Electronic Supplementary Material (ESI) for Chemical Communications.

Novel zwitterionic complexes arising from the coordination of an ambiphilic phosphorus-aluminum ligand to gold

Marc Devillard, Emmanuel Nicolas, Christian Appelt, Jana Backs, Sonia Mallet-Ladeira, Ghenwa Bouhadir, J. Chris Slootweg,* Werner Uhl* and Didier Bourissou**

SUPPLEMENTARY INFORMATION

Experimental details and spectroscopic data **S2**

NMR spectra **S9**

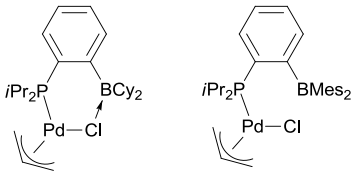
Determination of the activation barrier **S26**

Crystallographic data **S27**

Computational details **S28**

Theoretical results **S29**

Chart S1



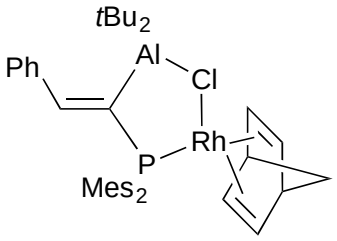
EXPERIMENTAL DETAILS AND SPECTROSCOPIC DATA

General comments:

All reactions and manipulations were carried out under an atmosphere of dry argon using standard Schlenk techniques. All solvents were sparged with argon and dried using an MBRAUN Solvent Purification System (SPS). ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded on a Bruker Avance 500 spectrometer. Chemical shifts are expressed with a positive sign, in parts per million, calibrated to residual ^{1}H (5.32 ppm) and ^{13}C (53.84 ppm) solvent signals and 85% H_3PO_4 (0 ppm) respectively. Mass spectra were recorded on a Waters LCT mass spectrometer. Melting points were measured with a Stuart SMP40 apparatus (resolution of 0.1 °C). The phosphine-alane ligand $Mes_2P(C{=}CHPh)Al\textit{t}Bu_2$ **1** was prepared as previously described.[1]

[1] Appelt, C.; Westenberg, H.; Bertini, F.; Ehlers, A. W.; Slootweg, J. C.; Lammertsma, K.; Uhl, W. *Angew. Chem. Int. Ed.* **2011**, *50*, 3925–3928.

[(Mes_2P(C=CHPh)Al*t*Bu_2)Rh(Cl)(nbd)] 2-Rh



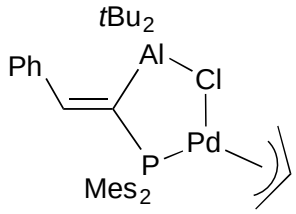
Toluene (3 mL) was added on a mixture of Mes_2P(C=CHPh)Al*t*Bu_2 **1** (70 mg, 0.136 mmol) and [Rh(nbd)(μ–Cl)]$_2$ (31.5 mg, 0.068 mmol, 0.5 equiv.) at -78 °C. The resulting suspension was allowed to warm to room temperature giving a clear orange solution. After removal of toluene under reduced pressure, crystals of the desired rhodium complex were obtained from a dichloromethane/pentane saturated solution at room temperature with a yield of 56 %. HRMS (ESI): exact mass (monoisotopic) calcd for $[C_{41}H_{54}AlPRhCl]^+$, 707.2834; found, 707.2831; Anal. Calcd. for $C_{41}H_{54}AlPRhCl$; C, 66.26; H, 7.32. Found: C, 66.56; H, 7.30; Melting point: 144.3 °C (decomposition).

^{1}H NMR (499.9 MHz, -80 °C, CD_2Cl_2, δ): 0.24 (s, 9H, *t*Bu), 0.36 (s, 9H, *t*Bu), 1.18 – 1.22 (m, 2H, $CH_{2\text{-nbd}}$), 1.50 (s, 3H, $CH_{3o\text{-Mes}}$), 1.80 (s, 3H, $CH_{3o\text{-Mes}}$), 2.20 (s, 3H, $CH_{3p\text{-Mes}}$), 2.22 (m, 2H, $H_{Csp2\text{-nbd}}$), 2.23 (s, 3H, $CH_{3p\text{-Mes}}$), 2.93 (s, 3H, $CH_{3o\text{-Mes}}$), 3.03 (m, 1H, CH_{nbd}), 3.69 (m, 2H, CH_{nbd} and $H_{Csp2\text{-nbd}}$), 3.88 (s, 3H, $CH_{3o\text{-Mes}}$), 4.83 (m, 1H, $H_{Csp2\text{-nbd}}$), 5.09 (m, 1H, $H_{Csp2\text{-nbd}}$), 6.67 (s, 1H, $CH_{m\text{-Mes}}$), 6.70 (s, 1H, $CH_{m\text{-Mes}}$), 7.06 (m, 2H, $CH_{m\text{-Mes}}$), 7.17 – 7.30 (m, 6H, CH_{Ph} and HCCP).

^{13}C {^{1}H} NMR (125.8 MHz, -80 °C, CD_2Cl_2, δ): 15.4 (d, $^3J_{CP}$ = 2.5 Hz, Al(C(CH$_3$)$_3$)$_2$), 16.7 (d, $^3J_{CP}$ = 3.8 Hz, Al(C(CH$_3$)$_3$)$_2$), 20.2 (s, $CH_{3p\text{-Mes}}$), 20.3 (s, $CH_{3p\text{-Mes}}$), 22.9 (s, $CH_{3o\text{-Mes}}$), 25.0 (d, $^3J_{CP}$ = 2.9 Hz, $CH_{3o\text{-Mes}}$), 27.4 (d, $^3J_{CP}$ = 8.9 Hz, $CH_{3o\text{-Mes}}$), 28.7 (d, $^3J_{CP}$ = 11.1 Hz, $CH_{3o\text{-Mes}}$), 30.1 (s, 3C, $CH_{3t\text{Bu}}$), 30.9 (s, 3C, $CH_{3t\text{Bu}}$), 48.5 (d, J_{CRh} = 10.6 Hz, $C_{sp2\text{-nbd}}$), 49.0 (s, CH_{nbd}), 51.1 (s, CH_{nbd}), 56.5 (d, J_{CRh} = 13.7 Hz, $C_{sp2\text{-nbd}}$), 62.8 (s, CH_{2nbd}), 76.9 (dd, J_{CP} = 9.0 Hz, $C_{sp2\text{-nbd}}$), 77.9 (d, J_{CP} = 9.5 Hz, $C_{sp2\text{-nbd}}$), 122.9 (d, $^1J_{CP}$ = 22.2 Hz, $C_{ipso\text{-Mes}}$), 126.9 (s, 2C, $CH_{o\text{-Ph}}$), 127.4 (s, $CH_{p\text{-Ph}}$), 127.7 (d, $^1J_{CP}$ = 41.2 Hz, $C_{ipso\text{-Mes}}$), 128.5 (s, 2C, $CH_{m\text{-Ph}}$), 130.2 (d, $^3J_{CP}$ = 6.2 Hz, $CH_{m\text{-Mes}}$), 130.3 (d, $^3J_{CP}$ = 7.0 Hz, $CH_{m\text{-Mes}}$), 130.4 (d, $^3J_{CP}$ = 7.5 Hz, $CH_{m\text{-Mes}}$), 130.8 (d, $^3J_{CP}$ = 9.7 Hz, $CH_{m\text{-Mes}}$), 137.8 (s, $C_{p\text{-Mes}}$), 139.9 (s, $C_{p\text{-Mes}}$), 140.1 (d, $^2J_{CP}$ = 4.0 Hz, $C_{o\text{-Mes}}$), 140.4 (d, $^2J_{CP}$ = 10.5 Hz, $C_{o\text{-Mes}}$), 140.9 (d, $^1J_{CP}$ = 27.5 Hz, HCCP), 141.0 (d, $^2J_{CP}$ = 19.6 Hz, $C_{o\text{-Mes}}$), 141.7 (d, $^3J_{CP}$ = 25.4 Hz, $C_{ipso\text{-Ph}}$), 144.1 (s, $C_{o\text{-Mes}}$), 150.9 (d, $^2J_{CP}$ = 11.4 Hz, HCCP).

^{31}P{^{1}H} NMR (202.5 MHz, -80 °C, CD_2Cl_2, δ): 27.5 (d, $^1J_{PRh}$ = 150.6 Hz).

[(Mes_2P(C=CHPh)Al*t*Bu_2)Pd(Cl)(allyl)] 2-Pd



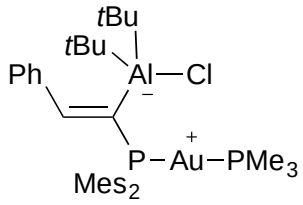
Toluene (3 mL) was added on a mixture of Mes_2P(C=CHPh)A/*t*Bu_2 **1** (70 mg, 0.136 mmol) and [Pd(allyl)(μ-Cl)]$_2$ (25.0 mg, 0.068 mmol, 0.5 equiv.) at -78 °C. The resulting mixture was allowed to warm to room temperature under stirring giving a thin black suspension in a yellowish solution. The solid was eliminated by filtration and the supernatant was concentrated to dryness under reduced pressure. Analytically pure pale yellow crystals of the desired palladium complex were obtained after two crystallizations from a saturated dichloromethane solution at room temperature with a yield of 59 %. HRMS (ESI): exact mass (monoisotopic) calcd for $[C_{37}H_{51}AlPPdCl]^+$, 657.25850; found, 657.2585; Anal. Calcd. for $C_{37}H_{51}AlPPdCl$; C, 63.88; H, 7.39. Found: C, 64.12; H, 7.35; Melting point: 148.6 °C (decomposition).

^{1}H NMR (499.9 MHz, 20 °C, CD_2Cl_2, δ): 0.46 (s, 9H, *t*Bu), 0.55 (s, 9H, *t*Bu), 2.29 (s, 6H, $CH_{3p\text{-Mes}}$), 2.32 (s, 6H, $CH_{3o\text{-Mes}}$), 2.56 (s, 6H, $CH_{3o\text{-Mes}}$), 2.60 (m, 1H, CH_{2allyl}), 2.70 (d br., 1H, J_{HH} = 12.0 Hz, CH_{2allyl}), 3.55 (dd, 1H, J_{PH} = 9.6 Hz, J_{HH} = 13.7 Hz, CH_{2allyl}), 4.45 (ddd, 1H, J_{HP} = 7.3 Hz, J_{HH} = 7.6 Hz, J_{HH} = 2.2 Hz, CH_{2allyl}), 5.55 (m, 1H, CH_{allyl}), 6.90 (d, 2H, $^4J_{HP}$ = 2.9 Hz, $CH_{m\text{-Mes}}$), 6.92 (d, 2H, $^4J_{HP}$ = 2.9 Hz, $CH_{m\text{-Mes}}$), 7.21 – 7.37 (m, 5H, CH_{Ph}), 7.43 (d, 1H, $^3J_{HP}$ = 38.2 Hz, HCCP).

^{13}C {^{1}H} NMR (125.8 MHz, 20 °C, CD_2Cl_2, δ): 17.2 (s br., 2C, Al(C(CH$_3$)$_3$)$_2$), 20.8 (d, $^5J_{CP}$ = 1.1 Hz, $CH_{3p\text{-Mes}}$), 20.9 (d, $^5J_{CP}$ = 1.1 Hz, $CH_{3p\text{-Mes}}$), 25.8 (d, 2C, $^3J_{CP}$ = 7.8 Hz, $CH_{3o\text{-Mes}}$), 26.2 (d, 2C, $^3J_{CP}$ = 8.7 Hz, $CH_{3o\text{-Mes}}$), 31.7 (s, 3C, $CH_{3t\text{Bu}}$), 31.8 (s, 3C, $CH_{3t\text{Bu}}$), 62.1 (d, J_{CP} = 5.7 Hz, CH_{2allyl}), 74.5 (d, J_{CP} = 30.0 Hz, CH_{2allyl}), 118.0 (d, J_{CP} = 30.0 Hz, CH_{allyl}), 128.0 (d, 2C, J_{CP} = 1.9 Hz, CH_{Ph}), 128.2 (s, $CH_{p\text{-Ph}}$), 128.3 (d, $^1J_{CP}$ = 36.2 Hz, $C_{ipso\text{-Mes}}$), 128.5 (d, $^2J_{CP}$ = 28.7 Hz, $C_{ipso\text{-Mes}}$), 129.1 (s, 2C, CH_{Ph}), 131.6 (d, 2C, $^3J_{CP}$ = 7.9 Hz, $CH_{m\text{-Mes}}$), 131.6 (d, 2C, $^3J_{CP}$ = 7.9 Hz, $CH_{m\text{-Mes}}$), 139.7 (d, $^4J_{CP}$ = 2.1 Hz, $C_{p\text{-Mes}}$), 140.6 (d, $^4J_{CP}$ = 2.1 Hz, $C_{p\text{-Mes}}$), 142.2 (d, $^3J_{CP}$ = 26.0 Hz, $C_{ipso\text{-Ph}}$), 142.3 (d, 4C, $^2J_{CP}$ = 8.4 Hz, $C_{o\text{-Mes}}$), 143.4 (d, $^1J_{CP}$ = 9.5 Hz, Al-C_{sp2}), 154.1 (d, $^2J_{CP}$ = 11.1 Hz, HCCP).

^{31}P{^{1}H} NMR (202.5 MHz, 20 °C, CD_2Cl_2, δ): 11.5.

[(Mes_2P(C=CHPh)Al(^{t}Bu$_2$)(Cl))AuPMe$_3$] 3-PMe$_3$



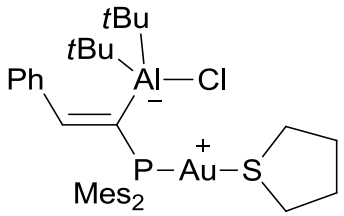
Dichloromethane (2 mL) was added on a mixture of trimethylphosphine gold(I) chloride (42.1 mg, 0.136 mmol) and Mes_2P(C=CHPh)Al*t*Bu$_2$ **1** (70 mg, 0.136 mmol, 1 equiv.) at -78 °C. The resulting mixture was allowed to warm to room temperature under stirring giving a thin dark suspension in a slightly yellow solution. After filtration of the suspension, the supernatant was concentrated to dryness under reduced pressure. Crystals of the expected gold(I) complex were obtained from a saturated solution in a mixture dichloromethane/pentane at -60 °C with a yield of 68 %. HRMS (ESI, (M-Cl)$^+$): exact mass (monoisotopic) calcd for $[C_{37}H_{55}AlP_2Au]^+$, 785.3260; found, 785.3278; Anal. Calcd. for $C_{37}H_{55}AlP_2AuCl$; C, 54.12; H, 6.75. Found: C, 53.92; H, 6.69; Melting point: 152.4 °C (decomposition).

^{1}H NMR (499.9 MHz, 20 °C, CD_2Cl_2, δ): 0.82 (s, 18H, *t*Bu), 1.56 (dd, 9H, $^2J_{HP}$ = 10.3 Hz, $^4J_{HP}$ = 2.0 Hz, P(CH_3)$_3$), 2.27 (s, 6H, $CH_{3p\text{-}Mes}$), 2.48 (s, 12H, $CH_{3o\text{-}Mes}$), 6.86 (d, 4H, $^4J_{HP}$ = 3.3 Hz, $CH_{m\text{-}Mes}$), 7.18 – 7.23 (m, 1H, CH_{Ph}), 7.26 – 7.32 (m, 4H, CH_{Ph}), 7.47 (d, 1H, $^3J_{HP}$ = 44.6 Hz, HCCP).

^{13}C {^{1}H} NMR (125.8 MHz, 20 °C, CD_2Cl_2, δ): 16.1 (dd, 3C, $^1J_{CP}$ = 34.3 Hz, $^3J_{CP}$ = 1.9 Hz, P(CH_3)$_3$), 17.8 (s br., 2C, Al(C(CH_3)$_3$)$_2$), 21.2 (d, 2C, $^5J_{CP}$ = 1.2 Hz, $CH_{3p\text{-}Mes}$), 25.8 (d, 4C, $^3J_{CP}$ = 8.5 Hz, $CH_{3o\text{-}Mes}$), 33.6 (s, 6C, $CH_{3t\text{Bu}}$), 127.7 (s, $CH_{p\text{-}Ph}$), 128.1 (d, 2C, J_{CP} = 1.8 Hz, CH_{Ph}), 128.6 (s, 2C, CH_{Ph}), 129.7 (dd, 2C, $^1J_{CP}$ = 39.8 Hz, $^3J_{CP}$ = 1.9 Hz, $C_{ipso\text{-}Mes}$), 131.3 (d, 2C, J_{CP} = 7.9 Hz, $C_{quat.Mes}$), 140.0 (d, 2C, J_{CP} = 2.3 Hz, $C_{quat.Mes}$), 143.0 (d, $^1J_{CP}$ = 30.6 Hz, Al-C_{sp2}), 143.2 (dd, 2C, J_{CP} = 8.9 Hz, J_{CP} = 1.3 Hz, $C_{quat.Mes}$), 148.2 (d br., $^3J_{CP}$ = 40.6 Hz, $C_{ipso\text{-}Ph}$), 155.6 (dd, $^4J_{CP}$ = 3.5 Hz, $^2J_{CP}$ = 7.7 Hz, HCCP).

^{31}P{^{1}H} NMR (202.5 MHz, 20 °C, CD_2Cl_2, δ): -1.48 (d, $^2J_{PP}$ = 330.6 Hz, P(CH_3)$_3$), 30.5 (d, $^2J_{PP}$ = 330.6 Hz, PMes_2).

[(Mes_2P(C=CHPh)Al(tBu_2)(Cl))Au(tht)] 3-tht



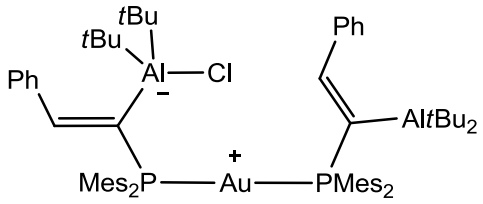
Dichloromethane (2 mL) was added on a mixture of AuCl(tht) (18.8 mg, 0.059 mmol) and **1** (30 mg, 0.059 mmol, 1 equiv.) at -78 °C. The suspension was allowed to warm up to room temperature leading to a black suspension in a colorless solution. After elimination of the thin black powder by filtration, the supernatant was concentrated and gave colorless crystals of the compound at -20 °C with 44 % yield.

^{1}H NMR (499.9 MHz, 20 °C, CD_2Cl_2, δ): 0.80 (s, 18H, *t*Bu), 2.13 (s br., 4H, CH_{2tht}), 2.28 (s, 6H, $CH_{3p\text{-}Mes}$), 2.49 (s, 12H, $CH_{3o\text{-}Mes}$), 3.40 (s br., 4H, SCH_{2tht}), 6.88 (d, 4H, $^{4}J_{HP}$ = 3.4 Hz, $CH_{m\text{-}Mes}$), 7.19 – 7.35 (m, 5H, CH_{Ph}), 7.48 (d, 1H, $^{3}J_{HP}$ = 47.3 Hz, HCCP).

^{13}C {^{1}H} NMR (125.8 MHz, 20 °C, CD_2Cl_2, δ): 17.8 (s br., 2C, Al($\underline{C}(CH_3)_3)_2$), 21.0 (s, 2C, $CH_{3p\text{-}Mes}$), 25.9 (d, 4C, $^{3}J_{CP}$ = 8.7 Hz, $CH_{3o\text{-}Mes}$), 31.1 (s, 2C, CH_{2tht}), 33.4 (s, 6C, Al($C(\underline{C}H_3)_3)_2$), 40.0 (s br., 2C, $^{3}J_{CP}$ = 1.8 Hz, SCH_{2tht}), 127.9 (s, $CH_{p\text{-}Ph}$), 128.1 (d, 2C, $^{4}J_{CP}$ = 2.0 Hz, $CH_{o\text{-}Ph}$), 128.6 (d, 2C, $^{1}J_{CP}$ = 45.6 Hz, $C_{ipso.Mes}$), 128.6 (s, 2C, $CH_{m\text{-}Ph}$), 131.4 (d, 4C, $^{3}J_{CP}$ = 8.3 Hz, CH_{Mes}), 140.4 (d, 2C, $^{4}J_{CP}$ = 2.3 Hz, $C_{p.Mes}$), 142.5 (d, J_{CP} = 32.2 Hz, $C_{quat.}$), 143.0 (d, 4C, $^{2}J_{CP}$ = 8.9 Hz, $C_{o\text{-}Mes}$), 147.2 (d, J_{CP} = 39.2 Hz, $C_{quat.}$), 155.8 (d, $^{2}J_{CP}$ = 7.4 Hz, H$\underline{C}$CP).

^{31}P{^{1}H} NMR (202.5 MHz, 20 °C, CD_2Cl_2, δ): 18.0.

[((Mes$_2$P(C=CHPh)Al(*t*Bu$_2$))$_2$Au(Cl)] 4



Dichloromethane (2 mL) was added on a mixture of **3-tht** (30 mg, 0.036 mmol) and **1** (18.5 mg, 0.036 mmol, 1 equiv.) at room temperature leading to a clear yellowish solution. After 5 minutes of stirring, the solution was filtered to remove some very thin black powder and the supernatant was concentrated to 0.5 mL. The product was precipitated as a white powder from this solution at -20 °C with a yield of 66 %. HRMS (ESI, (M-Cl)$^+$): exact mass (monoisotopic) calcd for $[C_{68}H_{92}Al_2P_2Au]^+$, 1221.5971; found, 1221.6016.

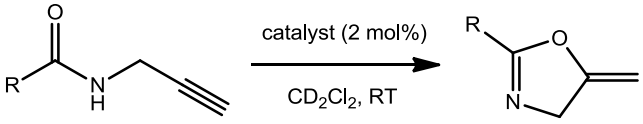
^{1}H NMR (499.9 MHz, 20 °C, CD_2Cl_2, δ): 0.52 (s, 36H, *t*Bu), 2.24 (s, 12H, $CH_{3p\text{-Mes}}$), 2.33 (s, 24H, $CH_{3o\text{-Mes}}$), 6.83 (s br., 8H, $CH_{m\text{-Mes}}$), 7.31 – 7.47(m, 10H, CH_{Ph}), 8.37 (s br., 2H, HCCP). ^{13}C{^{1}H} NMR shows only broad unresolved signals both at 20 and -60°C.

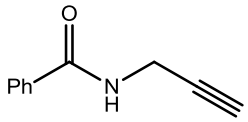
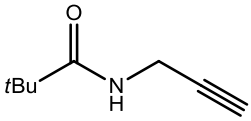
^{31}P{^{1}H} NMR (202.5 MHz, 20 °C, CD_2Cl_2, δ): 31.6 (s br.).

^{31}P{^{1}H} NMR (202.5 MHz, - 60 °C, CD_2Cl_2, δ): 25.2 (d br., $^2J_{PP}$ = 309.0 Hz), 36.1 (d br., $^2J_{PP}$ = 309.0 Hz).

Cyclization of propargylic amides

General procedure for the gold-catalyzed cycloisomerizations using 3-tht or Ph_3PAuCl as catalyst. An NMR tube was loaded with propargylamide (0.33 mmol) and **3-tht** or Ph_3PAuCl (2 mol %), and CD_2Cl_2 was added (0.67 mL). The catalytic reaction was monitored by ^1H NMR. The cyclized products were authenticated by comparison of their ^1H NMR data with those described in the literature.[2,3] The yields were determined by ^1H NMR using mesitylene as internal standard.



Substrate	Catalyst	Time (h)	Yield (%)
	**3-tht**	36 76	79 98
	Ph_3PAuCl	36	<1
	**3-tht**	4	99
	Ph_3PAuCl	5	0

[2] Doherty, S.; Knight, J. G.; Hashmi, A. S. K.; Smyth, C. H.; Ward, N. A. B.; Robson, K. J.; Tweedley, S.; Harrington, R. W.; Clegg, W. *Organometallics* **2010**, *29*, 4139-4147.

[3] Weyrauch, J. P.; Hashmi, A. S. K.; Schuster, A.; Hengst, T.; Shetter, S.; Littman, A.; Rudolph, M.; Hamzic, M.; Visus, J.; Rominger, F.; Frey, W.; Bats, J. W. *Chem. Eur. J.* **2010**, *16*, 956-963.

NMR SPECTRA

Figure 1. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Rh** (202.5 MHz, 193K) in CD_2Cl_2

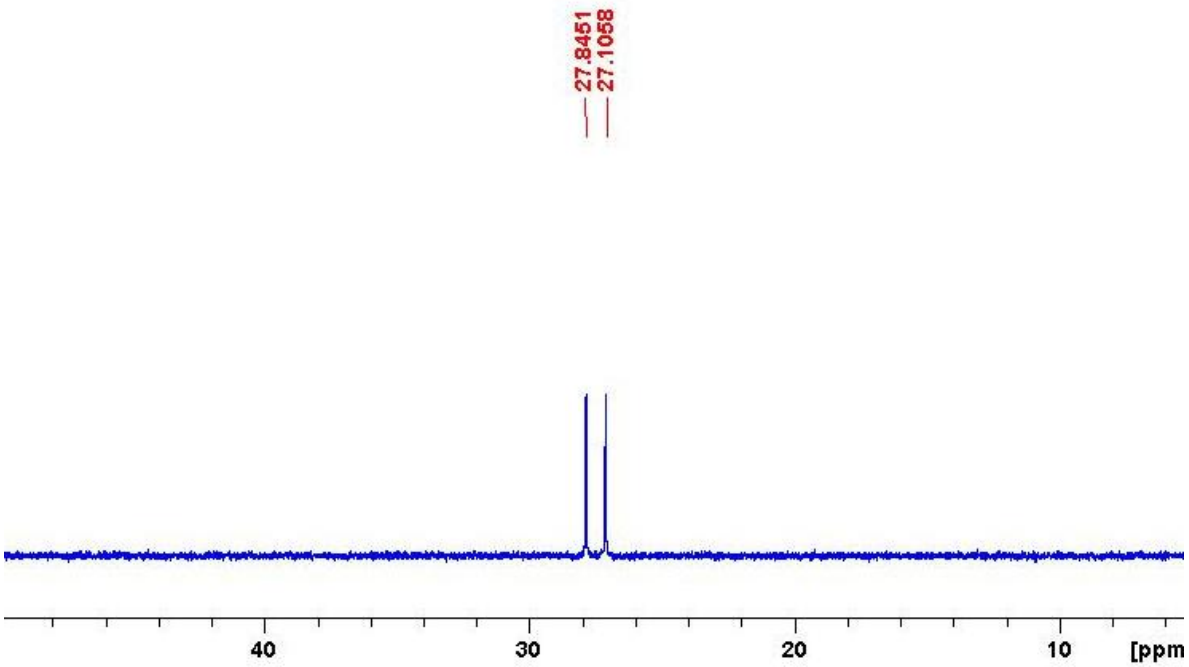
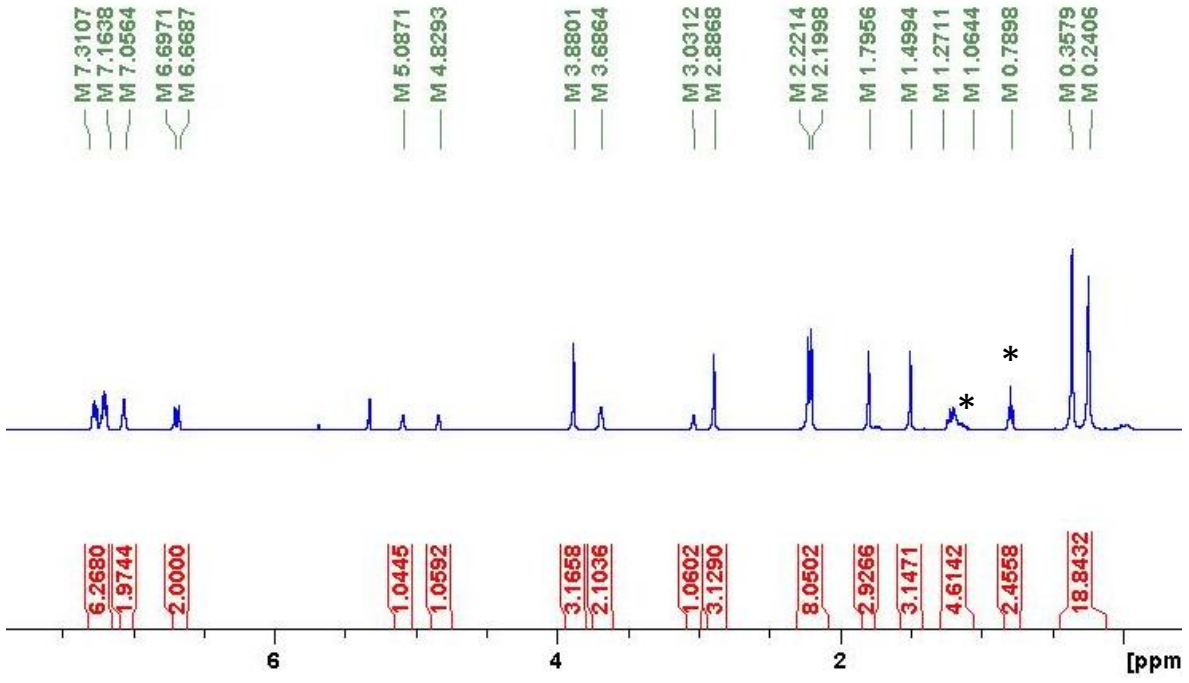


Figure 2. ^{1}H NMR spectrum of **2-Rh** (499.9 MHz, 193K) in CD_2Cl_2



* Signals attributed to pentane

Figure 3. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Rh** (125.8 MHz, 193K) in CD_2Cl_2

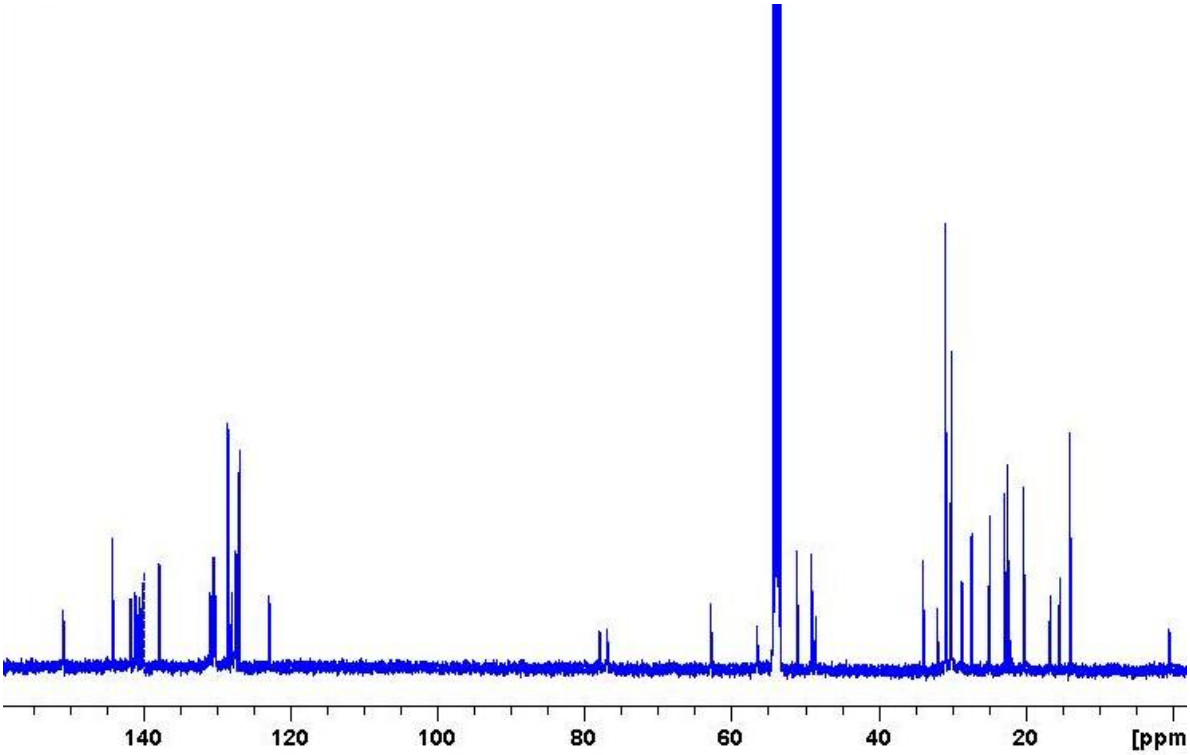


Figure 4. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Rh** (125.8 MHz, 193K) in CD_2Cl_2: zoom 1

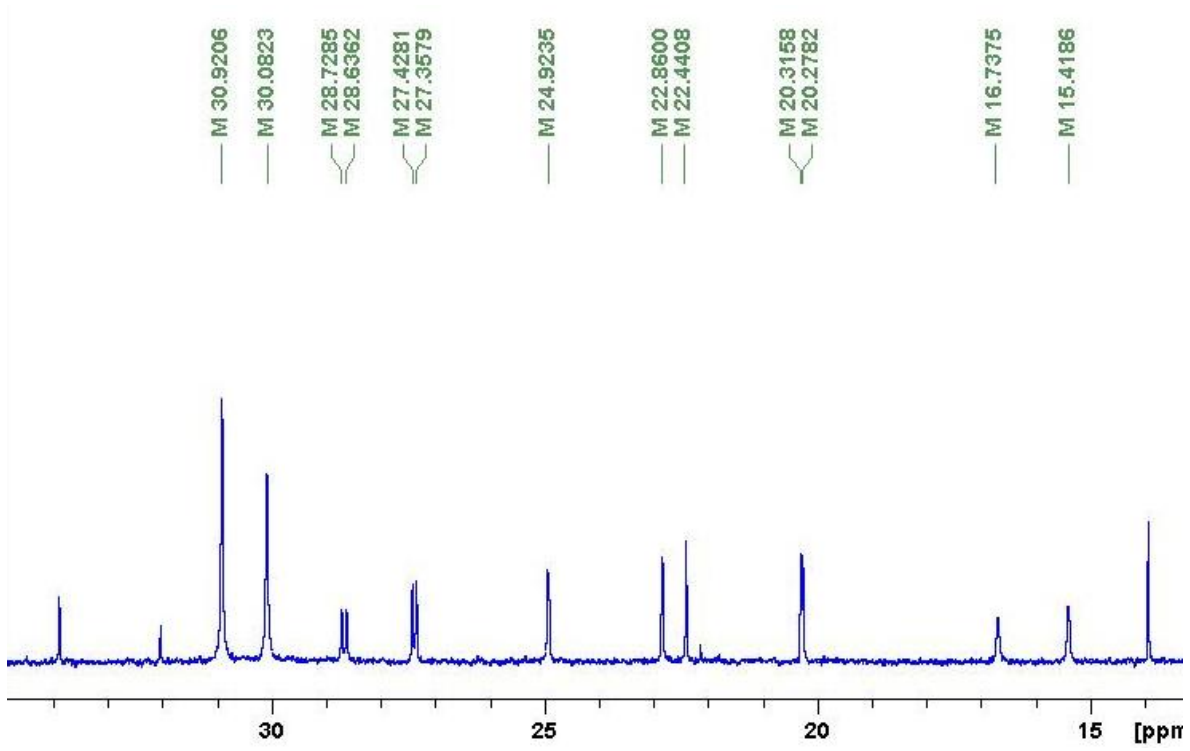


Figure 5. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Rh** (125.8 MHz, 193K) in CD_2Cl_2: zoom 2

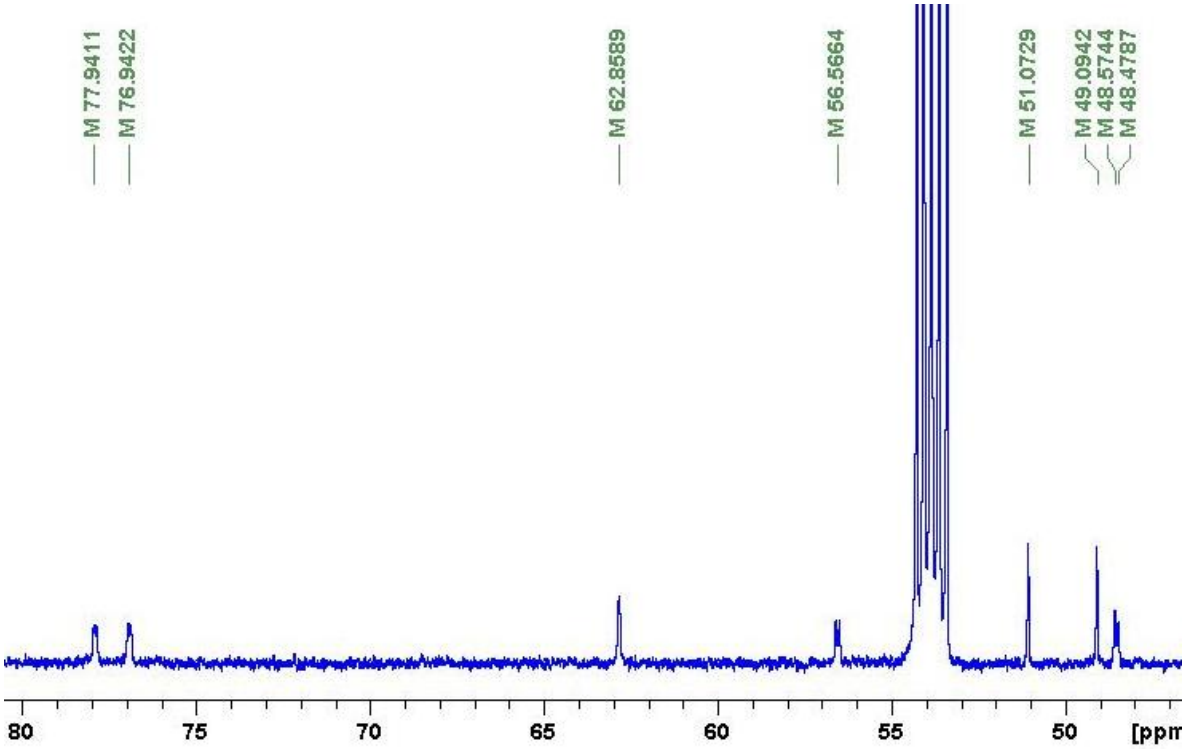


Figure 6. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Rh** (125.8 MHz, 193K) in CD_2Cl_2: zoom 3

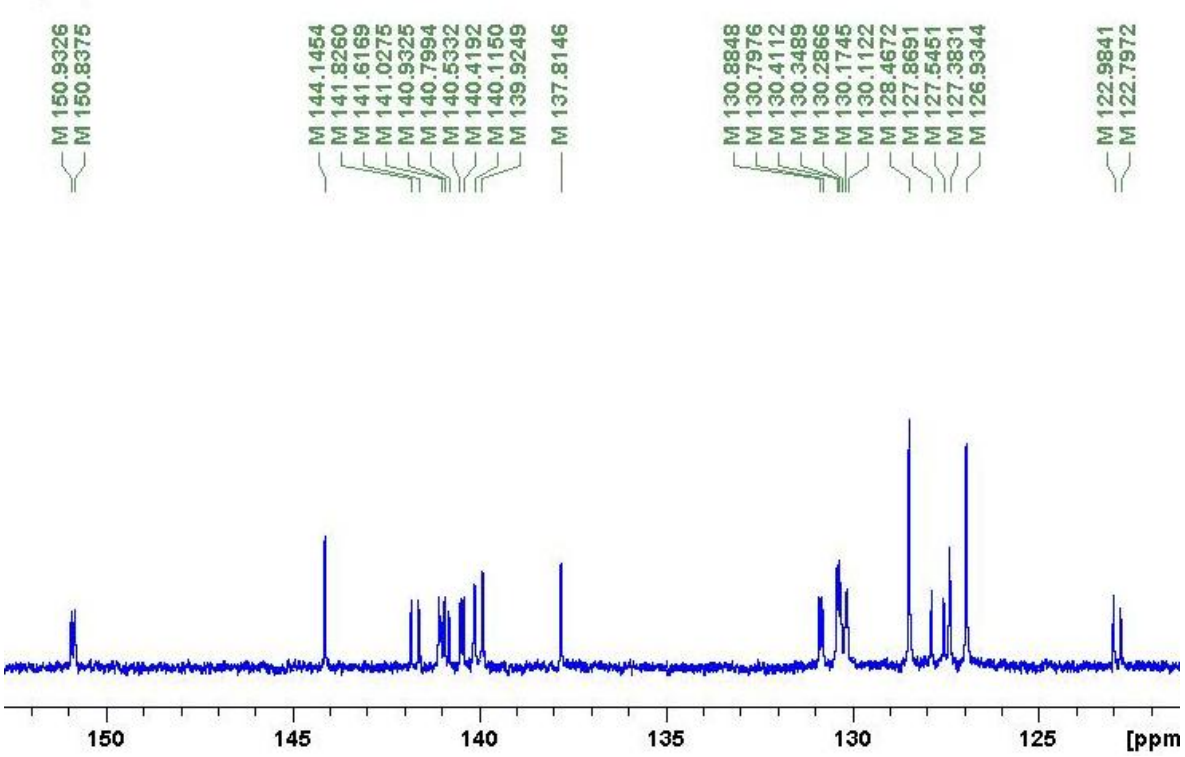


Figure 7. $^{31}P\{^{1}H\}$ NMR spectrum of **2-Pd** (202.5 MHz, 293 K) in CD_2Cl_2

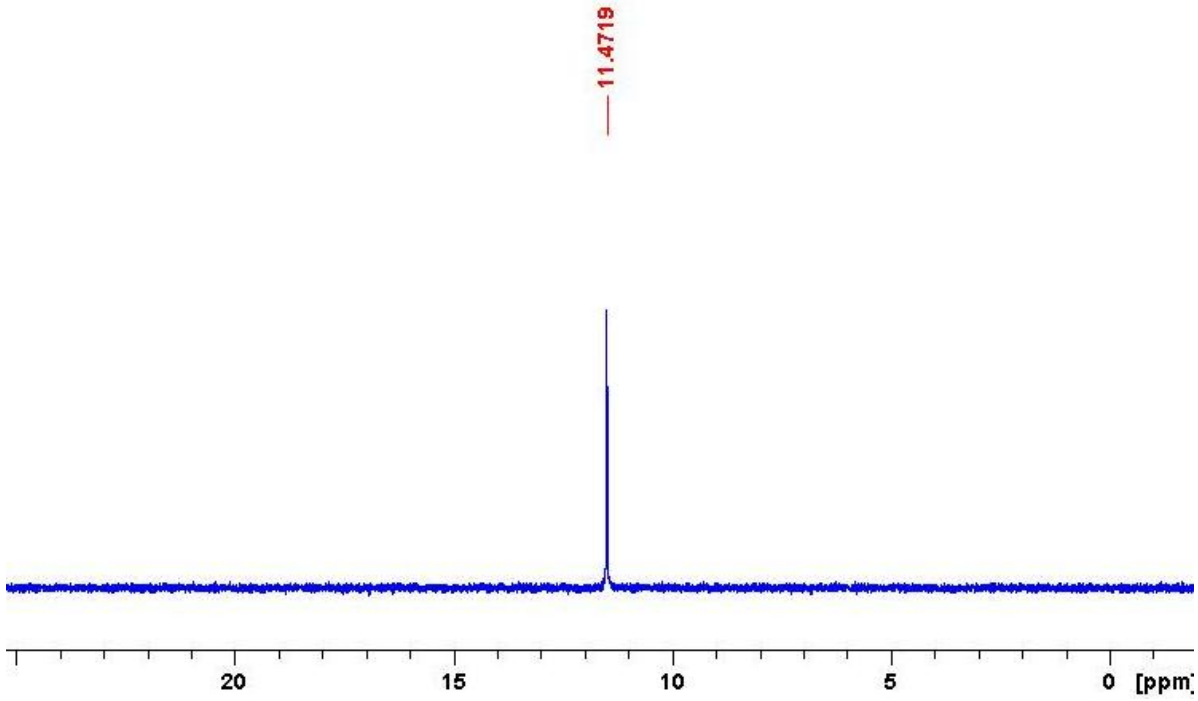
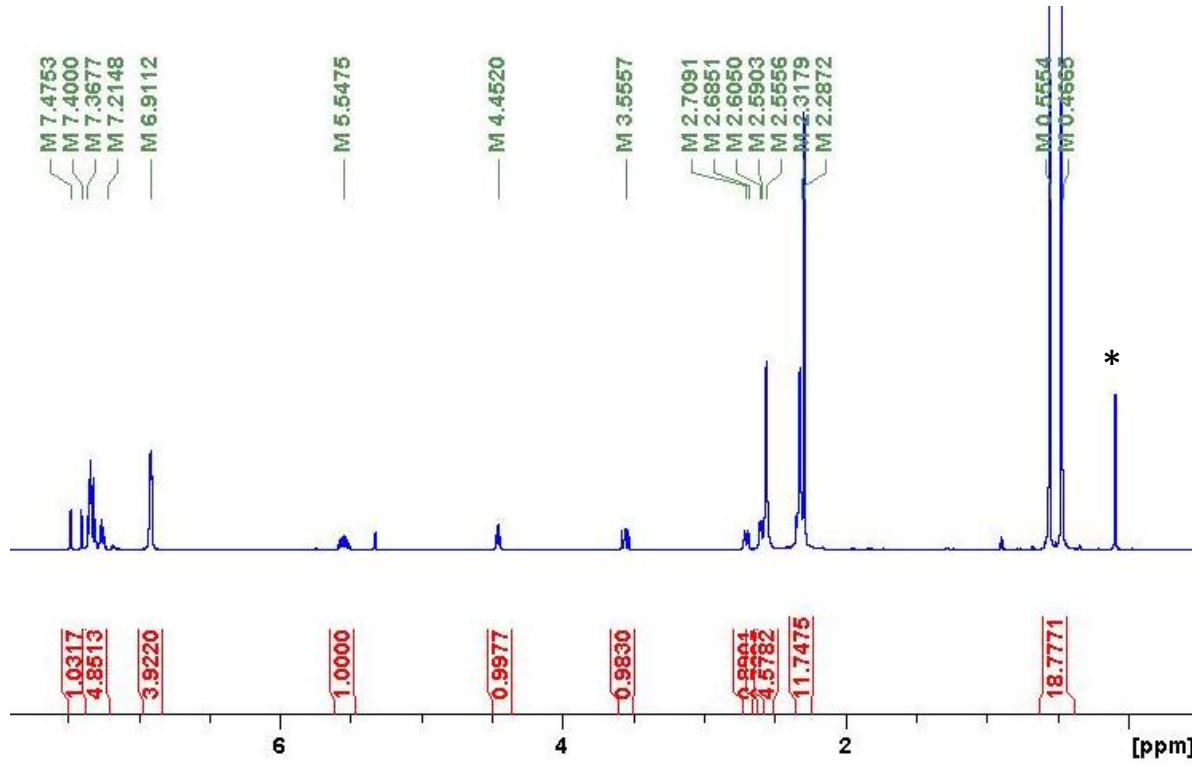


Figure 8. ^{1}H NMR spectrum of **2-Pd** (499.9 MHz, 293 K) in CD_2Cl_2



*Signal attributed to traces of grease

Figure 9.[1]H NMR spectrum of **2-Pd** (499.9 MHz, 293 K) in CD_2Cl_2: zoom 1

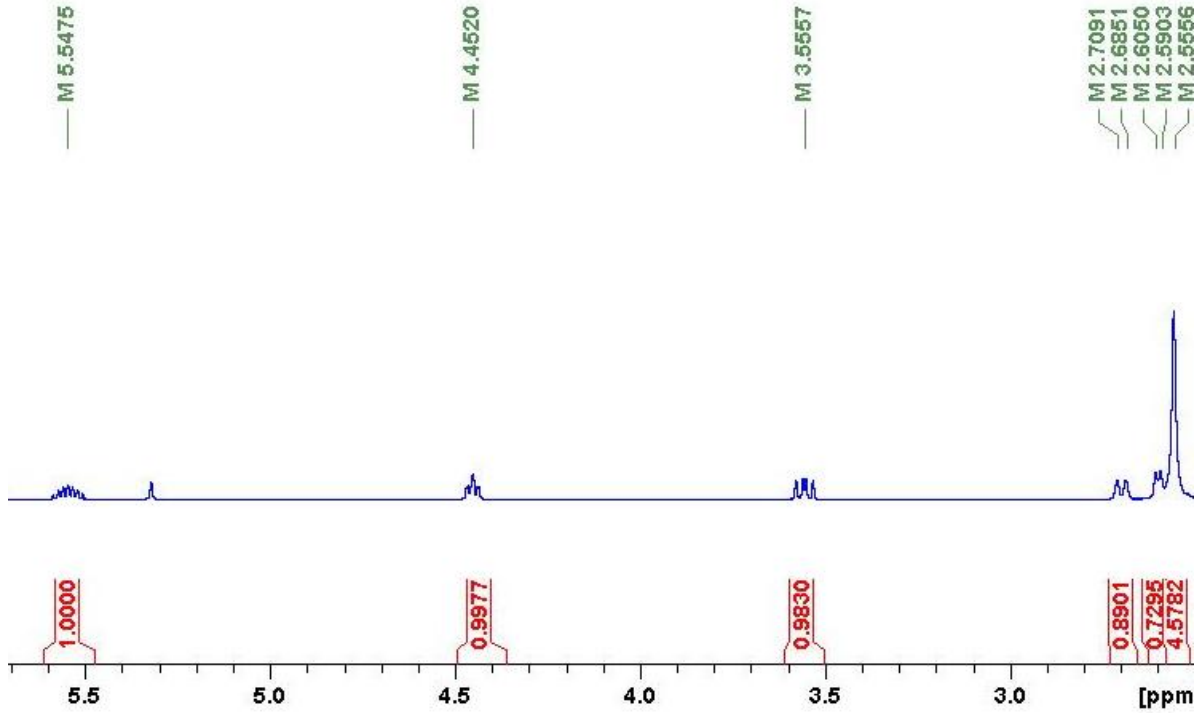


Figure 10.[1]H NMR spectrum of **2-Pd** (499.9 MHz, 293 K) in CD_2Cl_2: zoom 2

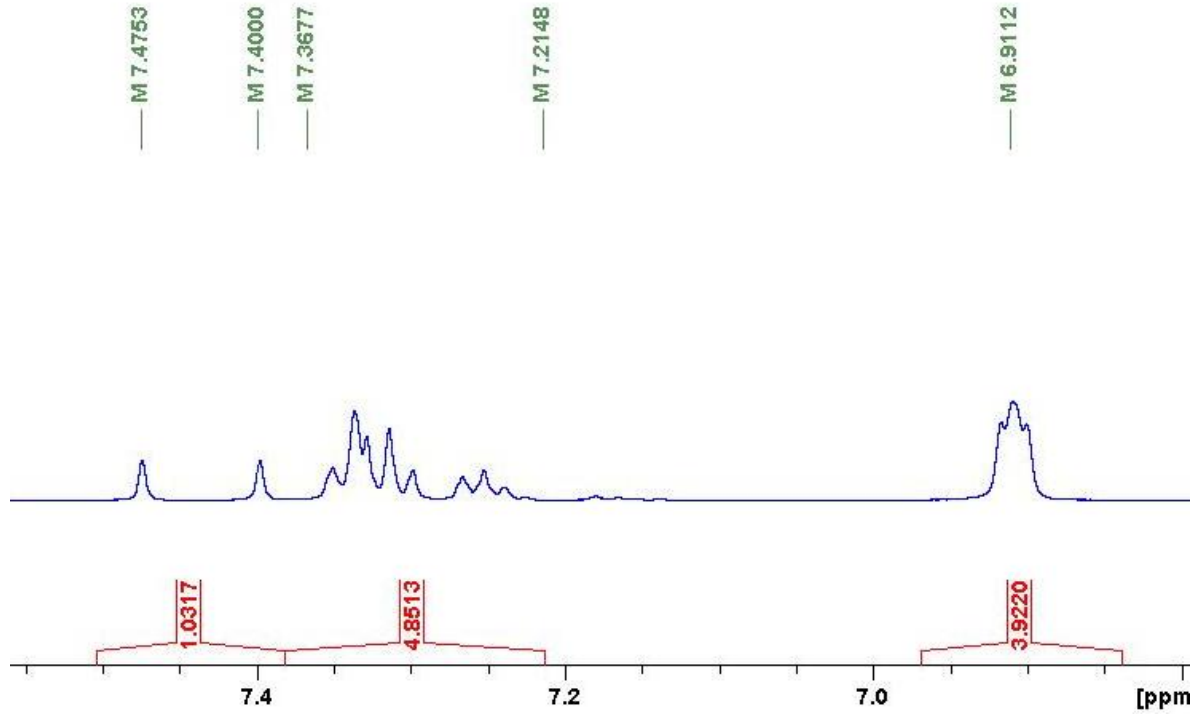


Figure 11. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Pd** (125.8 MHz, 293 K) in CD_2Cl_2

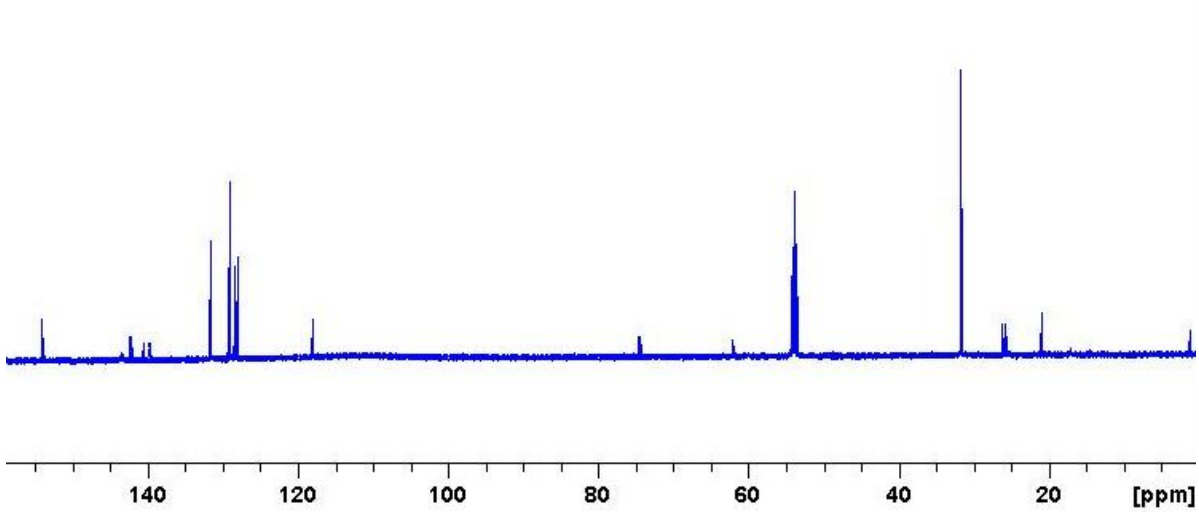


Figure 12. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Pd** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 1

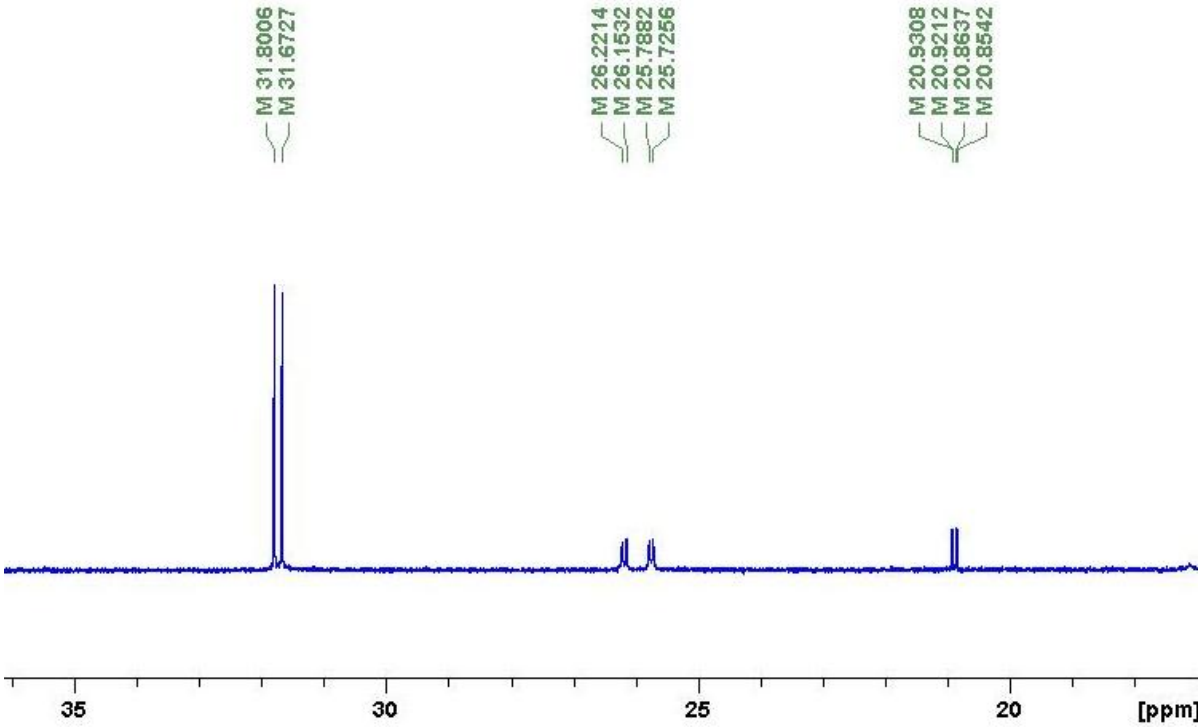


Figure 13. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Pd** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 2

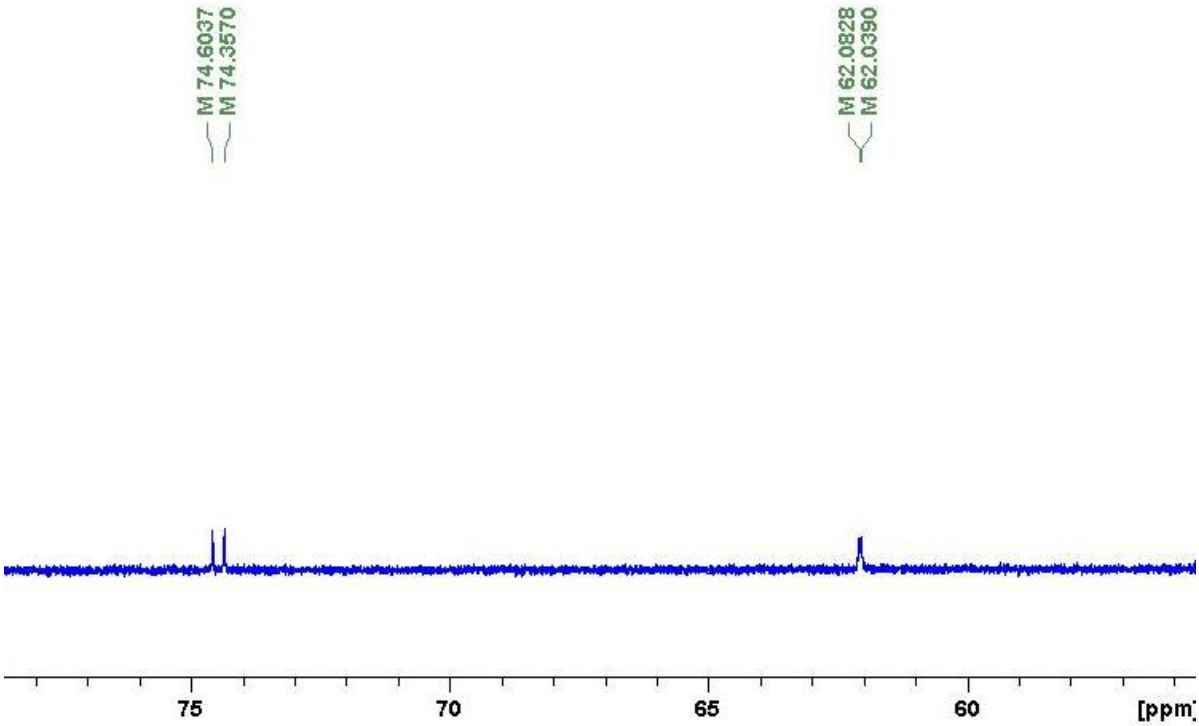


Figure 14. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Pd** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 3

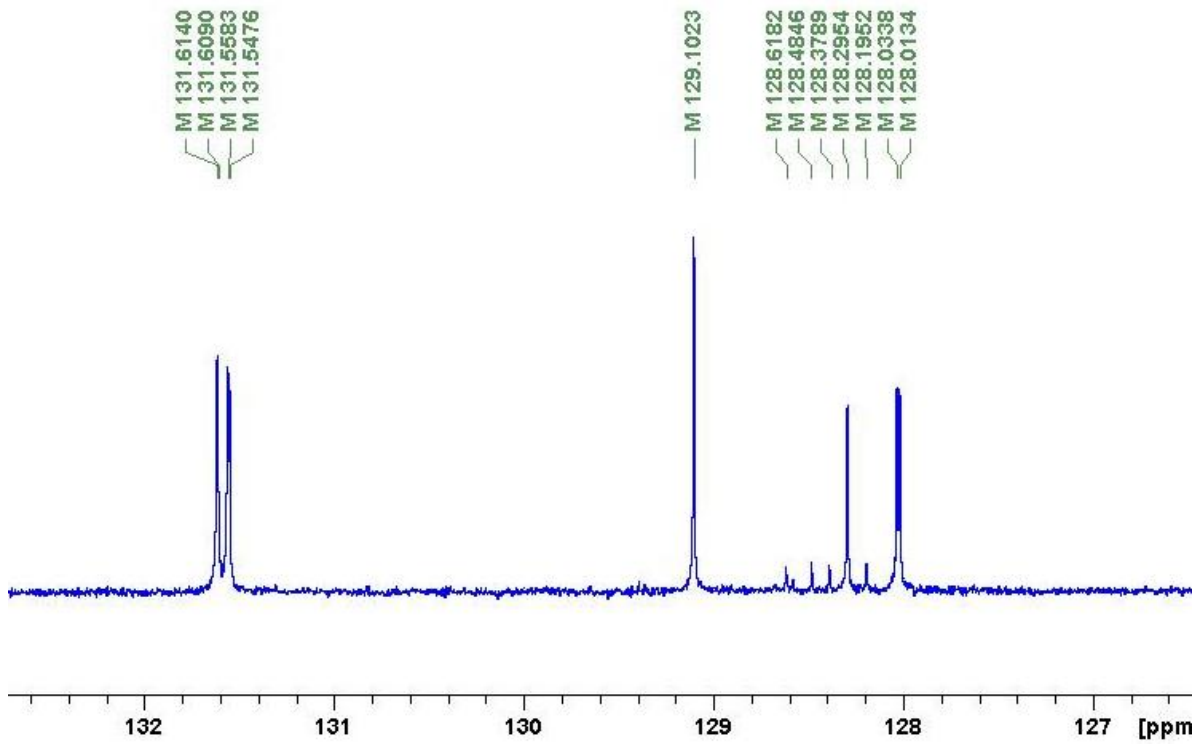


Figure 15. $^{13}C\{^{1}H\}$ NMR spectrum of **2-Pd** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 4

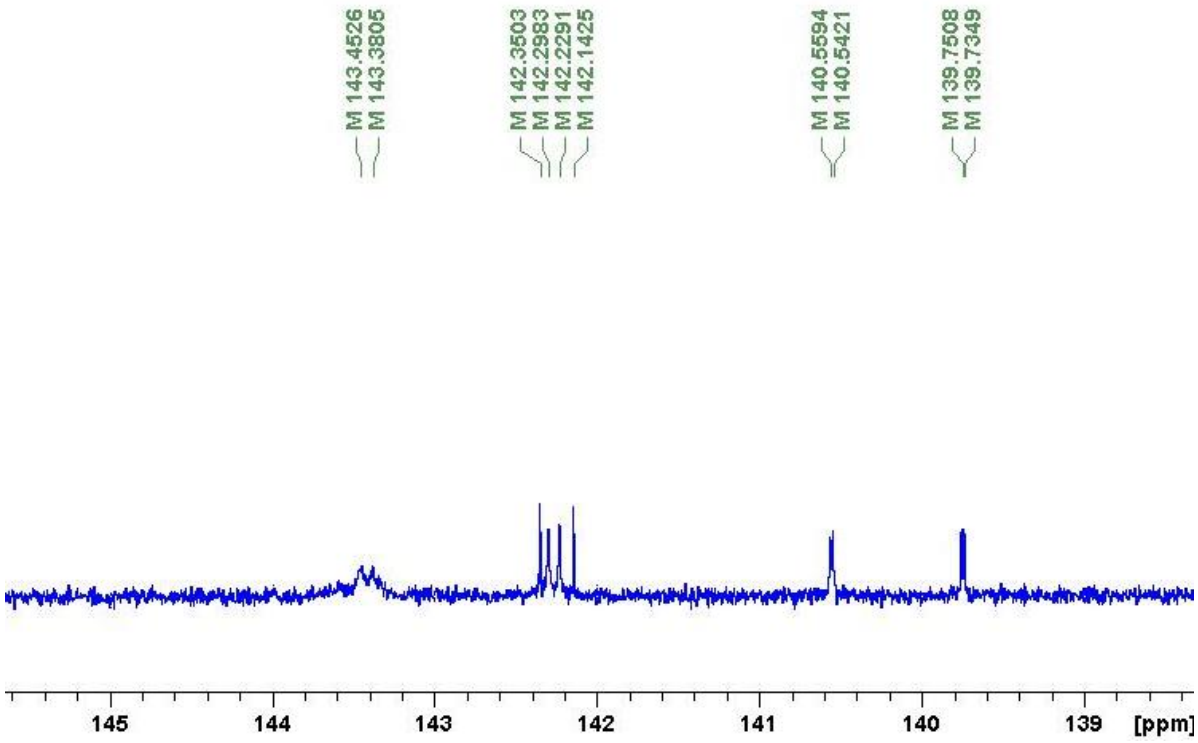


Figure 16. $^{31}P\{^{1}H\}$ NMR spectrum of **3-PMe$_3$** (202.5 MHz, 293 K) in CD_2Cl_2

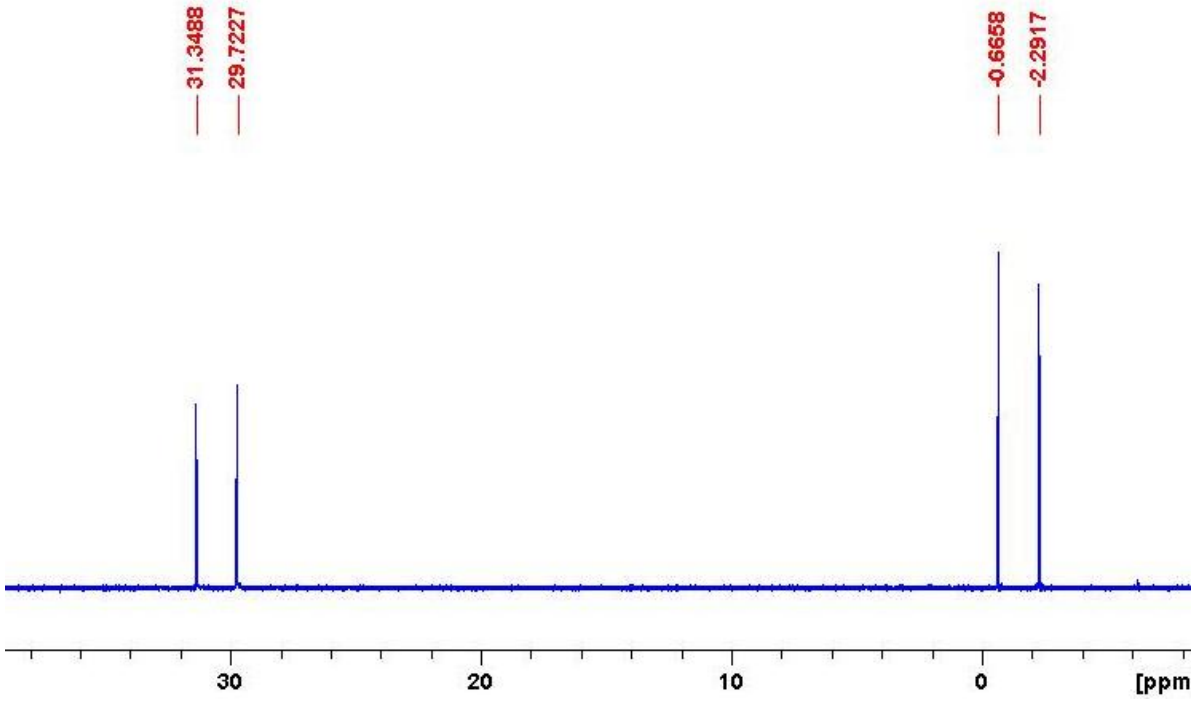
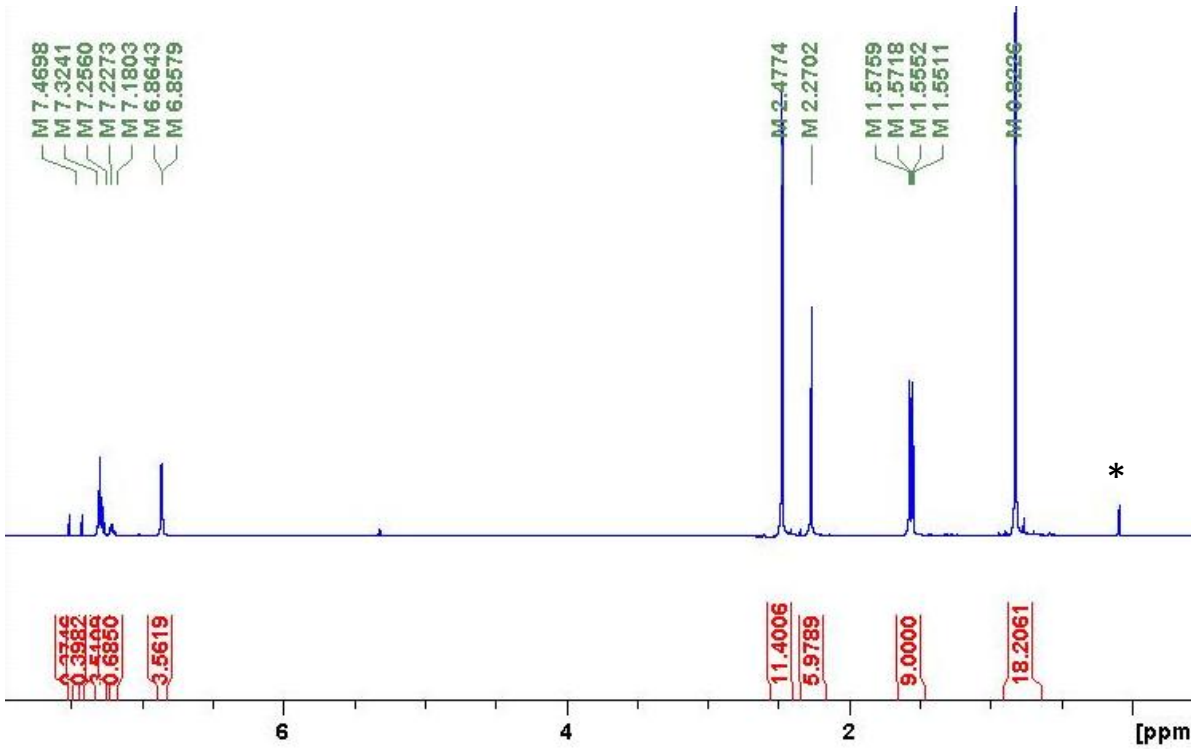


Figure 17. ^{1}H NMR spectrum of **3-PMe$_3$** (499.9 MHz, 293 K) in CD_2Cl_2



*Signal attributed to traces of grease

Figure 18. ^{1}H NMR spectrum of **3-PMe$_3$** (499.9 MHz, 293 K) in CD_2Cl_2: zoom

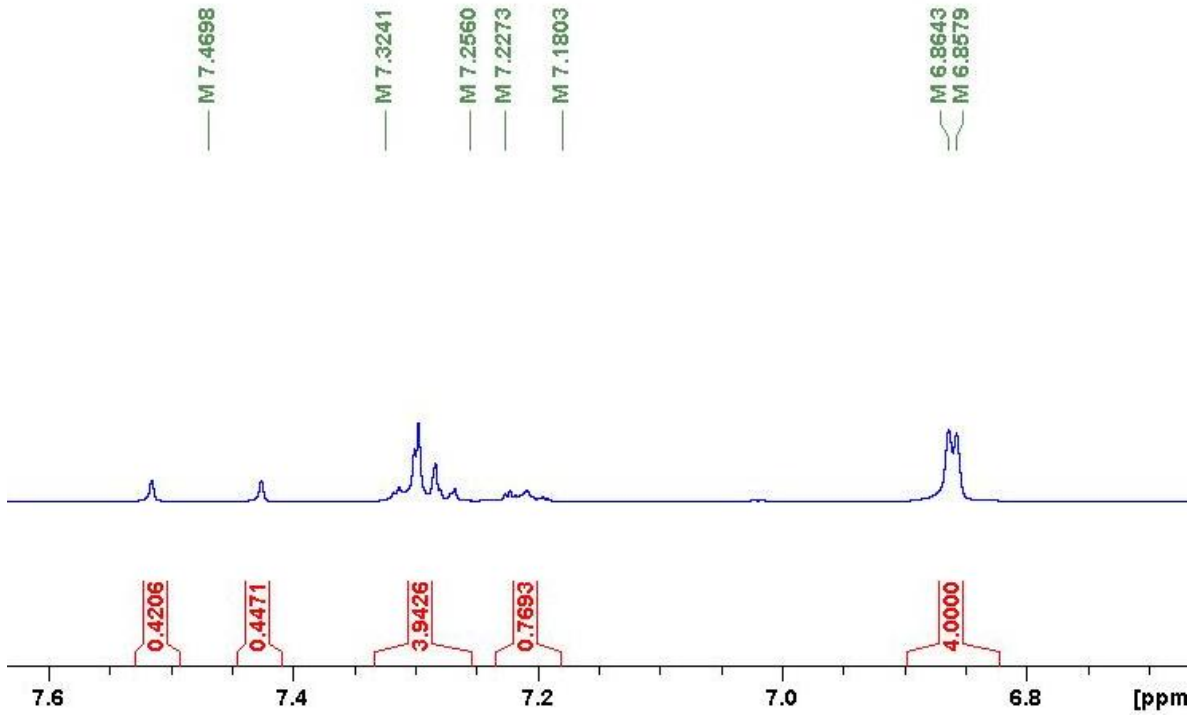


Figure 19. $^{13}C\{^{1}H\}$ NMR spectrum of **3-PMe$_3$** (125.8 MHz, 293 K) in CD_2Cl_2

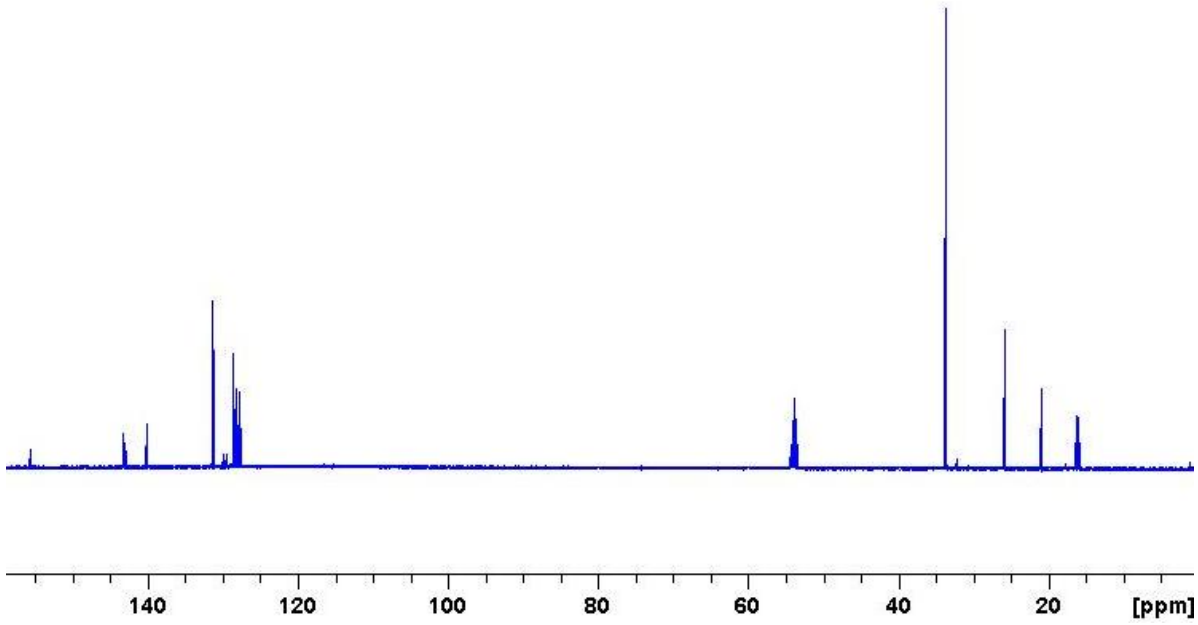


Figure 20. $^{13}C\{^{1}H\}$ NMR spectrum of **3-PMe$_3$** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 1

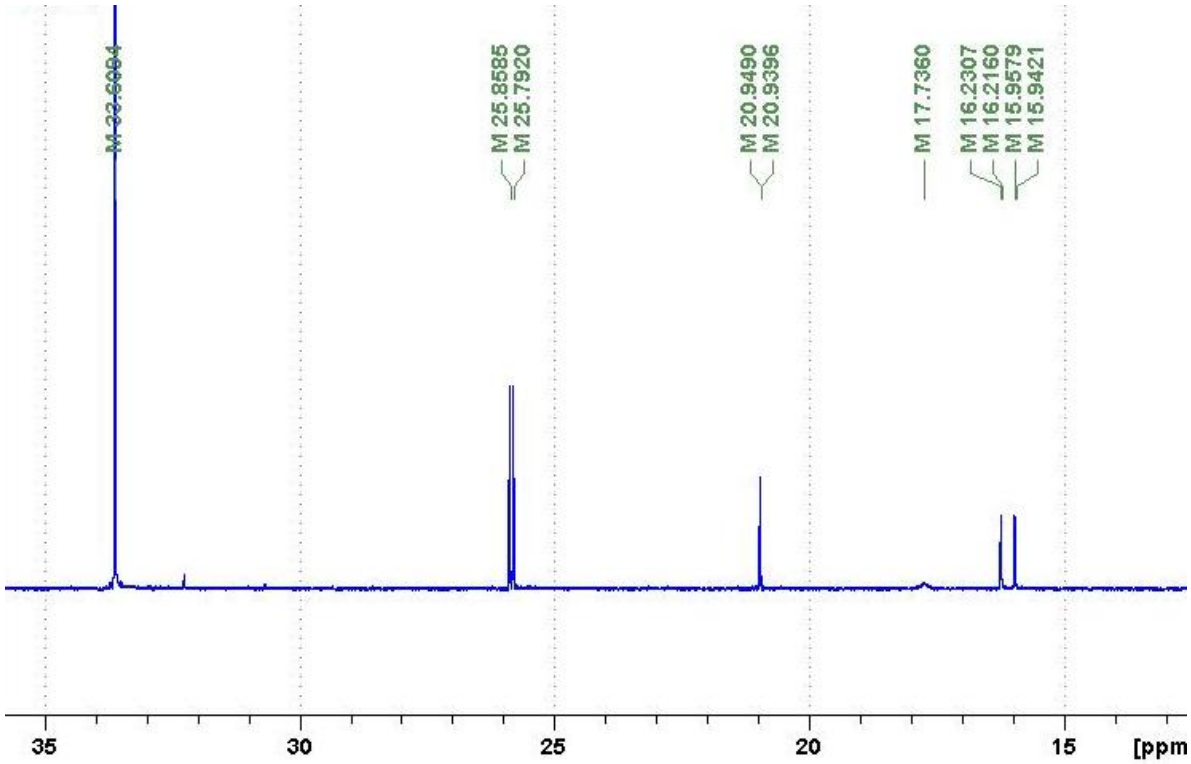


Figure 21. $^{13}C\{^{1}H\}$ NMR spectrum of **3-PMe$_3$** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 2

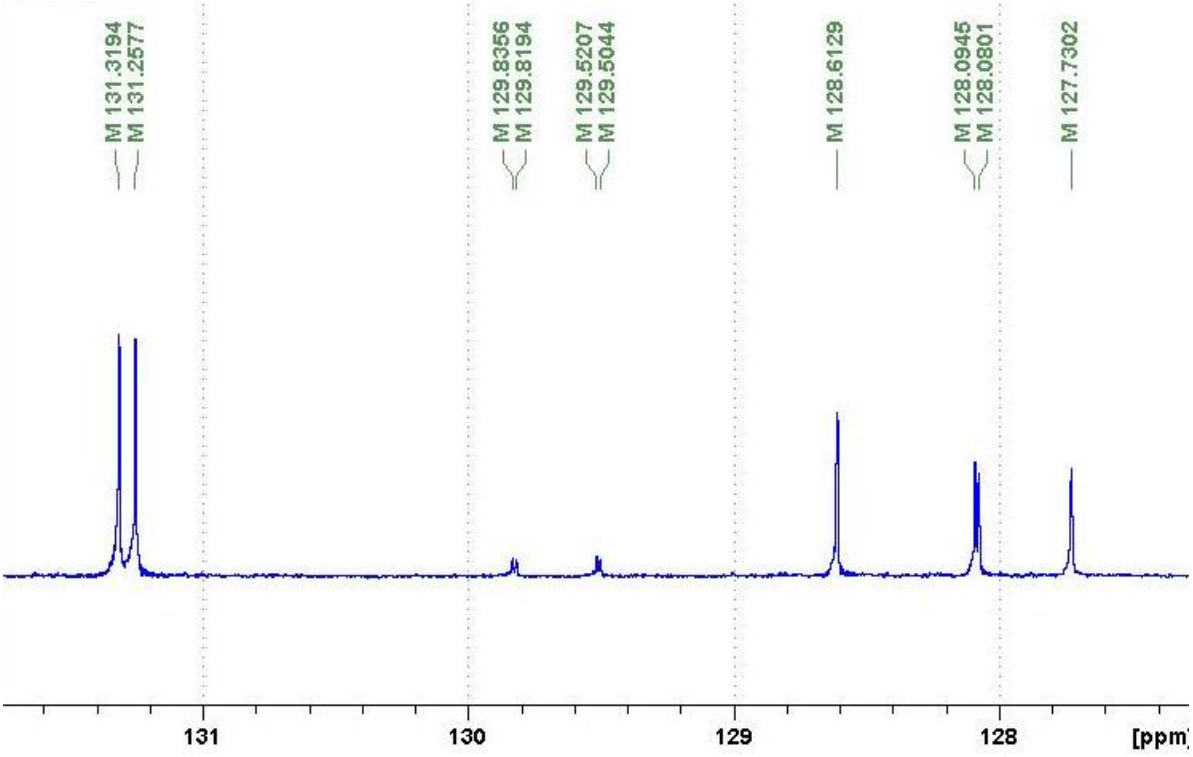


Figure 22. $^{13}C\{^{1}H\}$ NMR spectrum of **3-PMe$_3$** (125.8 MHz, 293 K) in CD_2Cl_2: zoom 3

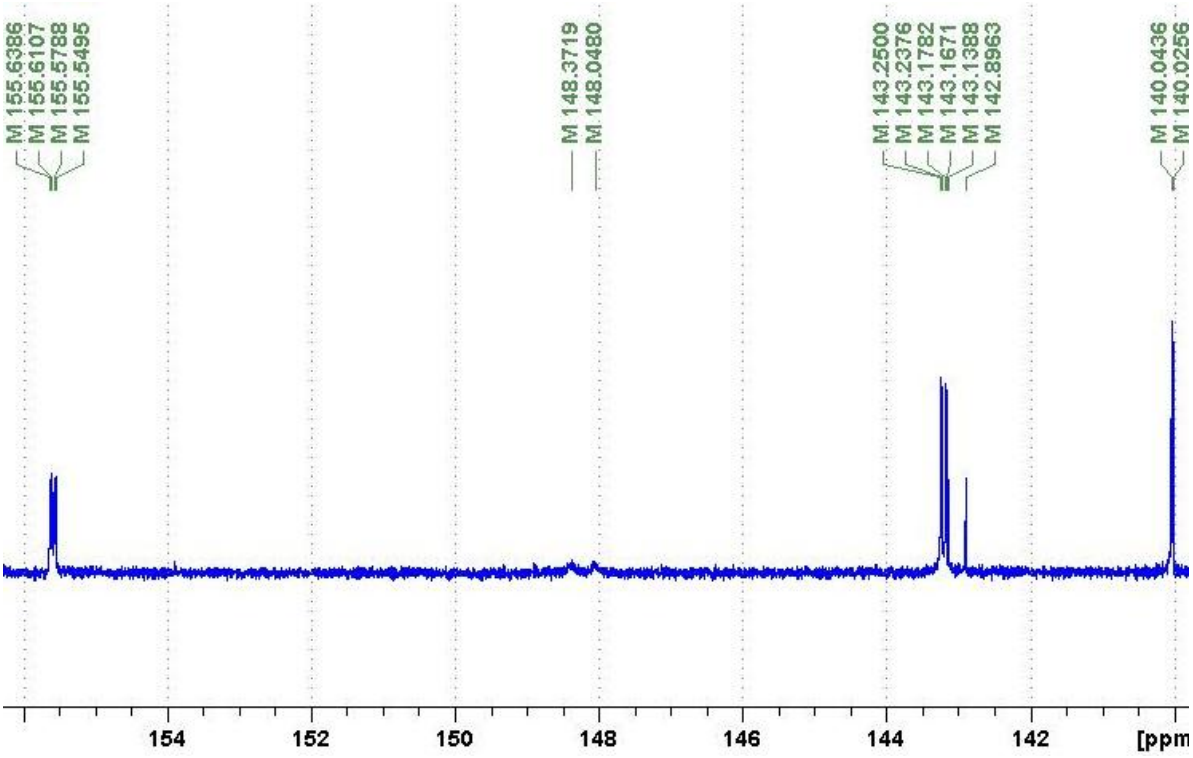


Figure 23. $^{31}P\{^{1}H\}$ NMR spectrum of **3-tht** (202.4-tht MHz, 20 °C) in CD_2Cl_2

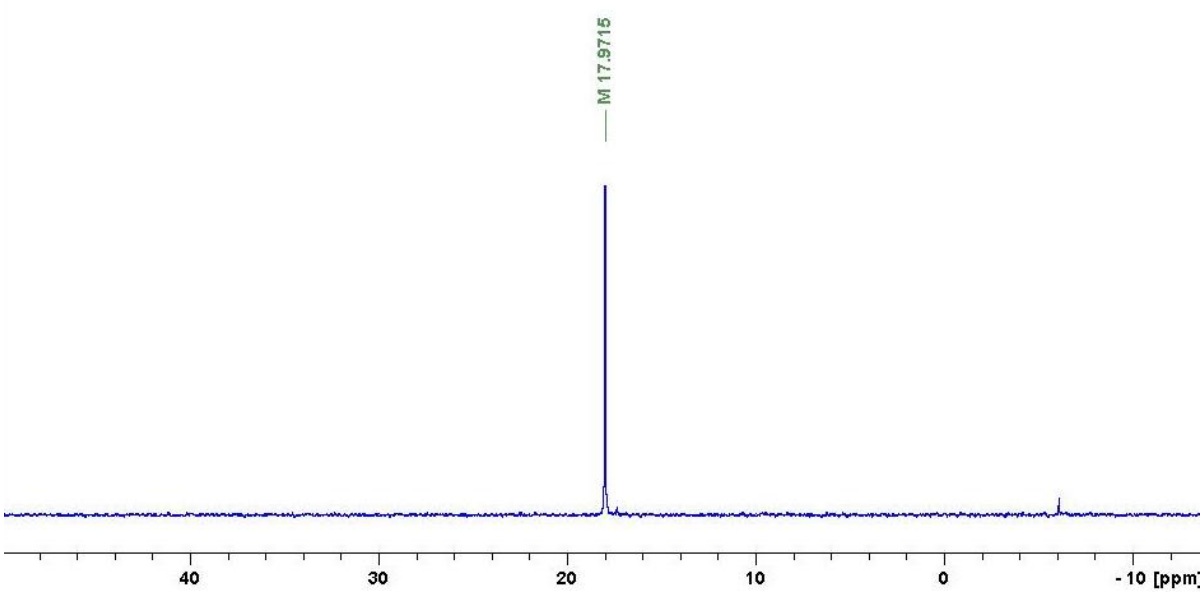


Figure 24. ^{1}H NMR spectrum of **3-tht** (499.9 MHz, 20 °C) in CD_2Cl_2

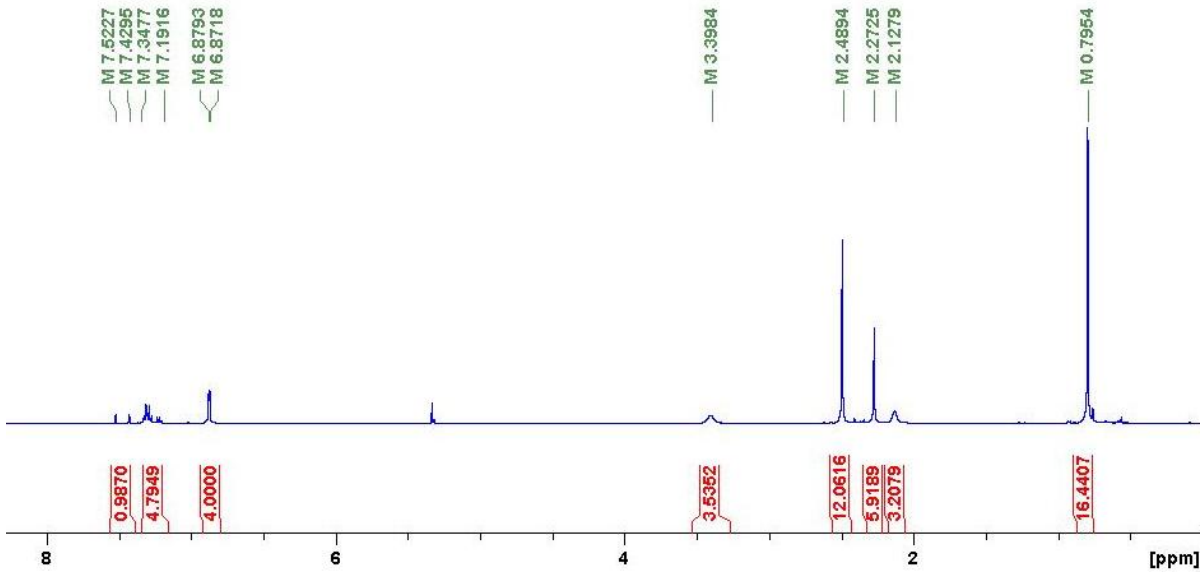


Figure 25. ^{1}H NMR spectrum of **3-tht** (499.9 MHz, 20 °C) in CD_2Cl_2: zoom 1

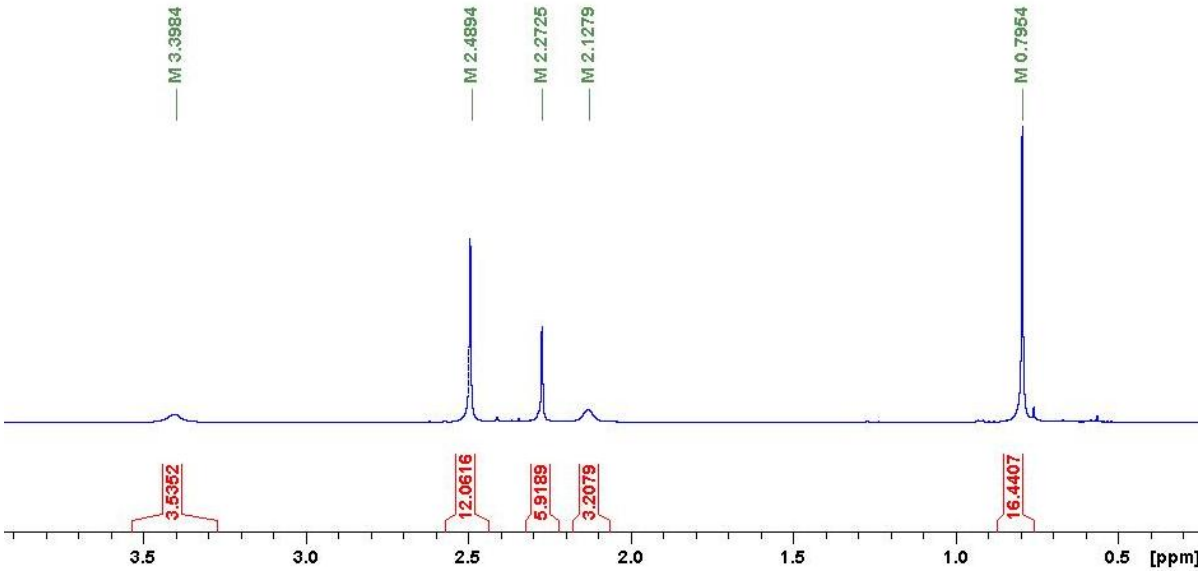


Figure 26. ^{1}H NMR spectrum of **3-tht** (499.9 MHz, 20 °C) in CD_2Cl_2: zoom 2

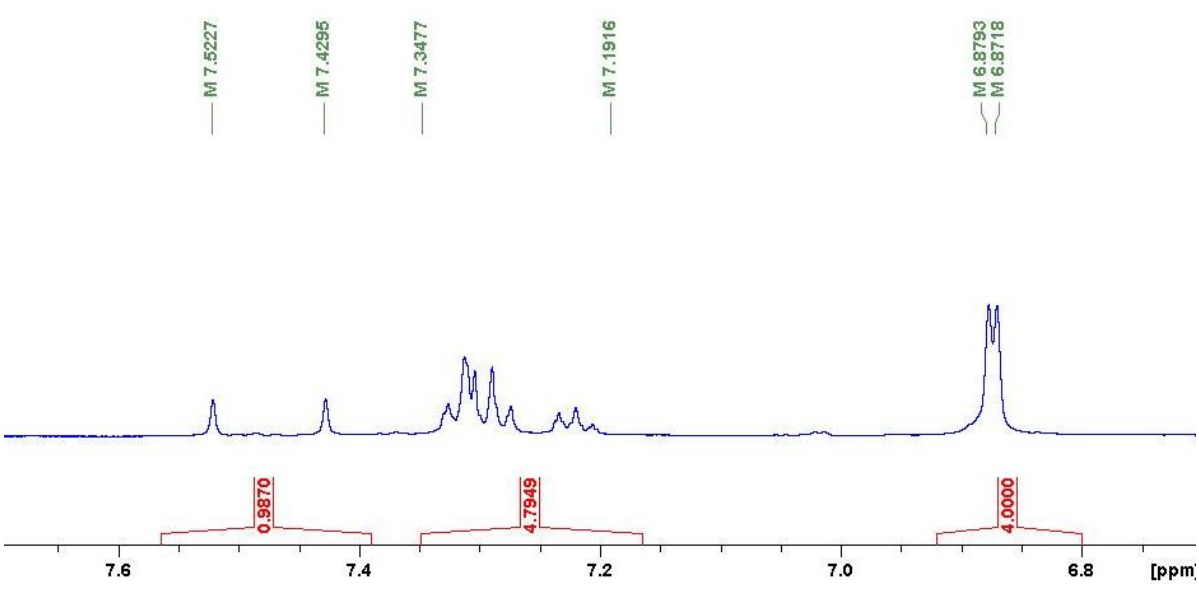


Figure 27. ^{1}H NMR and $^{1}H\{^{31}P\}$ spectra of **3-tht** (499.9 MHz, 20 °C) in CD_2Cl_2: zoom 2

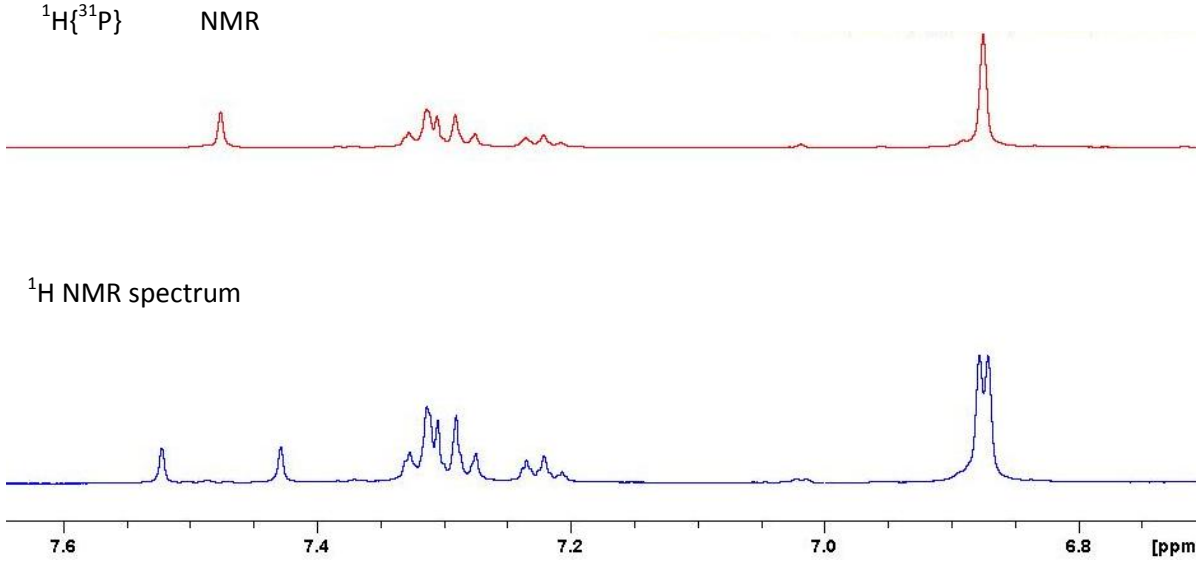


Figure 28. $^{13}C\{^{1}H\}$ NMR spectrum of **3-tht** (125.8 MHz, 20 °C) in CD_2Cl_2

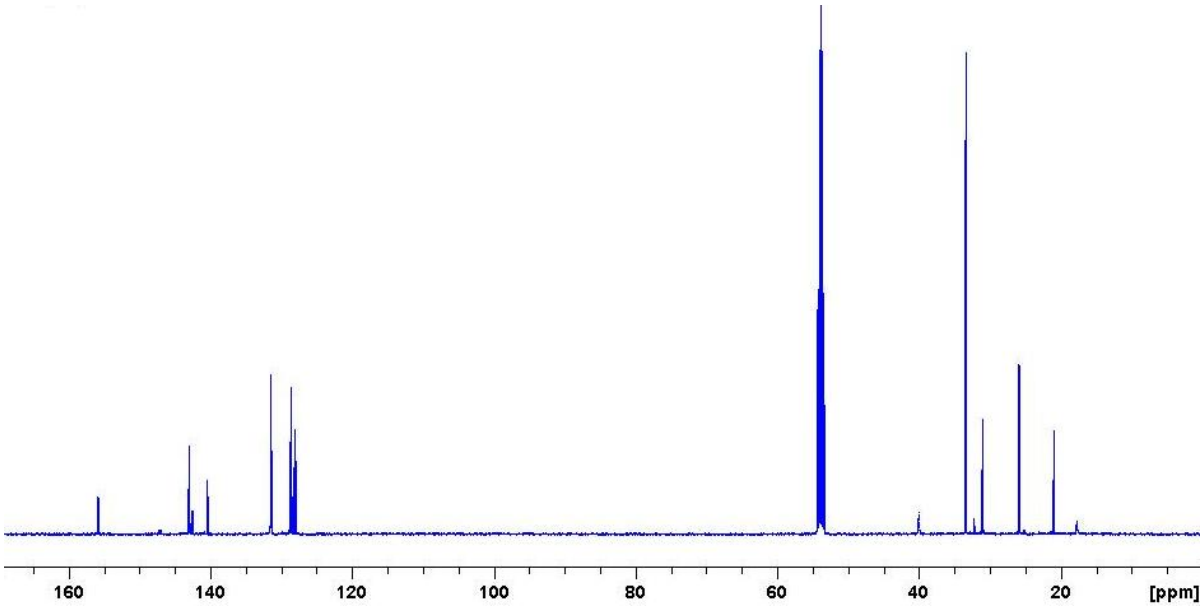


Figure 29. $^{13}C\{^{1}H\}$ NMR spectrum of **3-tht** (125.8 MHz, 20 °C) in CD_2Cl_2: zoom 1

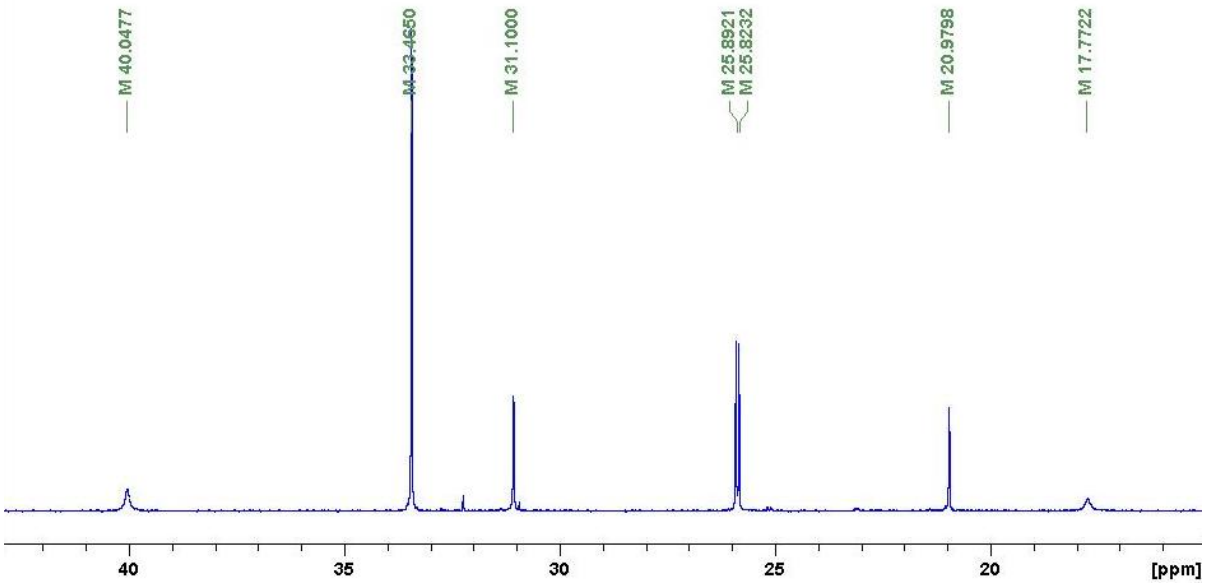


Figure 30. $^{13}C\{^{1}H\}$ NMR spectrum of **3-tht** (125.8 MHz, 20 °C) in CD_2Cl_2: zoom 2

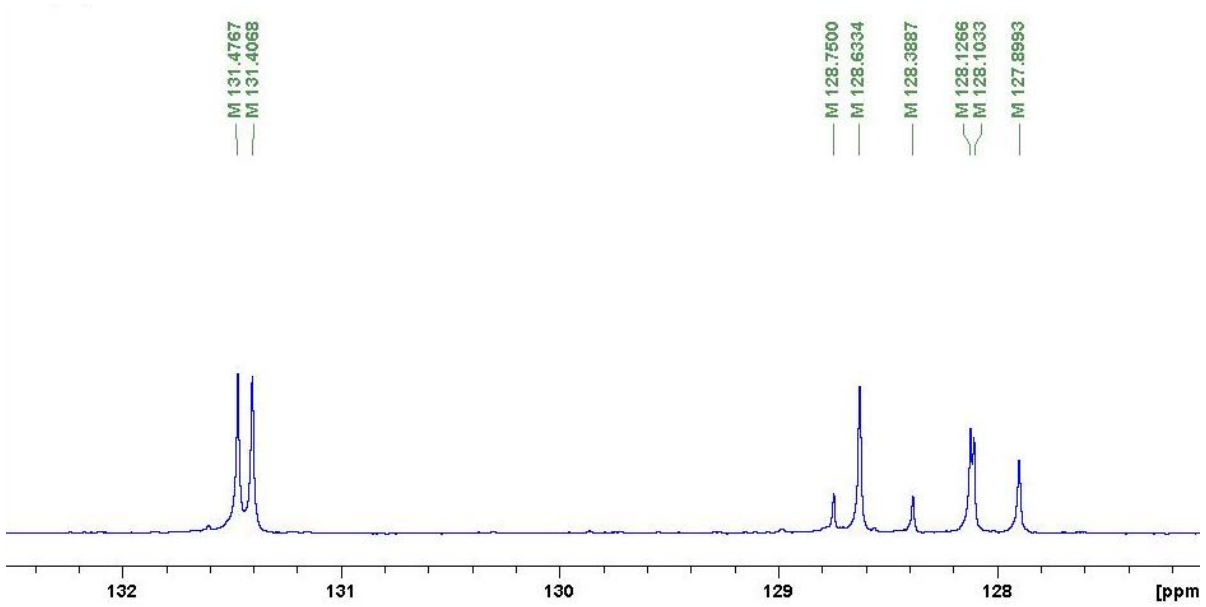


Figure 31. $^{13}C\{^{1}H\}$ NMR spectrum of **3-tht** (125.8 MHz, 20 °C) in CD_2Cl_2: zoom 3

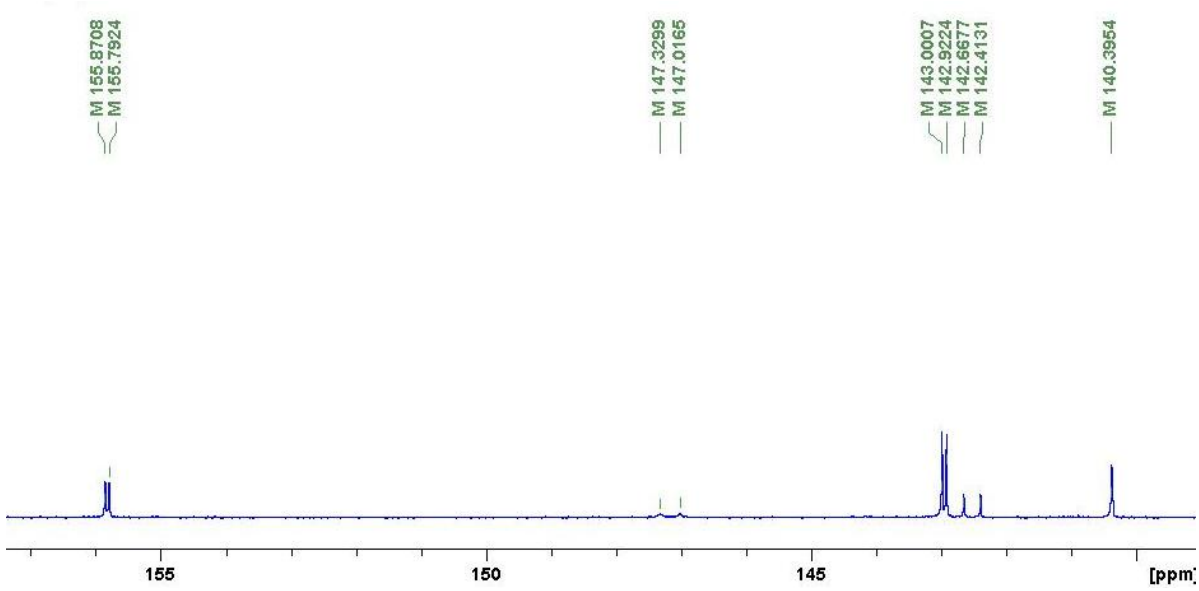
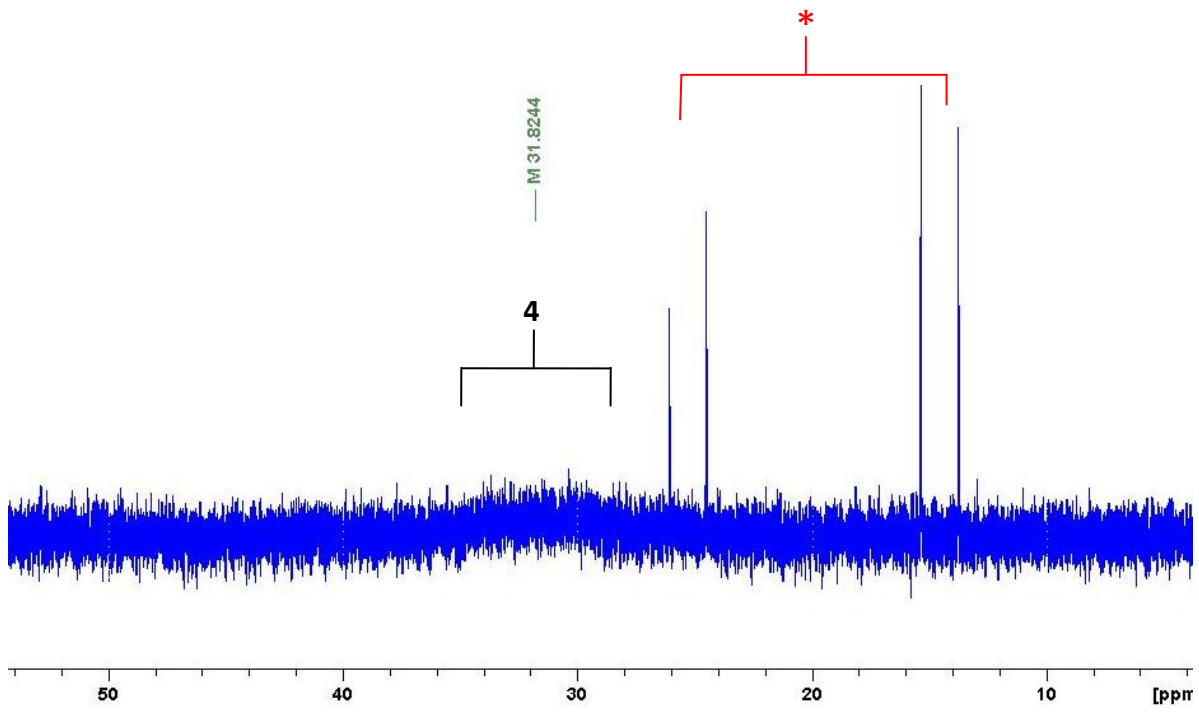


Figure 32. $^{31}P\{^{1}H\}$ NMR spectrum of **4** (202.4-tht MHz, 20 °C) in CD_2Cl_2



* AB spin system attributed to the hydrolysis product of **4** :

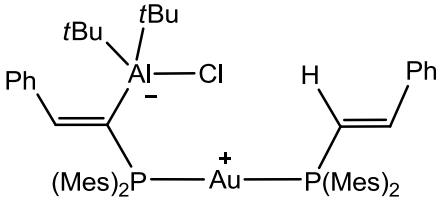
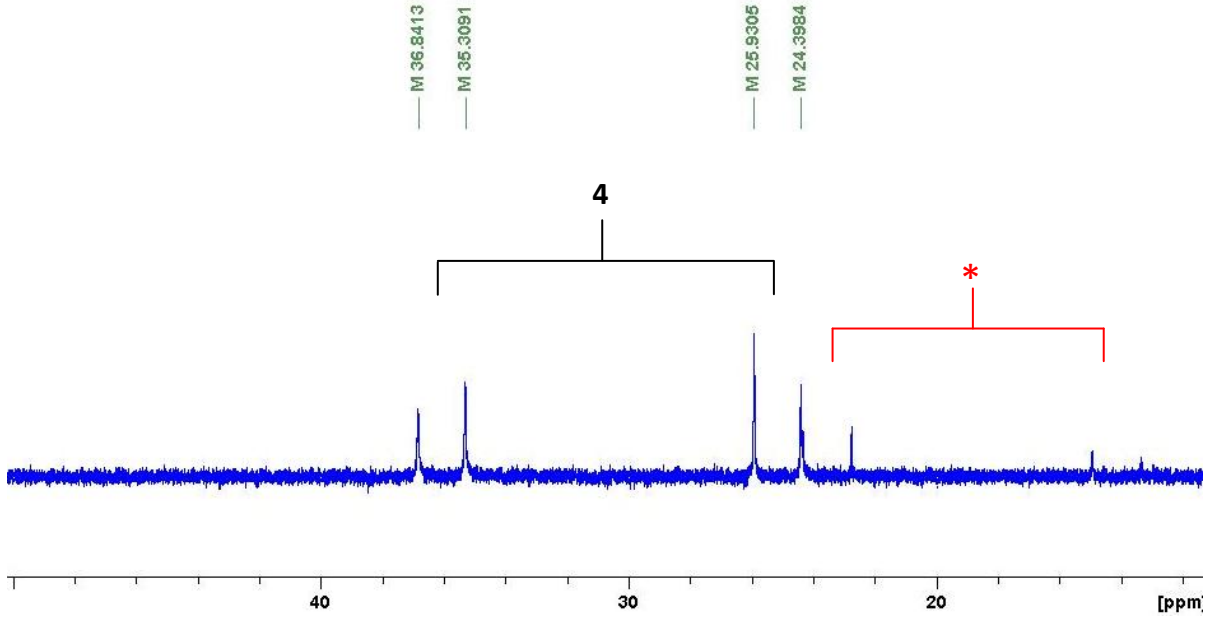
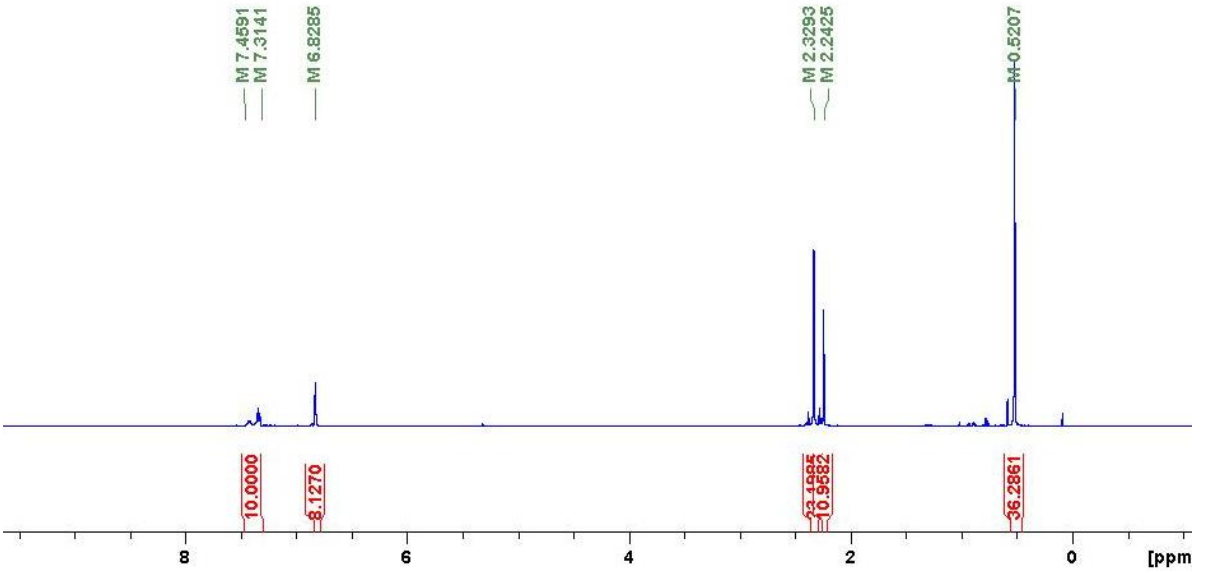


Figure 33. $^{31}P\{^{1}H\}$ NMR spectrum of **4** (202.4-tht MHz, -60 °C) in CD_2Cl_2



* AB spin system attributed to the hydrolysis product of **4** : [((Mes$_2$P(C=CHPh)Al(Cl)(*t*Bu$_2$)) Au ((Mes$_2$P(HC=CHPh)]

Figure 34. ^{1}H NMR spectrum of **4** (499.9 MHz, 20 °C) in CD_2Cl_2



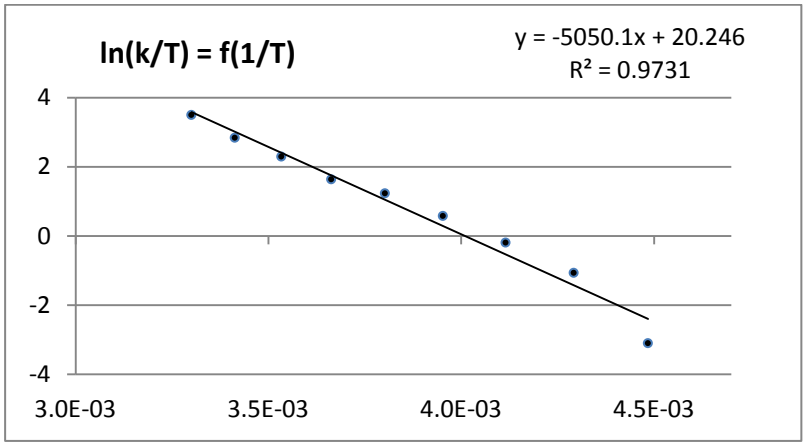
Determination of the activation barrier ($\Delta G^{\ddagger}$) for the chlorine shift in 4

A) The rate constant k (s^{-1}) of the exchange was estimated using the software DNMR based on the ^{31}P NMR spectra of **4** recorded at variable temperature.

Approximation : k = 0 s^{-1} at 213 K (temperature for which the exchange is frozen)

T (K)	k (s^{-1})
223	10
233	80
243	200
253	450
263	900
273	1400
283	2800
293	5000
303	10000

B) Eyring's plot : $\log\frac{k}{T} = f(\frac{1}{T})$



$(\Delta H^{\ddagger})/R$ = -5050.1 $J.mol^{-1}$, $\Delta H^{\ddagger}$ = 41986.5 $kJ.mol^{-1}$

$(\Delta S^{\ddagger})/R + \ln(k_B/h)$ = 20.246 $J.mol^{-1}.K^{-1}$, $\Delta S^{\ddagger}$ = -29.2 $J.mol^{-1}.K^{-1}$

at 303 K, $\Delta G^{\ddagger} = \Delta H^{\ddagger} - T\Delta S^{\ddagger}$ = 50.5 $kJ.mol^{-1}$ = 12.1 $kcal.mol^{-1}$

CRYSTALLOGRAPHIC DATA.

Crystallographic data were collected at 193 K on a Bruker-AXS APEX-II QUAZAR diffractometer equipped with a air-cooled microfocus source, using Mo K_α radiation (λ = 0.71073 Å). Semi-empirical absorption corrections were employed.[4] The structures were solved by direct methods (SHELXS 97),[5] and all non-hydrogen atoms were refined anisotropically using the least-squares method on F^2.[6]

2-Rh : $C_{41}H_{54}AlPRhCl$, *M* = 743.15, triclinic, *P-1*, *a* = 11.5935(14), *b* = 12.8808(17), *c* = 14.3137(18) Å, α = 80.717(6) °, β = 72.804(5) °, γ = 68.413(5) °, *V* = 1895.4(4) Å^3, *Z* = 2, crystal size 0.08 x 0.08 x 0.04 mm^3, 16245 reflections collected (4314 independent, R_{int} = 0.0579), 418 parameters, *R*1 [I>2σ(I)] = 0.0353, *wR*2 [all data] = 0.0754, largest diff. peak and hole: 0.306 and -0.337eÅ^{-3}.

2-Pd : $C_{37}H_{51}AlPPdCl$, *M* = 695.58, triclinic, *P-1*, *a* = 10.9029(12), *b* = 12.1216(14), *c* = 14.5288(16) Å, α = 91.146(3) °, β = 110.558(3) °, γ = 97.710(3) °, *V* = 1765.6(3) Å^3, *Z* = 2, crystal size 0.44 x 0.44 x 0.44 mm^3, 37893 reflections collected 7101 independent, R_{int} =0.0202, 433 parameters, *R*1 [I>2σ(I)] = 0.0222, *wR*2 [all data] = 0.0594, largest diff. peak and hole: 0.549 and -0.427eÅ^{-3}.

3-PMe$_3$: $C_{37}H_{55}AlP_2AuCl$, *M* = 860.20, monoclinic, *P2$_1$/c*, *a* = 9.6291(5), *b* = 23.6665(12), *c* = 17.7492(9) Å, α = 90 °, β = 97.902(2) °, γ = 90 °, *V* = 4006.4(4) Å^3, *Z* = 4, crystal size 0.08 x 0.04 x 0.02 mm^3, 64611 reflections collected 10792 independent, R_{int} =0.0541, 421 parameters, *R*1 [I>2σ(I)] = 0.0289, *wR*2 [all data] = 0.0550, largest diff. peak and hole: 0.658 and -0.608eÅ^{-3}.

3-tht : $C_{40}H_{58}AlPAuClS$, *M* = 860.20, monoclinic, *P2$_1$/c*, *a* = 9.6291(5), *b* = 23.6665(12), *c* = 17.7492(9) Å, α = 90 °, β = 97.902(2) °, γ = 90 °, *V* = 4006.4(4) Å^3, *Z* = 4, crystal size 0.08 x 0.04 x 0.02 mm^3, 64611 reflections collected 10792 independent, R_{int} =0.0541, 421 parameters, *R*1 [I>2σ(I)] = 0.0289, *wR*2 [all data] = 0.0550, largest diff. peak and hole: 0.658 and -0.608eÅ^{-3}.

Crystallographic data (excluding structure factors) have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1014327 (**2-Rh**), 1014328 (**2-Pd**), 1014329 (**3-PMe$_3$**) and 1014330 (**3-tht**). These data can be obtained free of charge via www.ccdc.cam.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223_336_033; or deposit@ccdc.cam.ac.uk).

[4] SADABS, Program for data correction, Bruker_AXS, **2003**, version 2.10.
[5] G. M. Sheldrick, *Acta Crystallogr.* **1990**, *A46*, 467–473.
[6] SHELXL–97, Program for Crystal Structure Refinement, G. M. Sheldrick, University of Göttingen, **1997**.

COMPUTATIONAL DETAILS.

Calculations were performed with the Gaussian09 suite of software, revision D.01,[7] using the B97D functional,[8] the 6-31G** basis set for all non–metallic atoms,[9] and the SDD basis set and associated electron core potential for Au,[10] augmented with a polarization function.[11] All geometries have been computed and optimized in the gas phase. The stationary points were characterized as minima by full vibration frequencies calculations (no imaginary frequency).

[7] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Rev D.01 **2009**.

[8] S. Grimme, *J. Comput. Chem.*, 2006, **27**, 1787.

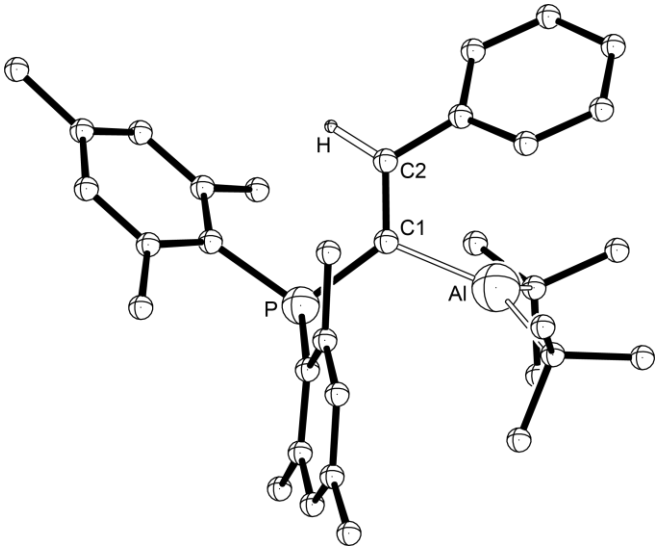
[9] W. J. Hehre, R. Ditchfield, and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257, P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213, M. M. Francl, *J. Chem. Phys.*, 1982, **77**, 3654.

[10] D. Andrae, U. Häussermann, M. Dolg, H. Stoll, and H. Preuss, *Theor. Chim. Acta*, 1990, **77**, 123–141.

[11] A. W. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp, and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 111–114.

THEORETICAL RESULTS.

($Mes_2PC(=CHPh)AltBu_2$) 1



Selected Bond Distances (Å) and Angles (°): P–C1 1.824, C1–C2 1.365, C1–Al 2.018; P–C1–C2 125.24, C2–C1–Al 112.95, P–C1–Al 118.99.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.210347	-0.592320	-0.039244
2	6	0	0.200334	-1.777264	-0.716165
3	15	0	-1.184304	0.081086	0.924395
4	13	0	2.074127	0.085563	0.333171
5	6	0	2.849740	1.834266	-0.321457
6	6	0	2.494350	2.201960	-1.777825
7	6	0	4.391312	1.803377	-0.191291
8	6	0	2.302828	2.954037	0.603198
9	6	0	2.958173	-0.885945	1.868309
10	6	0	4.365755	-1.416118	1.511281
11	6	0	3.085887	0.125412	3.037328
12	6	0	2.094002	-2.073861	2.346811
13	1	0	1.086387	-1.748519	2.647917
14	1	0	2.567788	-2.563544	3.220714
15	1	0	3.544065	-0.363923	3.919550
16	1	0	4.829440	-1.892639	2.398141
17	1	0	5.039379	-0.611244	1.178534
18	1	0	3.719693	0.986845	2.771337
19	1	0	2.102219	0.513306	3.355697
20	1	0	1.982151	-2.834213	1.558282
21	1	0	4.321162	-2.172640	0.712329
22	1	0	2.900317	3.202527	-2.026087
23	1	0	4.821710	2.776977	-0.498614
24	1	0	4.711216	1.612472	0.844793
25	1	0	1.407676	2.240883	-1.935780
26	1	0	4.842917	1.025176	-0.829398
27	1	0	2.930947	1.495087	-2.504243
28	1	0	2.765162	3.925897	0.337872
29	1	0	2.537193	2.762114	1.663916
30	1	0	1.214469	3.068922	0.504617
31	6	0	-1.261680	1.804521	0.227000
32	6	0	-1.125110	4.503738	-0.669539
33	6	0	-1.354054	2.878060	1.157483
34	6	0	-1.141971	2.094880	-1.160843

35	6	0	-1.070271	3.435544	-1.577834
36	6	0	-1.288805	4.202999	0.691302
37	6	0	-2.708538	-0.887913	0.449645
38	6	0	-4.846713	-2.670125	-0.218420
39	6	0	-3.874475	-0.401880	-0.214533
40	6	0	-2.698030	-2.249487	0.896715
41	6	0	-3.746440	-3.111107	0.530201
42	6	0	-4.902650	-1.307863	-0.541696
43	1	0	-5.786718	-0.922783	-1.056679
44	1	0	-3.712175	-4.149836	0.868790
45	1	0	-0.978117	3.648060	-2.645930
46	1	0	-1.357684	5.019748	1.413716
47	1	0	-0.695618	-2.403401	-0.808126
48	6	0	1.454861	-2.323136	-1.263915
49	6	0	4.035319	-3.280639	-1.974244
50	6	0	2.444979	-1.450279	-1.796263
51	6	0	1.770547	-3.697386	-1.161778
52	6	0	3.044045	-4.166287	-1.508437
53	6	0	3.725962	-1.923144	-2.134074
54	1	0	2.161301	-0.434442	-2.082090
55	1	0	4.463920	-1.232060	-2.544023
56	1	0	5.027330	-3.653809	-2.230168
57	1	0	3.275049	-5.227289	-1.399201
58	1	0	1.019788	-4.384405	-0.767664
59	6	0	-0.988194	5.935165	-1.140821
60	6	0	-1.520502	2.650034	2.650782
61	6	0	-1.129347	1.021577	-2.232786
62	6	0	-4.136410	1.059039	-0.544474
63	6	0	-5.944994	-3.623352	-0.638608
64	6	0	-1.632439	-2.801166	1.830431
65	1	0	-6.069807	-4.436436	0.092244
66	1	0	-6.907242	-3.101138	-0.746807
67	1	0	-5.712324	-4.089393	-1.611365
68	1	0	-5.211809	1.206245	-0.721488
69	1	0	-1.747161	0.159663	-1.952841
70	1	0	-3.604598	1.391253	-1.445906
71	1	0	-3.829041	1.727376	0.268685
72	1	0	-1.893623	-3.822065	2.143627
73	1	0	-0.632748	-2.828047	1.376055
74	1	0	-1.548162	-2.174370	2.732149
75	1	0	-1.499717	1.435315	-3.182502
76	1	0	-1.393275	6.063446	-2.155554
77	1	0	0.073489	6.233198	-1.170203
78	1	0	-1.507549	6.630337	-0.464950
79	1	0	-1.633710	3.610284	3.174058
80	1	0	-2.403118	2.030196	2.870283
81	1	0	-0.653960	2.120446	3.075352
82	1	0	-0.112614	0.639772	-2.403612

Harmonic Frequencies

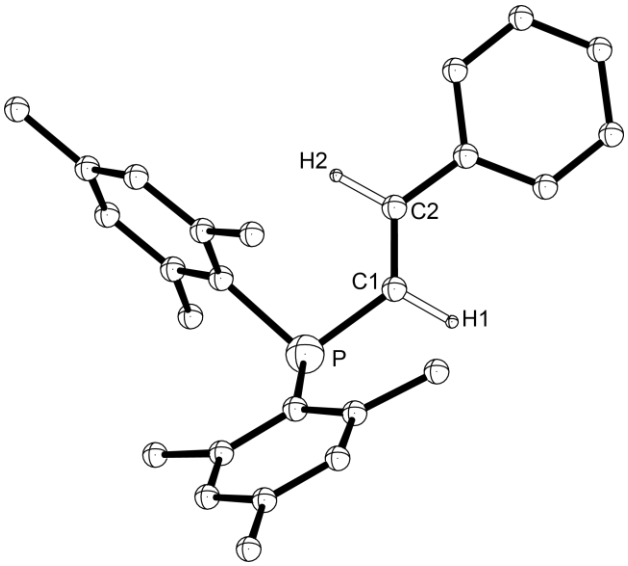
	1	2	3
	A	A	A
Frequencies --	20.9965	27.4943	30.6510
Red. masses --	3.9049	3.2400	4.5686
Frc consts --	0.0010	0.0014	0.0025
IR Inten --	0.0200	0.0690	0.1793

Thermochemistry

Sum of electronic and zero-point Energies=	-1905.481091
Sum of electronic and thermal Energies=	-1905.438576
Sum of electronic and thermal Enthalpies=	-1905.437632
Sum of electronic and thermal Free Energies=	-1905.555787

HF = -1906.16994558

$Mes_2PCH=CHPh$



Selected Bond Distances (Å) and Angles (°): P–C1 1.821, C1–C2 1.358, C1–H1 1.092; P–C1–C2 125.50, C2–C1–H1 119.15, P–C1–H1 114.42

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.185128	-0.940006	0.865038
2	6	0	-2.211488	-0.300684	0.247132
3	15	0	0.408106	-0.186583	1.321435
4	6	0	1.826436	-1.110880	0.528352
5	6	0	4.184433	-2.316184	-0.554149
6	6	0	3.103395	-0.489235	0.684872
7	6	0	1.755445	-2.367339	-0.139856
8	6	0	2.930612	-2.934079	-0.666499
9	6	0	4.244839	-1.096069	0.131826
10	6	0	0.361944	1.424634	0.379490
11	6	0	0.351258	3.961676	-0.913022
12	6	0	0.480883	1.507304	-1.035461
13	6	0	0.209906	2.619865	1.138683
14	6	0	0.211518	3.861076	0.480929
15	6	0	0.478027	2.775097	-1.648868
16	1	0	0.572154	2.830676	-2.736375
17	1	0	0.099338	4.771614	1.074855
18	1	0	2.856164	-3.891201	-1.189224
19	1	0	5.209636	-0.595952	0.248961
20	1	0	-2.024209	0.687477	-0.181961
21	6	0	-3.574721	-0.812512	0.064166
22	6	0	-6.224289	-1.721838	-0.396553
23	6	0	-4.046346	-2.011894	0.653261
24	6	0	-4.469567	-0.078464	-0.751748
25	6	0	-5.776688	-0.526684	-0.981784
26	6	0	-5.351083	-2.460076	0.423141
27	1	0	-3.388990	-2.588430	1.305261
28	1	0	-5.693308	-3.385687	0.889366
29	1	0	-7.242432	-2.072945	-0.570801
30	1	0	-6.446203	0.056990	-1.615918
31	1	0	-4.122268	0.850871	-1.208431
32	6	0	5.430779	-2.965030	-1.118332
33	6	0	3.298032	0.825731	1.419862
34	6	0	0.471925	-3.153317	-0.330854
35	6	0	0.603464	0.287987	-1.927136
36	6	0	0.330414	5.312052	-1.598256

37	6	0	0.039629	2.603520	2.647909
38	1	0	0.940754	6.045616	-1.049397
39	1	0	0.711327	5.243503	-2.627405
40	1	0	-0.695394	5.714450	-1.645927
41	1	0	0.381480	0.555608	-2.970265
42	1	0	-0.301471	-2.564536	-0.843448
43	1	0	-0.091290	-0.501177	-1.612640
44	1	0	1.616273	-0.138634	-1.886757
45	1	0	-0.076993	3.626756	3.033138
46	1	0	-0.845568	2.020782	2.945142
47	1	0	0.904066	2.139560	3.146545
48	1	0	0.664880	-4.057676	-0.925177
49	1	0	5.203369	-3.540064	-2.028513
50	1	0	5.877435	-3.664755	-0.391601
51	1	0	6.195215	-2.212955	-1.363686
52	1	0	4.366581	1.003730	1.606382
53	1	0	2.900478	1.676420	0.847017
54	1	0	2.774830	0.824561	2.389735
55	1	0	0.046803	-3.474481	0.632525
56	1	0	-1.356014	-1.929275	1.294227

Harmonic Frequencies

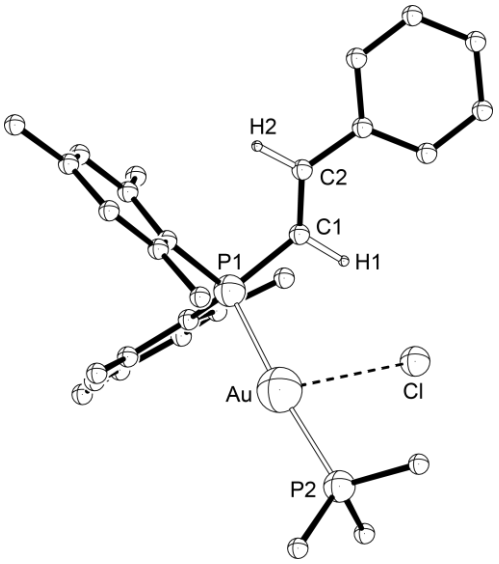
	1	2	3
	A	A	A
Frequencies --	23.6390	26.4501	27.1456
Red. masses --	3.7128	1.6836	4.1168
Frc consts --	0.0012	0.0007	0.0018
IR Inten --	0.1554	0.3064	0.0557

Thermochemistry

Sum of electronic and zero-point Energies=	-1348.389910
Sum of electronic and thermal Energies=	-1348.361552
Sum of electronic and thermal Enthalpies=	-1348.360608
Sum of electronic and thermal Free Energies=	-1348.451029

HF = -1348.85205060

[AuCl(PMe$_3$)(Mes$_2$PCHCHPh)] 3–H–PMe$_3$



Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): P1–Au 2.355, P2–Au 2.328, Au–Cl 3.184, P1–C1 1.804, C1–C2 1.354, C1–H 1.094, H–Cl 2.454; P1–Au–P2 172.30, P1–Au–Cl 92.02, P2–Au–Cl 80.55, Au–P1–C1 104.07, P1–C1–C2 125.07, C2–C1–H 122.20, P1–C1–H 111.70; C1–P1–Au–Cl 29.57.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.540343	-1.391172	-0.292762
2	1	0	3.179407	-0.697820	0.262730
3	6	0	1.285207	-1.017662	-0.635714
4	15	0	0.448129	0.467934	-0.046342
5	79	0	-1.661956	-0.305345	0.658846
6	17	0	-1.632674	-2.670507	-1.472679
7	6	0	0.014191	1.682254	-1.375783
8	6	0	-0.742694	3.648189	-3.280849
9	6	0	-0.481462	2.945888	-0.940163
10	6	0	0.061724	1.375909	-2.764868
11	6	0	-0.309585	2.375498	-3.681761
12	6	0	-0.837016	3.903931	-1.905985
13	1	0	-0.266961	2.138889	-4.747375
14	1	0	-1.210032	4.873168	-1.566303
15	6	0	1.672054	1.301411	1.053130
16	6	0	3.554422	2.619168	2.726681
17	6	0	1.558600	1.204092	2.468417
18	6	0	2.762863	2.015716	0.477391
19	6	0	3.675547	2.661774	1.330170
20	6	0	2.499642	1.871796	3.271657
21	1	0	4.512491	3.203833	0.883478
22	1	0	2.408207	1.793197	4.357382
23	6	0	-0.668787	3.317769	0.520210
24	1	0	-1.257190	4.242743	0.599172
25	1	0	0.290090	3.476073	1.034467
26	1	0	-1.202575	2.524213	1.068942
27	6	0	0.448396	0.020063	-3.318348
28	1	0	0.386703	0.031869	-4.415456
29	1	0	-0.225759	-0.768022	-2.944177
30	1	0	1.474108	-0.263025	-3.039526
31	6	0	0.479325	0.403494	3.171772
32	1	0	0.410362	-0.622258	2.780427
33	1	0	-0.514556	0.858943	3.034226

34	1	0	0.688760	0.349572	4.249527
35	6	0	3.010655	2.112495	-1.017796
36	1	0	4.053745	2.404394	-1.204901
37	1	0	2.354374	2.860583	-1.485954
38	1	0	2.824492	1.156623	-1.524814
39	15	0	-3.761763	-1.221069	1.074810
40	6	0	-4.797736	-1.220371	-0.445878
41	1	0	-4.978904	-0.184048	-0.762947
42	1	0	-5.756023	-1.732871	-0.269761
43	1	0	-4.207437	-1.739915	-1.215073
44	6	0	-4.799264	-0.431847	2.388798
45	1	0	-4.985949	0.616941	2.119160
46	1	0	-4.252237	-0.455270	3.341527
47	1	0	-5.760469	-0.956130	2.505592
48	6	0	-3.610698	-2.991594	1.553546
49	1	0	-3.059305	-3.067728	2.501067
50	1	0	-3.028949	-3.470779	0.752110
51	1	0	-4.601460	-3.459983	1.657654
52	6	0	3.140337	-2.690025	-0.622204
53	6	0	4.395075	-5.145097	-1.248155
54	6	0	4.517684	-2.886581	-0.366592
55	6	0	2.393456	-3.754727	-1.188611
56	6	0	3.021408	-4.965901	-1.496824
57	6	0	5.142059	-4.101222	-0.679279
58	1	0	5.094922	-2.071659	0.076492
59	1	0	1.323038	-3.638593	-1.369713
60	1	0	2.434797	-5.778082	-1.928857
61	1	0	6.206528	-4.233796	-0.478437
62	1	0	4.876430	-6.093931	-1.490893
63	6	0	-1.095769	4.707957	-4.302538
64	1	0	-1.741966	5.483566	-3.866239
65	1	0	-1.613419	4.268892	-5.168539
66	1	0	-0.187898	5.205908	-4.682956
67	6	0	4.529083	3.358614	3.617869
68	1	0	4.172714	4.382445	3.821476
69	1	0	5.517922	3.442770	3.143837
70	1	0	4.646766	2.852459	4.587180
71	1	0	0.595334	-1.694201	-1.148001

Harmonic Frequencies

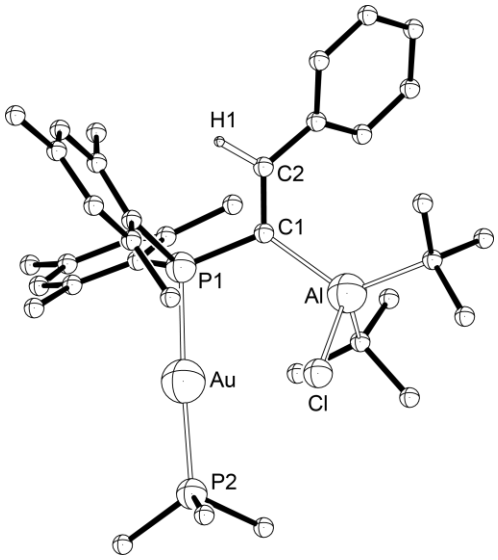
	1	2	3
	A	A	A
Frequencies --	15.5933	21.5274	24.0056
Red. masses --	5.7358	4.4880	6.2886
Frc consts --	0.0008	0.0012	0.0021
IR Inten --	1.1947	0.6428	3.2002

Thermochemistry

Sum of electronic and zero-point Energies=	-2405.811828
Sum of electronic and thermal Energies=	-2405.771684
Sum of electronic and thermal Enthalpies=	-2405.770740
Sum of electronic and thermal Free Energies=	-2405.888487

HF = -2406.38982134

[AuCl(PMe$_3$)(1)] 3–PMe$_3$



Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): P1–Au 2.356, P2–Au 2.332, Au–Cl 2.316, P1–C1 1.848, C1–C2 1.368, C1–Al 2.108, Al–Cl 2.316; P1–Au–P2 176.82, P1–Au–Cl 90.83, P2–Au–Cl 86.59, Au–P1–C1 111.06, P1–C1–C2 111.83, C2–C1–Al 125.90, P1–C1–Al 121.71, C1–Al–Cl 101.999, Al–C2–Au 90.36; C1–P1–Au–Cl 21.45, P1–C1–Al–Cl 42.03, Au–P1–Al–Cl 34.51, Au–P1–C–Al 7.32

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.277553	1.335109	-0.266102
2	1	0	-1.947564	2.334173	-0.578201
3	6	0	-1.380089	0.318467	-0.083848
4	13	0	-1.821478	-1.742569	-0.126456
5	15	0	0.360275	0.938235	-0.036948
6	79	0	1.895308	-0.827521	-0.313245
7	6	0	-1.391864	-2.693465	1.642419
8	6	0	-3.567467	-2.394028	-1.033694
9	17	0	-0.244646	-2.541533	-1.623346
10	6	0	0.891385	1.617146	1.623549
11	6	0	1.956964	2.487819	4.129343
12	6	0	2.222058	2.141989	1.705103
13	6	0	0.096563	1.566889	2.802912
14	6	0	0.653297	1.990367	4.024564
15	6	0	2.715604	2.561818	2.953181
16	1	0	0.032247	1.932451	4.921481
17	1	0	3.732584	2.959084	3.001047
18	6	0	0.488012	2.356258	-1.234295
19	6	0	0.719700	4.473670	-3.133086
20	6	0	0.799373	2.073517	-2.598124
21	6	0	0.222571	3.704475	-0.845847
22	6	0	0.355593	4.727253	-1.805014
23	6	0	0.915733	3.137128	-3.509023
24	1	0	0.150328	5.755910	-1.498839
25	1	0	1.152607	2.905456	-4.550187
26	6	0	-3.264068	-3.690311	-1.836301
27	1	0	-4.214356	-4.110535	-2.223721
28	1	0	-2.785369	-4.464163	-1.215606
29	1	0	-2.606976	-3.499703	-2.696058
30	6	0	-4.172261	-1.386888	-2.040625
31	1	0	-4.579333	-0.494205	-1.549369
32	1	0	-5.004066	-1.861873	-2.600329
33	1	0	-3.424817	-1.058989	-2.782959
34	6	0	-4.664979	-2.792481	-0.015371
35	1	0	-4.988292	-1.960366	0.622252
36	1	0	-4.325471	-3.610679	0.639469
37	1	0	-5.562540	-3.159757	-0.553722
38	6	0	-2.448855	-2.451931	2.750060

39	1	0	-2.490966	-1.403283	3.081907
40	1	0	-2.207266	-3.057372	3.647932
41	1	0	-3.458621	-2.739542	2.422456
42	6	0	-0.005774	-2.315606	2.213646
43	1	0	0.108413	-1.237199	2.404433
44	1	0	0.795448	-2.614365	1.521048
45	1	0	0.181637	-2.841142	3.174311
46	6	0	-1.374881	-4.217738	1.366584
47	1	0	-2.358328	-4.577743	1.026173
48	1	0	-1.114957	-4.779657	2.287791
49	1	0	-0.640366	-4.481254	0.589001
50	6	0	3.148684	2.331136	0.516844
51	1	0	4.116933	2.725642	0.855293
52	1	0	2.728371	3.031035	-0.217891
53	1	0	3.334869	1.387131	-0.019935
54	6	0	-1.353817	1.135573	2.837522
55	1	0	-1.688625	1.016422	3.877248
56	1	0	-1.512091	0.193887	2.306686
57	1	0	-2.007491	1.874246	2.349284
58	6	0	1.001207	0.674769	-3.148587
59	1	0	0.285061	-0.052378	-2.745276
60	1	0	2.010044	0.297424	-2.908880
61	1	0	0.900970	0.683645	-4.243337
62	6	0	-0.209303	4.143606	0.544571
63	1	0	-0.699367	5.125840	0.481607
64	1	0	0.646464	4.233542	1.229821
65	1	0	-0.915091	3.442713	1.005062
66	15	0	3.317923	-2.658118	-0.564041
67	6	0	2.664611	-4.171809	0.259014
68	1	0	2.652256	-4.019897	1.346370
69	1	0	3.274869	-5.053062	0.009676
70	1	0	1.630596	-4.311337	-0.083245
71	6	0	5.060240	-2.488225	0.029010
72	1	0	5.053150	-2.281944	1.108161
73	1	0	5.531469	-1.638436	-0.483855
74	1	0	5.639813	-3.403525	-0.166322
75	6	0	3.456317	-3.124190	-2.344726
76	1	0	3.914645	-2.294395	-2.900211
77	1	0	2.437849	-3.283027	-2.723695
78	1	0	4.057673	-4.036711	-2.475323
79	6	0	-3.718323	1.295736	0.002272
80	6	0	-6.479748	1.359016	0.597735
81	6	0	-4.582342	2.194645	-0.668046
82	6	0	-4.258180	0.456493	1.001265
83	6	0	-5.626979	0.489703	1.295989
84	6	0	-5.952293	2.213872	-0.387404
85	1	0	-4.164597	2.860743	-1.425841
86	1	0	-3.596365	-0.209469	1.551994
87	1	0	-6.027531	-0.165767	2.070414
88	1	0	-6.610060	2.896352	-0.928049
89	1	0	-7.546261	1.380649	0.826586
90	6	0	2.514057	2.964624	5.453485
91	1	0	3.598678	2.790927	5.515194
92	1	0	2.029493	2.451415	6.296752
93	1	0	2.346893	4.047164	5.584856
94	6	0	0.888223	5.598088	-4.132043
95	1	0	1.953874	5.852215	-4.260405
96	1	0	0.366806	6.507866	-3.801207
97	1	0	0.500133	5.312696	-5.121407

Harmonic Frequencies

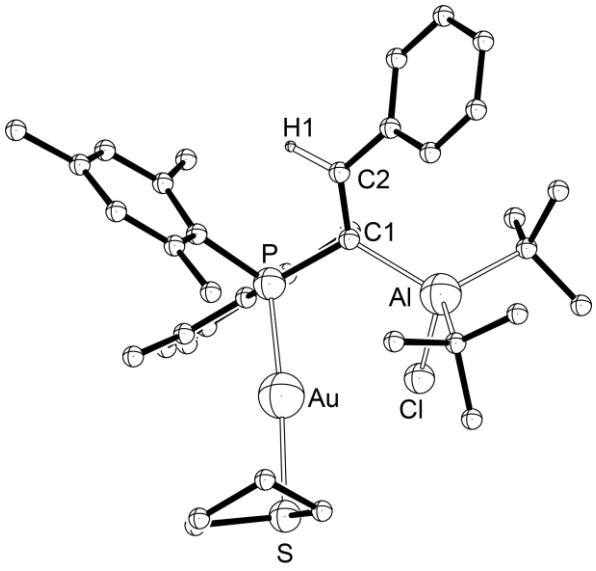
	1	2	3
	A	A	A
Frequencies --	18.0594	20.9094	27.3281
Red. masses --	4.4346	4.3062	4.4112
Frc consts --	0.0009	0.0011	0.0019
IR Inten --	0.7150	0.0364	0.2869

Thermochemistry

Sum of electronic and zero-point Energies=	-2962.940900
Sum of electronic and thermal Energies=	-2962.887700
Sum of electronic and thermal Enthalpies=	-2962.886756
Sum of electronic and thermal Free Energies=	-2963.027573

HF = -2963.74773157

[AuCl(1)(tht)] 3–tht



Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): P–Au 2.337, S–Au 2.456, Au–Cl 3.280, P–C1 1.840, C1–C2 1.365, C1–Al 2.094, Al–Cl 2.286; P–Au–S 174.21, Au–P–C1 106.32, P–C1–C2 113.17, C2–C1–Al 127.03, P–C1–Al 119.53, C1–Al–Cl 100.82; Au–P–Al–Cl 59.99, Au–P–C–Al 30.71, P–C–Al–Cl 29.59

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.325012	-1.303848	0.161730
2	13	0	-2.287870	-0.820864	0.859218
3	17	0	-0.870812	-1.263686	2.597887
4	15	0	0.536173	0.892851	0.050993
5	16	0	2.359931	-3.520507	0.381317
6	6	0	-1.296798	0.779127	-0.057995
7	6	0	-1.847445	1.735302	-0.862147
8	1	0	-1.265595	2.595300	-1.220160
9	6	0	-3.229875	1.734025	-1.374240
10	6	0	-3.967355	2.937091	-1.452241
11	1	0	-3.519370	3.862458	-1.083942
12	6	0	-5.267038	2.941939	-1.974239
13	1	0	-5.834816	3.873275	-2.008201
14	6	0	-5.837021	1.752451	-2.462755
15	1	0	-6.845228	1.760625	-2.879543
16	6	0	-5.100475	0.558847	-2.418637
17	1	0	-5.531333	-0.368704	-2.798237
18	6	0	-3.810880	0.551569	-1.874381
19	1	0	-3.232070	-0.366692	-1.837631
20	6	0	-4.055947	-0.412846	1.829074
21	6	0	-3.945873	0.798170	2.783847
22	1	0	-4.908241	0.954305	3.313080
23	1	0	-3.713467	1.729727	2.242113
24	1	0	-3.173718	0.640947	3.552192
25	6	0	-5.282506	-0.156055	0.924005
26	1	0	-5.440091	-0.957056	0.186961
27	1	0	-5.195071	0.791883	0.375389
28	1	0	-6.198610	-0.093368	1.547113
29	6	0	-4.375616	-1.651417	2.709695
30	1	0	-5.303387	-1.472866	3.290647
31	1	0	-3.565915	-1.863901	3.424136
32	1	0	-4.541453	-2.559991	2.108844
33	6	0	-2.323312	-2.536112	-0.321968
34	6	0	-1.461054	-2.483223	-1.601679
35	1	0	-0.396905	-2.307734	-1.372573
36	1	0	-1.768297	-1.691641	-2.303386
37	1	0	-1.522966	-3.446004	-2.153286
38	6	0	-1.798533	-3.712670	0.534859

39	1	0	-1.819713	-4.660058	-0.046661
40	1	0	-2.410748	-3.863787	1.436839
41	1	0	-0.769982	-3.531122	0.883271
42	6	0	-3.757954	-2.916155	-0.766709
43	1	0	-4.218701	-2.158024	-1.417673
44	1	0	-4.428938	-3.058143	0.092019
45	1	0	-3.741575	-3.868867	-1.335918
46	6	0	1.329870	1.678159	1.536937
47	6	0	0.584367	2.235289	2.611811
48	6	0	1.274052	2.763896	3.716426
49	1	0	0.688878	3.189121	4.534846
50	6	0	2.672464	2.771447	3.798882
51	6	0	3.390205	2.256217	2.711143
52	1	0	4.482258	2.281580	2.735673
53	6	0	2.758491	1.713892	1.577210
54	6	0	-0.922343	2.318677	2.628921
55	1	0	-1.265299	2.894657	3.499059
56	1	0	-1.358435	1.317849	2.692253
57	1	0	-1.327934	2.784371	1.721693
58	6	0	3.381297	3.306893	5.023799
59	1	0	4.392486	3.663516	4.778107
60	1	0	3.483736	2.519319	5.789015
61	1	0	2.818251	4.134657	5.479894
62	6	0	3.671035	1.265941	0.447626
63	1	0	3.536127	1.884799	-0.450618
64	1	0	3.482544	0.224456	0.142207
65	1	0	4.721277	1.339907	0.762521
66	6	0	1.149620	1.902962	-1.392221
67	6	0	1.324705	3.315583	-1.271965
68	6	0	1.884062	4.029279	-2.347573
69	1	0	2.011554	5.109388	-2.242113
70	6	0	2.255972	3.413251	-3.549816
71	6	0	1.992792	2.043210	-3.682138
72	1	0	2.207561	1.549467	-4.632959
73	6	0	1.434555	1.279587	-2.641924
74	6	0	0.909211	4.137489	-0.063645
75	1	0	1.674562	4.128284	0.725295
76	1	0	-0.020148	3.767979	0.385041
77	1	0	0.746433	5.180684	-0.370531
78	6	0	2.899384	4.202558	-4.668979
79	1	0	2.540478	5.242242	-4.680989
80	1	0	2.690875	3.748741	-5.648782
81	1	0	3.995037	4.234650	-4.545195
82	6	0	1.143348	-0.175187	-2.950168
83	1	0	1.076515	-0.322038	-4.037969
84	1	0	0.204055	-0.515186	-2.499347
85	1	0	1.944672	-0.830524	-2.571114
86	6	0	1.438262	-4.509038	-0.894356
87	1	0	1.695500	-5.566899	-0.742461
88	1	0	0.368328	-4.354753	-0.729846
89	6	0	1.947099	-3.977160	-2.235813
90	1	0	1.519035	-2.979185	-2.405424
91	1	0	1.634673	-4.635441	-3.060230
92	6	0	3.482253	-3.902247	-2.118227
93	1	0	3.927324	-3.315996	-2.934992
94	1	0	3.898682	-4.919537	-2.167411
95	6	0	3.843953	-3.269326	-0.750542
96	1	0	4.009716	-2.188554	-0.816774
97	1	0	4.714232	-3.743392	-0.279991

Harmonic Frequencies

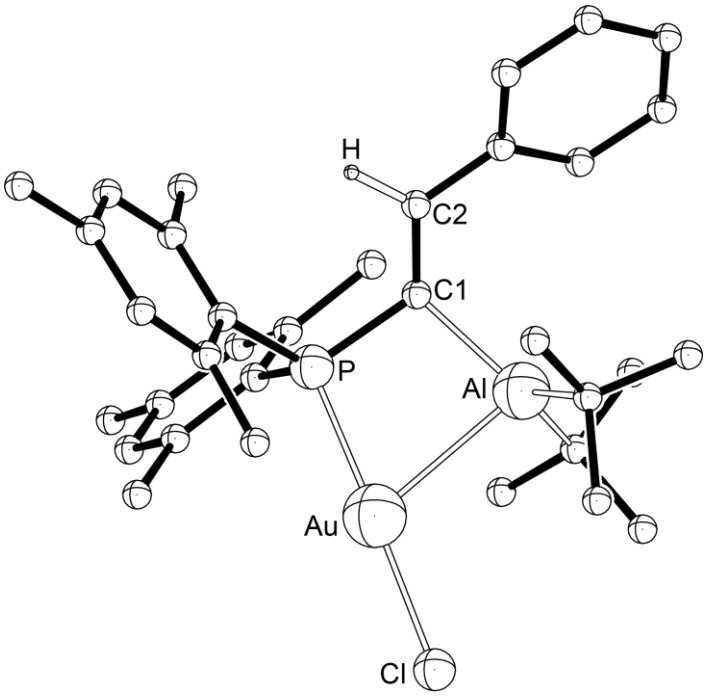
	1	2	3
	A	A	A
Frequencies --	20.3769	22.4026	28.7232
Red. masses --	4.4663	4.3316	4.6887
Frc consts --	0.0011	0.0013	0.0023
IR Inten --	0.5404	0.1618	0.1562

Thermochemistry

Sum of electronic and zero-point Energies= -3057.240274
Sum of electronic and thermal Energies= -3057.189036
Sum of electronic and thermal Enthalpies= -3057.188092
Sum of electronic and thermal Free Energies= -3057.325124

HF = -3058.04893381

[(1)AuCl]



Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): P–Au 2.322, Cl–Au 2.348, Au–Al 2.762, P–C1 1.812, C1–C2 1.359, C1–Al 2.024; P–Au–Cl 174.78, Au–P–C1 101.44, P–C1–C2 121.74, C2–C1–Al 129.48, P–C1–Al 102.84, C1–Al–Au 82.92, Al–Au–P 71.79, Al–Au–Cl 109.42; Au–P–C1–Al 9.52

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.014755	2.134285	0.954556
2	1	0	-0.268384	2.923780	0.796483
3	6	0	-0.734830	0.828652	0.701844
4	13	0	-1.967420	-0.657658	0.096382
5	15	0	0.874487	0.306986	0.052498
6	79	0	0.267228	-1.476961	-1.303992
7	6	0	-2.265830	-2.356078	1.146655
8	6	0	-3.193487	-0.057284	-1.398503
9	6	0	1.982389	-0.459462	1.329364
10	6	0	3.802351	-1.703279	3.129969
11	6	0	3.232018	-0.964260	0.856066
12	6	0	1.638075	-0.600210	2.704607
13	6	0	2.560748	-1.222053	3.566149
14	6	0	4.116418	-1.559093	1.771540
15	1	0	2.294590	-1.325972	4.620378
16	1	0	5.074750	-1.930958	1.402271
17	6	0	1.782201	1.763455	-0.647951
18	6	0	3.089485	4.093999	-1.641239
19	6	0	1.847865	2.005593	-2.053233
20	6	0	2.368596	2.702309	0.254287
21	6	0	3.005078	3.843572	-0.265649
22	6	0	2.500924	3.164419	-2.510158
23	1	0	3.443614	4.558145	0.434622
24	1	0	2.544621	3.343885	-3.586572
25	6	0	-3.173042	-1.081501	-2.557884
26	1	0	-3.896817	-0.771935	-3.337622
27	1	0	-3.447465	-2.092237	-2.224985
28	1	0	-2.179485	-1.154322	-3.023986
29	6	0	-2.789666	1.321798	-1.958952
30	1	0	-2.837938	2.110691	-1.194797
31	1	0	-3.470838	1.608922	-2.783751
32	1	0	-1.766288	1.307880	-2.365360
33	6	0	-4.642594	0.041840	-0.853320

34	1	0	-4.736655	0.812028	-0.072183
35	1	0	-4.994680	-0.916343	-0.437438
36	1	0	-5.332982	0.312843	-1.676539
37	6	0	-3.085528	-2.009378	2.417046
38	1	0	-2.518182	-1.372287	3.116538
39	1	0	-3.348934	-2.936195	2.963269
40	1	0	-4.031428	-1.494022	2.175728
41	6	0	-0.982221	-3.107669	1.572654
42	1	0	-0.288769	-2.485462	2.155866
43	1	0	-0.435950	-3.490540	0.697681
44	1	0	-1.253555	-3.979146	2.200581
45	6	0	-3.100330	-3.317174	0.266384
46	1	0	-4.054566	-2.865896	-0.048814
47	1	0	-3.339038	-4.237891	0.833739
48	1	0	-2.542235	-3.609630	-0.635616
49	6	0	3.668331	-0.921926	-0.597939
50	1	0	4.716804	-1.237444	-0.686658
51	1	0	3.575362	0.079201	-1.038591
52	1	0	3.064108	-1.610916	-1.210906
53	6	0	0.347455	-0.110837	3.336414
54	1	0	0.278178	-0.478719	4.369534
55	1	0	-0.535876	-0.457116	2.789312
56	1	0	0.285759	0.986424	3.363665
57	6	0	1.276041	1.085523	-3.114702
58	1	0	0.209006	0.878881	-2.957279
59	1	0	1.795488	0.114100	-3.131562
60	1	0	1.386968	1.539695	-4.108673
61	6	0	2.368376	2.547710	1.764785
62	1	0	2.625646	3.505252	2.238473
63	1	0	3.099032	1.793798	2.091236
64	1	0	1.389276	2.236044	2.146291
65	6	0	-2.335476	2.597861	1.399173
66	6	0	-4.916250	3.489125	2.136542
67	6	0	-2.743982	3.925286	1.134208
68	6	0	-3.231398	1.738262	2.078587
69	6	0	-4.510625	2.177491	2.438454
70	6	0	-4.026060	4.363282	1.489294
71	1	0	-2.054589	4.599052	0.621423
72	1	0	-2.905158	0.734633	2.353773
73	1	0	-5.187430	1.500575	2.961713
74	1	0	-4.333602	5.384853	1.261082
75	1	0	-5.913761	3.831483	2.415028
76	6	0	4.757569	-2.386477	4.084029
77	1	0	5.803487	-2.150321	3.837927
78	1	0	4.646696	-3.482096	4.027538
79	1	0	4.565513	-2.086111	5.124128
80	6	0	3.807337	5.314524	-2.174593
81	1	0	4.859103	5.077642	-2.406832
82	1	0	3.807035	6.131242	-1.438333
83	1	0	3.340370	5.677054	-3.101985
84	17	0	-0.247867	-3.408923	-2.535637

Harmonic Frequencies

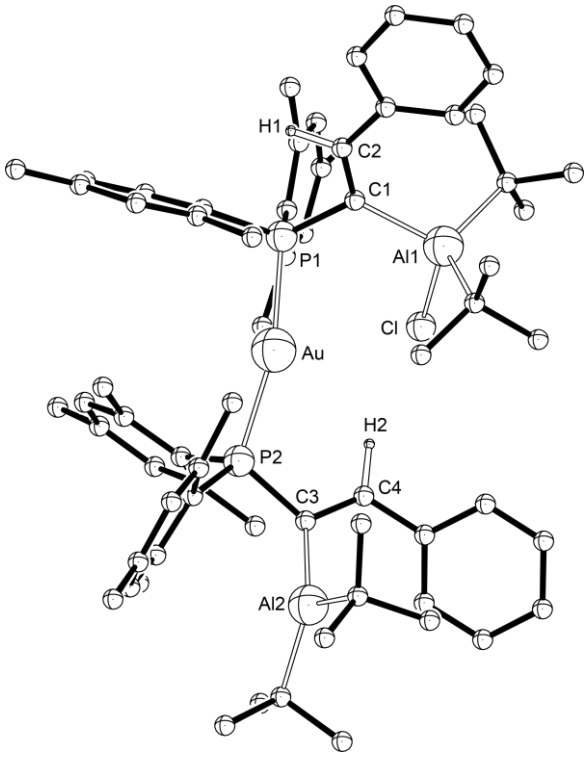
	1	2	3
	A	A	A
Frequencies --	23.5555	24.2150	25.3017
Red. masses --	4.4610	4.5709	4.1773
Frc consts --	0.0015	0.0016	0.0016
IR Inten --	0.1539	0.1414	0.1802

Thermochemistry

Sum of electronic and zero-point Energies=	-2502.003516
Sum of electronic and thermal Energies=	-2501.957776
Sum of electronic and thermal Enthalpies=	-2501.956832
Sum of electronic and thermal Free Energies=	-2502.082623

HF = -2502.69709279

[(1–Cl)Au(1)] 4



Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): Au–P1 2.349, P1–C1 1.826, C1–C2 1.366, C1–Al1 2.081, Al1–Cl 2.284, Au–Cl 3.448, Au–P2 2.359, P2–C3 1.823, C3–C4 1.366, C3–Al2 2.019; P1–Au–P2 164.09, Au–P1–C1 112.15, P1–C1–C2 114.16, P1–C1–Al1 115.31, C2–C1–Al1 130.52, C1–Al1–Cl 107.52, Al1–Cl–Au 87.20, Cl–Au–P2 113.86, Au–P2–C3 114.24, P2–C3–C4 115.01, P2–C3–Al2 122.98, C4–C3–Al2 117.95; Au–P1–C1–Al1 53.18, P1–C1–Al1–Cl 4.34, Au–P1–Al1–Cl 52.09, Au–P2–C3–Al2 140.41, Al1–P1–P2–Al2 13.11.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.178004	-0.563451	-0.048174
2	15	0	-2.157181	-0.857009	0.116042
3	15	0	2.504814	-0.873290	0.033102
4	17	0	1.412374	1.950700	1.962874
5	13	0	2.910038	2.394721	0.297063
6	13	0	-4.844980	1.173601	-0.133686
7	6	0	-2.811722	2.921089	1.614757
8	6	0	-1.999916	4.063939	1.432854
9	6	0	-4.620138	4.366327	2.408468
10	6	0	-4.118100	3.086332	2.132459
11	6	0	-3.820862	5.496927	2.179208
12	6	0	-2.507165	5.340414	1.699424
13	6	0	5.181548	1.172363	-2.378775
14	6	0	5.286043	2.569563	-2.209991
15	6	0	5.979869	0.568662	-3.382982
16	6	0	6.843896	1.328846	-4.181080
17	6	0	6.932720	2.717925	-3.992870
18	6	0	6.148574	3.332990	-3.000959
19	6	0	-2.129842	-2.273320	1.328416
20	6	0	-3.024906	-0.868816	3.320301
21	6	0	-2.149163	-3.188101	3.584594
22	6	0	-1.574732	-3.502891	0.856514
23	6	0	-1.232910	-3.775408	-0.597347
24	6	0	-1.579541	-4.391862	3.150506
25	6	0	-2.427618	-2.121788	2.710214
26	6	0	-1.317899	-4.530640	1.779890
27	6	0	-1.230904	-5.492113	4.128953
28	6	0	2.263826	-3.328426	-3.314848

29	6	0	2.806191	-3.697316	-0.586939
30	6	0	2.317683	-2.198758	-2.476888
31	6	0	2.636534	-2.371362	-1.090720
32	6	0	2.743506	-4.784295	-1.478206
33	6	0	2.491617	-4.627929	-2.847352
34	6	0	-4.487229	-1.937652	-1.098979
35	6	0	-3.191896	-1.381730	-1.329959
36	6	0	-3.675331	-1.343627	-3.717304
37	6	0	-5.353835	-2.130752	-2.190303
38	6	0	-2.769844	-1.121892	-2.663764
39	6	0	-4.978361	-1.817025	-3.504592
40	6	0	4.304448	0.299594	-1.588978
41	6	0	3.415318	0.581881	-0.590565
42	6	0	-3.063331	0.632860	0.648216
43	6	0	-2.290957	1.606777	1.215631
44	6	0	4.530262	3.247434	1.263805
45	6	0	4.892655	4.655753	0.727974
46	6	0	1.721260	3.491425	-0.981698
47	6	0	5.786219	2.345807	1.180629
48	6	0	2.477120	-1.258629	2.902786
49	6	0	3.251773	-1.182331	1.707661
50	6	0	-4.946097	-2.426594	0.260833
51	6	0	4.675745	-1.231866	1.803107
52	6	0	2.987533	-4.042930	0.880663
53	6	0	-5.953898	-1.965442	-4.650815
54	6	0	-6.696422	0.834840	0.643451
55	6	0	-1.381308	-0.636919	-3.019074
56	6	0	3.142133	-1.218223	4.141349
57	6	0	4.536040	-1.135237	4.253171
58	6	0	5.282400	-1.191944	3.070021
59	6	0	0.975237	-1.450027	2.963914
60	6	0	5.210151	-1.007297	5.600799
61	6	0	2.003222	-0.874153	-3.156238
62	6	0	2.463382	-5.817362	-3.782470
63	6	0	2.353734	3.896453	-2.331376
64	6	0	-6.730364	0.182868	2.044855
65	6	0	4.215342	3.423038	2.771750
66	6	0	1.295044	4.791111	-0.256239
67	6	0	-4.677508	2.430626	-1.710498
68	6	0	-7.363894	2.233241	0.757887
69	6	0	-7.582693	-0.005902	-0.310773
70	6	0	-5.764259	2.122575	-2.769805
71	6	0	-3.290805	2.336479	-2.385531
72	6	0	0.448317	2.675772	-1.316920
73	6	0	5.608363	-1.407882	0.618908
74	6	0	-4.858988	3.895255	-1.227658
75	1	0	-5.625722	4.477855	2.816144
76	1	0	-4.711637	2.204858	2.380238
77	1	0	-4.211121	6.493368	2.390321
78	1	0	4.689481	3.059218	-1.450571
79	1	0	5.913865	-0.512656	-3.527570
80	1	0	7.447819	0.839382	-4.947168
81	1	0	7.605038	3.314901	-4.611039
82	1	0	6.207365	4.410847	-2.842335
83	1	0	-2.304328	-0.038171	3.322998
84	1	0	-3.325385	-1.065751	4.358895
85	1	0	-3.903719	-0.515619	2.765361
86	1	0	-2.381890	-3.061677	4.644515
87	1	0	-0.453934	-3.091610	-0.968806
88	1	0	-0.848272	-4.797623	-0.710582
89	1	0	-2.106596	-3.656945	-1.253213
90	1	0	-0.893796	-5.466639	1.409101
91	1	0	-1.302018	-6.483682	3.658242
92	1	0	-0.196633	-5.373590	4.493674
93	1	0	-1.893849	-5.472148	5.006269
94	1	0	2.022190	-3.177697	-4.370151
95	1	0	2.878085	-5.791472	-1.076238
96	1	0	-3.349457	-1.123754	-4.736041
97	1	0	-6.345316	-2.546525	-2.001689
98	1	0	4.429661	-0.743088	-1.908178
99	1	0	-1.210207	1.484962	1.361954
100	1	0	4.055523	5.361313	0.850374
101	1	0	5.179625	4.662969	-0.335512
102	1	0	5.753898	5.067603	1.293006
103	1	0	5.593395	1.361812	1.635752
104	1	0	6.126741	2.182544	0.147632
105	1	0	6.628458	2.807837	1.735969
106	1	0	-4.735966	-1.708836	1.061369
107	1	0	-4.419040	-3.353787	0.529570
108	1	0	-6.023989	-2.631303	0.254655

109	1	0	2.948445	-5.133813	1.010908
110	1	0	3.943102	-3.684734	1.283894
111	1	0	2.195626	-3.599838	1.497969
112	1	0	-5.432467	-2.180860	-5.594531
113	1	0	-6.679362	-2.768752	-4.457003
114	1	0	-6.523698	-1.031901	-4.792829
115	1	0	-1.300029	-0.472230	-4.102244
116	1	0	-0.624408	-1.377678	-2.725383
117	1	0	-1.125609	0.303900	-2.513543
118	1	0	2.540679	-1.259379	5.052210
119	1	0	6.373314	-1.217841	3.123669
120	1	0	0.615186	-2.203221	2.249889
121	1	0	0.681970	-1.786267	3.968091
122	1	0	0.447283	-0.508248	2.759026
123	1	0	6.194485	-1.498809	5.604969
124	1	0	4.594118	-1.444445	6.400450
125	1	0	5.371018	0.055025	5.849202
126	1	0	1.316791	-1.051379	-3.995746
127	1	0	1.543600	-0.135445	-2.491389
128	1	0	1.783655	-5.642507	-4.629596
129	1	0	3.465608	-6.013281	-4.199540
130	1	0	2.142083	-6.729577	-3.258210
131	1	0	1.618638	4.449344	-2.952705
132	1	0	2.686838	3.021304	-2.911163
133	1	0	3.224616	4.557111	-2.194026
134	1	0	-6.144019	0.746353	2.789077
135	1	0	-6.353979	-0.849028	2.037050
136	1	0	-7.772632	0.147834	2.417826
137	1	0	3.341728	4.072835	2.936691
138	1	0	5.084120	3.883240	3.286449
139	1	0	4.003334	2.458771	3.257951
140	1	0	0.481210	5.308884	-0.806185
141	1	0	2.138879	5.495046	-0.181344
142	1	0	0.944624	4.594684	0.769114
143	1	0	-7.453508	2.720453	-0.224251
144	1	0	-8.385321	2.125164	1.170949
145	1	0	-6.806318	2.912400	1.420398
146	1	0	-7.214667	-1.034147	-0.422668
147	1	0	-7.640536	0.439894	-1.315813
148	1	0	-8.614409	-0.062074	0.087871
149	1	0	-5.679479	2.829583	-3.618099
150	1	0	-5.661718	1.102371	-3.175572
151	1	0	-6.779811	2.225848	-2.355614
152	1	0	-3.191117	3.126598	-3.154772
153	1	0	-3.156091	1.370528	-2.888845
154	1	0	-2.469781	2.467920	-1.665619
155	1	0	-0.242864	3.269131	-1.950000
156	1	0	0.699783	1.757957	-1.876182
157	1	0	-0.103896	2.369931	-0.416098
158	1	0	6.506240	-1.953186	0.944999
159	1	0	5.927302	-0.439560	0.211081
160	1	0	5.142247	-1.976518	-0.195386
161	1	0	-4.811165	4.573753	-2.101897
162	1	0	-5.826065	4.063245	-0.731360
163	1	0	-4.064093	4.196502	-0.530544
164	1	0	2.911371	-0.405393	-3.561495
165	1	0	-0.987126	3.935651	1.057339
166	1	0	-1.876525	6.214644	1.532640

Harmonic Frequencies

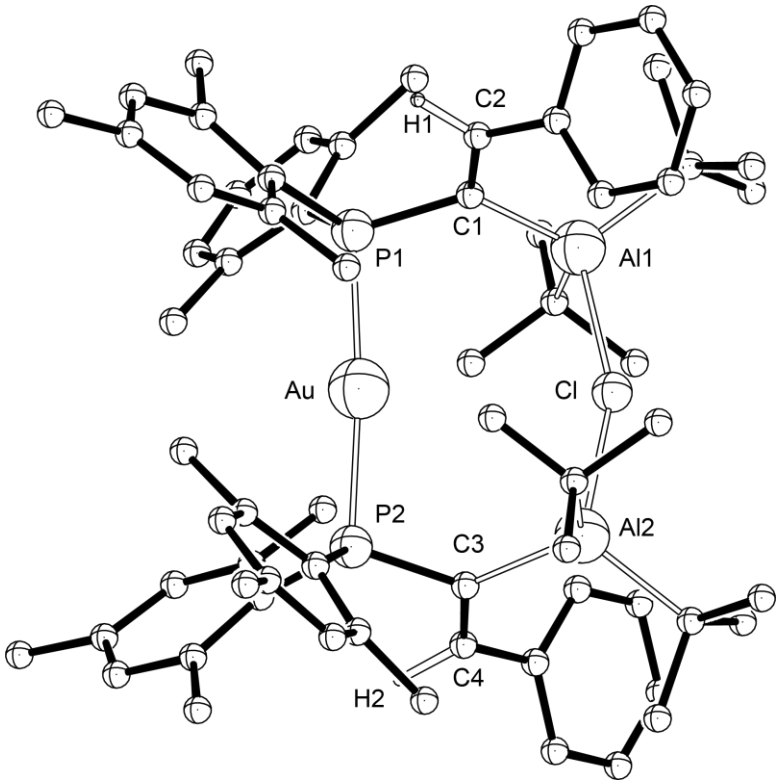
	1	2	3
	A	A	A
Frequencies --	11.3164	15.7836	17.8955
Red. masses --	4.9051	4.3572	4.1883
Frc consts --	0.0004	0.0006	0.0008
IR Inten --	0.1002	0.0483	0.0529

Thermochemistry

Sum of electronic and zero-point Energies= -4407.563346
Sum of electronic and thermal Energies= -4407.475875
Sum of electronic and thermal Enthalpies= -4407.474931
Sum of electronic and thermal Free Energies= -4407.688189

HF = -4408.95373050

[(1–Cl–1)Au] 5



The structure is C_2–symmetric around the Au–Cl axis.

Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): P1–Au 2.378, P1–C1 1.835, C1–C2 1.367, C1–Al1 2.107, Al1–Cl 2.445, Au–Cl 3.771; Au–P1–C1 103.31, P1–C1–C2 110.83, P1–C1–Al1 123.51, C2–C1–Al1 125.46, C2–Al1–Cl 104.68, Al1–Cl–Au 78.79, P1–Au–Cl 92.43; Au–P1–C1–Al1 57.18, P1–C1–Cl1–Cl 79.70, Au–P1–Al1–Cl 19.27, P1–Au–Cl–Al1 17.83.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.664468	0.799466	1.340914
2	1	0	-4.154729	-0.116103	1.705421
3	6	0	-2.892073	0.756013	0.213303
4	13	0	-2.231045	2.430994	-0.881391
5	15	0	-2.371025	-0.964626	-0.154823
6	79	0	0.000020	-0.863718	0.000013
7	15	0	2.371060	-0.964618	0.154880
8	6	0	-1.607699	2.194151	-2.844091
9	6	0	-3.454627	4.070042	-0.641110
10	17	0	0.000171	2.906866	-0.000378
11	13	0	2.231043	2.431255	0.881274
12	6	0	2.892062	0.756064	-0.213218
13	6	0	1.607482	2.194512	2.843898
14	6	0	3.454913	4.070121	0.641177
15	6	0	3.664537	0.799507	-1.340774
16	1	0	4.154885	-0.116032	-1.705233
17	6	0	2.817608	-1.584557	1.828216
18	6	0	3.300390	-2.447178	4.493182
19	6	0	3.868172	-0.999961	2.587978
20	6	0	2.090973	-2.688512	2.364610
21	6	0	2.341394	-3.082159	3.690754
22	6	0	4.076632	-1.437260	3.906323
23	1	0	1.782080	-3.928665	4.096894
24	1	0	4.880964	-0.978825	4.485794
25	6	0	3.013614	-2.245334	-1.064138
26	6	0	3.485801	-4.466590	-2.815537
27	6	0	3.964259	-3.258666	-0.716182

28	6	0	2.408797	-2.305164	-2.359034
29	6	0	2.651217	-3.408983	-3.194413
30	6	0	4.153283	-4.346558	-1.590381
31	1	0	2.177051	-3.424703	-4.178852
32	1	0	4.875499	-5.115694	-1.306113
33	6	0	-2.817835	-1.584533	-1.828110
34	6	0	-3.301219	-2.447310	-4.492909
35	6	0	-2.091328	-2.688485	-2.364593
36	6	0	-3.868615	-0.999982	-2.587674
37	6	0	-4.077393	-1.437385	-3.905908
38	6	0	-2.342029	-3.082196	-3.690696
39	1	0	-4.881918	-0.979037	-4.485184
40	1	0	-1.782760	-3.928666	-4.096960
41	6	0	-3.013360	-2.245457	1.064187
42	6	0	-3.484652	-4.467154	2.815229
43	6	0	-2.408315	-2.305347	2.358962
44	6	0	-3.963891	-3.258895	0.716252
45	6	0	-4.152467	-4.347016	1.590254
46	6	0	-2.650283	-3.409396	3.194170
47	1	0	-4.874609	-5.116226	1.305997
48	1	0	-2.175927	-3.425188	4.178517
49	6	0	1.526796	-1.223201	-2.940102
50	1	0	0.459296	-1.433499	-2.786213
51	1	0	1.688213	-1.158213	-4.025651
52	1	0	1.730875	-0.239259	-2.515438
53	6	0	4.864418	-3.250852	0.509095
54	1	0	4.356224	-3.607376	1.415433
55	1	0	5.250419	-2.249971	0.725179
56	1	0	5.726040	-3.908690	0.325604
57	6	0	4.827961	0.039182	2.040087
58	1	0	5.135429	-0.174849	1.009448
59	1	0	5.724650	0.088048	2.673598
60	1	0	4.384906	1.041872	2.024541
61	6	0	1.112720	-3.545063	1.574203
62	1	0	0.075332	-3.191107	1.671474
63	1	0	1.141922	-4.574873	1.959925
64	1	0	1.351508	-3.575708	0.504557
65	6	0	-1.526520	-1.223211	2.940046
66	1	0	-1.730666	-0.239335	2.515250
67	1	0	-0.458976	-1.433416	2.786322
68	1	0	-1.688099	-1.158141	4.025565
69	6	0	-4.864468	-3.250868	-0.508720
70	1	0	-5.725902	-3.908924	-0.325119
71	1	0	-4.356523	-3.607019	-1.415344
72	1	0	-5.250726	-2.249986	-0.724351
73	6	0	-4.828327	0.039168	-2.039637
74	1	0	-5.725154	0.087934	-2.672963
75	1	0	-4.385320	1.041887	-2.024277
76	1	0	-5.135569	-0.174789	-1.008920
77	6	0	-1.112890	-3.545011	-1.574390
78	1	0	-1.351710	-3.576009	-0.504762
79	1	0	-0.075584	-3.190780	-1.671522
80	1	0	-1.141841	-4.574725	-1.960385
81	6	0	-3.823476	1.919905	2.285739
82	6	0	-5.086171	2.253858	2.823954
83	6	0	-2.675955	2.569320	2.787620
84	6	0	-5.199286	3.246763	3.805004
85	1	0	-5.977324	1.742047	2.455229
86	6	0	-2.785859	3.539196	3.792793
87	1	0	-1.701447	2.300795	2.390306
88	6	0	-4.047738	3.887898	4.297097
89	1	0	-6.182657	3.515185	4.194699
90	1	0	-1.883992	4.024013	4.165560
91	1	0	-4.137226	4.650113	5.072633
92	6	0	3.823299	1.919878	-2.285714
93	6	0	5.085883	2.253773	-2.824243
94	6	0	2.675686	2.569347	-2.787305
95	6	0	5.198809	3.246693	-3.805292
96	1	0	5.977096	1.741911	-2.455735
97	6	0	2.785401	3.539279	-3.792450
98	1	0	1.701254	2.300840	-2.389783
99	6	0	4.047172	3.887929	-4.297053
100	1	0	6.182094	3.515075	-4.195231
101	1	0	1.883471	4.024158	-4.164981
102	1	0	4.136511	4.650181	-5.072569
103	6	0	3.506225	-2.850209	5.936352
104	1	0	4.555071	-2.721047	6.241614
105	1	0	2.890592	-2.223892	6.603371
106	1	0	3.216413	-3.897739	6.104999
107	6	0	-3.677411	-5.676776	3.702916

108	1	0	-4.673788	-6.121082	3.563100
109	1	0	-2.933076	-6.456111	3.467283
110	1	0	-3.555484	-5.415656	4.764408
111	6	0	3.679098	-5.675953	-3.703462
112	1	0	4.675475	-6.120160	-3.563336
113	1	0	2.934762	-6.455448	-3.468363
114	1	0	3.557593	-5.414566	-4.764937
115	6	0	-3.507496	-2.850278	-5.936031
116	1	0	-4.557743	-2.727266	-6.239082
117	1	0	-2.897215	-2.219430	-6.603703
118	1	0	-3.211605	-3.895839	-6.106245
119	6	0	-0.755872	3.416568	-3.295480
120	1	0	0.037616	3.678544	-2.584274
121	1	0	-0.270752	3.169977	-4.261179
122	1	0	-1.365280	4.312684	-3.462052
123	6	0	-2.716801	2.035181	-3.914237
124	1	0	-3.229769	1.070107	-3.843023
125	1	0	-3.474301	2.833145	-3.867957
126	1	0	-2.264769	2.074198	-4.925682
127	6	0	-0.689494	0.963878	-2.932712
128	1	0	-1.237248	0.025293	-2.786592
129	1	0	-0.188228	0.903709	-3.919708
130	1	0	0.096760	1.007874	-2.168396
131	6	0	-3.333059	4.910839	0.650913
132	1	0	-2.288145	5.169808	0.884783
133	1	0	-3.890155	5.861110	0.525358
134	1	0	-3.762677	4.405043	1.518612
135	6	0	-3.209965	5.055835	-1.811866
136	1	0	-3.345040	4.585435	-2.794989
137	1	0	-3.932385	5.893134	-1.743365
138	1	0	-2.198556	5.489051	-1.776908
139	6	0	-4.922429	3.581312	-0.759328
140	1	0	-5.111006	3.078457	-1.723691
141	1	0	-5.191597	2.886277	0.050275
142	1	0	-5.617681	4.442802	-0.705283
143	6	0	3.334152	4.910756	-0.651023
144	1	0	3.763828	4.404658	-1.518510
145	1	0	2.289431	5.170160	-0.885269
146	1	0	3.891629	5.860791	-0.525398
147	6	0	3.210105	5.056195	1.811659
148	1	0	3.344490	4.585865	2.794908
149	1	0	3.932932	5.893161	1.743403
150	1	0	2.198907	5.489859	1.776140
151	6	0	4.922539	3.580972	0.760027
152	1	0	5.618065	4.442251	0.706160
153	1	0	5.110583	3.078161	1.724516
154	1	0	5.191795	2.885766	-0.049406
155	6	0	0.689299	0.964224	2.932528
156	1	0	-0.096925	1.008160	2.168171
157	1	0	1.237077	0.025651	2.786465
158	1	0	0.187984	0.904084	3.919501
159	6	0	2.716471	2.035712	3.914191
160	1	0	3.473910	2.833732	3.867936
161	1	0	2.264318	2.074772	4.925581
162	1	0	3.229550	1.070682	3.843121
163	6	0	0.755533	3.416922	3.295059
164	1	0	-0.037798	3.678838	2.583654
165	1	0	0.270194	3.170336	4.260652
166	1	0	1.364851	4.313070	3.461758

Harmonic Frequencies

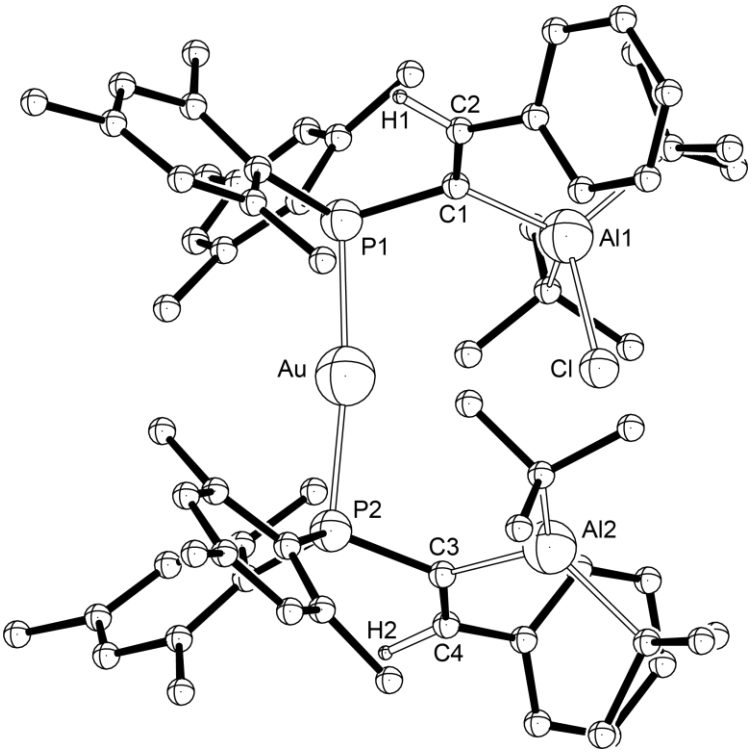
	1	2	3
	A	A	A
Frequencies --	17.6727	22.9056	24.0404
Red. masses --	4.6406	4.4447	4.1686
Frc consts --	0.0009	0.0014	0.0014
IR Inten --	0.0118	0.0275	0.0222

Thermochemistry

Sum of electronic and zero-point Energies=	-4407.543901
Sum of electronic and thermal Energies=	-4407.458704
Sum of electronic and thermal Enthalpies=	-4407.457759
Sum of electronic and thermal Free Energies=	-4407.660660

HF = -4408.94110922

$TS_{4–5}$



Selected Bond Distances (Å), Angles (°) and Dihedral Angles (°): P1–Au 2.379, Au–P2 2.381, P2–C3 1.830, C3–C4 1.369, C3–Al2 2.067, Al2–Cl 3.095, Cl–Al1 2.342, Al1–C1 2.120, C1–C2 1.368, C1–P1 1.832, Au–Cl 3.841; Au–P1–C1 103.57, P1–C1–C2 110.69, C2–C1–Al1 125.39, P1–C1–Al1 123.57, C1–Al1–Cl 103.65, Al1–Cl–Al2 153.50, Cl–Al2–C3 96.67, Al2–C3–P2 124.11, Al2–C3–C4 124.18 C4–C3–P2 111.66 C3–P2–Au 104.14 P2–Au–P1 173.37; Au–P1–Al1–Cl 22.31, Au–P2–Al2–Cl 17.70.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.565520	0.862135	1.509691
2	1	0	-4.008968	-0.050101	1.936945
3	6	0	-2.897845	0.808299	0.317020
4	13	0	-2.316989	2.485687	-0.841730
5	15	0	-2.391524	-0.910554	-0.064169
6	79	0	-0.014435	-0.813717	-0.026067
7	15	0	2.358636	-0.990631	0.041372
8	6	0	-1.764881	2.207383	-2.826296
9	6	0	-3.655249	4.041972	-0.604758
10	17	0	-0.194625	3.022764	-0.010970
11	13	0	2.674885	2.325375	0.917186
12	6	0	2.943850	0.702179	-0.333684
13	6	0	1.838986	2.189342	2.792680
14	6	0	4.062043	3.818522	0.627889
15	6	0	3.534028	0.771255	-1.567408
16	1	0	3.910154	-0.146003	-2.043239
17	6	0	2.830354	-1.636527	1.702230
18	6	0	3.331558	-2.572410	4.346095
19	6	0	3.900432	-1.093526	2.464754
20	6	0	2.090260	-2.740336	2.227748
21	6	0	2.349579	-3.167906	3.541017
22	6	0	4.118904	-1.566705	3.770494
23	1	0	1.777579	-4.011644	3.934828
24	1	0	4.941487	-1.138297	4.347651
25	6	0	2.925408	-2.272137	-1.205856
26	6	0	3.317972	-4.506631	-2.952144
27	6	0	3.909955	-3.265892	-0.904338
28	6	0	2.246284	-2.348942	-2.461417
29	6	0	2.450063	-3.462965	-3.294272

30	6	0	4.060778	-4.362927	-1.772662
31	1	0	1.919085	-3.496669	-4.248717
32	1	0	4.810460	-5.118075	-1.524154
33	6	0	-2.905668	-1.568299	-1.707115
34	6	0	-3.523576	-2.517451	-4.316301
35	6	0	-2.214170	-2.696245	-2.240990
36	6	0	-3.983763	-0.998039	-2.438107
37	6	0	-4.260242	-1.479249	-3.728672
38	6	0	-2.530989	-3.132204	-3.539676
39	1	0	-5.084716	-1.028959	-4.285634
40	1	0	-1.997397	-3.996681	-3.942718
41	6	0	-2.965506	-2.183057	1.199744
42	6	0	-3.385141	-4.370684	3.005060
43	6	0	-2.289882	-2.239742	2.457964
44	6	0	-3.956795	-3.177814	0.921120
45	6	0	-4.119903	-4.250498	1.818627
46	6	0	-2.505672	-3.328702	3.320265
47	1	0	-4.874961	-5.005608	1.586564
48	1	0	-1.974981	-3.343099	4.275606
49	6	0	1.333692	-1.274075	-3.009189
50	1	0	0.272859	-1.506580	-2.843599
51	1	0	1.478195	-1.188839	-4.095908
52	1	0	1.523845	-0.291537	-2.574015
53	6	0	4.879445	-3.215177	0.264797
54	1	0	4.435433	-3.578847	1.201695
55	1	0	5.240089	-2.197654	0.448505
56	1	0	5.751371	-3.845071	0.037364
57	6	0	4.887197	-0.059939	1.952446
58	1	0	5.012211	-0.078292	0.865818
59	1	0	5.868364	-0.226392	2.420288
60	1	0	4.584642	0.960344	2.232663
61	6	0	1.077008	-3.560391	1.443276
62	1	0	0.050726	-3.190662	1.585642
63	1	0	1.100341	-4.599933	1.802313
64	1	0	1.278696	-3.569268	0.366597
65	6	0	-1.352445	-1.171510	2.973868
66	1	0	-1.517173	-0.199406	2.506067
67	1	0	-0.300603	-1.446187	2.813725
68	1	0	-1.493310	-1.048909	4.057516
69	6	0	-4.922493	-3.159686	-0.252303
70	1	0	-5.790128	-3.791752	-0.014466
71	1	0	-4.473026	-3.539269	-1.180105
72	1	0	-5.291484	-2.150520	-0.459677
73	6	0	-4.895245	0.079776	-1.887387
74	1	0	-5.815365	0.134500	-2.485706
75	1	0	-4.420244	1.066123	-1.926863
76	1	0	-5.165424	-0.089244	-0.838121
77	6	0	-1.204002	-3.536193	-1.473879
78	1	0	-1.396250	-3.542005	-0.395265
79	1	0	-0.171598	-3.186641	-1.622848
80	1	0	-1.249930	-4.574617	-1.834147
81	6	0	-3.668914	2.003116	2.439661
82	6	0	-4.885196	2.293783	3.097579
83	6	0	-2.511397	2.724533	2.802885
84	6	0	-4.949550	3.310985	4.057815
85	1	0	-5.781768	1.727754	2.836632
86	6	0	-2.569480	3.720182	3.786772
87	1	0	-1.570848	2.500678	2.309546
88	6	0	-3.789075	4.023775	4.410394
89	1	0	-5.900865	3.543193	4.539733
90	1	0	-1.660779	4.261881	4.050950
91	1	0	-3.838747	4.806238	5.169364
92	6	0	3.620447	1.938545	-2.458799
93	6	0	4.779138	2.167174	-3.237343
94	6	0	2.489384	2.758841	-2.661276
95	6	0	4.820064	3.220917	-4.156784
96	1	0	5.649174	1.521283	-3.102306
97	6	0	2.520619	3.791849	-3.608542
98	1	0	1.583303	2.570140	-2.090333
99	6	0	3.686844	4.032988	-4.349580
100	1	0	5.727849	3.403056	-4.734343
101	1	0	1.630291	4.400787	-3.759785
102	1	0	3.713529	4.840979	-5.082268
103	6	0	3.547492	-3.013868	5.776327
104	1	0	4.597763	-2.890257	6.078791
105	1	0	2.933902	-2.407748	6.463576
106	1	0	3.261204	-4.066312	5.918115
107	6	0	-3.554942	-5.564062	3.919283
108	1	0	-4.565643	-5.990126	3.837033

109	1	0	-2.838982	-6.361621	3.657806
110	1	0	-3.373919	-5.290871	4.969288
111	6	0	3.469729	-5.726528	-3.833624
112	1	0	4.478494	-6.157013	-3.750738
113	1	0	2.751683	-6.510748	-3.539971
114	1	0	3.277395	-5.482677	-4.888670
115	6	0	-3.803508	-2.969145	-5.732422
116	1	0	-4.865995	-2.844361	-5.988663
117	1	0	-3.220126	-2.370084	-6.451500
118	1	0	-3.527521	-4.023818	-5.878691
119	6	0	-0.989050	3.466583	-3.308708
120	1	0	-0.213094	3.784686	-2.600178
121	1	0	-0.491464	3.237981	-4.272921
122	1	0	-1.655461	4.320821	-3.481800
123	6	0	-2.873053	1.967660	-3.880431
124	1	0	-3.319936	0.971199	-3.796321
125	1	0	-3.681706	2.713609	-3.830464
126	1	0	-2.438169	2.027433	-4.898946
127	6	0	-0.783526	1.025014	-2.910263
128	1	0	-1.273880	0.067797	-2.691891
129	1	0	-0.333118	0.943613	-3.920882
130	1	0	0.040140	1.146057	-2.194103
131	6	0	-3.487818	4.936387	0.647277
132	1	0	-2.442461	5.247486	0.801538
133	1	0	-4.096508	5.856131	0.529821
134	1	0	-3.833834	4.442548	1.559093
135	6	0	-3.545319	4.995997	-1.821744
136	1	0	-3.697382	4.481285	-2.780963
137	1	0	-4.318097	5.786899	-1.743003
138	1	0	-2.565449	5.497130	-1.857684
139	6	0	-5.100741	3.483115	-0.596068
140	1	0	-5.346314	2.966533	-1.539401
141	1	0	-5.262638	2.779047	0.234355
142	1	0	-5.831572	4.309450	-0.483827
143	6	0	3.784115	4.846479	-0.495789
144	1	0	3.912663	4.417284	-1.492295
145	1	0	2.769989	5.272181	-0.430995
146	1	0	4.503551	5.684283	-0.405031
147	6	0	4.208754	4.643602	1.933409
148	1	0	4.403841	4.023493	2.819973
149	1	0	5.062040	5.341575	1.826163
150	1	0	3.315503	5.253622	2.130296
151	6	0	5.438670	3.161078	0.343164
152	1	0	6.206681	3.948183	0.211457
153	1	0	5.774400	2.521171	1.176044
154	1	0	5.422080	2.553679	-0.572239
155	6	0	0.773522	1.080137	2.814682
156	1	0	0.023620	1.219680	2.027587
157	1	0	1.223902	0.088754	2.676101
158	1	0	0.241655	1.069691	3.785860
159	6	0	2.820169	1.875871	3.953448
160	1	0	3.657709	2.585328	4.023915
161	1	0	2.265677	1.938870	4.910378
162	1	0	3.226501	0.859628	3.896933
163	6	0	1.152079	3.532067	3.169653
164	1	0	0.422068	3.867318	2.422677
165	1	0	0.613347	3.394704	4.127849
166	1	0	1.886427	4.334490	3.323710

Harmonic Frequencies

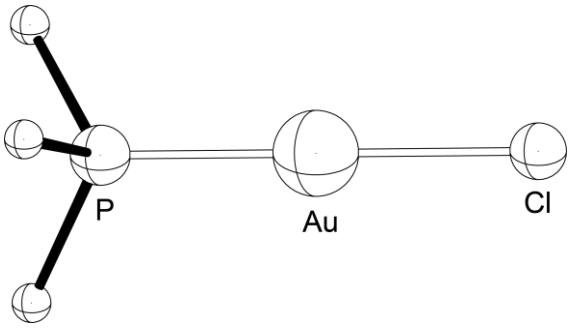
	1	2	3
	A	A	A
Frequencies --	-43.3344	20.5795	22.4989
Red. masses --	4.9064	4.4605	4.5808
Frc consts --	0.0054	0.0011	0.0014
IR Inten --	11.9433	0.0408	0.0541

Thermochemistry

Sum of electronic and zero-point Energies=	-4407.540039
Sum of electronic and thermal Energies=	-4407.455015
Sum of electronic and thermal Enthalpies=	-4407.454071
Sum of electronic and thermal Free Energies=	-4407.656676

HF = -4408.93540699

[AuCl(PMe$_3$)]



Selected Bond Distances (Å) and Angles (°): P–Au 2.263, Au–Cl 2.334; P–Au–Cl 179.96

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.001244	0.000000	0.063260
2	79	0	-0.001018	0.000000	2.326386
3	6	0	1.685709	0.000000	-0.689932
4	1	0	2.228802	-0.890915	-0.347068
5	1	0	2.228802	0.890915	-0.347068
6	1	0	1.626298	0.000000	-1.788937
7	6	0	-0.843142	1.461656	-0.690535
8	1	0	-0.341259	2.376368	-0.347390
9	1	0	-1.886085	1.488202	-0.347323
10	1	0	-0.813681	1.410988	-1.789662
11	6	0	-0.843142	-1.461656	-0.690536
12	1	0	-0.341259	-2.376369	-0.347391
13	1	0	-0.813681	-1.410988	-1.789662
14	1	0	-1.886085	-1.488202	-0.347324
15	17	0	0.000987	0.000001	4.660637

Harmonic Frequencies

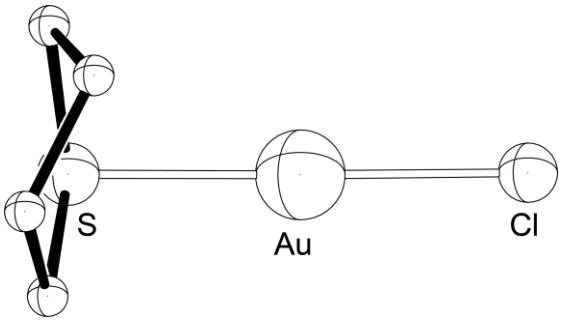
	1	2	3
	A	A	A
Frequencies --	63.4398	63.5329	157.6861
Red. masses --	7.3951	7.5997	1.0220
Frc consts --	0.0175	0.0181	0.0150
IR Inten --	0.3998	0.4003	0.0087

Thermochemistry

```
 Sum of electronic and zero-point Energies=          -1057.384962
 Sum of electronic and thermal Energies=             -1057.374371
 Sum of electronic and thermal Enthalpies=           -1057.373427
 Sum of electronic and thermal Free Energies=        -1057.422853

HF =  -1057.49799124
```

[AuCl(tht)]



Selected Bond Distances (Å) and Angles (°): S–Au 2.355, Au–Cl 2.311; S–Au–Cl 179.31.

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.084448	-1.152772	0.751643
2	6	0	0.134834	0.393181	0.432195
3	6	0	-1.192459	0.960233	-0.118040
4	6	0	-2.109573	-0.226846	-0.469530
5	1	0	-2.445362	-2.168398	0.554756
6	1	0	-2.612305	-0.719613	1.613147
7	1	0	0.584421	1.020040	1.211930
8	1	0	0.868948	0.199190	-0.356521
9	1	0	-1.676997	1.578737	0.652797
10	1	0	-0.994349	1.598375	-0.990849
11	1	0	-3.136305	0.101828	-0.689196
12	1	0	-1.716442	-0.771468	-1.341817
13	16	0	-0.275609	-1.281528	1.205388
14	79	0	0.489655	-2.798822	-0.425726
15	17	0	1.214369	-4.296394	-2.030185

Harmonic Frequencies

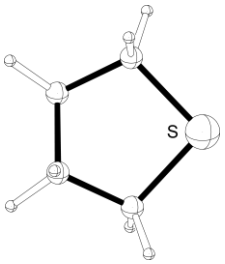
	1	2	3
	A	A	A
Frequencies --	47.8112	73.9841	85.6620
Red. masses --	3.5334	7.5216	7.0558
Frc consts --	0.0048	0.0243	0.0305
IR Inten --	1.3289	0.6896	0.3157

Thermochemistry

Sum of electronic and zero-point Energies=	-1151.674335
Sum of electronic and thermal Energies=	-1151.665350
Sum of electronic and thermal Enthalpies=	-1151.664406
Sum of electronic and thermal Free Energies=	-1151.711338

HF = -1151.78797997

tht



Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.102569	-1.577470	-0.197612
2	6	0	2.092932	-0.024005	0.171456
3	6	0	0.805286	0.714927	-0.239976
4	6	0	-0.370294	-0.136450	0.274189
5	1	0	-0.391128	-1.706925	-1.251116
6	1	0	-0.629842	-2.325296	0.409757
7	1	0	2.343990	0.177923	1.223102
8	1	0	2.952224	0.245824	-0.456930
9	1	0	0.789485	1.735949	0.172022
10	1	0	0.754630	0.786947	-1.337949
11	1	0	-0.394119	-0.105563	1.374985
12	1	0	-1.340070	0.226422	-0.100574
13	16	0	1.734178	-1.842115	-0.030825

Harmonic Frequencies

	1	2	3
	A	A	A
Frequencies --	117.0182	282.1089	460.5471
Red. masses --	2.3065	1.6359	5.7689
Frc consts --	0.0186	0.0767	0.7209
IR Inten --	2.2185	0.0154	0.3093

Thermochemistry

Sum of electronic and zero-point Energies=	-555.207882
Sum of electronic and thermal Energies=	-555.202608
Sum of electronic and thermal Enthalpies=	-555.201664
Sum of electronic and thermal Free Energies=	-555.236599

HF = -555.318752164