Amidine functionalized phosphines: tuneable ligands for transition metals

Supplementary material.

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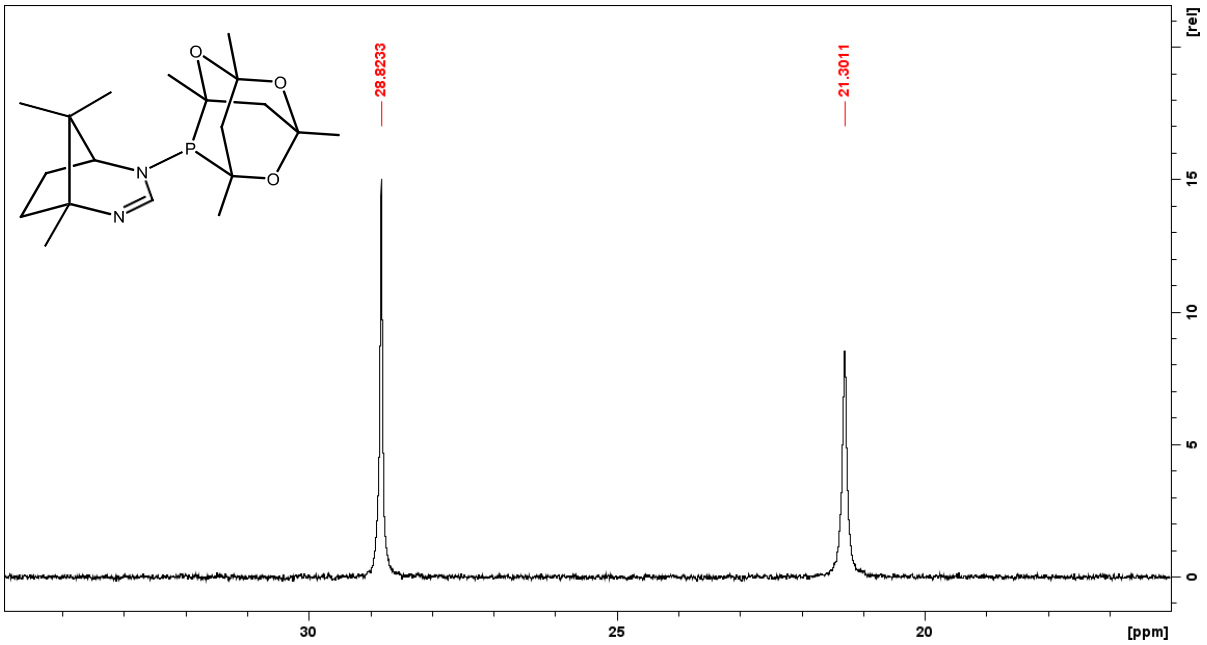
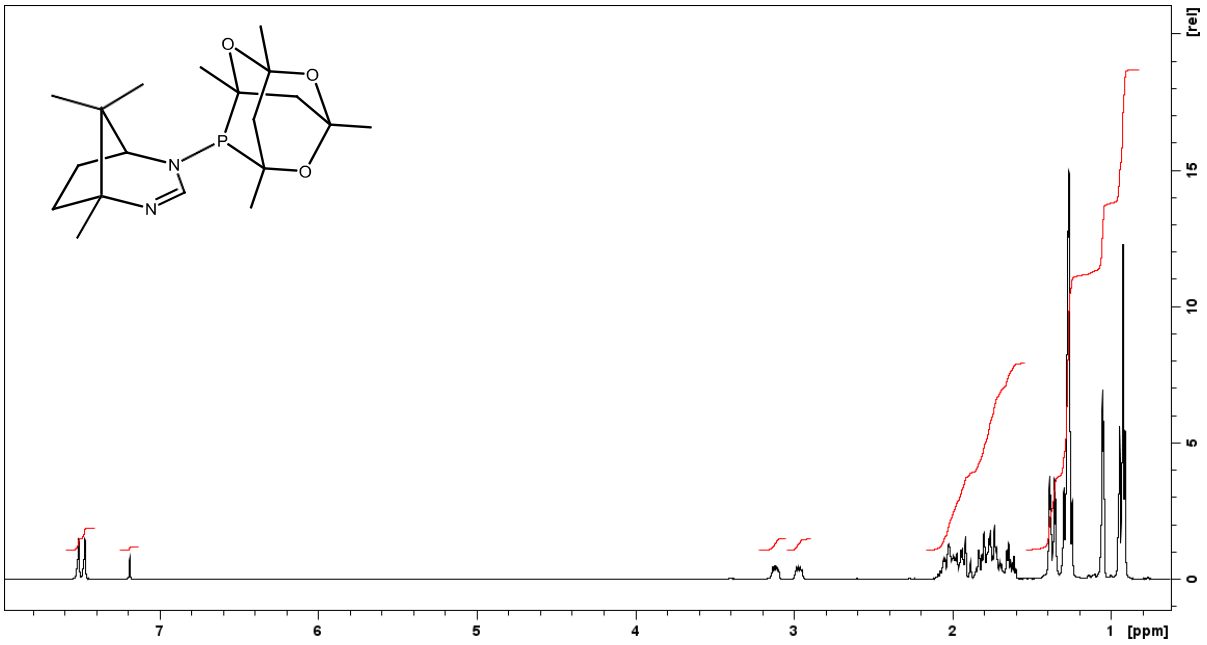
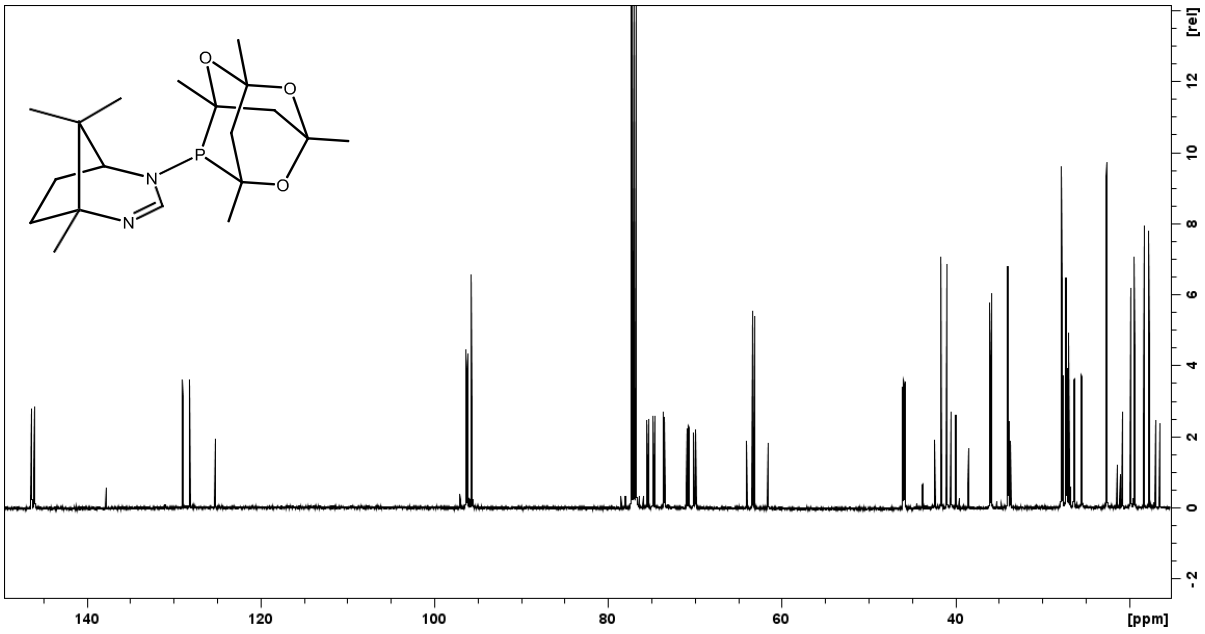
$^{31}P\{^{1}H\}$ NMR spectrum of α,β-CgPAm recorded at 162 MHz in $CDCl_3$.



^{1}H NMR spectrum of α,β-CgPAm recorded at 400 MHz in $CDCl_3$.



$^{13}C\{^{1}H\}$ NMR spectrum of α,β-CgPAm recorded at 100 MHz in $CDCl_3$.



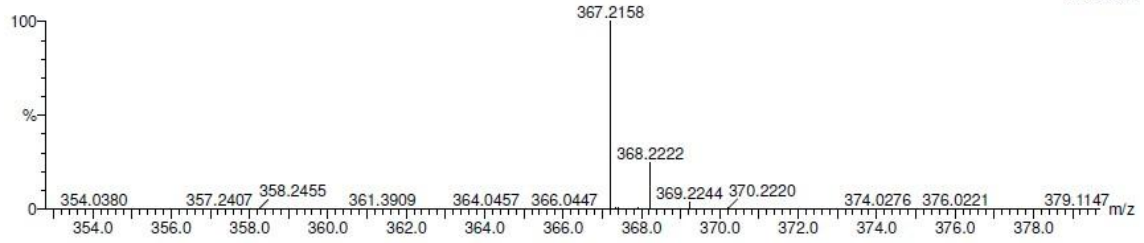
HRMS (ES^+) spectrum of α,β-CgPAm.

Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-19 H: 0-32 N: 0-2 O: 0-3 P: 0-1

24-Jan-2017
PDN_MS14077_ESP 10 (1.278) Cm (10-1:4)

CgPAM

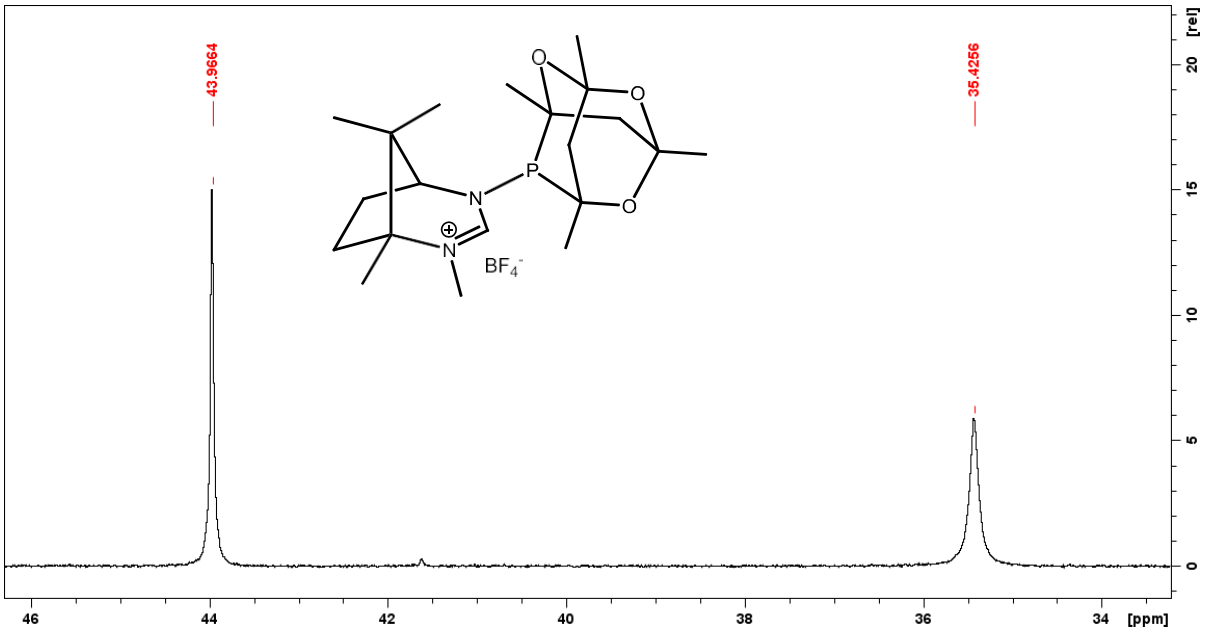
School of Chemistry Cardiff University
1: TOF MS ES+
5.70e+005



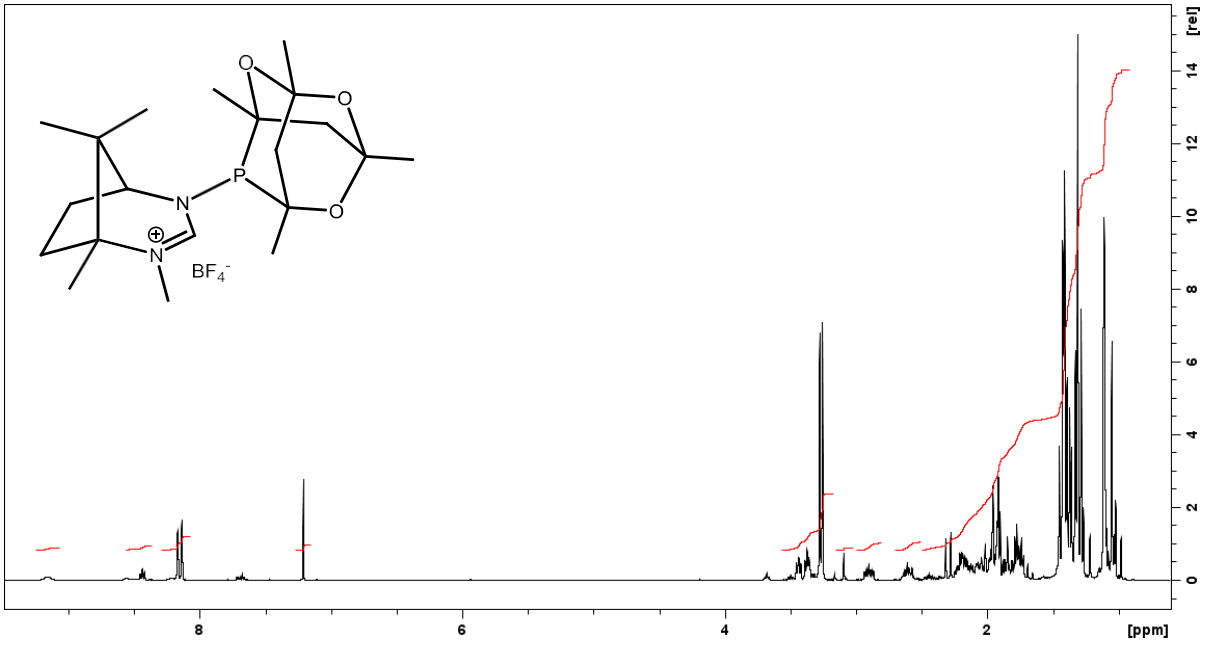
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
367.2158	367.2151	0.7	1.9	5.5	783.5	0.0	C19 H32 N2 O3 P

1.2 NMR and mass spectra of [α,β-CgPAmMe]BF_4.

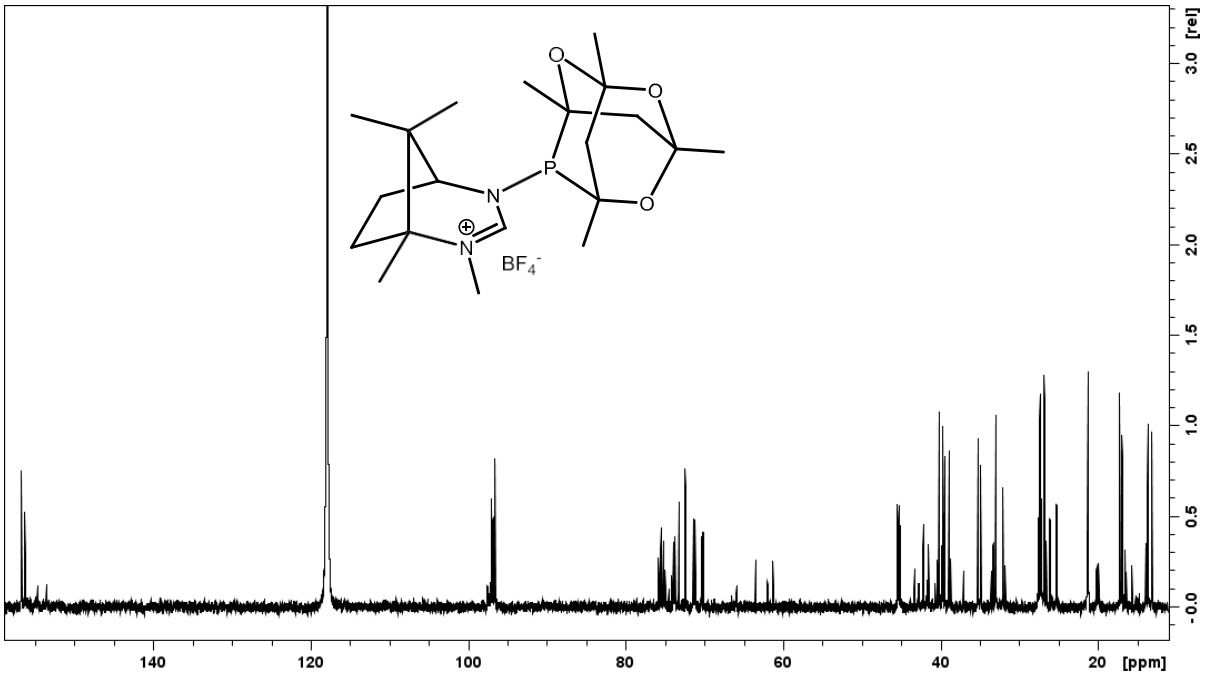
$^{31}P\{^1H\}$ NMR spectrum of [α,β-CgPAmMe]BF_4 recorded at 162 MHz in $CDCl_3$.



^1H NMR spectrum of [α,β-CgPAmMe]BF_4 recorded at 400 MHz in $CDCl_3$.

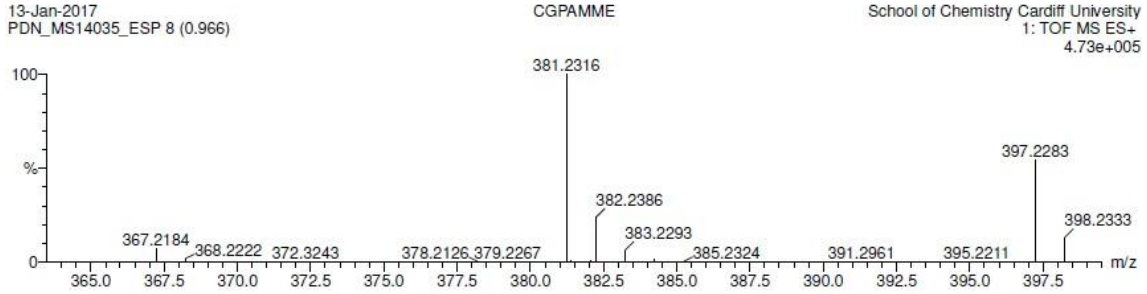


$^{13}C\{^{1}H\}$ NMR spectrum of [α,β-CgPAmMe]BF_4 recorded at 100 MHz in CD_3CN.



HRMS (ES^+) spectrum of [α,β-CgPAmMe]BF_4.

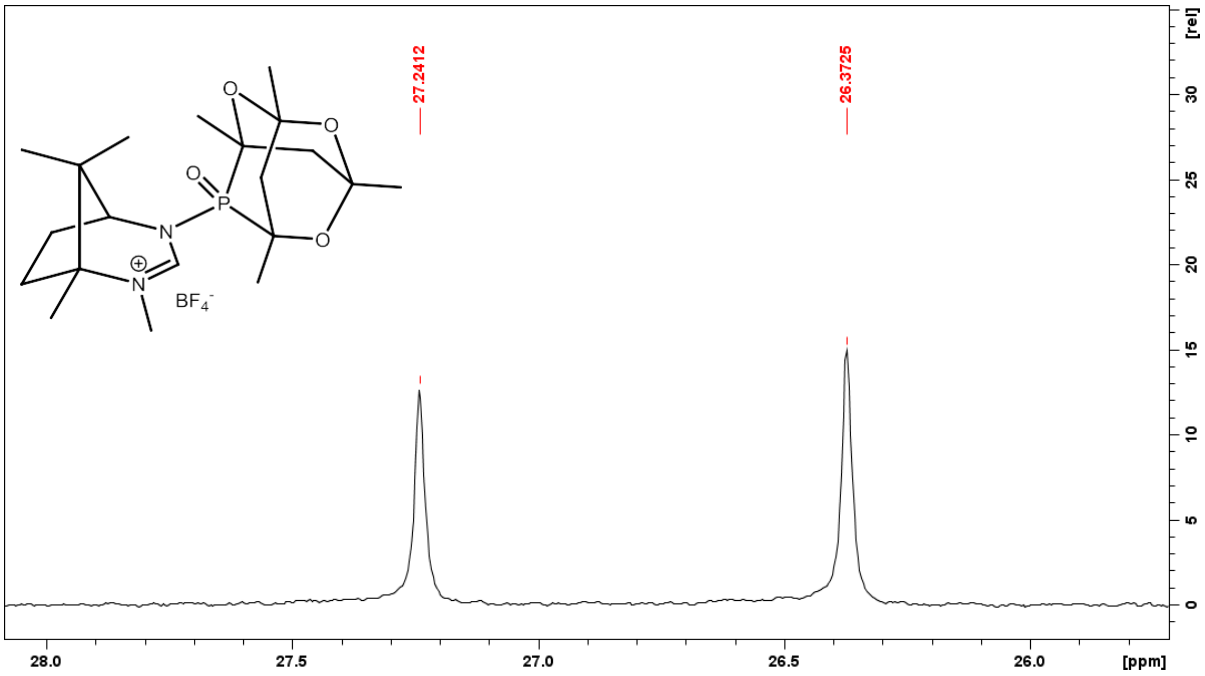
Monoisotopic Mass, Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-34 N: 0-2 O: 0-3 P: 0-1



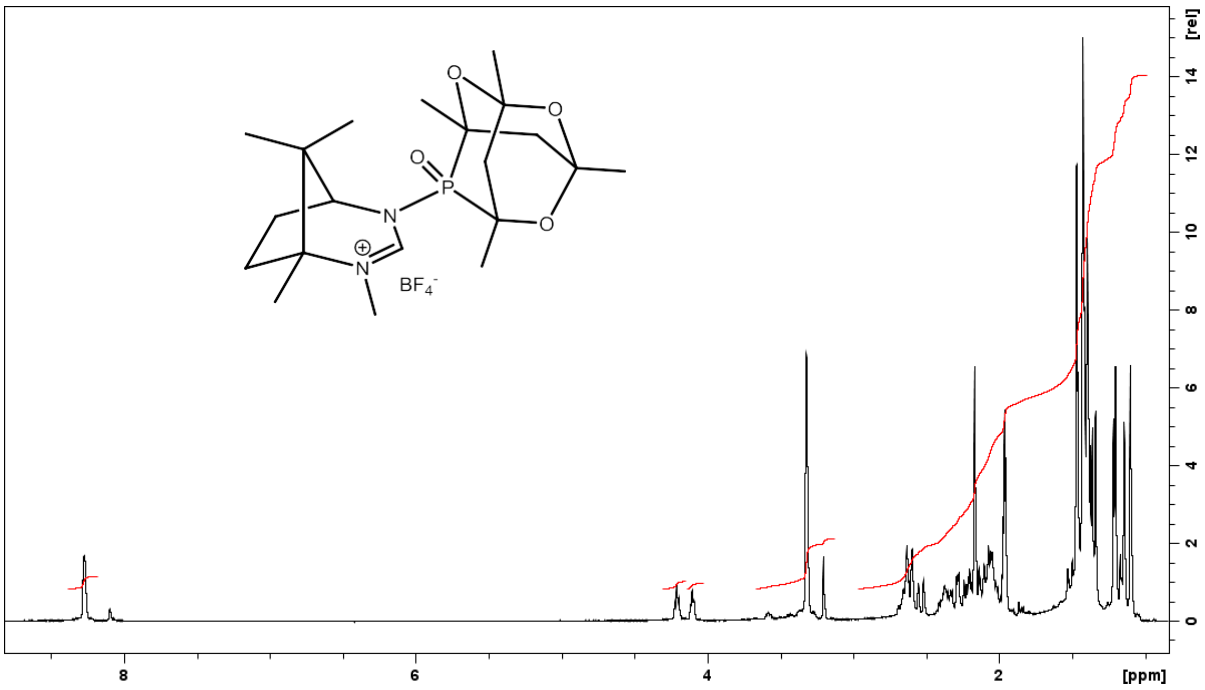
Minimum:				-1.5			
Maximum:		5.0	10.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
381.2316	381.2307	0.9	2.4	5.5	796.5	0.0	C20 H34 N2 O3 P

1.3 NMR and mass spectra of [α,β-CgP(O)AmMe]BF_4.

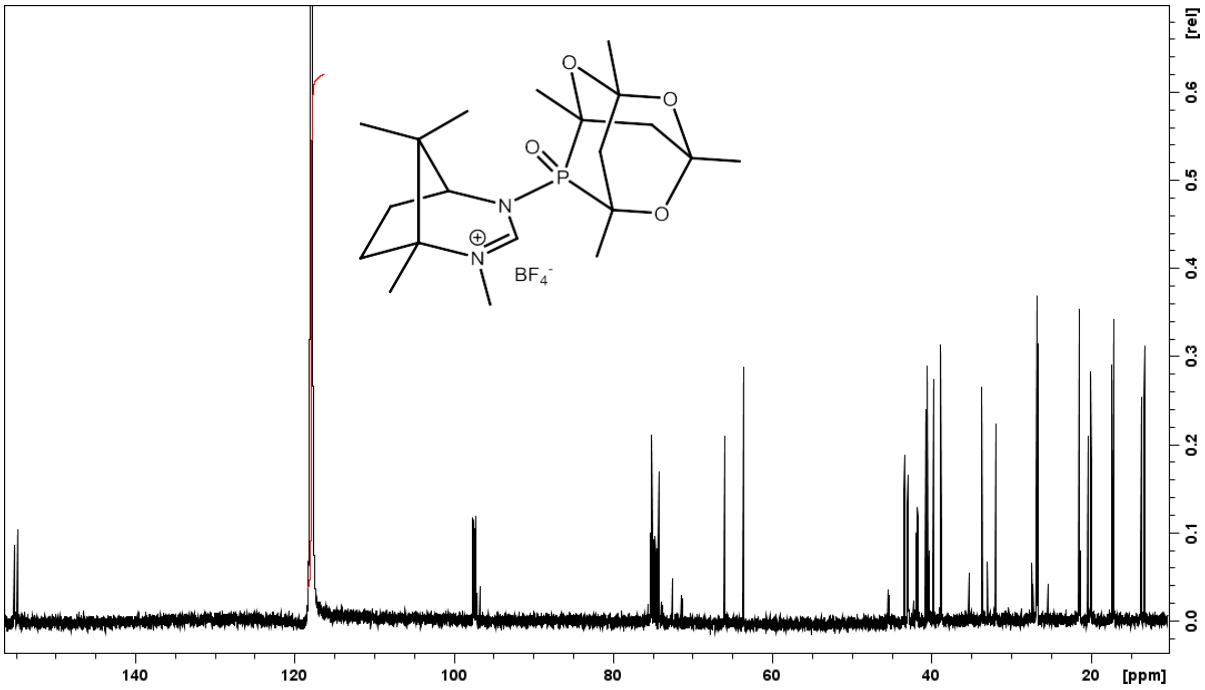
$^{31}P\{^1H\}$ NMR spectrum of [α,β-CgP(O)AmMe]BF_4 recorded at 162 MHz in CD_3CN.



^1H NMR spectrum of [α,β-CgP(O)AmMe]BF_4 recorded at 400 MHz in CD_3CN.



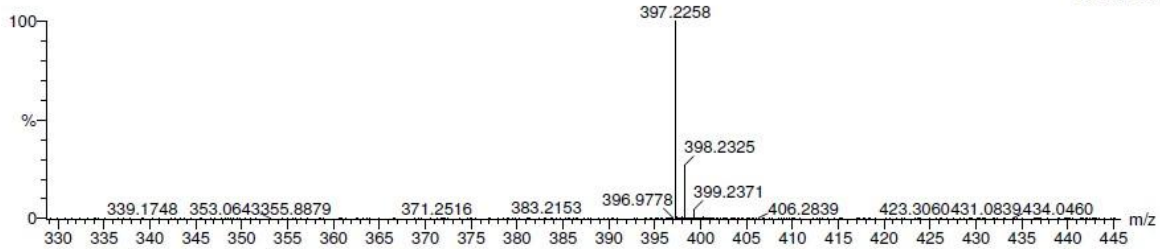
^{13}C NMR spectrum of [α,β-CgP(O)AmMe]BF_4 recorded at 100 MHz in CD_3CN.



HRMS (ES^+) spectrum of [α,β-CgP(O)AmMe]BF_4.

Monoisotopic Mass, Odd and Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-34 N: 0-2 O: 0-4 P: 0-1

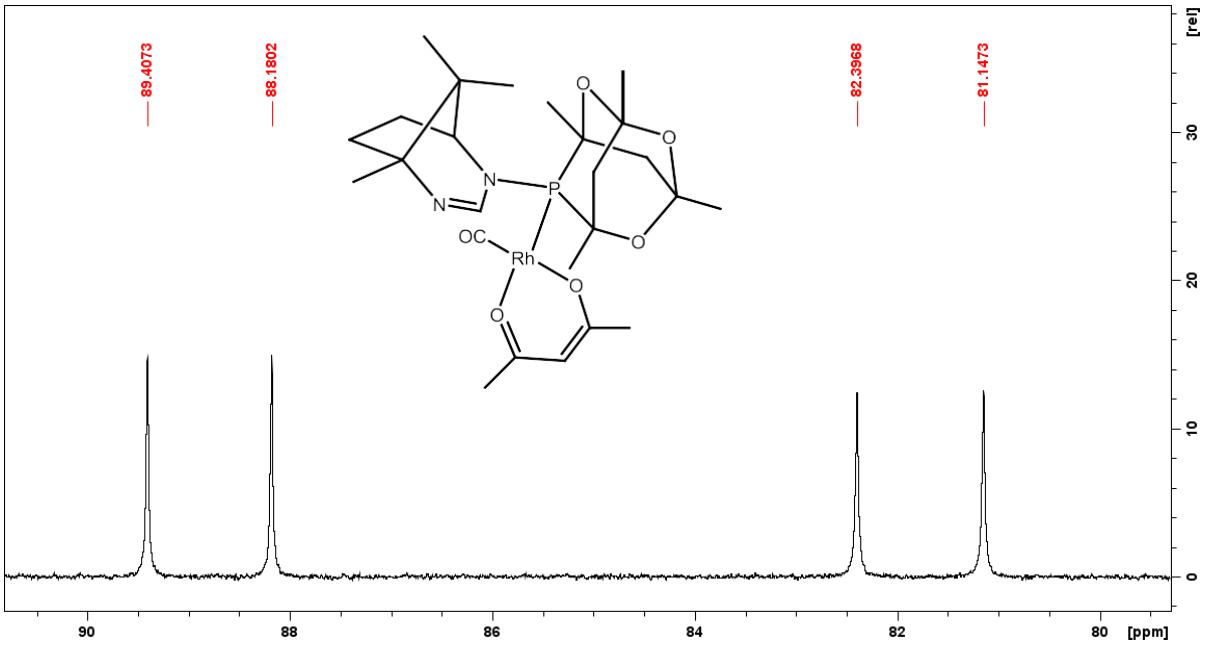
21-Jun-2017 CgPAmMeO School of Chemistry Cardiff University
PDN_MS17372_ESP2 9 (1.180) Cm (9-1:4) 1: TOF MS ES+
2.23e+005



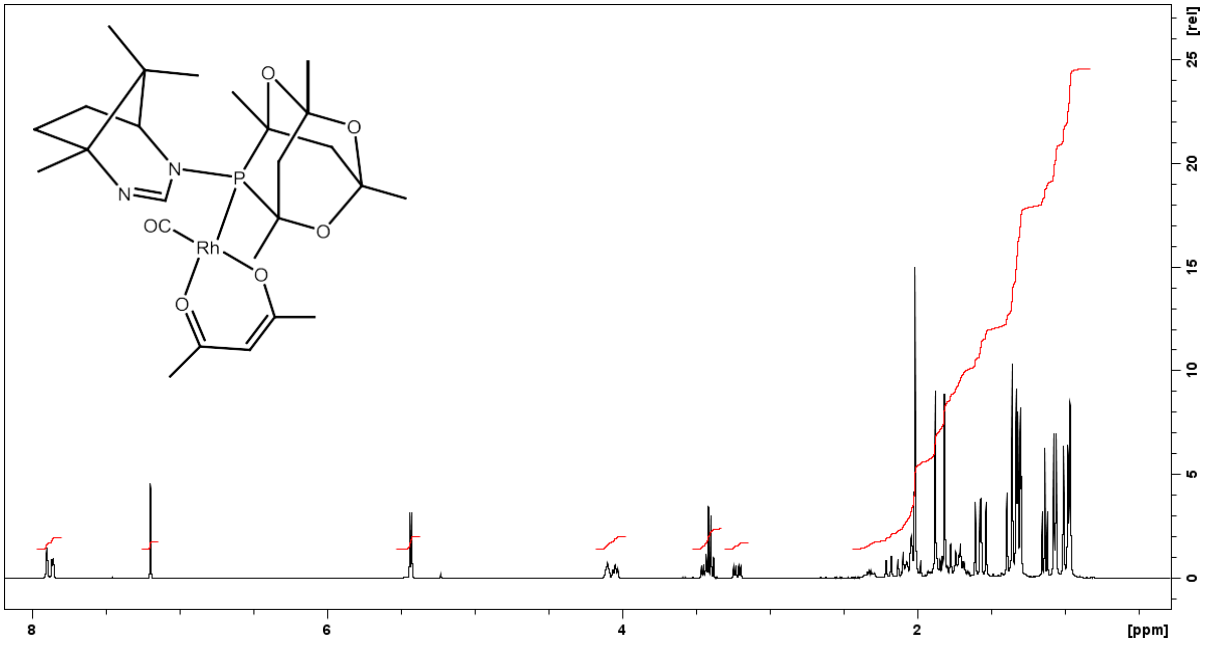
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
397.2258	397.2256	0.2	0.5	5.5	625.2	0.0	C20 H34 N2 O4 P

1.4 NMR, mass and IR spectra of [Rh(α,β-CgPAm)(acac)CO].

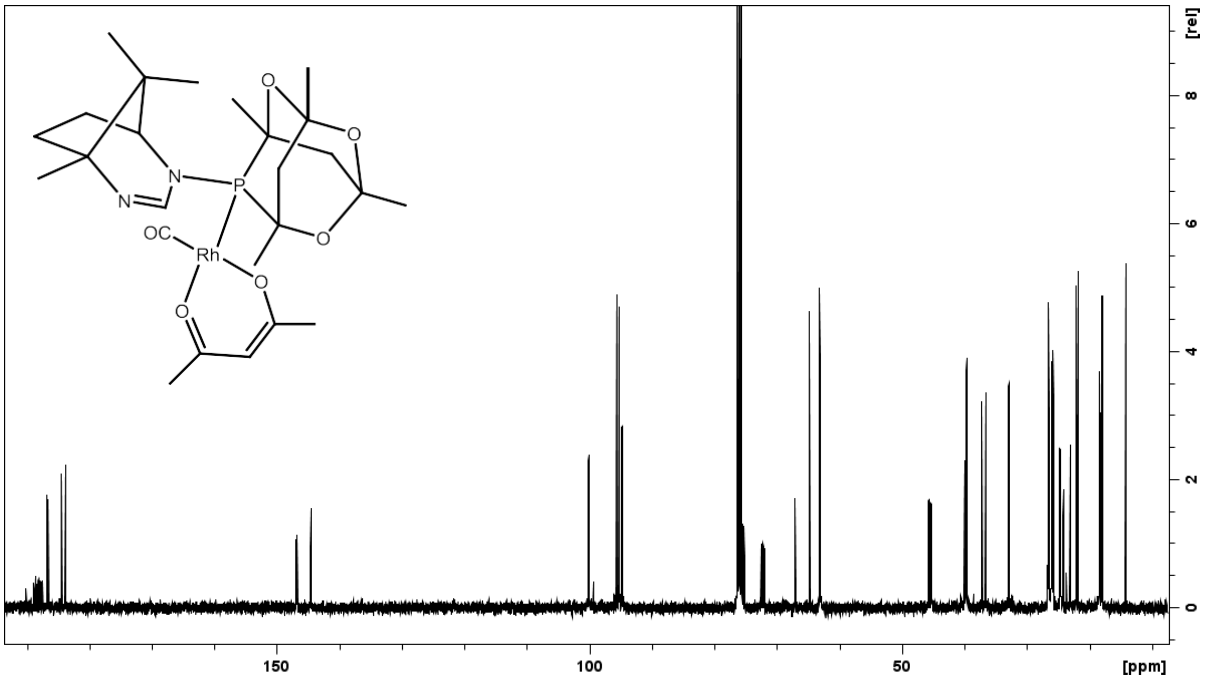
$^{31}P\{^{1}H\}$ NMR spectrum of [Rh(α,β-CgPAm)(acac)CO] recorded at 162 MHz in $CDCl_3$.



^{1}H NMR spectrum of [Rh(α,β-CgPAm)(acac)CO] recorded at 400 MHz in $CDCl_3$.



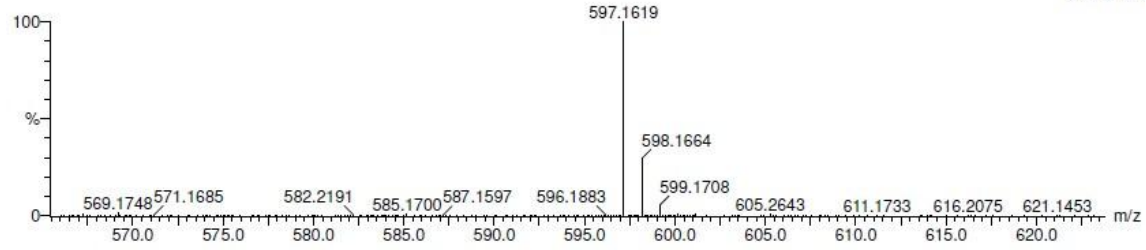
$^{13}C\{^{1}H\}$ NMR spectrum of [Rh(α,β-CgPAm)(acac)CO] recorded at 100 MHz in $CDCl_3$.



HRMS (ES^+) spectrum of [Rh(α,β-CgPAm)(acac)CO].

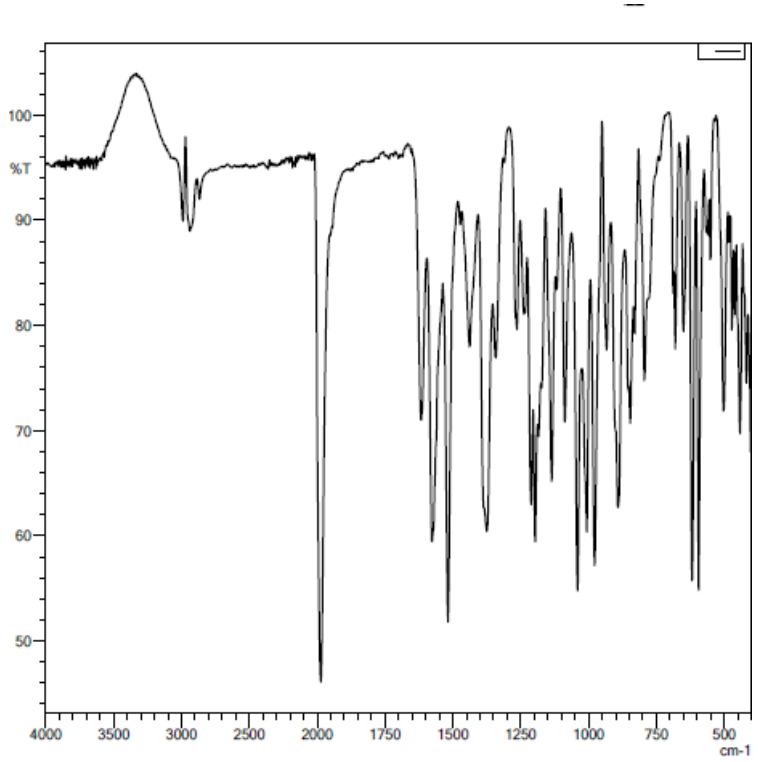
Monoisotopic Mass, Odd and Even Electron Ions
82 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-39 N: 0-2 O: 0-6 P: 0-1 103Rh: 0-1

10-May-2017 CgPAmRh School of Chemistry Cardiff University
PDN_MS17122_ESP2 6 (0.622) Cm (6-1:4) 3: TOF MS ES+
1.65e+005



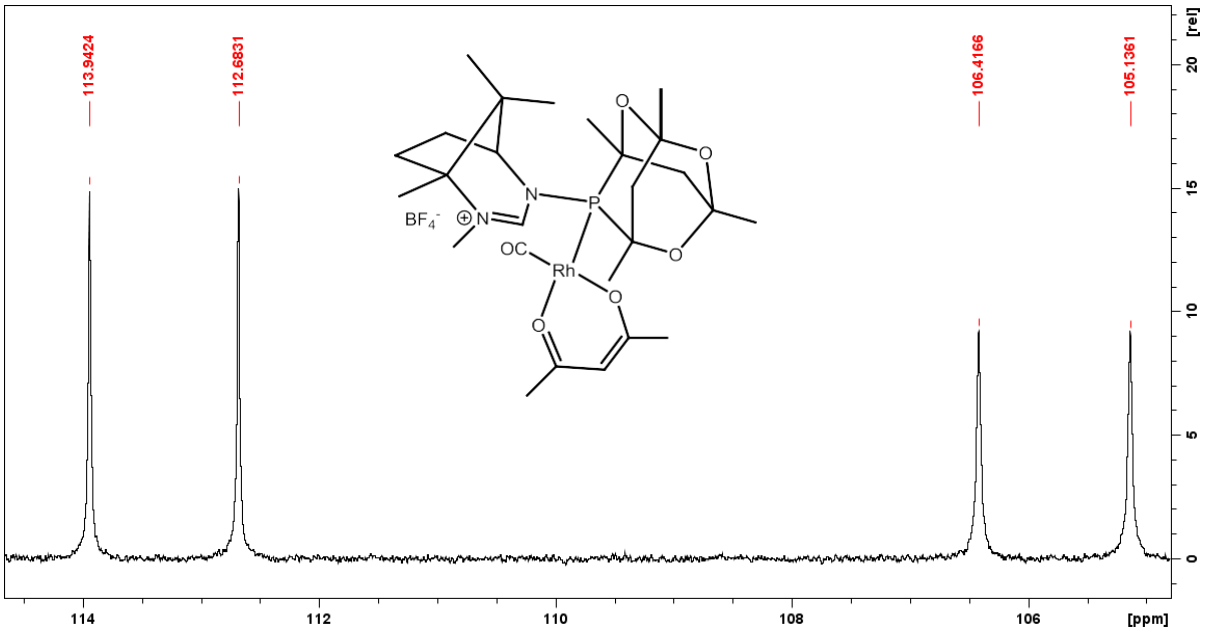
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
597.1619	597.1601	1.8	3.0	8.0	360.0	0.0	C25 H39 N2 O6 P 103Rh

IR spectrum of [Rh(α,β-CgPAm)(acac)CO].

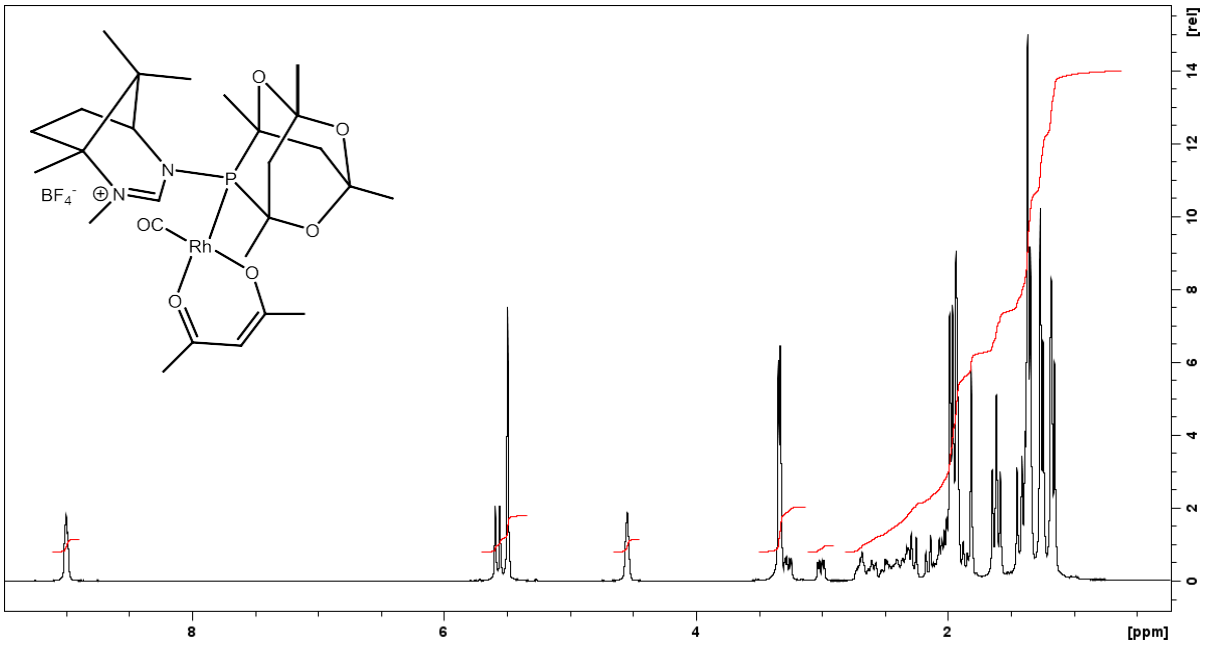


1.5 NMR, mass and IR spectra of [Rh(α,β-CgPAmMe)(acac)CO]BF_4.

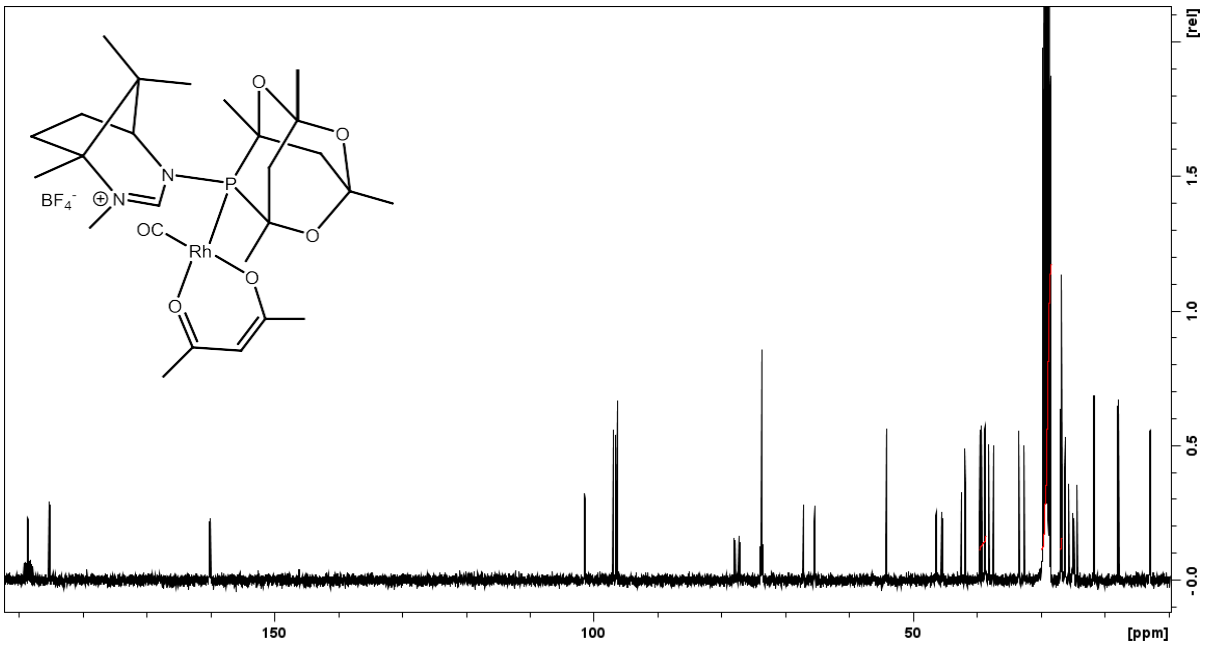
$^{31}P\{^{1}H\}$ NMR spectrum of [Rh(α,β-CgPAmMe)(acac)CO]BF_4 recorded at 162 MHz in d_6-acetone.



^{1}H NMR spectrum of [Rh(α,β-CgPAmMe)(acac)CO]BF_4 recorded at 400 MHz in d_6-acetone.

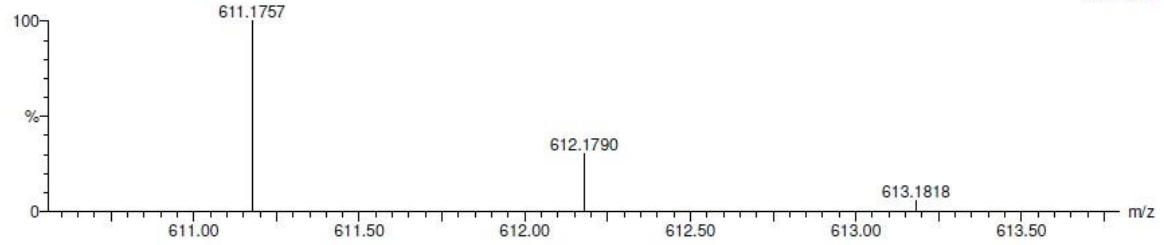


^{13}C{^{1}H} NMR spectrum of [Rh(α,β-CgPAmMe)(acac)CO]BF_4 recorded at 100 MHz in d_6-acetone.



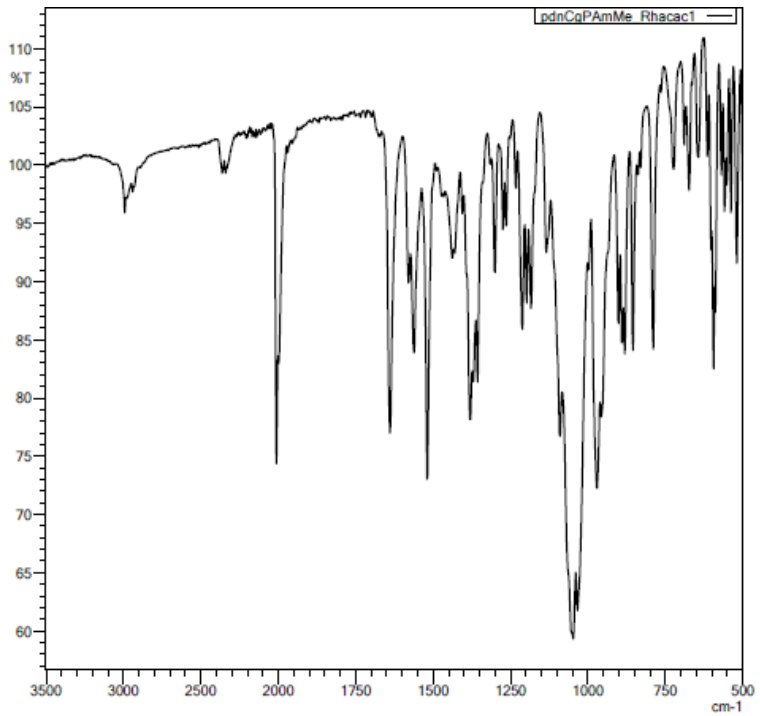
HRMS (ES^+) spectrum of $[Rh(\alpha,\beta\text{-CgPAmMe})(acac)CO]BF_4$.

Monoisotopic Mass, Odd and Even Electron Ions
82 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-26 H: 0-41 N: 0-2 O: 0-6 P: 0-1 Rh: 0-1
13-Jan-2017 GCPAMMERH School of Chemistry Cardiff University
PDN_MS14034_ESP (0.138) Is (0.50,1.00) C26H41O6N2PRh 1: TOF MS ES+
7.29e+012



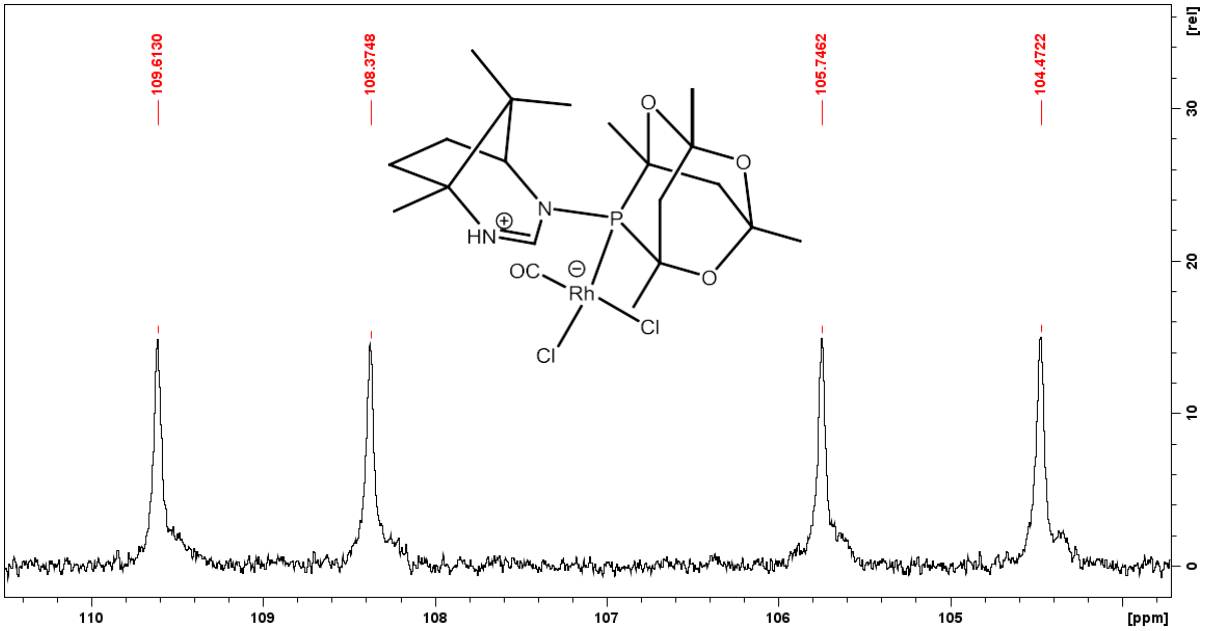
Minimum:				-1.5							
Maximum:		5.0	10.0	100.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
611.1757	611.1757	0.0	0.0	8.0	183.3	0.0	C26	H41	N2	O6	P Rh

IR spectrum of $[Rh(\alpha,\beta\text{-CgPAmMe})(acac)CO]BF_4$.

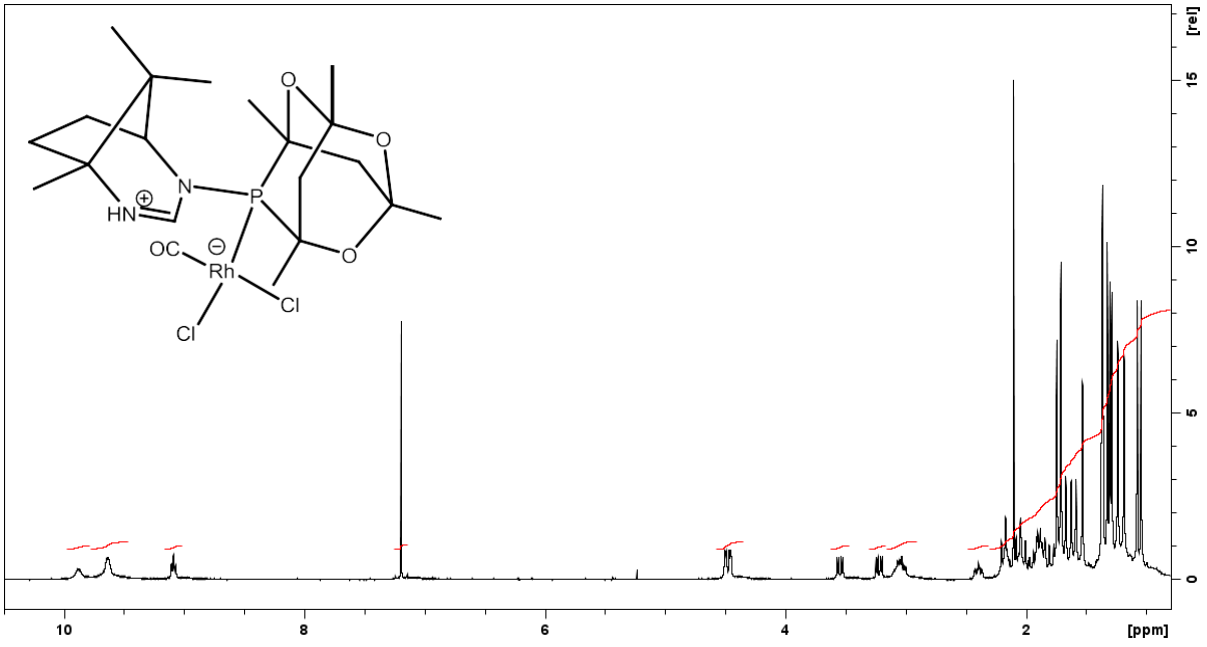


1.6 NMR, mass and IR spectra of [Rh(α,β-CgPAmH)(CO)(Cl)$_2$].

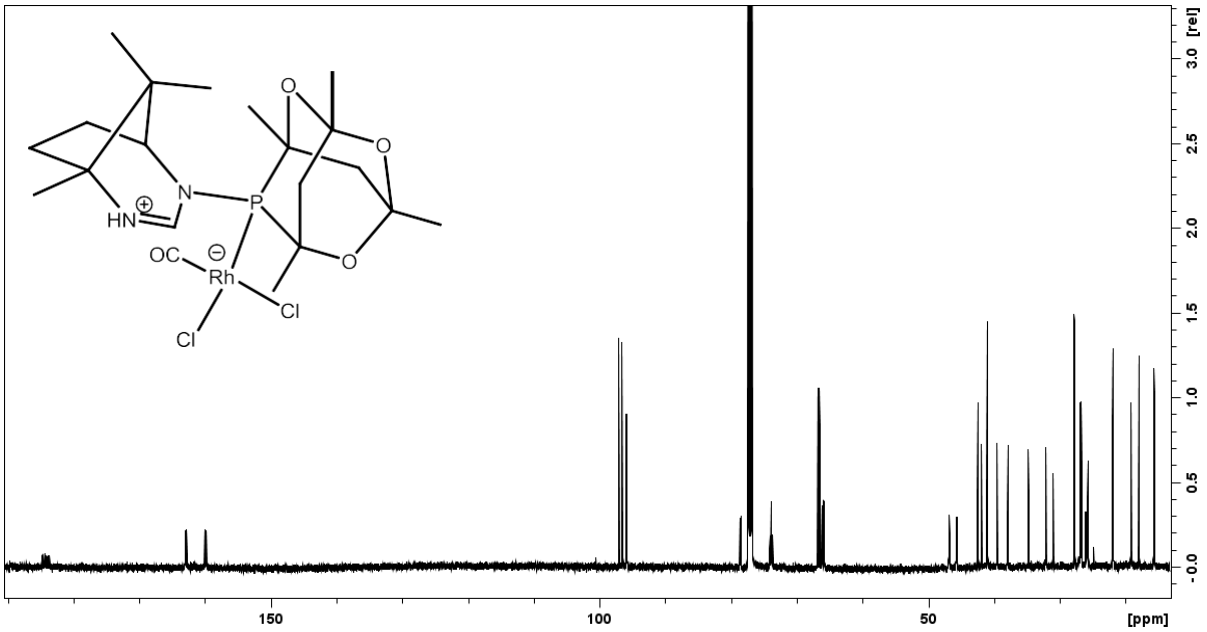
$^{31}P\{^{1}H\}$ NMR spectrum of [Rh(α,β-CgPAmH)(CO)(Cl)$_2$] recorded at 162 MHz in $CDCl_3$.



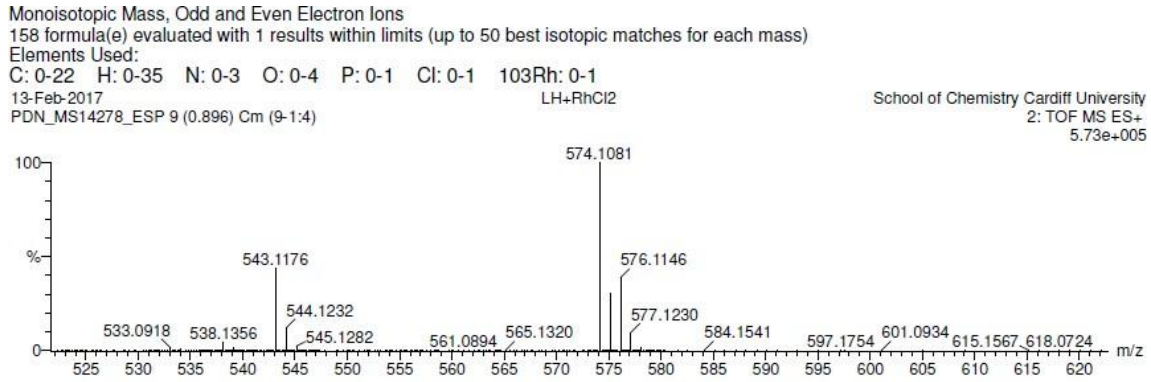
^{1}H NMR spectrum of [Rh(α,β-CgPAmH)(CO)(Cl)$_2$] recorded at 400 MHz in $CDCl_3$.



$^{13}C\{^{1}H\}$ NMR spectrum of [Rh(α,β-CgPAmH)(CO)$(Cl)_2$] recorded at 100 MHz in $CDCl_3$.

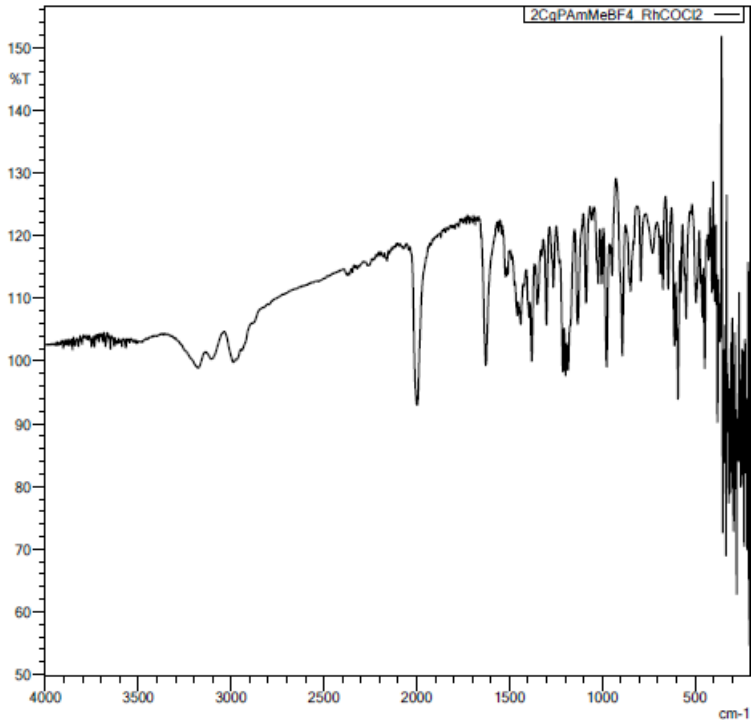


HRMS (ES^{+}) spectrum of [Rh(α,β-CgPAmH)(CO)$(Cl)_2$].



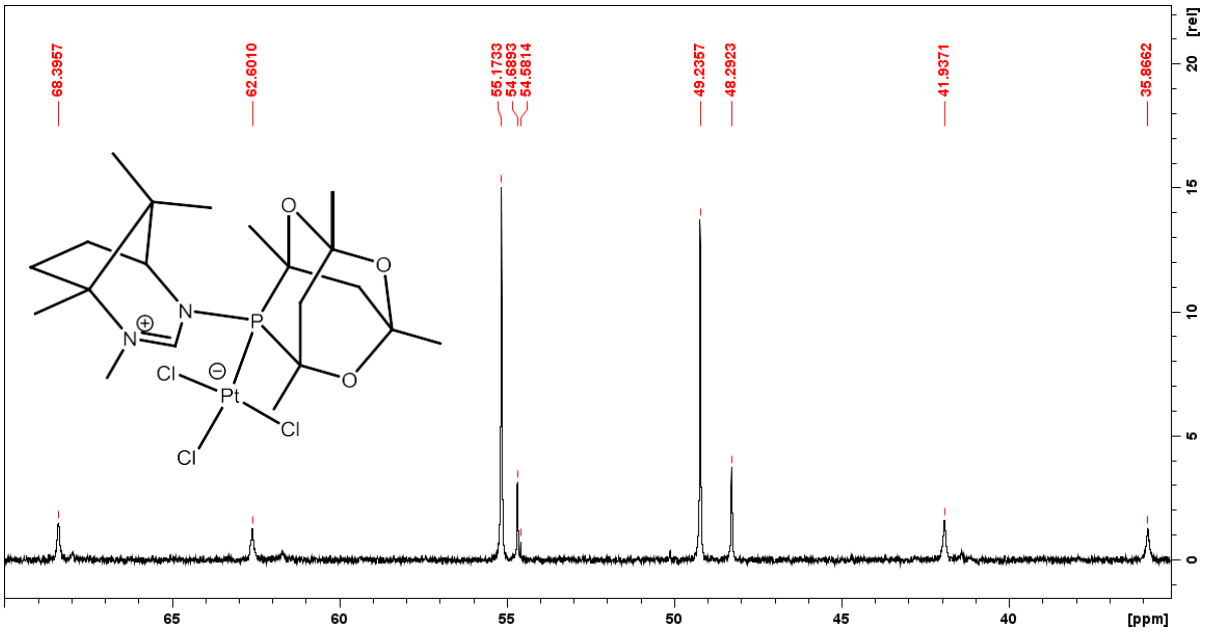
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
574.1081	574.1109	-2.8	-4.9	7.0	599.7	0.0	C22 H35 N3 O4 P Cl 103Rh

IR spectrum of [Rh(α,β-CgPAmH)(CO)(Cl)$_2$].

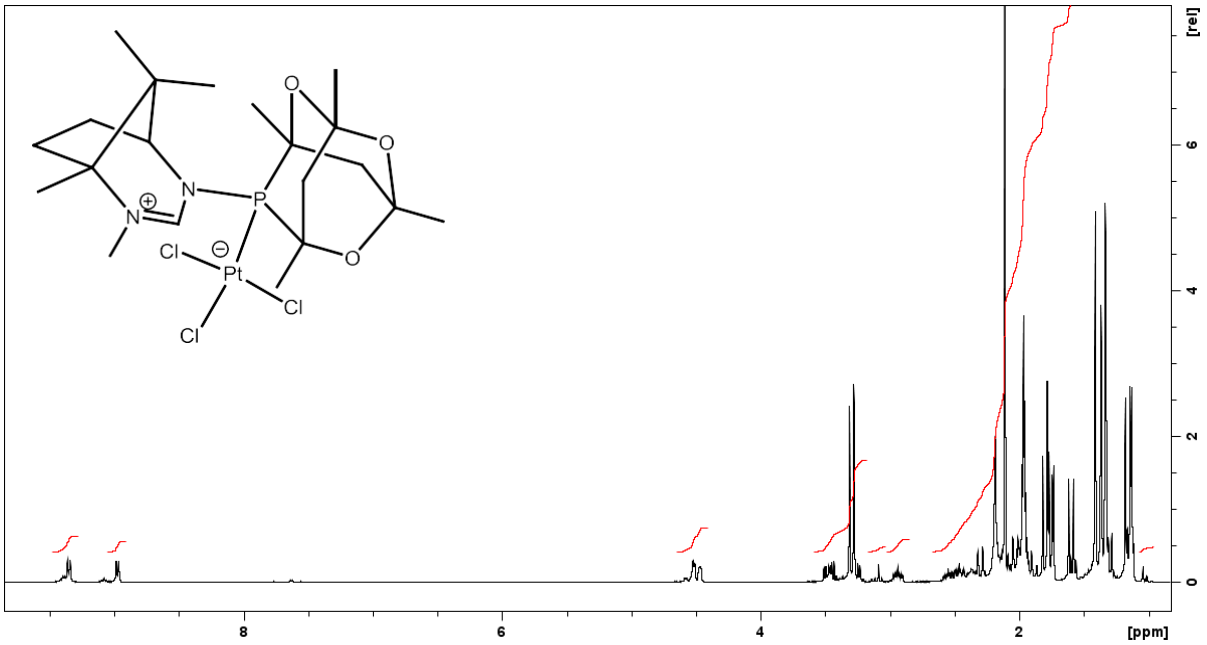


1.7 NMR, mass and IR spectra of [Pt(α,β-CgPAmMe)Cl$_3$].

$^{31}P\{^{1}H\}$ NMR spectrum of [Pt(CgPAmMe)Cl$_3$] recorded at 162 MHz in CD_3CN.



^{1}H NMR spectrum of [Pt(α,β-CgPAmMe)Cl_3] recorded at 400 MHz in CD_3CN.



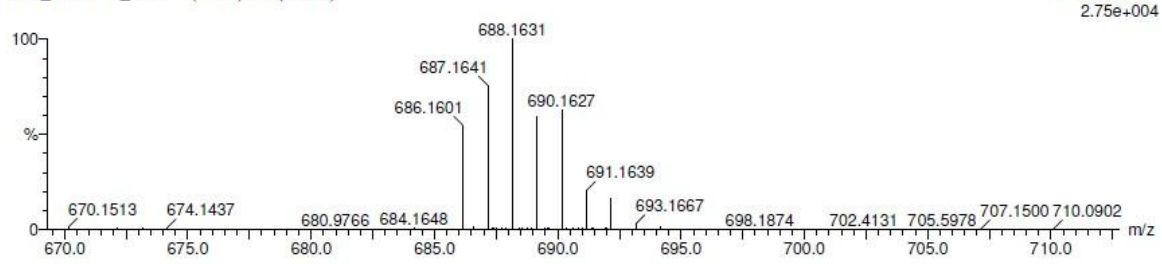
HRMS (ES^{+}) spectrum of [Pt(α,β-CgPAmMe)Cl_3].

Monoisotopic Mass, Odd and Even Electron Ions
190 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-22 H: 0-37 N: 0-3 O: 0-3 P: 0-1 Cl: 0-2 194Pt: 0-1

10-Feb-2017
PDN_MS14273_ESP 17 (1.762) Cm (17-1:4)

CgPAmMePt

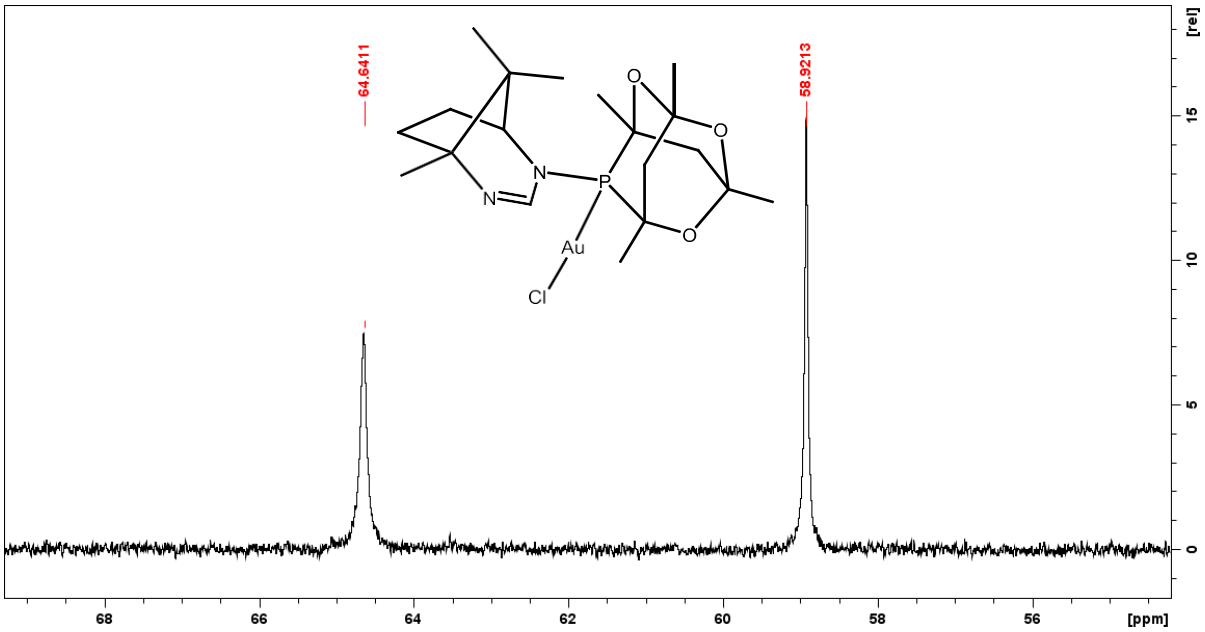
School of Chemistry Cardiff University
3: TOF MS ES+
2.75e+004



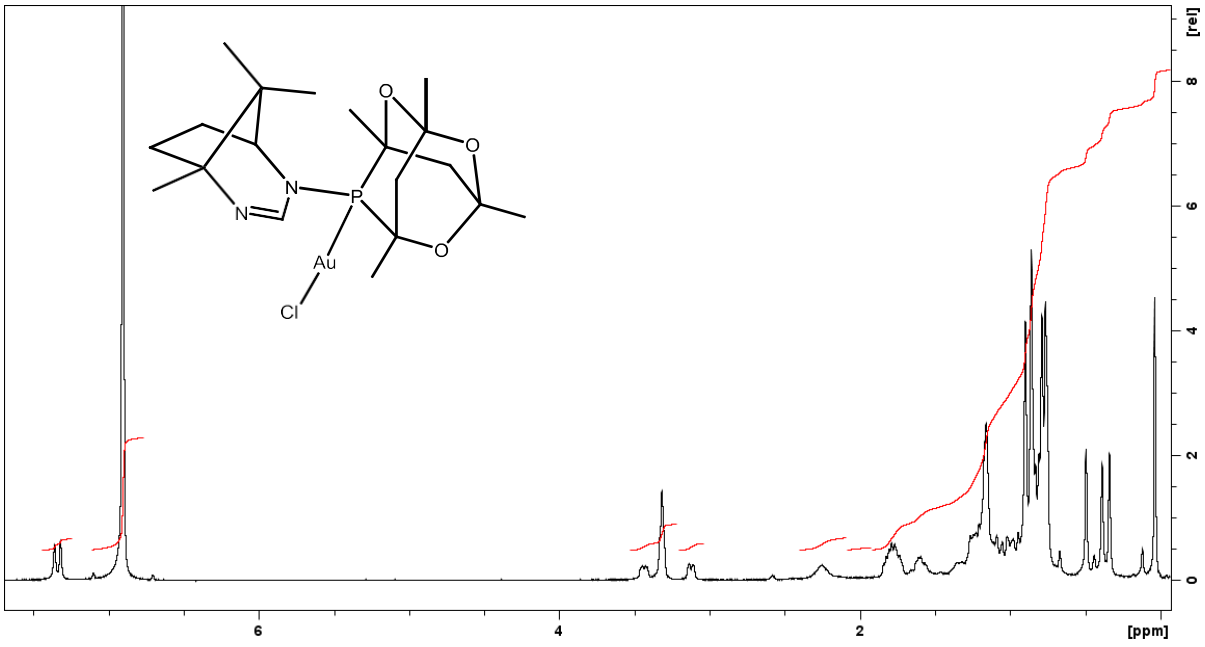
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
686.1601	686.1576	2.5	3.6	6.5	412.9	0.0	C22 H37 N3 O3 P Cl2 194Pt

1.8 NMR and mass spectra of [Au(α,β-CgPAm)Cl].

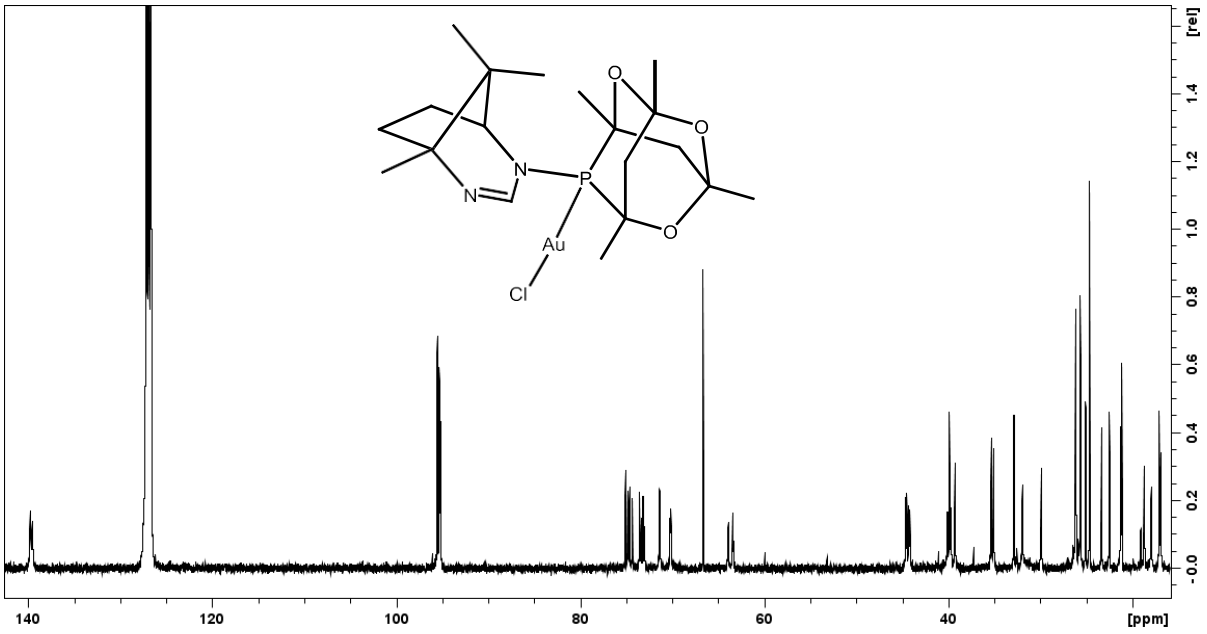
$^{31}P\{^{1}H\}$ NMR spectrum of [Au(α,β-CgPAm)Cl] recorded at 162 MHz in C_6D_6.



^{1}H NMR spectrum of [Au(α,β-CgPAm)Cl] recorded at 400 MHz in C_6D_6.



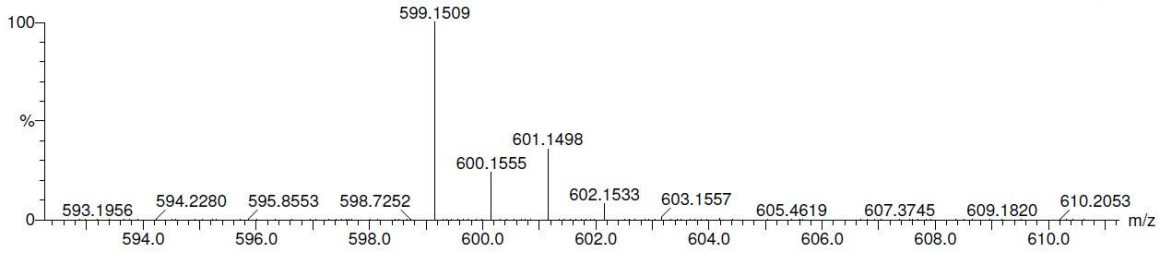
$^{13}C\{^{1}H\}$ NMR spectrum of [Au(α,β-CgPAm)Cl] recorded at 100 MHz in C_6D_6.



HRMS (ES^+) spectrum of [Pt(α,β-CgPAmMe)Cl_3].

Monoisotopic Mass, Odd and Even Electron Ions
94 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-19 H: 0-32 N: 0-2 O: 0-3 P: 0-1 35Cl: 0-1 197Au: 0-1

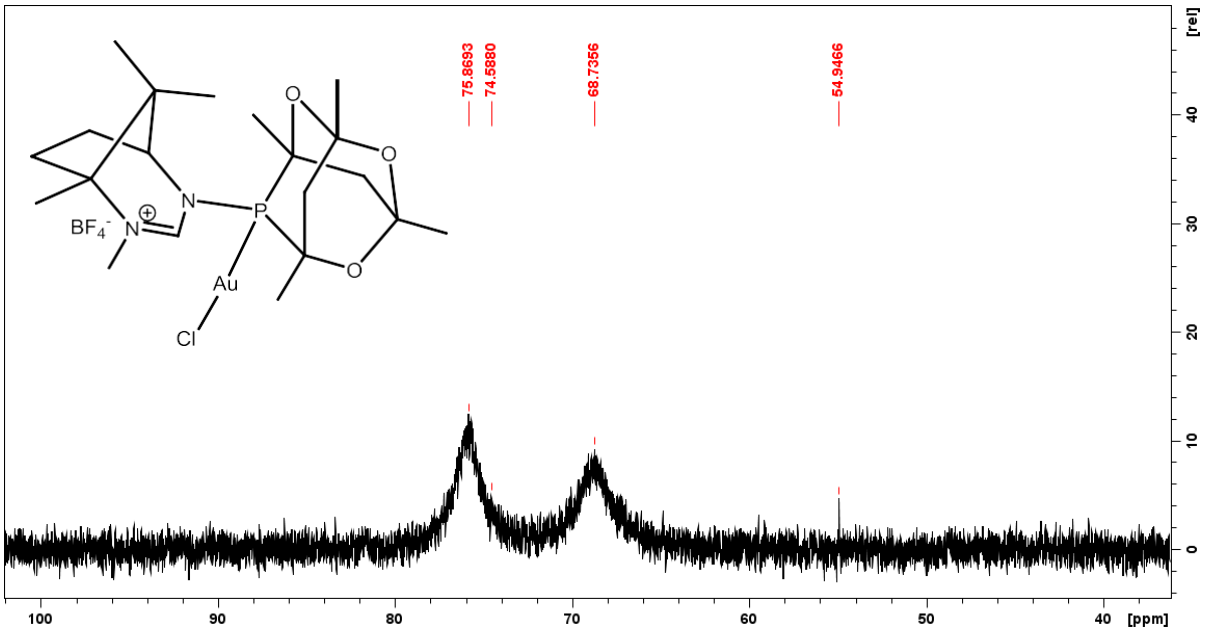
21-Feb-2017 CgPAmAy School of Chemistry Cardiff University
PDN_MS14362_ESP3 9 (0.897) Cm (9-1:4) 2: TOF MS ES+
5.88e+005



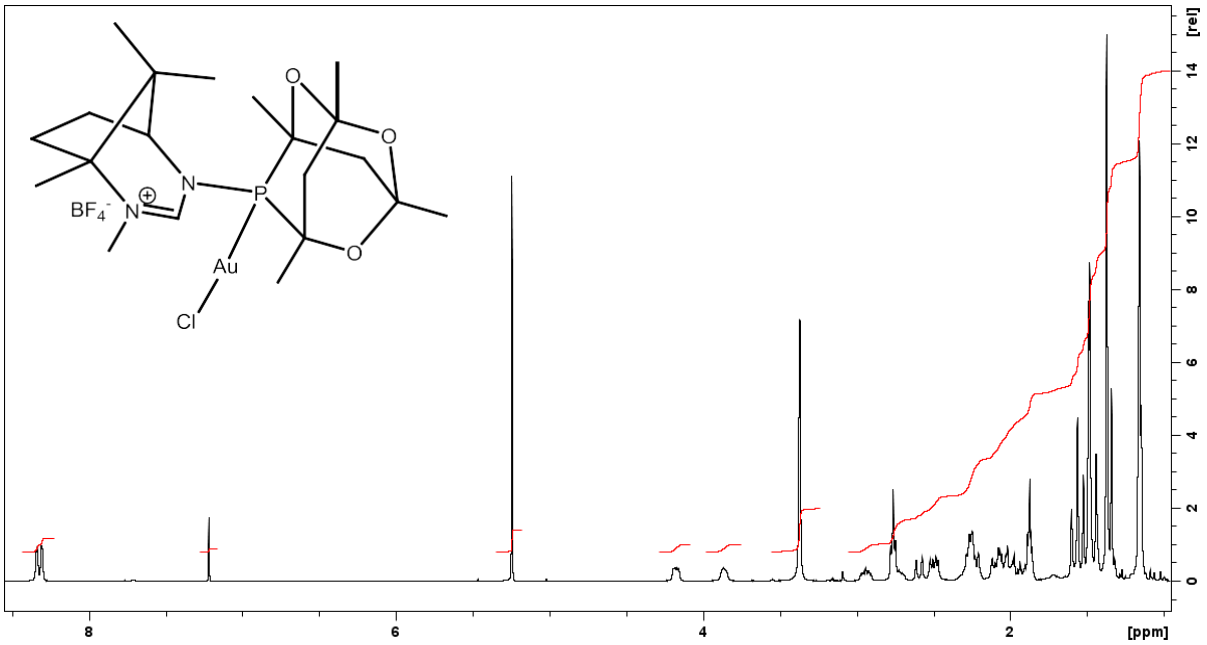
Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
599.1509	599.1505	0.4	0.7	5.5	562.5	0.0	C19 H32 N2 O3 P 35Cl 197Au

1.9 NMR and mass spectra of [Au(α,β-CgPAmMe)Cl]BF_4.

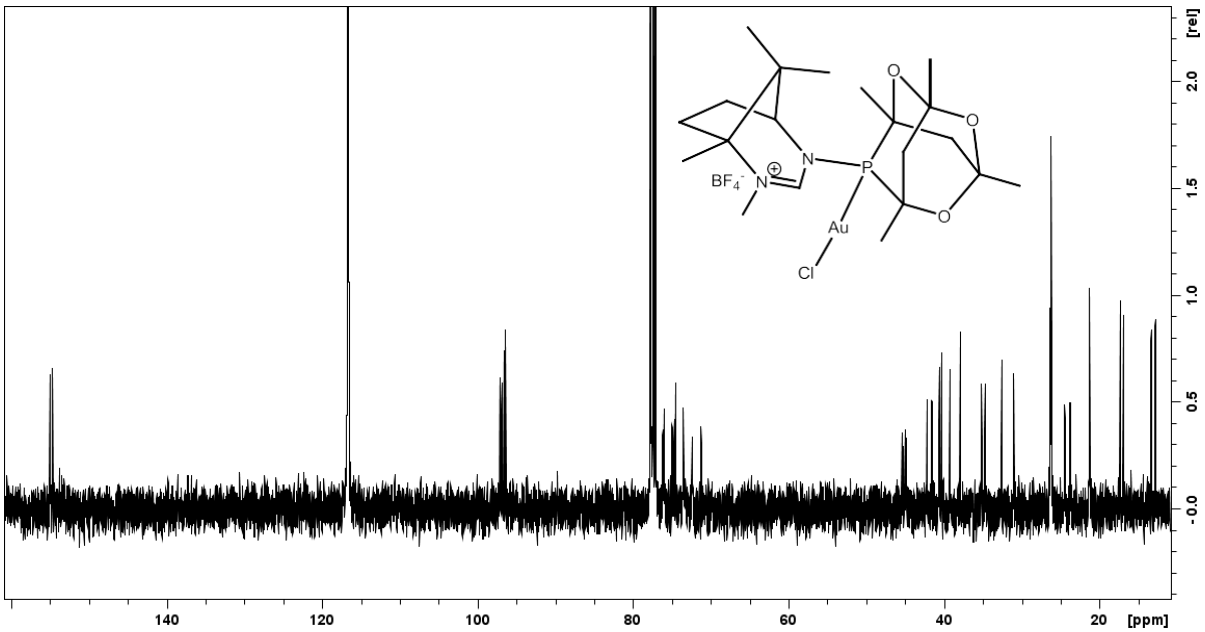
$^{31}P\{^1H\}$ NMR spectrum of [Au(α,β-CgPAmMe)Cl]BF_4 recorded at 162 MHz in $CDCl_3$.



^1H NMR spectrum of [Au(α,β-CgPAmMe)Cl]BF_4 recorded at 400 MHz in $CDCl_3$.



$^{13}C\{^{1}H\}$ NMR spectrum of [Au(α,β-CgPAmMe)Cl]BF_4 recorded at 100 MHz in $CDCl_3$.



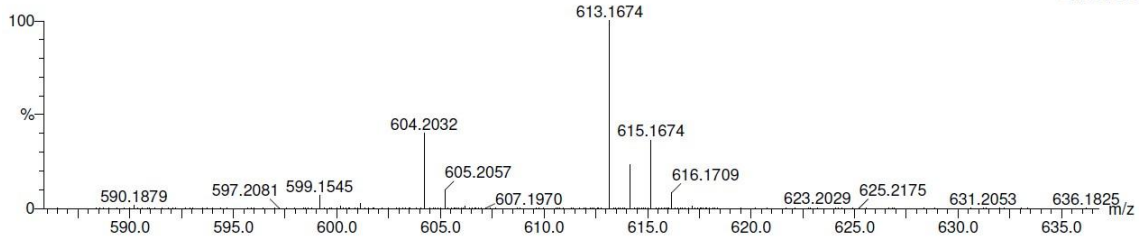
HRMS (ES^+) spectrum of [Au(α,β-CgPAmMe)Cl].

Monoisotopic Mass, Odd and Even Electron Ions
94 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-20 H: 0-34 N: 0-2 O: 0-3 P: 0-1 Cl: 0-1 197Au: 0-1

24-Jan-2017
PDN_MS14078_ESP 6 (0.622) Cm (6-1:4)

CgAmMeAu

School of Chemistry Cardiff University
3: TOF MS ES+
2.79e+005



Minimum:				-1.5			
Maximum:		5.0	5.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
613.1674	613.1661	1.3	2.1	5.5	444.9	0.0	C20 H34 N2 O3 P Cl 197Au

2. Crystallographic studies.

Crystallographic studies were undertaken of a single crystal mounted in paratone and studied on an Agilent SuperNova Dual Atlas three-circle diffractometer using Mo-Kα or Cu-Kα radiation and a CCD detector. Measurements were carried out at 150(2) K with temperatures maintained using an Oxford cryostream unless otherwise stated. Data were collected and integrated and data corrected for absorption using a numerical absorption correction based on gaussian integration over a multifaceted crystal model within CrysAlisPro.[1] The structures were solved by direct methods and refined against F^2 within SHELXL-2013.[2] A summary of crystallographic data are available as ESI and the structures deposited with the Cambridge Structural Database (CCDC deposition numbers 1550609–1550613). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

In all cases, structures were solved in a monoclinic crystal system as a 2-component inversion twin with two crystallographically independent diastereomers in the asymmetric unit other than [CgP(O)AmMe]BF_4 where four molecules were present in the asymmetric unit. All structures were refined anisotropically with various disordered solvent molecules or BF_4^- counterions being modelled over various positions. In the case of [Rh(CgPAmH)(CO)Cl_2] SQUEEZE[3] protocols were utilized due to two severely disordered CH_2Cl_2 solvate molecules whereby a solvent accessible void of 332 Å^3 consisting of 80 e^- was found per asymmetric unit consistent with the inclusion of two CH_2Cl_2 solvent molecules.

2.1 Table 1. Crystallographic refinement data.

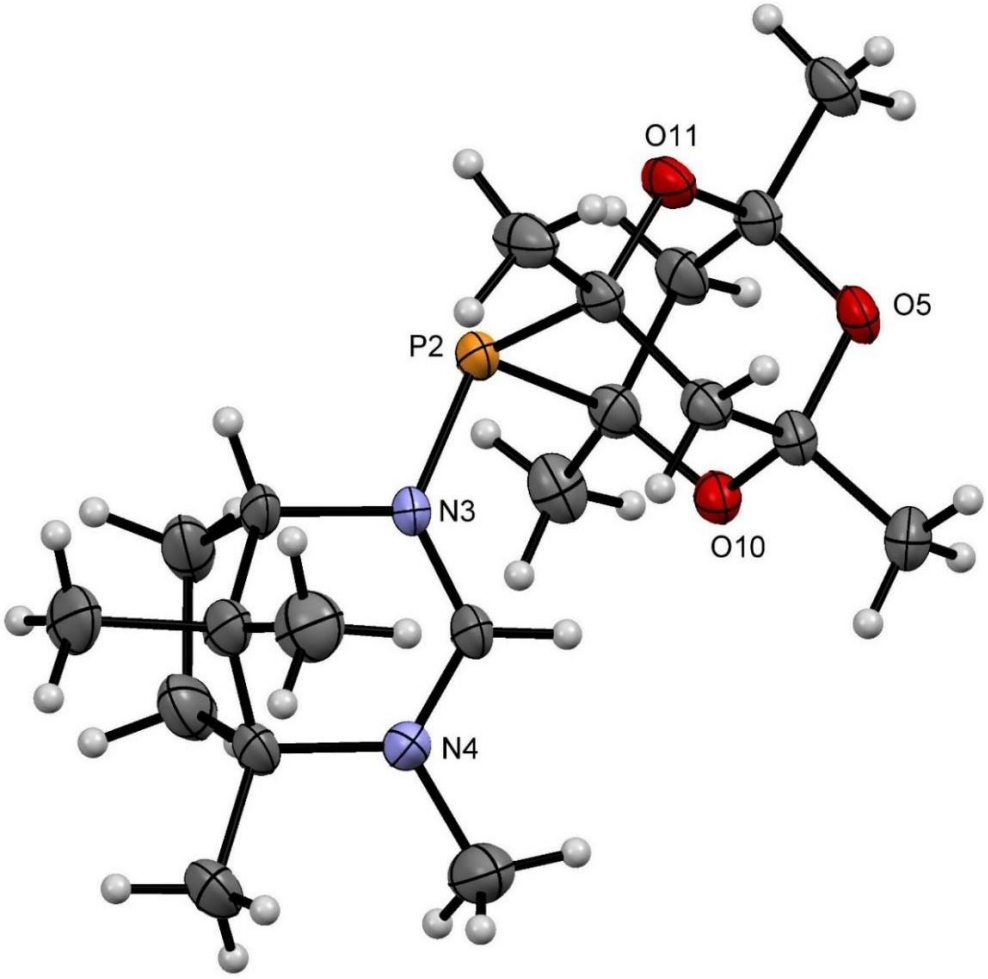
Compound	[α,β-CgPAmMe]BF_4	[α,β-CgP(O)AmMe]BF_4	[Rh(α,β-CgPAm)(acac)(CO)]BF_4
Empirical Formula	$C_{20}H_{34}BF_4N_2O_3P$	$C_{20}H_{34}BF_4N_2O_4P$	$C_{27}H_{43}BCl_2F_4N_2O_6PRh$
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	*P*21	*P*21	*P*21
a/Å	19.4905(5)	14.2214(3)	8.4507(2)
b/Å	7.7502(2)	23.4406(4)	32.6387(6)
c/Å	15.2759(4)	14.2488(2)	12.2306(3)
α/°	90	90	90
β/°	96.808(2)	93.0250(10)	97.379(2)
γ/°	90	90	90
V/Å^3	2291.25(11)	4743.34(14)	3345.50(13)
Z	4	8	4
T /K	150(2)	150(2)	150(2)
D_c/g.cm^{-3}	1.357	1.356	1.555
Crystal size/mm	0.240 x 0.180 x 0.063	0.145 x 0.122 x 0.081	0.171 x 0.142 x 0.102
Total data	15730	15875	29150
Unique data	8248	10088	11751
R_{int}	0.0605	0.0262	0.0368
$R_1[F^2>2\ \sigma(F^2)]$	0.0713	0.0527	0.0279
wR2 (all data)	0.2058	0.1520	0.0594

GoF	1.036	1.041	1.048
$\rho_{min}/\rho_{max}/eÅ^{-3}$	-0.445/1.166	-0.888/0.902	-0.442/0.386
CCDC code	1550609	1550610	1550611

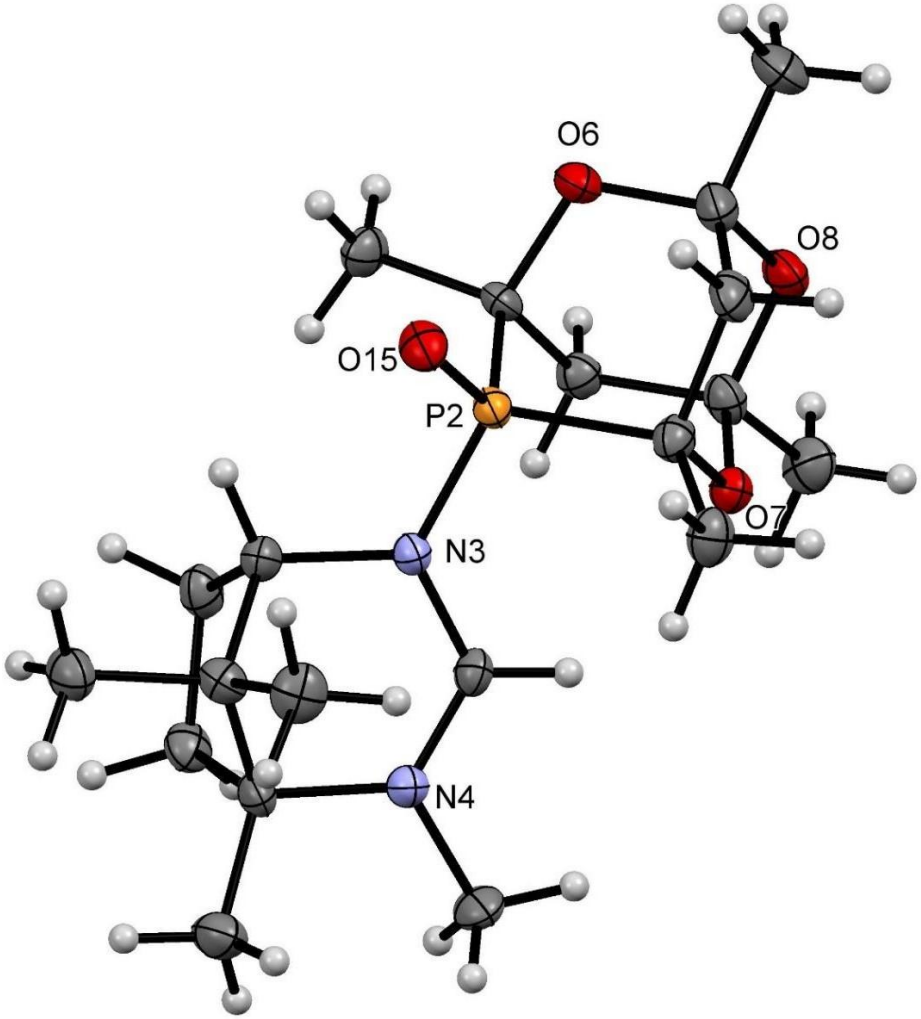
Compound	[Rh(α,β-CgPAmH)(CO)Cl_2]	[Pt(α,β-CgPAmMe)Cl_3]
Empirical Formula	$C_{20}H_{32}Cl_2N_2O_4PRh$	$C_{23}H_{40}Cl_3N_2O_4PPt$
Crystal System	Monoclinic	Monoclinic
Space Group	*C*2	*P*21
a/Å	20.8539(5)	10.2699(4)
b/Å	12.8581(3)	18.0168(6)
c/Å	22.0217(6)	15.4569(5)
α/°	90	90
β/°	103.783(3)	103.602(4)
γ/°	90	90
V/Å^3	5734.9(2)	2779.79(17)
Z	8	4
T /K	150(2)	150(2)
D_c/g.cm^{-3}	1.319	1.771
Crystal size/mm	0.237 x 0.175 x 0.099	0.228 x 0.162 x 0.088
Total data	27505	28866
Unique data	12693	13257
R_{int}	0.0312	0.0521
$R_1[F^2>2\ \sigma(F^2)]$	0.0230	0.0392
wR2 (all data)	0.0547	0.0898
GoF	1.030	1.042
$\rho_{min}/\rho_{max}/eÅ^{-3}$	-0.370/0.325	-1.527/1.674
CCDC code	1550612	1550613

2.2 Thermal ellipsoid plots.

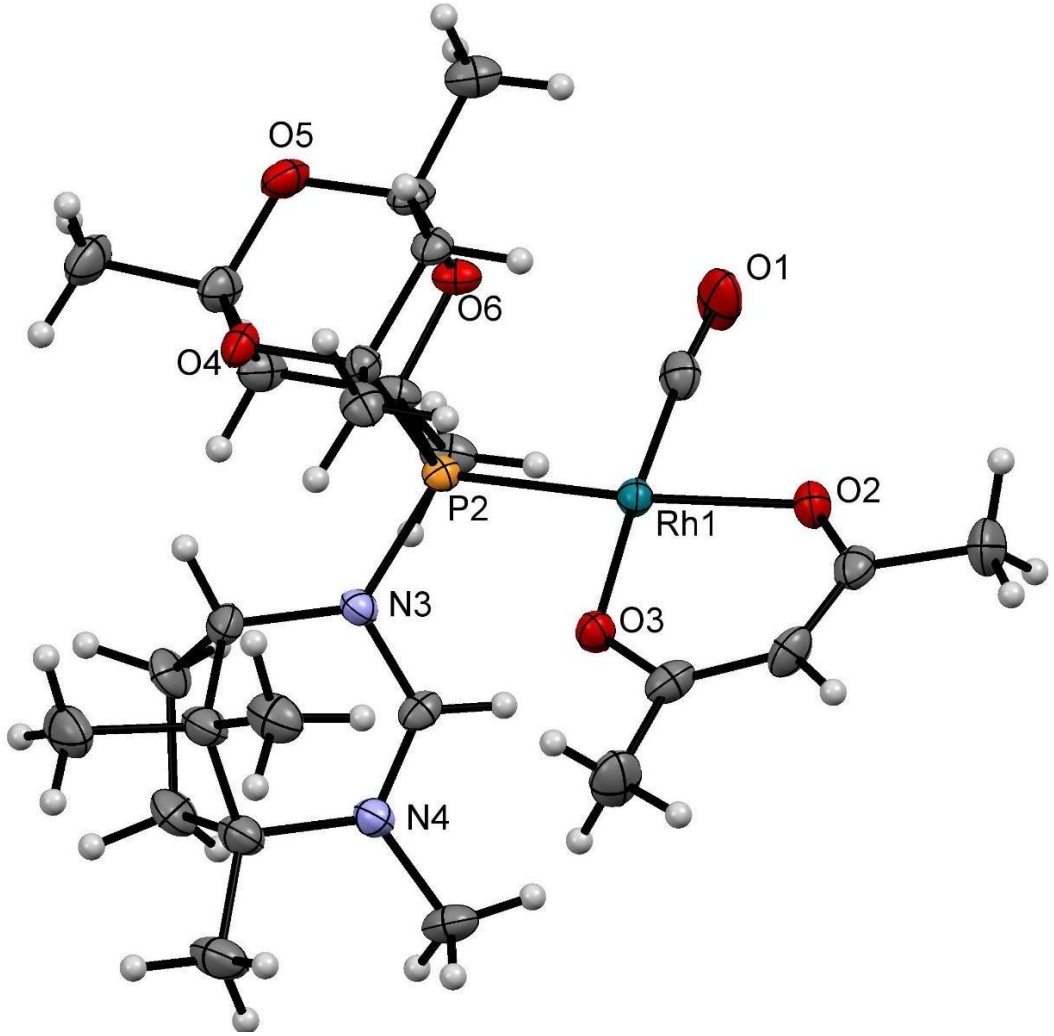
Thermal ellipsoid plot (ellipsoids drawn at 50% probability) of [α,β-CgPAmMe]BF_4. One of two diastereomers in the asymmetric unit with BF_4^- counterion omitted for clarity.



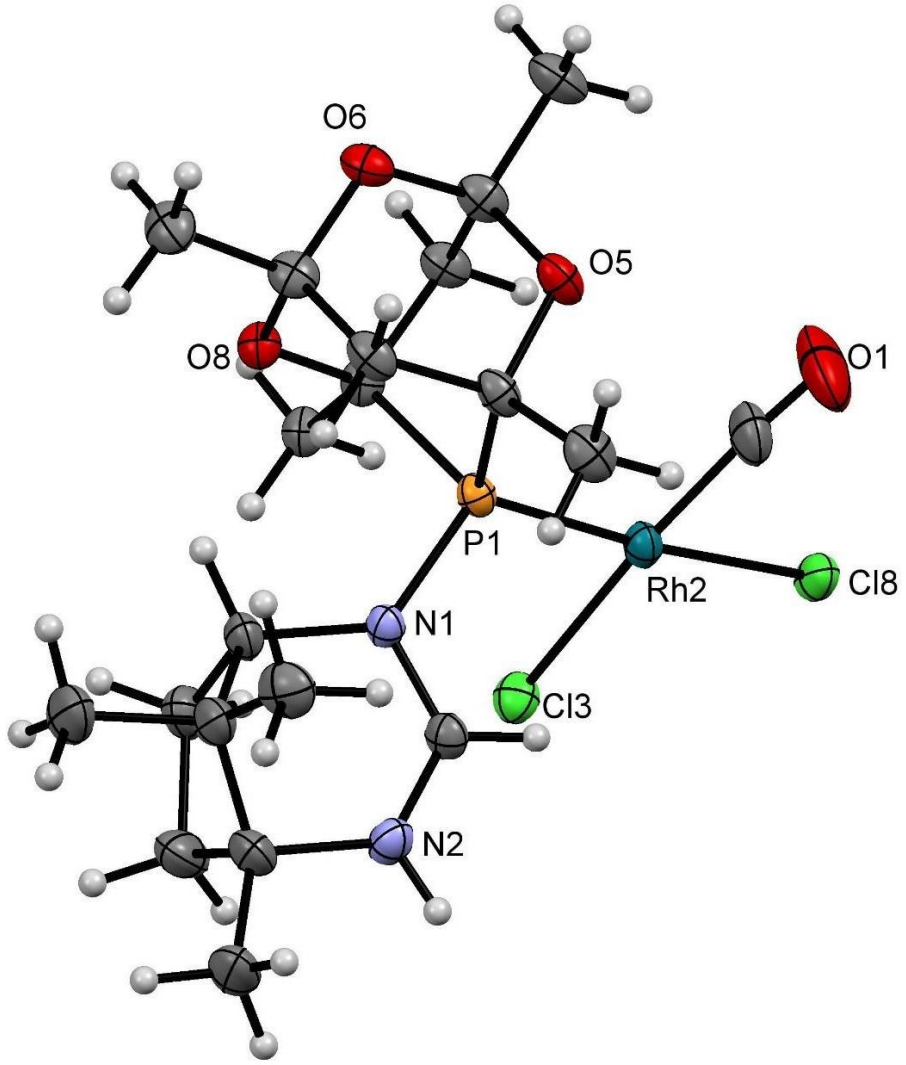
Thermal ellipsoid plot (ellipsoids drawn at 50% probability) of [α,β-CgP(O)AmMe]BF_4. One of four molecules in the asymmetric unit with BF_4^- counterion omitted for clarity.



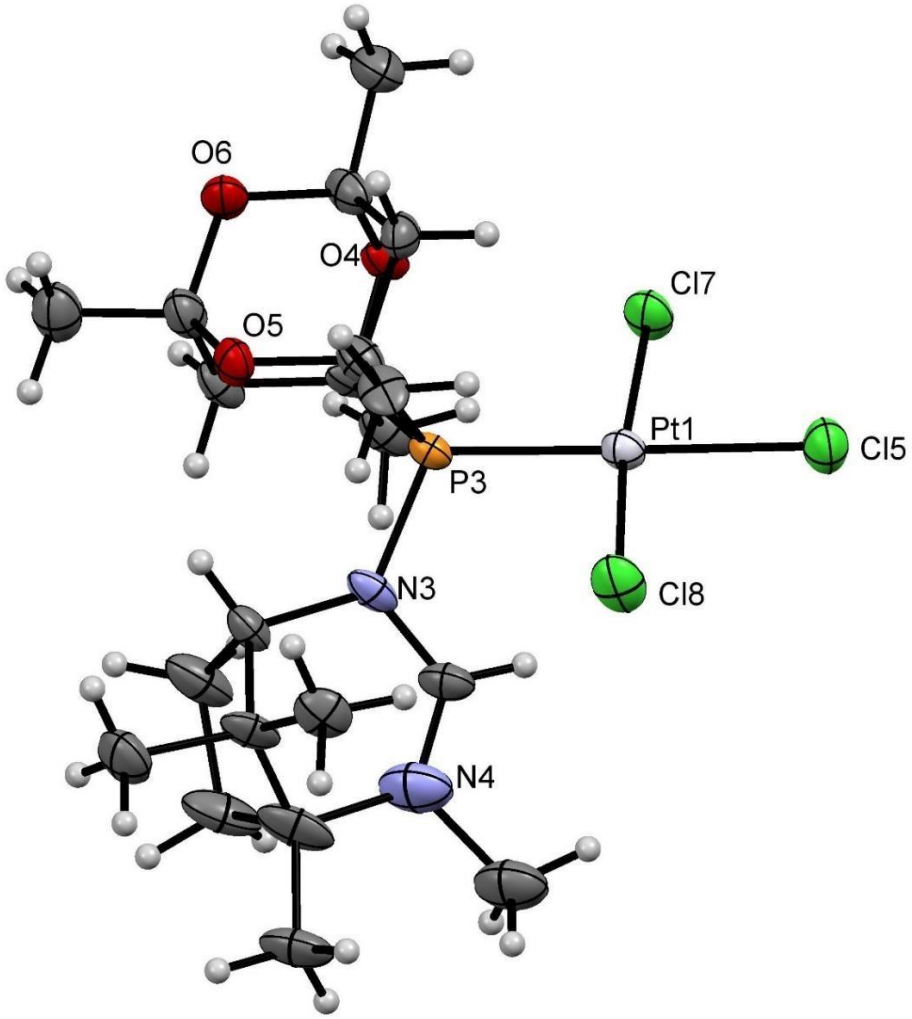
Thermal ellipsoid plot (ellipsoids drawn at 50% probability) of [Rh(α,β-CgPAm)(acac)(CO)]BF_4PAmMe]BF_4. One of two diastereomers in the asymmetric unit with BF_4^- counterion and CH_2Cl_2 solvate molecule omitted for clarity.



Thermal ellipsoid plot (ellipsoids drawn at 50% probability) of [Rh(α,β-CgPAmH)(CO)Cl_2]. One of two diastereomers in the asymmetric unit.



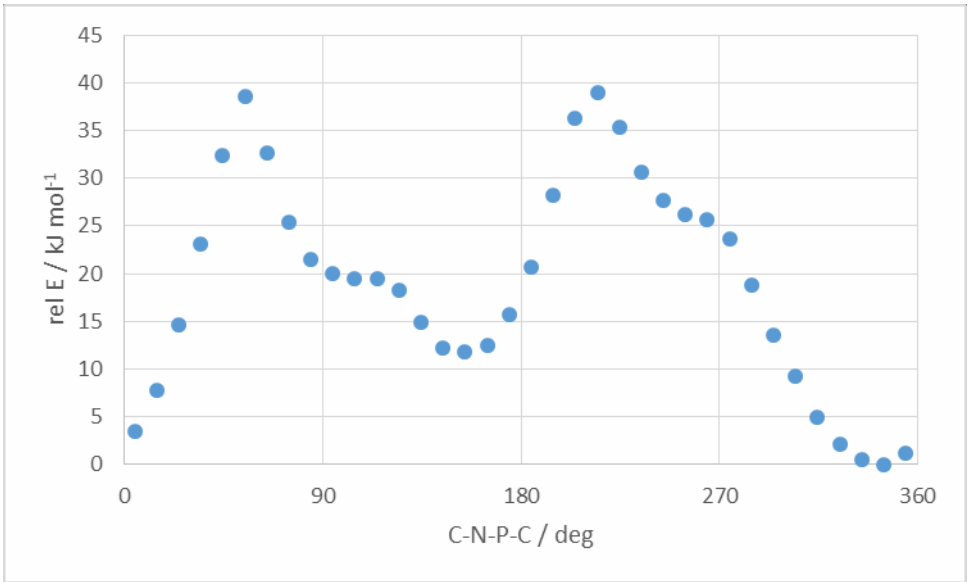
Thermal ellipsoid plot (ellipsoids drawn at 50% probability) of [Pt(α,β-CgPAmMe)Cl_3]. One of two diastereomers in the asymmetric unit. Acetone solvate molecules omitted for clarity.



3. DFT details.

All DFT calculations were performed using the Gaussian09 software,[4] with the B3LYP[5] functional and a basis set consisting of Stuttgart-Dreseden ECP/basis on Pt[6] and 6-31G* on all remaining atoms.[7] All structures were fully geometry optimised without symmetry constraint, and confirmed as minima *via* harmonic frequency calculation. Natural bond orbital (NBO) analysis[8] was also carried out in Gaussian.

3.1 Potential energy surface for P—N rotation in [α,β-CgPAmMe]⁺



3.2 NBO data for [Pt(α,β-CgPAmMe)(Cl)$_3$]

NBO1: Occupancy 1.84 Bond Pt 1 - P 2:

25% Pt: 0.51 (6s), -0.36 (6px), 0.63 (6py), -0.30 (5dxy), 0.18 (5d xz), -0.21 (5d x2-y2), -0.20 (5dz2)

75% P: 0.60 (3s), 0.41 (3px), -0.68 (3py)

Donor NBO	Acceptor NBO	E(2) / kcal/mol	E(j)-E(i) /au	F(i,j) /au
LP (2) Pt	RY*(1) P	11.44	4.03	0.192
LP (2) Pt	RY*(2) P	10.09	2.89	0.153
LP (2) Pt	RY*(3) P	4.77	2.05	0.089
LP (2) Pt	RY*(4) P	3.65	1.67	0.070
LP (2) Pt	RY*(5) P	0.77	1.02	0.025

LP (2) Pt	RY*(6) P	1.40	1.31	0.038
LP (2) Pt	RY*(8) P	1.12	1.32	0.035
LP (2)Pt	RY*(9) P	1.36	1.56	0.041

NBO data for $[Pt(PPh_3)(Cl)_3]$

NBO1: Occupancy 1.82 Bond (1)Pt 1 - P 2

26% Pt 0.51 (6s), 0.71 (6py), 0.46 (5dx2-y2)

74%) P 0.55 (3s), -0.82 (3px), -0.1142 (3py)

Donor NBO	Acceptor NBO	E(2) / kcal/mol	E(j)-E(i) /au	F(i,j) /au
LP (2) Pt	RY*(1) P	11.75	5.61	0.229
LP (2) Pt	RY*(2) P	5.84	1.98	0.096
LP (2) Pt	RY*(3) P	5.59	2.25	0.100
LP (2) Pt	RY*(8) P	0.57	1.20	0.024

Cartesian coordinates for α,β-CgPAm

C	3.42590000	-0.10230000	-0.78710000
C	2.23570000	0.89460000	-0.69350000
N	1.03010000	0.18390000	-0.18320000
C	1.30220000	-0.69500000	0.86850000
N	2.45830000	-0.96420000	1.34810000
C	3.64680000	-0.30160000	0.75320000
C	3.67600000	1.15490000	1.28790000
C	2.71410000	1.93960000	0.34550000
P	-0.47880000	0.44050000	-1.03290000
C	-1.64310000	1.42080000	0.13260000
O	-2.91640000	1.42240000	-0.55780000
C	-3.61780000	0.17810000	-0.59610000
O	-3.77360000	-0.36410000	0.71420000
C	-2.51900000	-0.59320000	1.35350000
C	-1.81670000	0.76410000	1.50370000
C	-2.85650000	-0.85570000	-1.43990000
C	-1.49130000	-1.15710000	-0.79020000
O	-1.72170000	-1.50680000	0.59440000
C	4.87260000	-1.12030000	1.15240000
C	-2.81180000	-1.28010000	2.67390000
C	-5.00780000	0.48940000	-1.11870000
C	-0.82280000	-2.37440000	-1.41760000
C	-1.23490000	2.88290000	0.23070000
C	3.10300000	-1.39060000	-1.55810000
C	4.62270000	0.57180000	-1.49110000
H	0.43070000	-1.20560000	1.27070000

H	1.97550000	1.33760000	-1.65880000
H	4.80930000	-2.14000000	0.75740000
H	4.92520000	-1.19530000	2.24370000
H	5.79980000	-0.66240000	0.79200000
H	-1.15380000	3.32850000	-0.76590000
H	-0.27160000	2.98350000	0.74010000
H	-1.98870000	3.44030000	0.79910000
H	-1.88040000	-1.47900000	3.21210000
H	-3.32260000	-2.22760000	2.48320000
H	-3.45450000	-0.64560000	3.29020000
H	-2.44710000	1.40460000	2.13310000
H	-0.84990000	0.64700000	2.00330000
H	-4.94340000	0.92390000	-2.12030000
H	-5.49180000	1.20610000	-0.45010000
H	-5.60860000	-0.42330000	-1.15820000
H	-2.73340000	-0.49170000	-2.46500000
H	-3.44240000	-1.78250000	-1.46790000
H	0.12280000	-2.61020000	-0.92210000
H	-0.62600000	-2.20030000	-2.48030000
H	-1.48320000	-3.24350000	-1.31910000
H	4.69160000	1.56610000	1.25910000
H	3.34950000	1.17420000	2.33170000
H	1.86500000	2.37130000	0.88170000
H	3.22950000	2.76760000	-0.15290000
H	2.75150000	-1.15320000	-2.56990000
H	2.34150000	-1.99900000	-1.06830000
H	4.00260000	-2.00840000	-1.66150000
H	4.94970000	1.49830000	-1.01170000
H	4.36150000	0.81150000	-2.52970000
H	5.48330000	-0.10500000	-1.52080000

Cartesian coordinates for α,β-CgPAmMe

P	-0.697234	-1.098536	0.636052
N	0.895559	-0.406215	0.083633
N	2.401490	1.349695	-0.278898
C	1.178495	0.879849	-0.090871
H	0.352052	1.584456	-0.052187
C	2.050116	-1.354979	-0.025728
H	1.723280	-2.304512	0.401202
C	3.593944	0.402608	-0.314121
C	2.574547	2.775139	-0.589522
H	3.233312	3.251533	0.138856
H	1.601933	3.269331	-0.560120
H	2.998746	2.898228	-1.590682
C	4.888945	1.164035	-0.049927
H	4.883621	1.666069	0.922561
H	5.095932	1.907537	-0.824853

H	5.721872	0.457388	-0.057233
C	-2.521401	1.263589	-0.770649
C	-3.768428	-0.407638	0.353512
C	-1.610496	0.421011	1.347275
C	-1.807234	-1.143187	-0.925067
C	-1.454792	-2.312081	-1.833566
H	-1.458696	-3.252299	-1.274270
H	-0.468892	-2.174949	-2.289797
H	-2.197423	-2.386934	-2.635282
C	-2.704327	2.607561	-1.447082
H	-1.739072	3.016672	-1.760735
H	-3.178300	3.303332	-0.750433
H	-3.344000	2.495500	-2.326185
O	-3.095582	-1.454402	-0.366610
O	-1.708850	1.508100	0.402478
O	-3.806185	0.796663	-0.406537
C	-1.867867	0.196524	-1.660772
H	-2.486699	0.077088	-2.557508
H	-0.871501	0.512161	-1.988468
C	-5.197453	-0.871436	0.545587
H	-5.216483	-1.807857	1.109516
H	-5.658981	-1.034571	-0.431355
H	-5.768279	-0.112241	1.086408
C	-3.025967	-0.103653	1.660347
H	-2.985710	-0.995869	2.293776
H	-3.570397	0.678082	2.201947
C	-0.944064	0.986886	2.597013
H	0.057585	1.378573	2.396823
H	-0.864544	0.217157	3.370828
H	-1.551992	1.810851	2.984745
C	3.539112	-0.309809	-1.689293
H	4.526348	-0.699768	-1.951981

H	3.257719	0.387778	-2.483983
C	2.498806	-1.458298	-1.502507
H	1.648848	-1.364341	-2.182586
H	2.948254	-2.436655	-1.691817
C	3.276270	-0.745421	0.705014
C	3.001890	-0.283408	2.145042
H	2.671499	-1.131798	2.753949
H	2.241444	0.496430	2.223530
H	3.918342	0.103726	2.602115
C	4.409218	-1.795277	0.763866
H	4.736253	-2.153212	-0.215192
H	4.067698	-2.664669	1.336026
H	5.284432	-1.393512	1.282517

Cartesian coordinates for [Pt(CgPAmMe)$(Cl)_3$]

Pt	1.487279	-1.538286	0.060550
P	0.357845	0.433122	-0.079263
Cl	2.601060	-3.591570	0.309818
Cl	3.097053	-0.981228	-1.570151
Cl	-0.069890	-2.308895	1.738029
O	1.523635	4.018389	0.283526
O	2.124864	2.170854	-1.052097
O	-0.262942	2.798244	1.227020
N	-2.947850	-1.642742	-0.743852
C	2.031889	1.966530	1.387437
H	2.256848	2.526518	2.302363
H	2.645683	1.060580	1.373460
C	0.758245	1.287169	-2.790271
H	1.439505	0.441382	-2.900090
H	1.079942	2.092667	-3.460135
H	-0.254565	0.983344	-3.080091
N	-1.421221	0.085833	-0.298710

C	-0.095838	3.059272	-1.185042
H	-1.156296	2.851481	-1.329630
H	0.211734	3.771464	-1.959877
C	0.775019	1.802529	-1.357012
C	0.529079	1.607103	1.409905
C	0.148576	3.701211	0.184337
C	-4.867381	1.234176	0.972171
H	-5.656014	0.736612	1.545261
H	-5.331885	1.696567	0.097336
H	-4.470750	2.038184	1.601907
C	-1.720110	-1.172964	-0.623663
H	-0.890361	-1.850945	-0.801973
C	3.795131	3.326336	0.138401
H	3.935849	3.982364	-0.724685
H	4.460027	2.464006	0.043398
H	4.038644	3.878455	1.050308
C	-0.625949	4.987137	0.409738
H	-0.384532	5.384500	1.398987
H	-1.702914	4.801668	0.353592
H	-0.349348	5.726049	-0.347238
C	2.354573	2.857531	0.182084
C	-3.324321	-0.449744	1.949866
H	-3.108712	0.306647	2.711994
H	-2.447113	-1.095023	1.866399
H	-4.156648	-1.051765	2.332097
C	0.119009	1.020937	2.751755
H	-0.949774	0.802453	2.782115
H	0.343334	1.758300	3.530812
H	0.657514	0.093212	2.955103
C	-2.592808	1.000388	-0.101821
H	-2.238543	1.867811	0.451583
C	-3.731847	0.238837	0.638779

C	-4.140976	-0.741153	-0.512133
C	-3.218161	1.327495	-1.483947
H	-3.713873	2.302480	-1.454047
H	-2.456311	1.380073	-2.264086
C	-5.398926	-1.564550	-0.248495
H	-5.669141	-2.185361	-1.107966
H	-6.235790	-0.886127	-0.064810
H	-5.292691	-2.212570	0.626633
C	-4.243492	0.182405	-1.752213
H	-4.021340	-0.370100	-2.670291
H	-5.261683	0.569238	-1.855501
C	-3.120195	-3.038176	-1.169635
H	-3.679099	-3.600453	-0.419223
H	-2.137691	-3.498104	-1.282754
H	-3.649262	-3.083722	-2.126862

Cartesian coordinates for $[Pt(PPh3)(Cl)_3]$

Pt	5.203767	12.335262	13.344627
P	4.362318	13.741620	11.768409
Cl	5.989670	10.847995	15.039451
Cl	7.461459	12.719226	12.718488
Cl	2.955228	11.859969	14.041139
C	5.509842	14.413241	10.479971
C	6.557609	15.258892	10.882900
C	5.380132	14.101353	9.120450
C	7.435529	15.794939	9.942995
H	6.692086	15.486943	11.934413
C	6.269337	14.631260	8.180455
H	4.582963	13.445498	8.787302
C	7.295334	15.482389	8.588134
H	8.241752	16.445116	10.273167
H	6.153016	14.376964	7.129481

H	7.986479	15.896011	7.857252
C	3.611443	15.301583	12.437777
C	3.482295	16.458621	11.650303
C	3.162838	15.334104	13.767452
C	2.907278	17.617297	12.175629
H	3.843954	16.461474	10.626496
C	2.589172	16.495749	14.288907
H	3.256062	14.444603	14.381569
C	2.458645	17.638183	13.497659
H	2.817480	18.504102	11.552331
H	2.248448	16.503946	15.321197
H	2.015635	18.542191	13.909514
C	3.020798	12.969670	10.753099
C	1.978458	13.706264	10.174365
C	3.084453	11.586201	10.526594
C	1.022811	13.074335	9.375804
H	1.901734	14.773972	10.354314
C	2.134294	10.958442	9.720321
H	3.867557	11.007165	11.007095
C	1.100962	11.700078	9.143647
H	0.214545	13.657391	8.940307
H	2.193301	9.885035	9.559379
H	0.354637	11.207820	8.524257

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