403000	0.453619000	-0.576754000
C	1.658947000	0.299566000	2.756861000
H	1.580471000	1.405335000	2.675885000
H	2.056581000	0.055831000	3.764632000
H	2.387600000	-0.066757000	2.014138000
C	-1.383475000	-2.970370000	-1.613664000
H	-1.543711000	-2.529747000	-2.621753000
H	-1.613621000	-4.054507000	-1.678643000
H	-2.104295000	-2.523645000	-0.908190000

H_2O

O	2.690132000	7.167205000	10.675903000
H	2.690132000	7.926184000	11.288194000
H	2.690132000	6.408226000	11.288194000

12.2 XYZ coordinates of the molecules present in Fig. 12

G'



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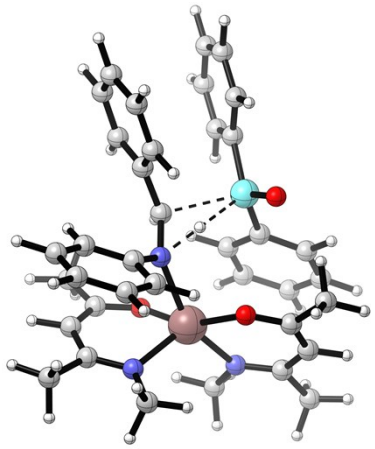
O	5.327891000	1.931171000	7.536933000
N	8.113698000	0.323905000	8.024698000
N	6.599252000	2.389240000	10.326795000

C	10.404178000	2.374297000	8.323074000
C	10.470110000	0.982655000	8.191801000
H	11.483347000	0.562320000	8.158589000
C	9.417220000	0.031243000	8.044999000
C	11.657192000	3.203579000	8.330093000
H	11.666492000	3.811743000	7.395140000
H	12.574987000	2.590318000	8.377571000
H	11.638242000	3.910859000	9.184356000
C	9.826326000	-1.414776000	7.889411000
H	9.365169000	-2.047462000	8.675767000
H	10.922390000	-1.532796000	7.942100000
H	9.475806000	-1.815399000	6.915513000
C	4.254304000	2.505100000	9.635906000
H	3.253494000	2.689357000	10.048107000
C	4.278226000	2.210016000	8.266223000
C	5.308769000	2.544820000	10.608566000
C	2.984125000	2.195157000	7.487736000
H	3.009329000	2.991917000	6.713781000
H	2.094359000	2.345678000	8.125037000
H	2.887836000	1.231977000	6.946401000
C	4.905078000	2.796439000	12.042230000
H	5.206652000	1.949352000	12.693534000
H	3.814466000	2.936134000	12.140952000
H	5.417662000	3.698555000	12.436579000
C	5.402021000	6.306460000	6.758156000
C	4.509103000	6.353001000	5.656447000
C	5.796934000	7.524029000	7.373731000
C	3.998982000	7.571547000	5.197124000
C	5.293612000	8.739234000	6.901528000
C	4.387805000	8.767537000	5.823269000
H	4.228881000	5.414827000	5.153665000
H	6.505047000	7.518113000	8.210914000
H	3.305949000	7.592084000	4.343382000
H	5.607536000	9.678778000	7.379229000
H	3.991361000	9.729456000	5.465463000
C	5.910709000	4.982705000	7.100374000
H	5.611099000	4.189522000	6.392644000
C	5.942328000	5.720688000	10.088004000
C	6.991206000	5.367928000	9.211357000
C	6.226393000	6.440587000	11.256125000
H	5.407328000	6.717421000	11.936850000
C	8.321002000	5.714554000	9.516504000
C	7.550462000	6.811542000	11.555446000
H	9.129978000	5.392793000	8.847848000
H	7.771301000	7.379119000	12.471404000
C	8.590285000	6.447867000	10.683500000
H	9.627735000	6.732692000	10.913676000
H	4.914860000	5.414266000	9.842916000
N	6.682877000	4.575661000	8.065791000
C	7.610992000	2.481929000	11.375334000
H	7.654252000	3.505996000	11.805612000
H	7.421888000	1.768058000	12.203915000
H	8.605479000	2.256504000	10.948232000
C	7.121781000	-0.738167000	7.872913000
H	7.295627000	-1.340221000	6.957044000
H	7.126041000	-1.429997000	8.743543000
H	6.116484000	-0.286729000	7.792185000
P	9.355352000	4.498514000	5.530521000
O	10.870574000	4.588869000	5.460149000
H	8.799988000	4.889764000	6.787184000
C	8.358916000	5.545473000	4.419643000
C	7.909666000	5.093626000	3.160778000
C	8.070767000	6.864182000	4.833497000
C	7.163832000	5.949332000	2.335092000
C	7.335501000	7.719736000	4.001283000
C	6.876760000	7.260094000	2.754943000

H	8.141950000	4.070837000	2.826921000
H	8.423286000	7.223221000	5.813461000
H	6.812390000	5.595276000	1.354650000
H	7.113876000	8.745510000	4.328558000
H	6.297616000	7.930605000	2.101877000
C	8.766171000	2.781177000	5.242304000
C	7.404954000	2.413986000	5.129182000
C	9.766253000	1.806753000	5.058196000
C	7.050055000	1.085463000	4.841425000
C	9.407556000	0.483076000	4.755878000
C	8.054032000	0.121813000	4.648185000
H	6.616840000	3.177765000	5.186702000
H	10.819834000	2.117134000	5.128989000
H	5.988090000	0.813302000	4.757395000
H	10.193792000	-0.269298000	4.590895000
H	7.778636000	-0.912450000	4.391622000

$TS_{G'H'}$



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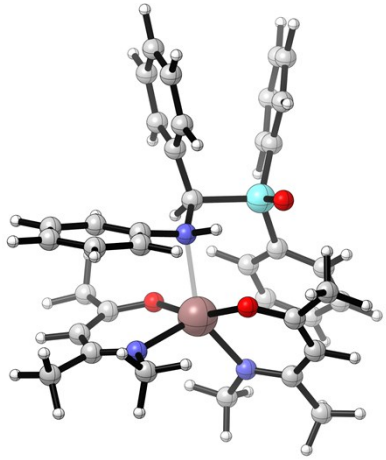
O	5.513218000	1.840792000	7.781168000
N	8.307256000	0.342203000	8.093442000
N	6.605728000	2.247922000	10.638288000
C	10.530629000	2.460886000	8.325580000
C	10.626305000	1.122738000	7.916686000
H	11.624895000	0.789105000	7.606355000
C	9.606584000	0.130364000	7.848791000
C	11.718972000	3.378771000	8.238798000
H	11.455961000	4.194573000	7.531215000
H	12.637552000	2.866654000	7.899908000
H	11.902973000	3.852411000	9.224583000
C	10.039761000	-1.266826000	7.469040000
H	9.821173000	-1.979956000	8.291353000
H	11.120914000	-1.307402000	7.250991000
H	9.482907000	-1.629240000	6.581364000
C	4.371184000	2.692862000	9.741468000
H	3.383998000	3.056565000	10.054962000
C	4.456562000	2.296427000	8.398540000
C	5.337558000	2.631891000	10.797152000
C	3.226392000	2.375339000	7.524443000
H	3.422117000	3.056271000	6.668866000
H	2.330251000	2.728921000	8.065153000
H	3.017015000	1.375856000	7.091200000
C	4.878285000	3.047360000	12.173214000
H	5.011488000	2.228862000	12.910577000
H	3.817121000	3.348856000	12.171058000
H	5.487715000	3.906035000	12.526730000
C	6.143323000	6.247653000	6.697857000

C	5.055204000	6.491762000	5.834173000
C	6.904916000	7.334562000	7.186420000
C	4.722768000	7.803926000	5.470609000
C	6.565895000	8.643150000	6.824119000
C	5.474162000	8.880944000	5.968948000
H	4.474711000	5.645283000	5.438359000
H	7.774333000	7.150217000	7.834401000
H	3.875026000	7.987158000	4.794226000
H	7.161708000	9.485214000	7.205305000
H	5.213092000	9.911266000	5.684762000
C	6.515928000	4.849134000	6.997718000
H	5.928388000	4.085616000	6.453886000
C	5.581925000	5.880234000	9.746278000
C	6.813178000	5.247930000	9.458448000
C	5.428751000	6.604542000	10.936003000
H	4.467393000	7.094887000	11.151121000
C	7.881910000	5.350866000	10.374581000
C	6.489777000	6.699144000	11.854960000
H	8.834455000	4.858676000	10.127798000
H	6.363727000	7.267225000	12.788536000
C	7.714234000	6.069946000	11.568101000
H	8.554133000	6.149936000	12.275673000
H	4.745124000	5.786201000	9.040282000
N	6.956998000	4.423059000	8.315014000
C	7.514838000	2.181360000	11.779529000
H	7.651560000	3.176621000	12.253917000
H	7.151263000	1.473765000	12.554299000
H	8.507339000	1.831857000	11.439443000
C	7.350510000	-0.757933000	7.982675000
H	7.351511000	-1.200216000	6.964420000
H	7.569725000	-1.568714000	8.709544000
H	6.331995000	-0.376729000	8.176440000
P	8.416450000	4.552498000	5.484731000
O	9.717192000	5.093748000	6.064308000
H	7.769504000	4.685461000	7.211461000
C	7.683530000	5.474462000	4.129232000
C	6.716449000	4.919897000	3.262502000
C	8.035526000	6.840418000	4.034401000
C	6.093547000	5.740771000	2.311385000
C	7.402659000	7.649004000	3.082688000
C	6.428888000	7.103429000	2.226772000
H	6.462923000	3.850689000	3.315713000
H	8.799055000	7.251361000	4.710913000
H	5.346402000	5.312097000	1.626472000
H	7.672692000	8.712421000	3.005815000
H	5.933526000	7.743362000	1.481154000
C	8.381042000	2.767225000	5.160686000
C	7.184105000	2.018827000	5.051403000
C	9.630093000	2.135045000	4.965501000
C	7.241035000	0.661389000	4.707816000
C	9.672638000	0.780277000	4.606753000
C	8.482662000	0.046817000	4.467395000
H	6.203230000	2.474843000	5.245060000
H	10.555122000	2.718625000	5.078904000
H	6.308423000	0.085080000	4.624086000
H	10.644614000	0.294644000	4.435697000
H	8.521526000	-1.011692000	4.169229000

H’



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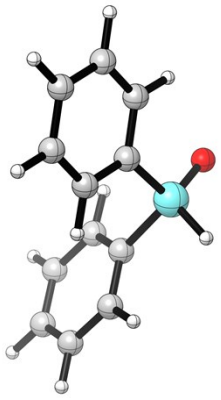
O	9.517879000	3.099572000	8.908893000
O	5.477130000	2.225347000	7.950093000
N	8.270388000	0.483383000	8.050713000
N	6.839665000	2.385929000	10.705136000
C	10.547868000	2.551558000	8.327747000
C	10.587107000	1.246051000	7.813788000
H	11.560380000	0.921742000	7.423246000
C	9.556341000	0.263765000	7.751723000
C	11.744783000	3.453195000	8.216528000
H	11.471226000	4.262950000	7.505347000
H	12.649391000	2.931360000	7.856212000
H	11.953536000	3.930890000	9.194725000
C	9.957960000	-1.126386000	7.318087000
H	9.796694000	-1.851190000	8.143839000
H	11.021889000	-1.163405000	7.027699000
H	9.342778000	-1.474129000	6.464119000
C	4.456649000	2.305750000	10.143992000
H	3.467467000	2.319779000	10.618966000
C	4.439974000	2.252999000	8.746935000
C	5.554135000	2.377883000	11.059246000
C	3.119877000	2.237635000	8.014885000
H	3.042312000	3.142413000	7.374665000
H	2.249959000	2.207619000	8.695489000
H	3.080303000	1.362961000	7.333395000
C	5.212189000	2.470643000	12.526590000
H	5.700051000	1.660554000	13.106644000
H	4.122910000	2.416535000	12.694419000
H	5.582411000	3.431673000	12.940754000
C	6.362282000	6.435215000	6.581366000
C	5.259866000	6.736544000	5.758814000
C	7.184570000	7.480402000	7.046989000
C	4.988849000	8.062672000	5.392769000
C	6.904959000	8.808389000	6.691570000
C	5.812602000	9.101615000	5.857999000
H	4.622813000	5.921002000	5.382691000
H	8.059780000	7.256823000	7.674204000
H	4.130591000	8.287422000	4.742259000
H	7.550768000	9.618454000	7.061270000
H	5.600390000	10.142757000	5.572546000
C	6.735123000	4.991043000	6.813565000
H	5.864714000	4.325208000	6.643194000
C	5.364072000	5.459944000	9.422053000
C	6.753279000	5.286223000	9.310260000
C	4.825008000	5.949429000	10.621320000
H	3.737292000	6.091189000	10.705077000
C	7.601855000	5.608486000	10.385388000
C	5.662315000	6.262657000	11.704828000

H	8.687891000	5.458002000	10.280776000
H	5.233769000	6.653500000	12.639532000
C	7.053150000	6.095043000	11.580718000
H	7.719075000	6.355889000	12.416936000
H	4.705604000	5.223760000	8.576556000
N	7.338299000	4.694373000	8.132466000
C	7.888716000	2.471312000	11.720159000
H	7.770520000	3.376283000	12.351696000
H	7.890932000	1.581139000	12.385700000
H	8.873584000	2.535920000	11.221575000
C	7.292170000	-0.599276000	7.974547000
H	7.231566000	-1.027477000	6.952746000
H	7.532750000	-1.420777000	8.682185000
H	6.290355000	-0.207211000	8.227910000
P	8.144360000	4.558320000	5.616966000
O	9.447356000	4.984186000	6.295070000
H	8.359730000	4.903993000	8.068362000
C	7.742569000	5.446455000	4.094651000
C	6.806316000	4.954229000	3.163615000
C	8.306948000	6.729073000	3.937907000
C	6.416708000	5.762011000	2.084630000
C	7.907790000	7.529983000	2.859224000
C	6.959380000	7.050445000	1.938857000
H	6.384023000	3.944062000	3.276139000
H	9.044206000	7.086571000	4.671718000
H	5.688398000	5.384246000	1.351110000
H	8.338679000	8.534328000	2.736144000
H	6.646880000	7.683472000	1.094603000
C	8.049301000	2.772982000	5.267405000
C	6.829936000	2.064128000	5.176716000
C	9.266406000	2.130573000	4.947894000
C	6.830260000	0.727571000	4.749518000
C	9.255243000	0.798493000	4.511943000
C	8.039540000	0.100374000	4.403991000
H	5.878822000	2.540814000	5.451389000
H	10.208930000	2.690459000	5.036168000
H	5.879975000	0.178261000	4.678624000
H	10.201252000	0.302662000	4.248683000
H	8.034039000	-0.939735000	4.044401000

$Ph_2P(=O)H$

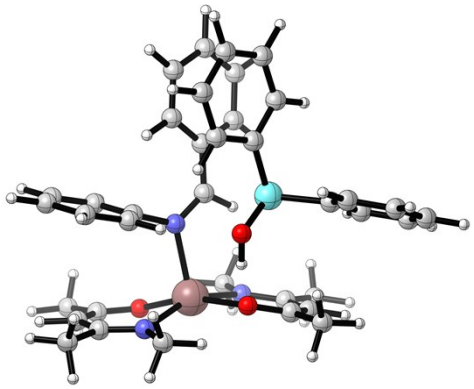


P	7.959708000	4.362247000	5.402504000
O	9.159385000	5.007864000	6.064173000
C	8.386829000	-0.167324000	4.528393000
C	9.511806000	0.676707000	4.515505000
C	7.117676000	0.351417000	4.837800000
H	10.506030000	0.264940000	4.283943000
H	6.240100000	-0.312646000	4.863316000
C	9.369660000	2.043063000	4.799920000
C	6.971078000	1.718273000	5.125878000

H	10.241327000	2.715850000	4.809314000
H	5.980021000	2.123254000	5.388115000
C	8.094929000	2.566865000	5.093911000
H	8.501391000	-1.238655000	4.302469000
C	6.631168000	4.556218000	2.877059000
C	7.564952000	5.109812000	3.775288000
C	6.384703000	5.190923000	1.650092000
H	5.658499000	4.758693000	0.944424000
C	8.258863000	6.288238000	3.440199000
C	7.071081000	6.372769000	1.318167000
H	8.994454000	6.687244000	4.156739000
H	6.876747000	6.866910000	0.353900000
C	8.008145000	6.919242000	2.210985000
H	8.547534000	7.842112000	1.948522000
H	6.105961000	3.620175000	3.124539000
H	6.704125000	4.429625000	6.113156000

12.3 XYZ coordinates of the molecules present in Fig. 13

G



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O	8.953091000	1.832796000	8.298800000
O	5.112057000	1.658526000	10.210689000
N	6.455961000	0.238198000	7.834773000
N	7.710035000	3.067063000	10.816944000
C	9.463986000	0.878682000	7.553887000
C	8.734159000	-0.175676000	7.008957000
H	9.310315000	-0.879001000	6.394805000
C	7.335987000	-0.455879000	7.106000000
C	10.942707000	1.003308000	7.308548000
H	11.174842000	2.018468000	6.928350000
H	11.317445000	0.259102000	6.583819000
H	11.485942000	0.885552000	8.269713000
C	6.836619000	-1.635878000	6.303490000
H	6.374093000	-2.398366000	6.963717000
H	7.656381000	-2.113556000	5.740176000
H	6.048008000	-1.326135000	5.586976000
C	5.497233000	3.383630000	11.838151000
H	4.984988000	3.969920000	12.610720000
C	4.708746000	2.438514000	11.171620000
C	6.890459000	3.646464000	11.706977000
C	3.263774000	2.250069000	11.559751000
H	2.614829000	2.448873000	10.681458000
H	2.954620000	2.902838000	12.395435000
H	3.094822000	1.190786000	11.843076000
C	7.476597000	4.649264000	12.673125000
H	8.212777000	4.168517000	13.350520000
H	6.688312000	5.112159000	13.291098000
H	8.015916000	5.450527000	12.129504000

C	5.429234000	4.388616000	5.552736000
C	5.053773000	3.827052000	4.305186000
C	5.366760000	5.796688000	5.716379000
C	4.593923000	4.638093000	3.263321000
C	4.918371000	6.603658000	4.665171000
C	4.523310000	6.030962000	3.443909000
H	5.132369000	2.737499000	4.161704000
H	5.682132000	6.263205000	6.655338000
H	4.296832000	4.188371000	2.304463000
H	4.886728000	7.694576000	4.797886000
H	4.172228000	6.674227000	2.623120000
C	5.911323000	3.450493000	6.564123000
H	6.034211000	2.410698000	6.215433000
C	4.614780000	5.179620000	9.001638000
C	5.910073000	4.847756000	8.561710000
C	4.424546000	6.327723000	9.784285000
H	3.412237000	6.591864000	10.124389000
C	7.014710000	5.645118000	8.916417000
C	5.520080000	7.133511000	10.138169000
H	8.011223000	5.363798000	8.545770000
H	5.365916000	8.032860000	10.752467000
C	6.811596000	6.791295000	9.699757000
H	7.670354000	7.427009000	9.964372000
H	3.769479000	4.534202000	8.723449000
N	6.119348000	3.626915000	7.848174000
C	9.139004000	3.382418000	10.859975000
H	9.331014000	4.441213000	10.578474000
H	9.563484000	3.216251000	11.871362000
H	9.676920000	2.737776000	10.146552000
C	5.042442000	-0.158279000	7.817039000
H	4.607056000	-0.067160000	6.798184000
H	4.907972000	-1.210105000	8.147493000
H	4.474842000	0.483573000	8.511234000
P	8.652281000	3.788797000	5.655546000
O	9.417529000	4.189826000	7.102814000
C	12.045758000	1.717669000	3.245137000
C	12.276102000	2.992415000	3.797362000
C	10.792345000	1.100980000	3.390280000
H	13.258056000	3.474584000	3.675209000
H	10.613480000	0.105944000	2.955865000
C	11.255119000	3.651921000	4.495769000
C	9.770081000	1.755482000	4.098470000
H	11.428501000	4.649285000	4.927680000
H	8.790805000	1.269827000	4.238750000
C	9.996188000	3.031871000	4.651512000
H	12.850579000	1.205456000	2.696281000
C	8.119794000	5.549428000	3.568029000
C	8.509274000	5.455010000	4.922054000
C	7.872925000	6.802753000	2.992790000
H	7.569523000	6.869126000	1.937261000
C	8.648300000	6.628448000	5.691353000
C	8.010647000	7.972576000	3.762282000
H	8.964191000	6.552541000	6.740585000
H	7.816722000	8.956187000	3.308440000
C	8.403283000	7.882689000	5.107657000
H	8.524133000	8.796827000	5.708679000
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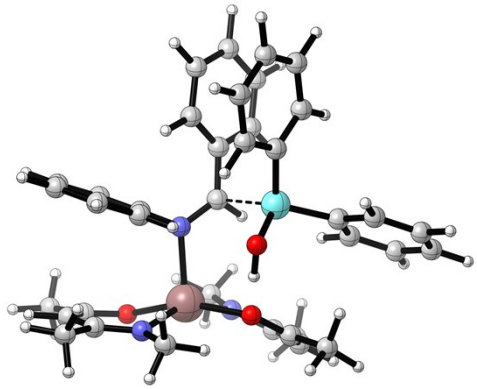

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N	7.732703000	3.086046000	10.748808000
C	9.633072000	0.908663000	7.613471000
C	8.990920000	-0.274502000	7.258417000
H	9.632776000	-1.056736000	6.834720000
C	7.589477000	-0.564902000	7.262443000
C	11.104050000	1.095457000	7.361865000
H	11.246631000	1.907616000	6.617002000
H	11.589440000	0.178753000	6.982158000
H	11.610608000	1.419185000	8.294183000
C	7.170229000	-1.860017000	6.605045000
H	6.562926000	-2.479793000	7.296447000
H	8.045221000	-2.448341000	6.279285000
H	6.531493000	-1.663785000	5.718150000
C	5.501016000	3.253032000	11.760144000
H	4.949080000	3.797983000	12.535829000
C	4.778046000	2.259989000	11.084829000
C	6.874920000	3.606327000	11.639560000
C	3.348840000	1.973300000	11.473383000
H	2.681945000	2.189721000	10.612381000
H	3.013967000	2.560938000	12.346630000
H	3.238945000	0.892083000	11.695035000
C	7.393620000	4.637963000	12.614010000
H	8.159103000	4.203995000	13.290497000
H	6.575211000	5.044284000	13.232468000
H	7.877612000	5.476243000	12.073564000
C	5.673442000	4.478277000	5.429247000
C	5.369301000	3.929974000	4.160672000
C	5.451542000	5.859489000	5.644058000
C	4.831653000	4.727676000	3.142184000
C	4.919281000	6.654622000	4.620291000
C	4.601352000	6.094940000	3.371572000
H	5.560966000	2.860695000	3.975061000
H	5.713734000	6.321740000	6.601898000
H	4.591157000	4.281874000	2.165518000
H	4.759947000	7.727768000	4.800096000
H	4.182847000	6.725338000	2.572694000
C	6.284025000	3.561680000	6.421872000
H	6.404323000	2.529435000	6.048491000
C	4.567802000	5.067200000	8.895074000
C	5.893564000	4.828899000	8.485654000
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C	5.295114000	7.066133000	10.081194000
H	7.953169000	5.495076000	8.559674000
H	5.059379000	7.942303000	10.703316000
C	6.619761000	6.822829000	9.676894000

H	7.423742000	7.511194000	9.979707000
H	3.779875000	4.366546000	8.583767000
N	6.204474000	3.638644000	7.758413000
C	9.140583000	3.476580000	10.798848000
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H	9.573504000	3.321262000	11.808617000
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H	4.956563000	-0.240194000	6.548834000
H	5.005347000	-1.096772000	8.126400000
H	4.602016000	0.636794000	8.083819000
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C	11.166279000	1.246455000	3.247090000
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C	10.866253000	3.447459000	4.243704000
C	9.116008000	1.751830000	4.450322000
H	11.235499000	4.462157000	4.456598000
H	8.132522000	1.439784000	4.833094000
C	9.595714000	3.050288000	4.719003000
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C	8.268222000	5.897212000	3.702352000
C	8.639785000	5.775687000	5.060096000
C	8.077304000	7.167256000	3.143171000
H	7.784029000	7.259475000	2.086965000
C	8.821934000	6.931442000	5.849313000
C	8.255526000	8.319102000	3.930086000
H	9.117756000	6.830452000	6.902576000
H	8.103277000	9.315480000	3.488458000
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H	8.787777000	9.101076000	5.889520000
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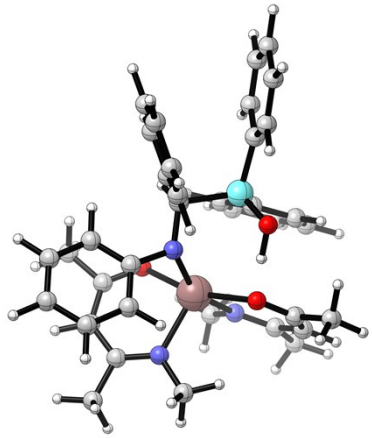
H



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N	7.544880000	2.382218000	10.469247000
C	10.797085000	2.618377000	7.646873000
C	10.871973000	1.231460000	7.661775000
H	11.875846000	0.812817000	7.513725000
C	9.827094000	0.256810000	7.812729000
C	12.022645000	3.454128000	7.388070000

H	11.864190000	4.075873000	6.481308000
H	12.932946000	2.843741000	7.249813000
H	12.179590000	4.160759000	8.229401000
C	10.258745000	-1.191087000	7.752879000
H	9.984097000	-1.727647000	8.685013000
H	11.348382000	-1.285499000	7.603784000
H	9.743124000	-1.721340000	6.924725000
C	5.101113000	2.237521000	10.490067000
H	4.247273000	2.334646000	11.172303000
C	4.764815000	2.003814000	9.147512000
C	6.375882000	2.353943000	11.117674000
C	3.308685000	1.911891000	8.756992000
H	3.093895000	2.668780000	7.974535000
H	2.624409000	2.073708000	9.608874000
H	3.103626000	0.917371000	8.308797000
C	6.387637000	2.476706000	12.622679000
H	6.989738000	1.669480000	13.088808000
H	5.367021000	2.436025000	13.040062000
H	6.851248000	3.438339000	12.925611000
C	6.280760000	6.285534000	6.096971000
C	5.306735000	6.660608000	5.152956000
C	7.107158000	7.269030000	6.674466000
C	5.165205000	8.004873000	4.777940000
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C	5.995423000	8.983836000	5.350003000
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H	7.603655000	9.380151000	6.761477000
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C	6.203442000	5.059663000	8.777803000
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H	2.995871000	5.925943000	9.670593000
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C	4.716563000	6.012482000	10.998341000
H	7.938019000	5.252964000	10.065913000
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C	6.106968000	5.824144000	11.102263000
H	6.625598000	6.067114000	12.043056000
H	4.290184000	5.080578000	7.725599000
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H	8.870226000	3.456147000	11.763501000
H	8.936071000	1.672769000	11.936926000
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H	7.653670000	-1.311497000	7.365458000
H	7.766514000	-1.086027000	9.143789000
H	6.565154000	-0.148522000	8.191841000
P	7.935290000	4.324987000	5.265801000
O	9.310159000	4.860272000	5.880916000
C	8.077296000	-0.245490000	4.648212000
C	9.246544000	0.525869000	4.524875000
C	6.861818000	0.360850000	5.007848000
H	10.198185000	0.047764000	4.249954000
H	5.949419000	-0.242264000	5.121006000
C	9.204352000	1.908830000	4.743490000
C	6.806449000	1.743510000	5.235118000
H	10.113861000	2.517202000	4.636318000
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C	7.980711000	2.521669000	5.096371000
H	8.114334000	-1.329039000	4.458903000
C	6.962208000	4.456263000	2.672142000

C	7.742280000	5.091599000	3.660989000
C	6.678935000	5.139214000	1.480005000
H	6.074793000	4.652090000	0.700300000
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C	7.171721000	6.440106000	1.281565000
H	8.841557000	6.880456000	4.250703000
H	6.943851000	6.973349000	0.346392000
C	7.957653000	7.063333000	2.267752000
H	8.342187000	8.080683000	2.106586000
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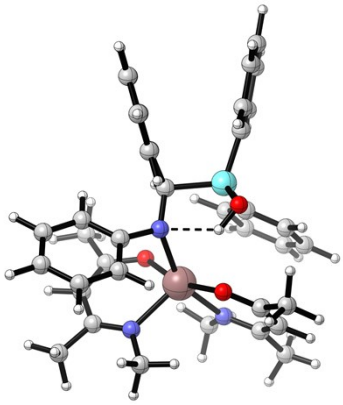

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N	7.267795000	2.359402000	10.490330000
C	10.803869000	2.609028000	7.890206000
C	10.887075000	1.229032000	7.671522000
H	11.885786000	0.848002000	7.421268000
C	9.865705000	0.232295000	7.759126000
C	12.027792000	3.475953000	7.730715000
H	11.832215000	4.240110000	6.949292000
H	12.932348000	2.901720000	7.460542000
H	12.215711000	4.029952000	8.673500000
C	10.310586000	-1.202092000	7.582651000
H	10.084808000	-1.798667000	8.491266000
H	11.394760000	-1.268080000	7.385398000
H	9.767608000	-1.689070000	6.746244000
C	4.844534000	2.342413000	10.149676000
H	3.906103000	2.504512000	10.694627000
C	4.696624000	2.055943000	8.786415000
C	6.020316000	2.435259000	10.957236000
C	3.309430000	1.991307000	8.190212000
H	3.209747000	2.769785000	7.403496000
H	2.509480000	2.137079000	8.938155000
H	3.165084000	1.011922000	7.689103000
C	5.819227000	2.646578000	12.438647000
H	6.278583000	1.825841000	13.028142000
H	4.748383000	2.704556000	12.697541000
H	6.309136000	3.590044000	12.756072000
C	6.110506000	6.122150000	6.153706000
C	5.047205000	6.341928000	5.257559000
C	6.876346000	7.215765000	6.604035000
C	4.752721000	7.638453000	4.810331000
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C	5.518081000	8.726926000	5.262225000
H	4.451864000	5.487515000	4.898503000
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C	6.504203000	4.697001000	6.507835000
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C	5.304422000	5.517914000	9.058284000
C	6.665283000	5.161963000	8.908257000
C	4.855370000	6.121776000	10.241847000
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C	7.559934000	5.439549000	9.970766000
C	5.744345000	6.373351000	11.300654000
H	8.622764000	5.182593000	9.839370000
H	5.385666000	6.848701000	12.225514000
C	7.101651000	6.031137000	11.155880000
H	7.815058000	6.249680000	11.965930000
H	4.591287000	5.306529000	8.249504000
N	7.175703000	4.495767000	7.765673000
C	8.406710000	2.434815000	11.399196000
H	8.436035000	3.403352000	11.943116000
H	8.391162000	1.619635000	12.154337000
H	9.345465000	2.345428000	10.820563000
C	7.633362000	-0.638590000	8.111220000
H	7.686131000	-1.330701000	7.245411000
H	7.824493000	-1.229173000	9.034194000
H	6.605889000	-0.236438000	8.159552000
P	7.870866000	4.254760000	5.291090000
O	9.211263000	4.850084000	5.959214000
C	8.272364000	-0.264910000	4.530426000
C	9.412869000	0.557225000	4.532575000
C	7.007046000	0.271793000	4.825998000
H	10.402235000	0.130529000	4.312568000
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C	9.295101000	1.924595000	4.812120000
C	6.872707000	1.638103000	5.108052000
H	10.181755000	2.574269000	4.811613000
H	5.886387000	2.045114000	5.371240000
C	8.020374000	2.465989000	5.095172000
H	8.370095000	-1.335333000	4.294028000
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C	7.661276000	5.045738000	3.703958000
C	6.602205000	5.081451000	1.520015000
H	6.033060000	4.576219000	0.725632000
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C	7.751487000	7.063056000	2.362277000
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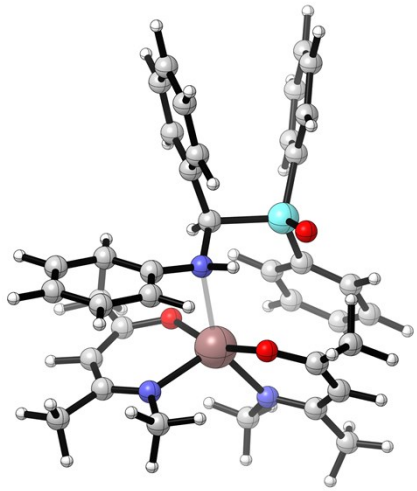

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N	8.578104000	0.407422000	8.045530000
N	7.140821000	2.453615000	10.541653000
C	10.757727000	2.594936000	8.032619000
C	10.847733000	1.245238000	7.658936000
H	11.824614000	0.927325000	7.271799000
C	9.864292000	0.215527000	7.731012000
C	11.901900000	3.536215000	7.781325000
H	11.561698000	4.249491000	6.998762000
H	12.821199000	3.023387000	7.445630000
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C	10.322641000	-1.192690000	7.432702000
H	10.223492000	-1.830692000	8.336245000
H	11.378224000	-1.210527000	7.111409000
H	9.700038000	-1.659942000	6.643563000
C	4.747511000	2.220117000	10.078971000
H	3.775298000	2.226047000	10.587835000
C	4.687271000	2.052640000	8.692269000
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C	3.346188000	1.907763000	8.014387000
H	3.199157000	2.745410000	7.299357000
H	2.502217000	1.895096000	8.727476000
H	3.330384000	0.973987000	7.415419000
C	5.574304000	2.611637000	12.411248000
H	6.106515000	1.863029000	13.033319000
H	4.493537000	2.536946000	12.620735000
H	5.925237000	3.612271000	12.738879000
C	6.343902000	6.156581000	6.151102000
C	5.195631000	6.355521000	5.361103000
C	7.145939000	7.261885000	6.498273000
C	4.858102000	7.640331000	4.912121000
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H	5.937040000	4.039173000	6.386789000
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C	6.870160000	5.231227000	8.944281000
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H	3.868413000	5.989402000	10.394870000
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C	5.816538000	6.332110000	11.301503000
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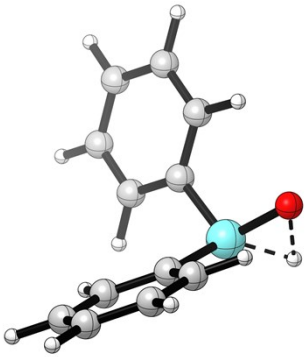
H	5.401790000	6.770401000	12.221342000
C	7.208820000	6.224545000	11.134679000
H	7.890105000	6.580247000	11.922119000
H	4.802652000	5.012686000	8.299492000
N	7.441863000	4.578613000	7.792251000
C	8.219449000	2.664074000	11.506661000
H	8.074812000	3.602954000	12.080400000
H	8.293885000	1.822993000	12.229620000
H	9.180855000	2.744525000	10.966017000
C	7.652106000	-0.720110000	8.121692000
H	7.583595000	-1.265703000	7.157568000
H	7.952322000	-1.443807000	8.909317000
H	6.639631000	-0.348357000	8.363443000
P	8.165701000	4.278935000	5.265341000
O	9.472071000	4.820695000	5.845942000
C	8.228919000	-0.278745000	4.491771000
C	9.415105000	0.475779000	4.495927000
C	7.001197000	0.330274000	4.804623000
H	10.375464000	-0.004650000	4.257416000
H	6.074078000	-0.261638000	4.815326000
C	9.378631000	1.844107000	4.797812000
C	6.952783000	1.701814000	5.096157000
H	10.297924000	2.447804000	4.802920000
H	5.988610000	2.165948000	5.346412000
C	8.142995000	2.465093000	5.086432000
H	8.260197000	-1.349279000	4.237888000
C	6.714777000	4.384009000	2.844401000
C	7.656993000	5.004015000	3.689140000
C	6.242134000	5.071637000	1.716314000
H	5.509964000	4.591898000	1.049402000
C	8.143767000	6.295328000	3.397233000
C	6.707236000	6.368059000	1.436382000
H	8.887691000	6.754871000	4.064567000
H	6.329736000	6.905130000	0.553381000
C	7.661338000	6.975739000	2.271185000
H	8.031768000	7.985690000	2.042863000
H	6.353234000	3.367202000	3.060050000
H	8.449433000	4.828269000	7.676283000

12.4 XYZ coordinates of the molecules present in Fig. FS112

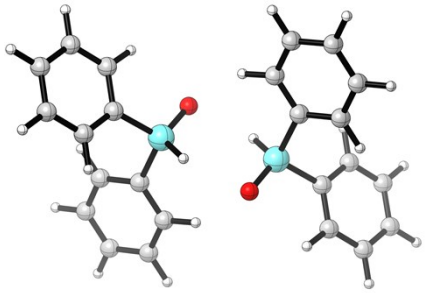
Monomer$TS_{P(V)-P(III)}$



P	7.870578000	4.321486000	5.353009000
O	9.280238000	4.927783000	5.893662000
C	8.459585000	-0.203265000	4.548691000
C	9.549233000	0.638939000	4.830224000
C	7.153027000	0.317472000	4.526318000

H	10.570227000	0.227716000	4.860414000
H	6.298347000	-0.345489000	4.322111000
C	9.338766000	2.003443000	5.082541000
C	6.935093000	1.681759000	4.771808000
H	10.170752000	2.684597000	5.325615000
H	5.908186000	2.081128000	4.776739000
C	8.032553000	2.528793000	5.030308000
H	8.627390000	-1.274084000	4.355922000
C	6.437168000	4.611385000	2.886176000
C	7.462266000	5.075714000	3.737333000
C	6.185251000	5.272649000	1.676195000
H	5.388659000	4.908142000	1.009229000
C	8.228304000	6.202307000	3.372916000
C	6.952204000	6.393903000	1.309105000
H	9.027416000	6.537851000	4.053632000
H	6.750924000	6.909001000	0.357488000
C	7.974585000	6.853778000	2.155320000
H	8.578351000	7.728262000	1.867471000
H	5.843457000	3.725147000	3.156015000
H	8.011283000	4.987538000	6.664427000

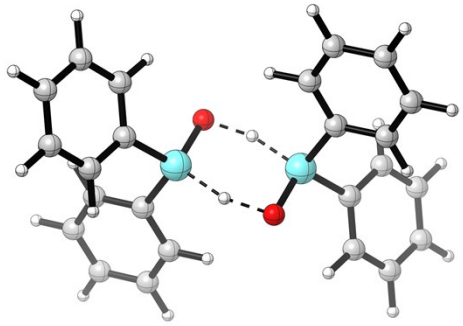
Dimer P(V)



P	5.515965134	4.977530648	7.470861189
O	5.003227715	6.404033821	7.261621493
H	6.934535341	4.824137941	7.369539491
P	7.185536250	7.191391417	5.068746346
O	7.697589311	5.764584079	5.277538254
H	5.767009034	7.345455020	5.169711359
C	7.822901619	8.426407739	6.251012582
C	7.139907038	8.642060867	7.467483676
C	9.037115967	9.097303503	5.991308062
C	7.670840188	9.537459828	8.409765777
C	9.561441971	9.986969239	6.941072695
C	8.877083571	10.209553954	8.149183323
H	6.209040321	8.082123675	7.662540680
H	9.568909751	8.927827619	5.041844152
H	7.137533628	9.709365051	9.357523006
H	10.508741828	10.509490868	6.738604770
H	9.288692764	10.909922704	8.892723819
C	7.627390610	7.837920356	3.417443364
C	8.401562995	7.019855062	2.573499573
C	7.209772370	9.112317970	2.982035611
C	8.760594749	7.478041722	1.294952421
C	7.568871266	9.564949672	1.703563298
C	8.344855786	8.747989381	0.860587296
H	8.711271831	6.029641638	2.940945308
H	6.610833774	9.755410788	3.647583721
H	9.366074737	6.839819250	0.632732646
H	7.244416530	10.559530064	1.362208821
H	8.626158381	9.104956437	-0.141776256
C	5.074871789	4.331418773	9.122541926
C	4.300725254	5.149520017	9.966472732

C	5.493061630	3.057310485	9.558245150
C	3.942289812	4.691659936	11.245306241
C	5.134554436	2.605001440	10.836998416
C	4.358597071	3.421999503	11.679965562
H	3.990529334	6.139488492	9.598776336
H	6.091957078	2.414175631	8.892701787
H	3.336823853	5.329909593	11.907513098
H	5.459440567	1.610638845	11.178577378
H	4.077745516	3.065281652	12.682544914
C	4.878813922	3.741776537	6.289272463
C	5.561243088	3.526172645	5.072493829
C	3.665145804	3.070208728	6.549865074
C	5.030369961	2.630107078	4.130808796
C	3.140870486	2.179887505	5.600689848
C	3.824714842	1.957312129	4.392286251
H	6.491599230	4.086706420	4.876706336
H	3.133749258	3.239669352	7.499551184
H	5.563264901	2.458223419	3.182817255
H	2.193998855	1.656854328	5.803850531
H	3.413159372	1.256400960	3.649226559

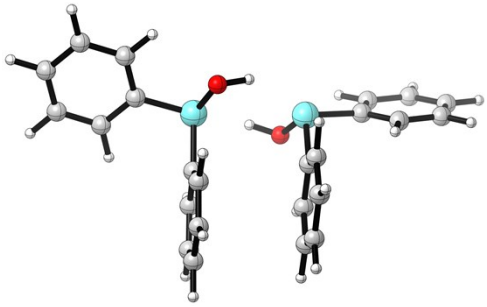
Dimer$TS_{P(V)-P(III)}$



P	5.534854000	4.935958000	7.106702000
O	4.823897000	6.348011000	6.861789000
H	7.028692000	5.191614000	6.528361000
P	7.167382000	7.232672000	5.433695000
O	7.878325000	5.820610000	5.678590000
H	5.673576000	6.977029000	6.011949000
C	7.901875000	8.527408000	6.500165000
C	7.254792000	8.791079000	7.726885000
C	9.093283000	9.208099000	6.174553000
C	7.795370000	9.730720000	8.618472000
C	9.629479000	10.146970000	7.068847000
C	8.981117000	10.408937000	8.289278000
H	6.325075000	8.251601000	7.970875000
H	9.597286000	9.003510000	5.217020000
H	7.287701000	9.936637000	9.573179000
H	10.560127000	10.677293000	6.815065000
H	9.403357000	11.147921000	8.987947000
C	7.568154000	7.755893000	3.734002000
C	8.266010000	6.865735000	2.893819000
C	7.154057000	9.012644000	3.242960000
C	8.552736000	7.235166000	1.569249000
C	7.442809000	9.375225000	1.919244000
C	8.141958000	8.486951000	1.080789000
H	8.584052000	5.894669000	3.302849000
H	6.612431000	9.710726000	3.901515000
H	9.101230000	6.540592000	0.913988000
H	7.121958000	10.356693000	1.538250000
H	8.367109000	8.773864000	0.042349000
C	5.134120000	4.412780000	8.806423000
C	4.436204000	5.302924000	9.646571000
C	5.548297000	3.156074000	9.297516000

C	4.149498000	4.933525000	10.971154000
C	5.259563000	2.793524000	10.621243000
C	4.560354000	3.681785000	11.459663000
H	4.118103000	6.273954000	9.237502000
H	6.089970000	2.458003000	8.638989000
H	3.600956000	5.628088000	11.626387000
H	5.580477000	1.812092000	11.002277000
H	4.335219000	3.394897000	12.498114000
C	4.800289000	3.641192000	6.040306000
C	5.447298000	3.377487000	4.813554000
C	3.608905000	2.960505000	6.366007000
C	4.906673000	2.437820000	3.922025000
C	3.072659000	2.021605000	5.471772000
C	3.720950000	1.759605000	4.251310000
H	6.377002000	3.916958000	4.569494000
H	3.104960000	3.165120000	7.323564000
H	5.414286000	2.231875000	2.967294000
H	2.142029000	1.491285000	5.725626000
H	3.298672000	1.020596000	3.552690000

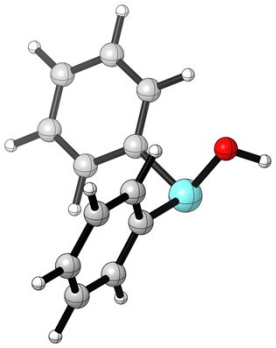
Dimer P(III)



P	5.399819000	4.334877000	5.710053000
O	4.224093000	5.527020000	5.571671000
H	7.234304000	5.174922000	4.556451000
P	6.688430000	7.272730000	4.609672000
O	7.782045000	6.003128000	4.480410000
H	4.630884000	6.235276000	5.002326000
C	6.911260000	7.855994000	6.342701000
C	5.887650000	8.623924000	6.933074000
C	8.053628000	7.515701000	7.092849000
C	6.025996000	9.089361000	8.250931000
C	8.179331000	7.965197000	8.414463000
C	7.173004000	8.760857000	8.991396000
H	4.973088000	8.850644000	6.360354000
H	8.827580000	6.884387000	6.630976000
H	5.227139000	9.695262000	8.706113000
H	9.066229000	7.688014000	9.004237000
H	7.276602000	9.111321000	10.029435000
C	7.630050000	8.546807000	3.675745000
C	8.363888000	8.161126000	2.533528000
C	7.566861000	9.911156000	4.030858000
C	9.027733000	9.127997000	1.762648000
C	8.227572000	10.873968000	3.252619000
C	8.958672000	10.486287000	2.116477000
H	8.426617000	7.095289000	2.266838000
H	7.016651000	10.220105000	4.933012000
H	9.603948000	8.816322000	0.877588000
H	8.179710000	11.935168000	3.542909000
H	9.478276000	11.242869000	1.509010000
C	6.109813000	4.631091000	7.385599000
C	5.418970000	5.386081000	8.353153000
C	7.388803000	4.117260000	7.677970000
C	5.994884000	5.598447000	9.613141000
C	7.954693000	4.315732000	8.948197000

C	7.256183000	5.054829000	9.916224000
H	4.436972000	5.811284000	8.097778000
H	7.951370000	3.571481000	6.902331000
H	5.459352000	6.196422000	10.366149000
H	8.951945000	3.909639000	9.175782000
H	7.703986000	5.225460000	10.907289000
C	4.305001000	2.896192000	6.044525000
C	4.803254000	1.764958000	6.725942000
C	2.983379000	2.885012000	5.552767000
C	3.987220000	0.639533000	6.914365000
C	2.169614000	1.756849000	5.748495000
C	2.668589000	0.631691000	6.425965000
H	5.827669000	1.770687000	7.129874000
H	2.596489000	3.774753000	5.034973000
H	4.380948000	-0.235599000	7.454106000
H	1.135890000	1.759733000	5.369905000
H	2.028874000	-0.251177000	6.578792000

P(III) or $Ph_2P{-}OH$



P	7.363321000	4.285442000	5.567359000
O	8.851859000	4.931974000	6.067226000
C	8.800040000	0.002488000	4.382126000
C	9.606003000	0.809615000	5.201284000
C	7.574200000	0.499857000	3.904160000
H	10.569632000	0.429214000	5.573794000
H	6.938625000	-0.126247000	3.258523000
C	9.191528000	2.107197000	5.546726000
C	7.158183000	1.795395000	4.243642000
H	9.821528000	2.750783000	6.178573000
H	6.203174000	2.181078000	3.852896000
C	7.966670000	2.610235000	5.065041000
H	9.125451000	-1.013735000	4.113107000
C	5.935277000	5.085590000	3.278651000
C	7.209814000	5.024542000	3.877502000
C	5.788668000	5.598609000	1.978272000
H	4.791682000	5.637333000	1.512315000
C	8.332561000	5.513731000	3.178839000
C	6.910802000	6.076709000	1.282268000
H	9.321009000	5.477865000	3.662133000
H	6.796283000	6.485890000	0.267111000
C	8.180566000	6.040459000	1.887932000
H	9.059556000	6.421201000	1.344962000
H	5.050570000	4.735585000	3.835798000
H	8.682756000	5.479133000	6.856541000

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