Bulky *N*-Phosphinomethyl-Functionalized *N*-Heterocyclic Carbene (NHCP) Chelate Ligands: Synthesis, Molecular Geometry, Electronic Structure and their Ruthenium Alkylidene Complexes

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Supporting Information

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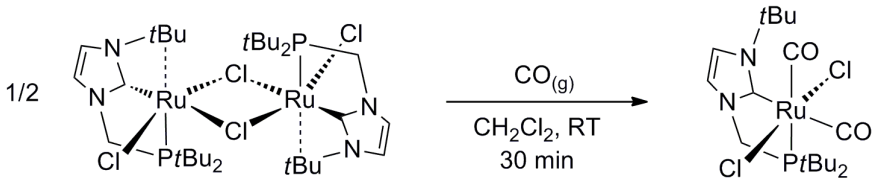
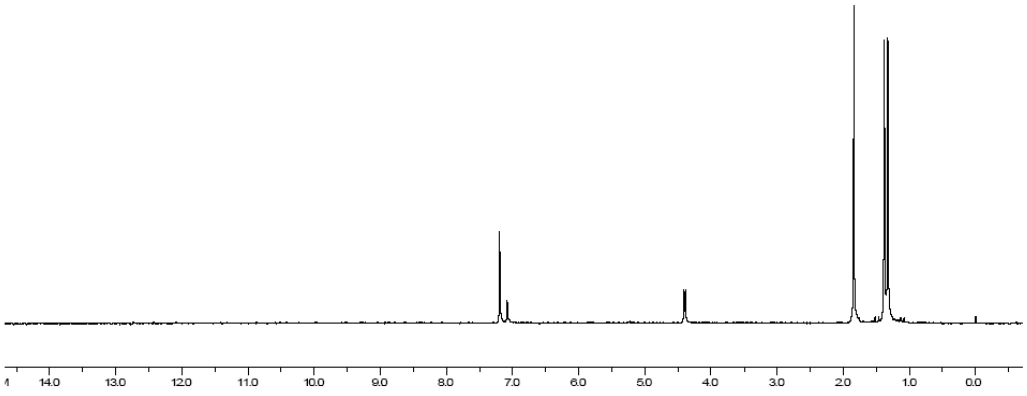
1. Synthesis of A

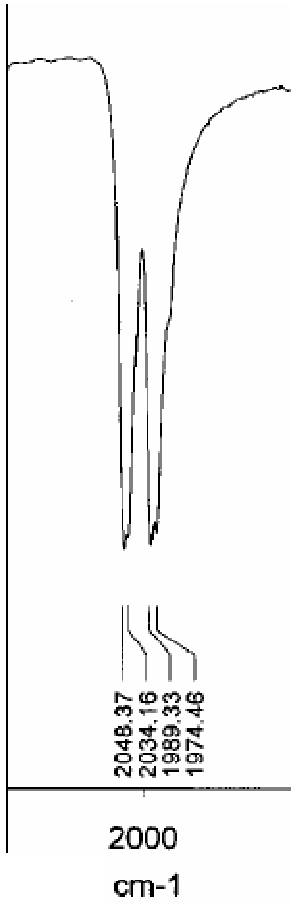


Complex **6** (43.0 mg, 47.3 μmol) was dissolved in dichloromethane (10 mL) in a Schlenk tube and cooled to liquid nitrogen temperature under vacuum and then filled up with CO(g). This procedure was repeated three times, then the system was allowed to warm up to room temperature under the CO(g) atmosphere. After 30 minutes of reaction the color had changed from green to yellow and the CO atmosphere was replaced by argon. The solvent was evaporated to a volume of ca. 1 mL and pentane (10 mL) was added furnishing a precipitate, which was washed with pentane (3 x 10 mL) and dried in vacuum to yield a yellow solid in 73 % yield (35.2 mg). Crystals suitable for X-ray diffraction were obtained from a solution of A in benzene by slow evaporation of the solvent. Mp: 163 °C. ^{1}H NMR (250.1 MHz, $CDCl_3$): 7.19 (s, 1H, N(C*H*)$_2$N), 7.07 (d, $^{3}J_{H,H}$ = 2.0 Hz, 2H, N(C*H*)$_2$N), 4.40 (d, $^{2}J_{H,H}$ = 5.36 Hz, 2H, N(CH_2)P), 1.84 (s, 9H, N-*s*Bu), 1.35 (d, $^{3}J_{H,P}$ = 13.1 Hz). ^{31}P{^{1}H} NMR (101.2 MHz, $CDCl_3$): 65.8 (s). MS (FAB+), m/z (%): 447,2 (75) $[M-Cl-CO]^+$; 412,2 (5) $[M-2Cl-CO]^+$; 383,2 (10) $[M-2Cl-2CO]^+$. IR (KBr), ν(CO) = 2048.37, 1989.33 cm^{-1} and 2034.16, 1974.46 cm^{-1}. Anal. Calcd. for $C_{18}H_{32}Cl_2N_4O_2PRu$: C, 42.07; H, 6.15; N, 5.47; P, 6.06. Found: C, 42.27; H, 6.13; N, 5.48; P, 6.06.

X-ray diffraction parameters. Yellow crystals (polyhedron), 0.17 x 0.14 x 0.14 mm^3, monoclinic, $P2_1/c$, Z=1, a=17.733(3) Å, b=18.438(3) Å, c=14.015(2) Å, α=90°, β=90.649(3)°, γ=90°, V=4582.3(12) Å^3, ρ=1.48 g/cm^3, T=200(2) K, θ_{max}= 28.4°, 48201 reflections measured, 11436 unique (R_{int}=0.0323), 10329 observed (I >2σ(I)), μ=1.00 mm^{-1}, T_{min}=0.77, T_{max}=0.84, 487 parameters refined, goodness of fit 1.03 for observed reflections, final residual values R1(F)=0.026, wR(F^2)=0.066 for observed reflections, residual electron density −0.59 to 0.75 eÅ^{-3}.



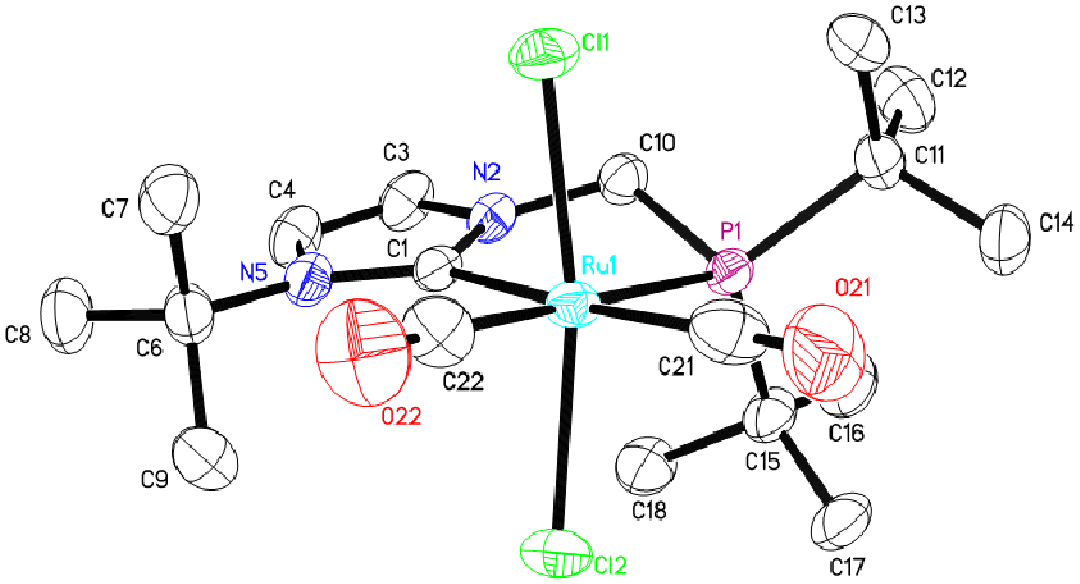
^{1}H NMR spectrum of *trans*-[$RuCl_2$($^{t\text{Bu}}$NHCP$^{t\text{Bu}}$)$(CO)_2$] in $CDCl_3$.



Solid state IR spectrum of *trans*-[$RuCl_2$($^{t\text{Bu}}$NHCP$^{t\text{Bu}}$)$(CO)_2$] **A** (KBr), CO region

As expected, single crystal X-ray diffraction analysis reveals a somewhat distorted octahedral ruthenium(II)- $^{t\text{Bu}}$NHCP$^{t\text{Bu}}$ complex with the chloro ligands *trans* to each other and the $^{t\text{Bu}}$NHCP$^{t\text{Bu}}$

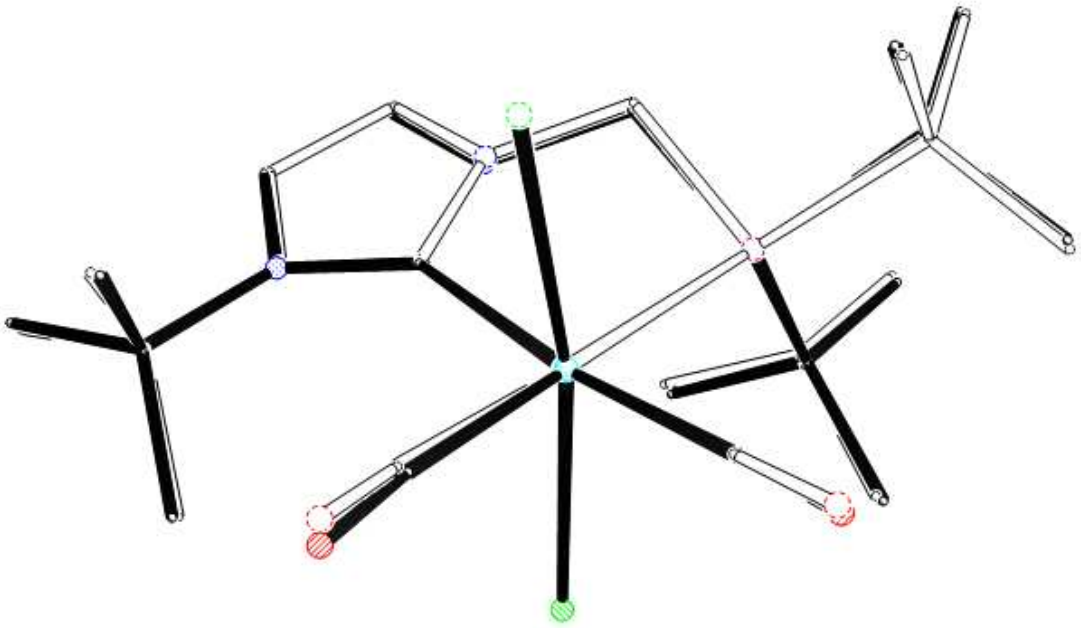
ligand coplanar with the two *cis* CO ligands. The two Ru-C_{CO} distances Ru-C21 and Ru-C22 are equal, of the two carbonyl C-O bond lengths the one *trans* to the NHC-unit is somewhat shorter than the one opposite to the *t*Bu_2P ligand arm, indicative of the NHC exerting the weaker *trans*-influence.



ORTEP plot of **A**. Thermal ellipsoids are at 50 % probability level. Most hydrogen atoms are omitted for clarity. Selected bond lengths and angles:

Ru1-Cl1	2.4137(6)	C22-Ru1-Cl1	86.21(7)
Ru1-Cl2	2.4166(6)	C21-Ru1-Cl2	89.15(7)
Ru1-P1	2.4521(6)	C22-Ru1-Cl2	84.85(7)
Ru1-C1	2.1649(18)	C1-Ru1-Cl2	93.23(5)
Ru1-C21	1.924(2)	Cl1-Ru1-Cl2	169.44(2)
Ru1-C22	1.924(2)	C21-Ru1-P1	91.50(8)
C21-O21	1.087(3)	C22-Ru1-P1	178.10(7)
C22-O22	1.127(3)	C1-Ru1-P1	80.42(5)
C21-Ru1-C22	86.88(10)	Cl1-Ru1-P1	92.98(2)
C21-Ru1-C1	171.77(9)	Cl2-Ru1-P1	96.12(2)
C22-Ru1-C1	101.17(8)	O21-C21-Ru1	178.1(2)
C21-Ru1-Cl1	95.96(7)	O22-C22-Ru1	173.1(2)

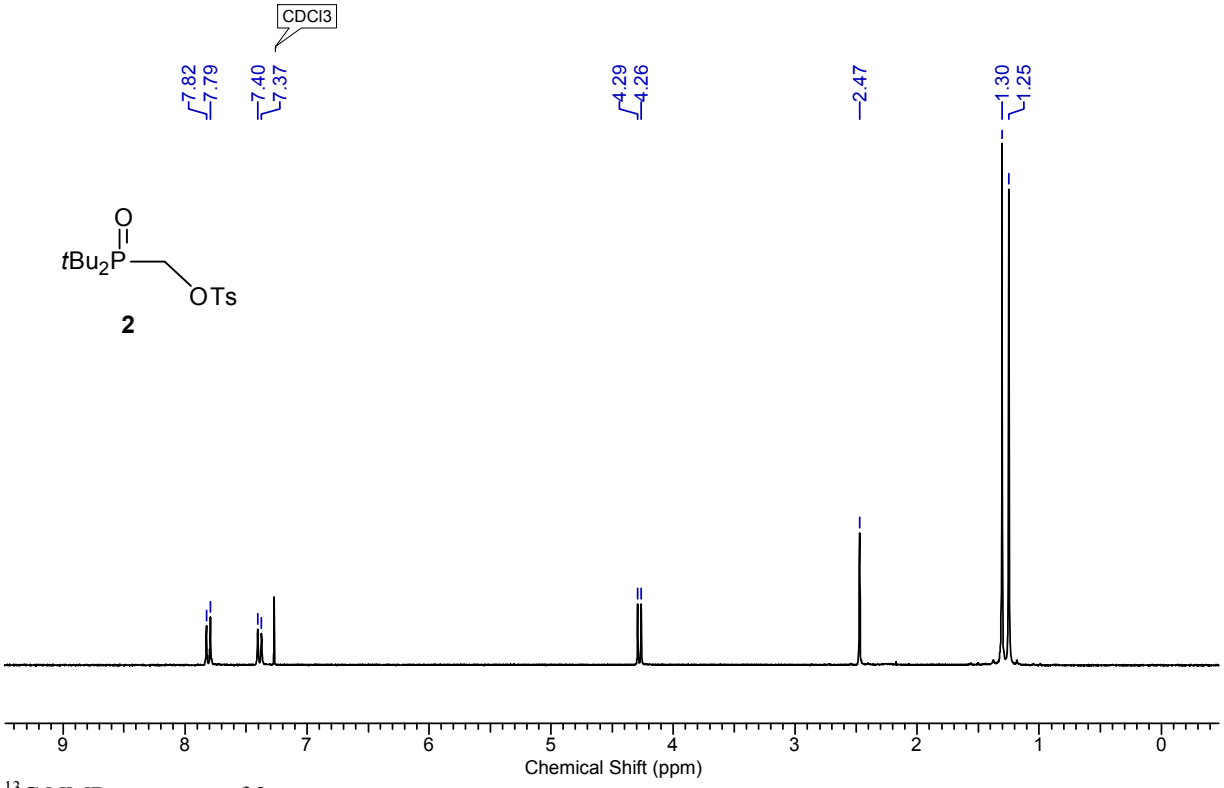
The X-ray crystal structure can account for the observed two sets of bands for the ν(CO) stretching frequencies in the solid state IR spectrum (KBr) by revealing two independent molecules in the unit cell. A superposition of their molecular structures is shown here:



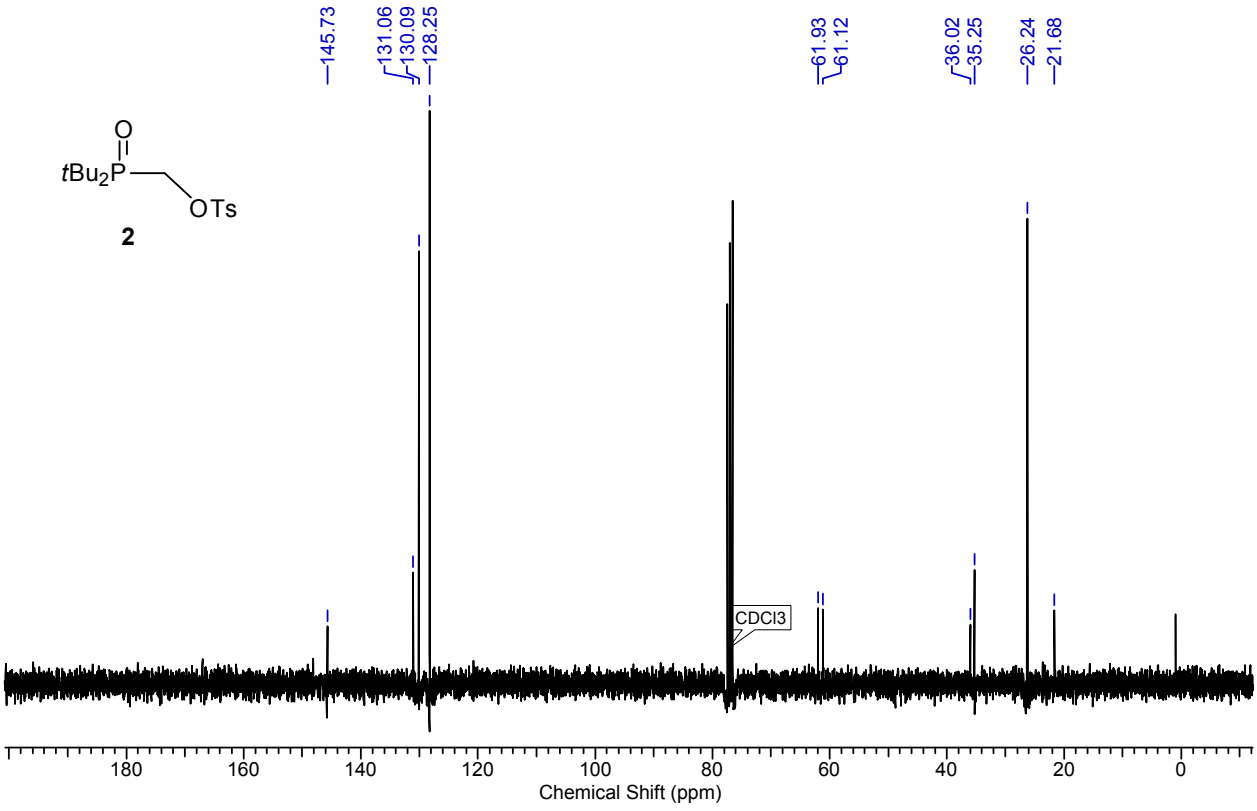
Although the differences in bond lengths and angles are subtle, the different environments of the molecules in the crystal lattice can explain the two sets of signals in the IR spectrum.

2. NMR spectra

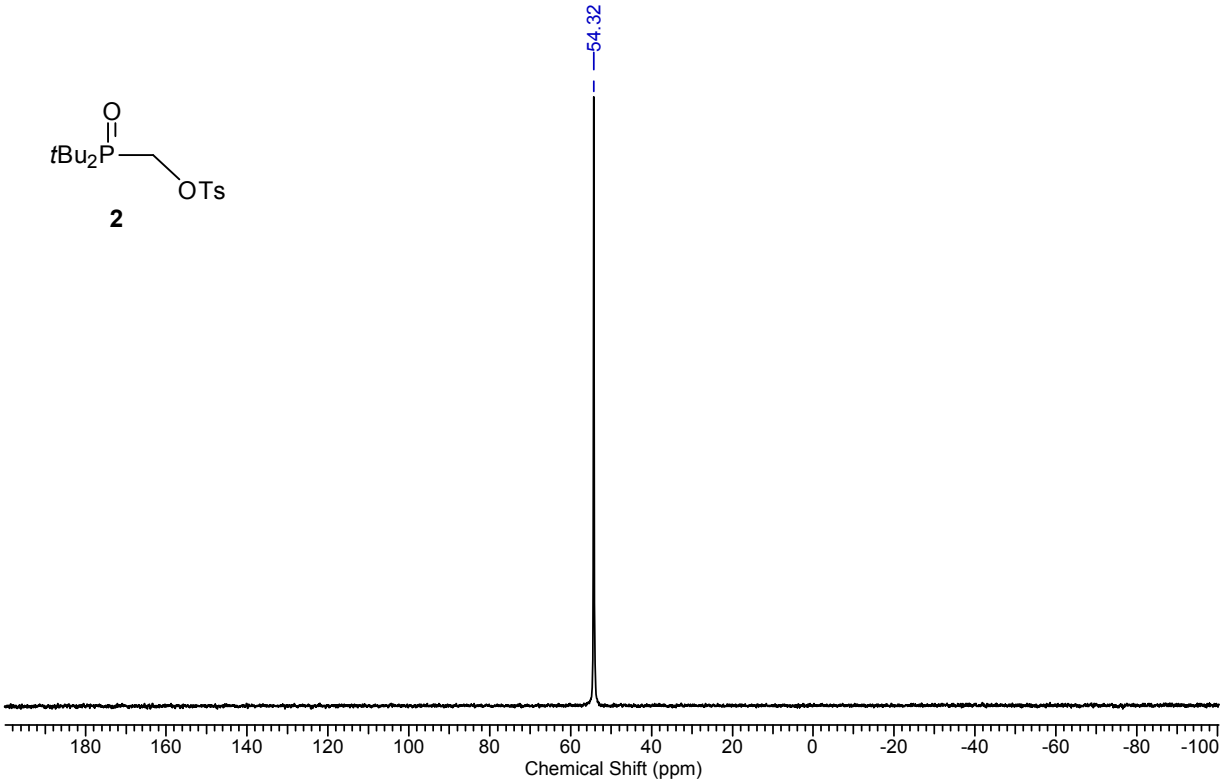
^{1}H NMR spectrum of **2**



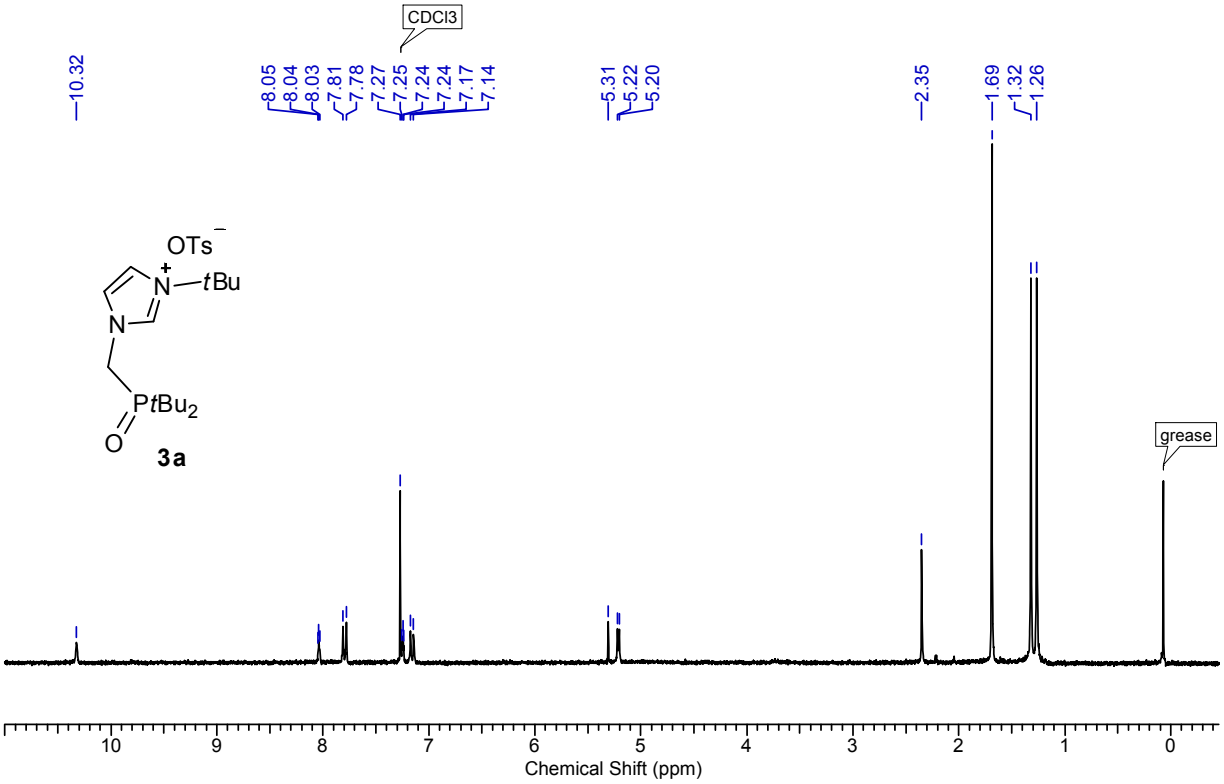
^{13}C NMR spectrum of **2**



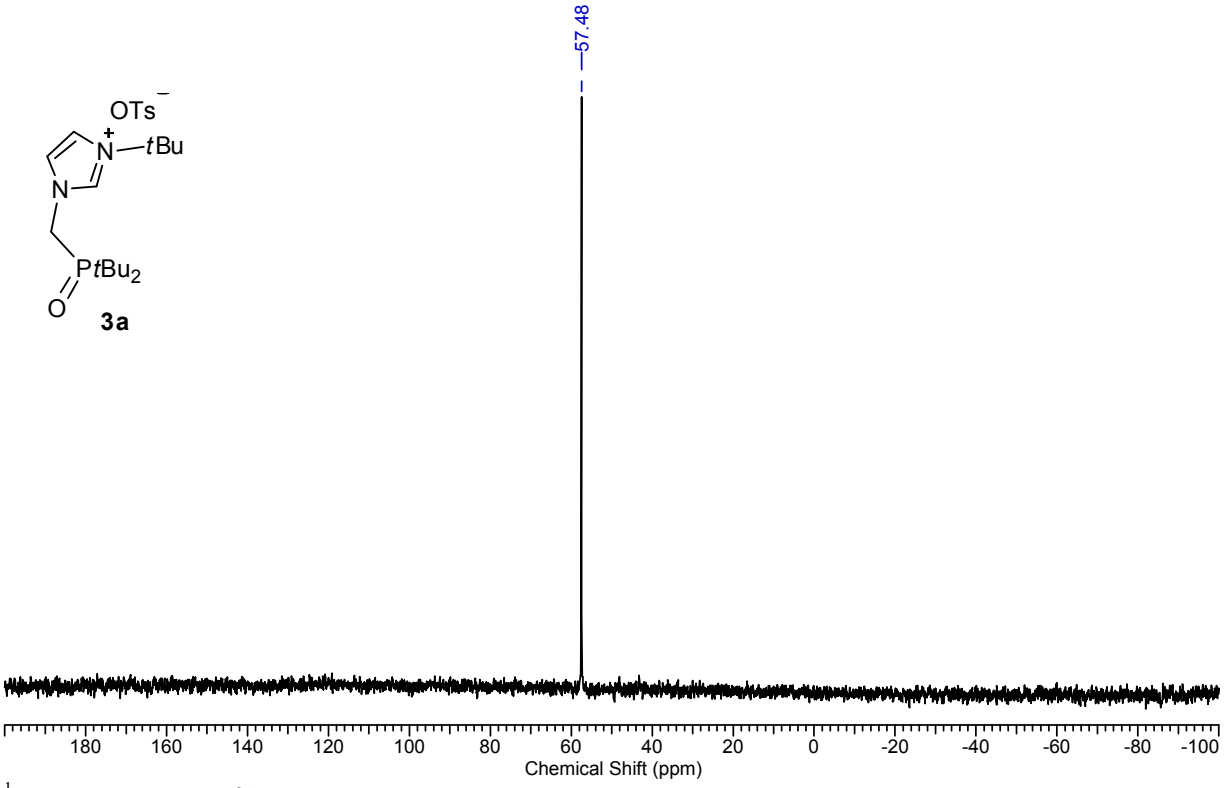
^{31}P NMR spectrum of **2**



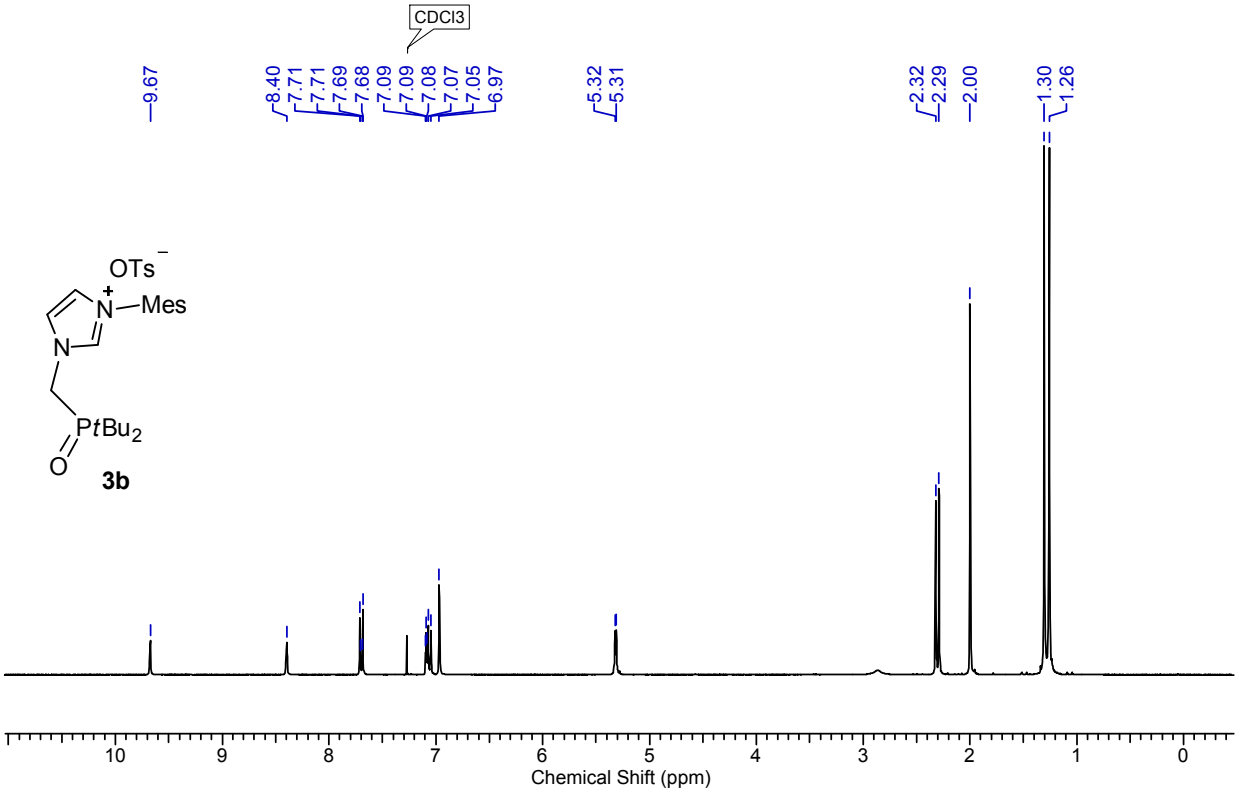
^{1}H NMR spectrum of **3a**



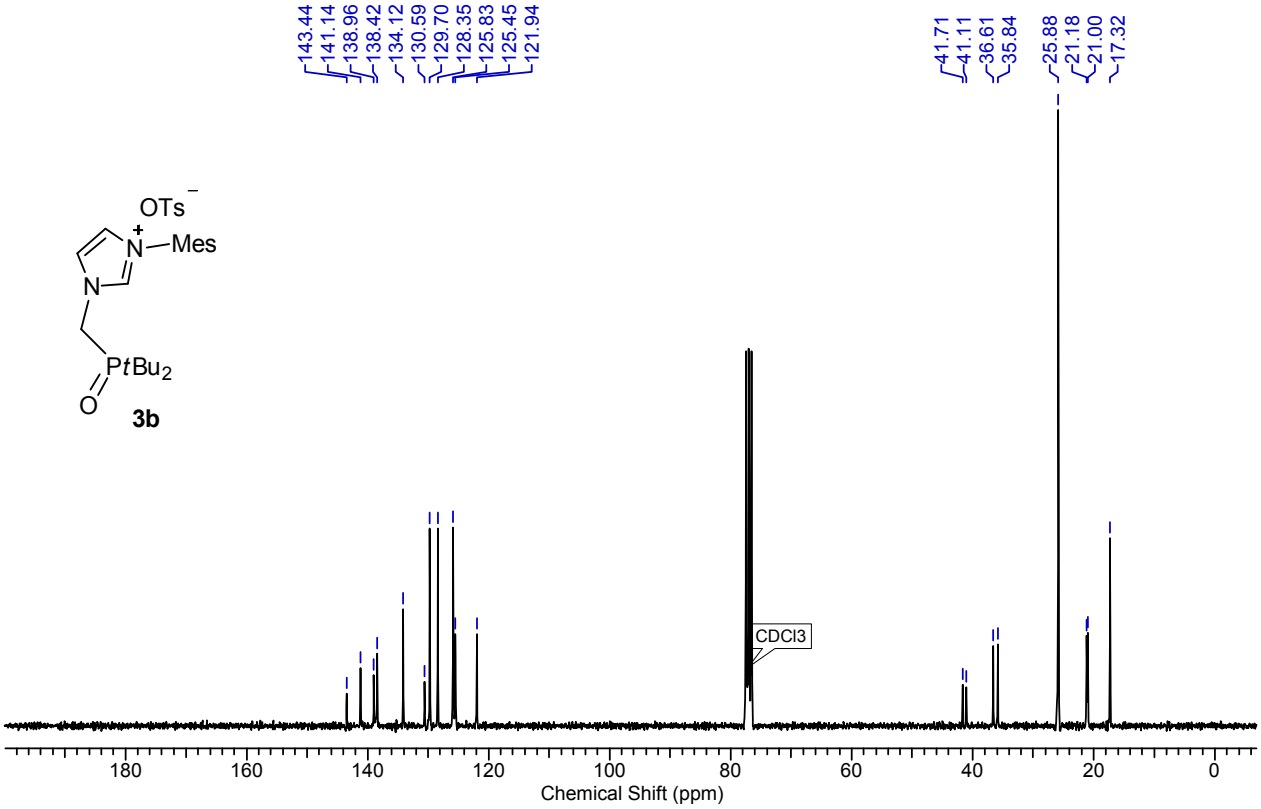
^{31}P NMR spectrum of **3a**



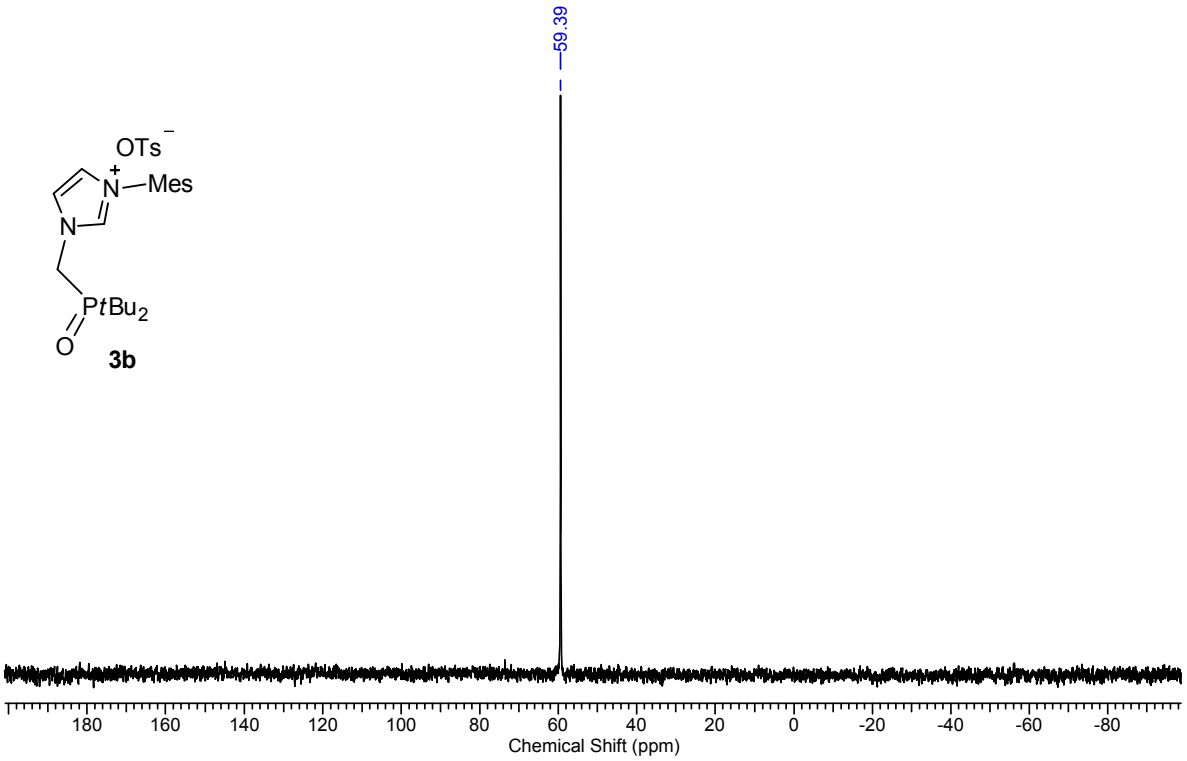
^{1}H NMR spectrum of **3b**



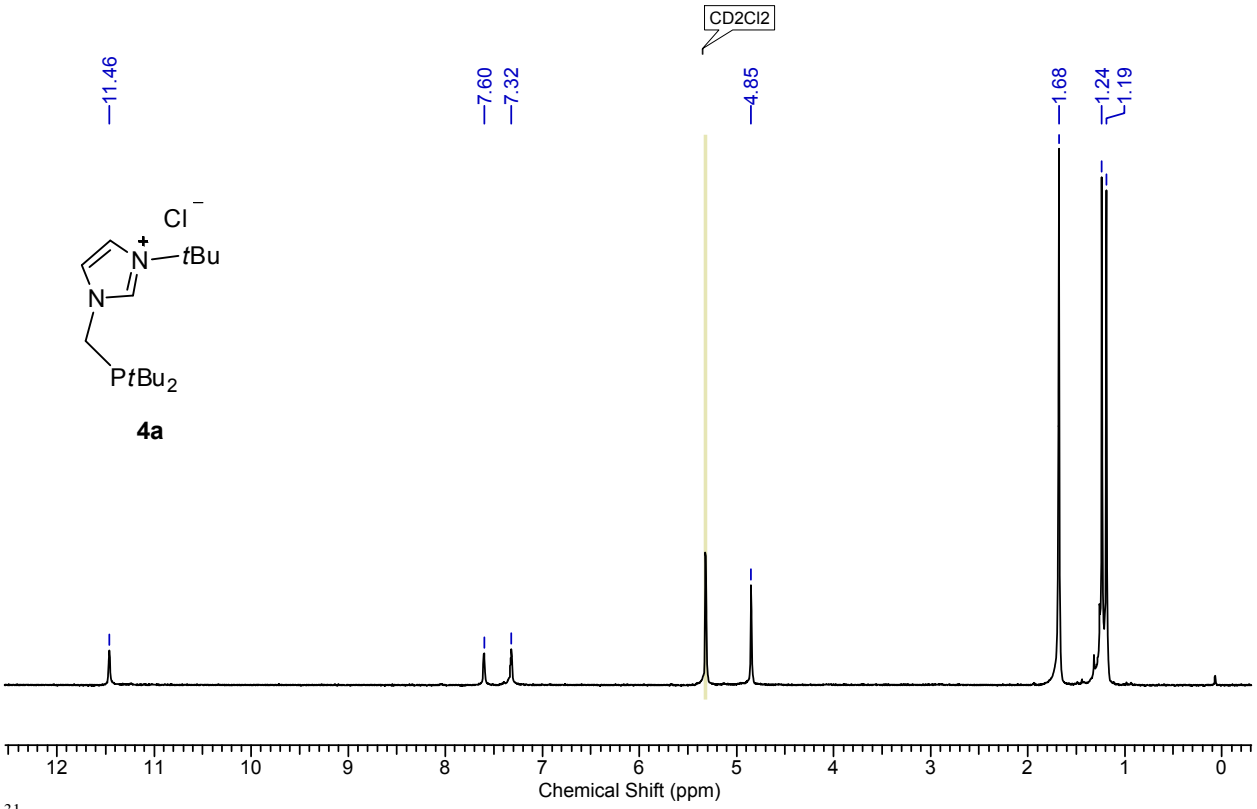
^{13}C NMR spectrum of **3b**



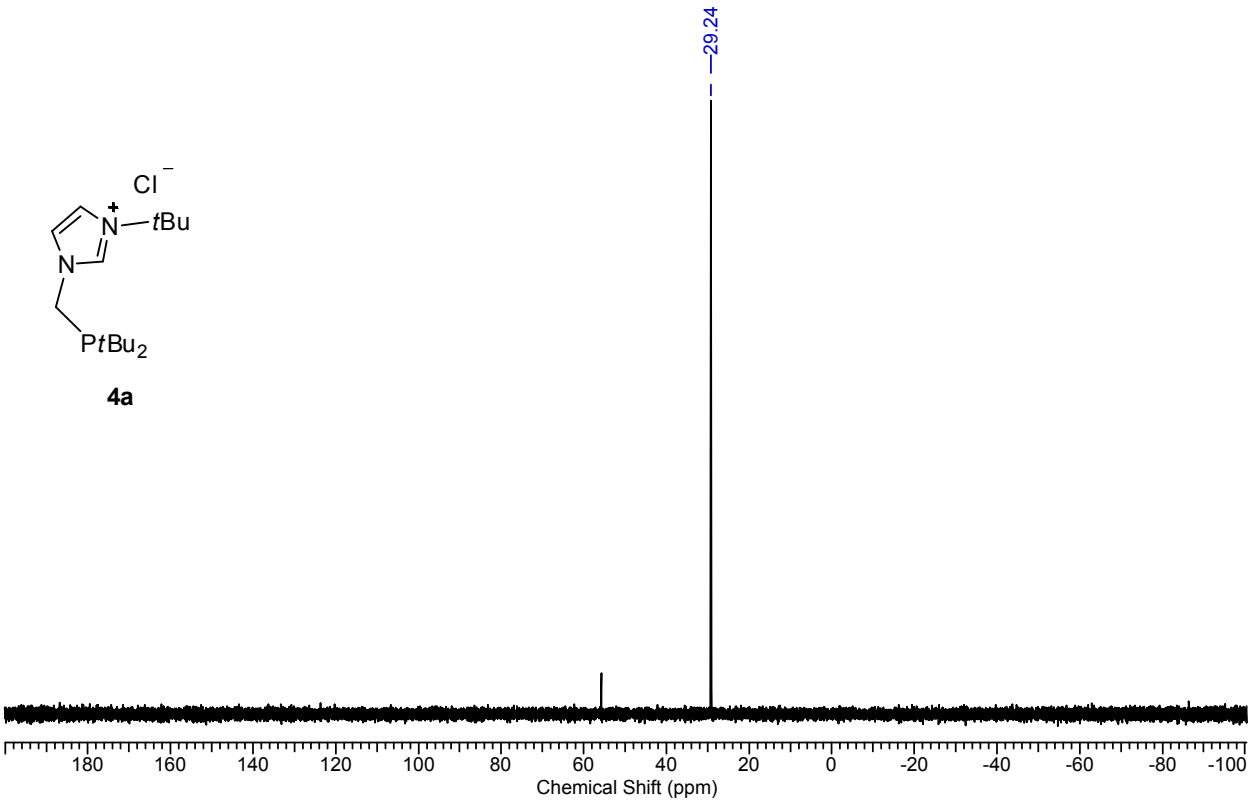
^{31}P NMR spectrum of **3b**



^{1}H NMR spectrum of **4a**



^{31}P NMR spectrum of **4a**



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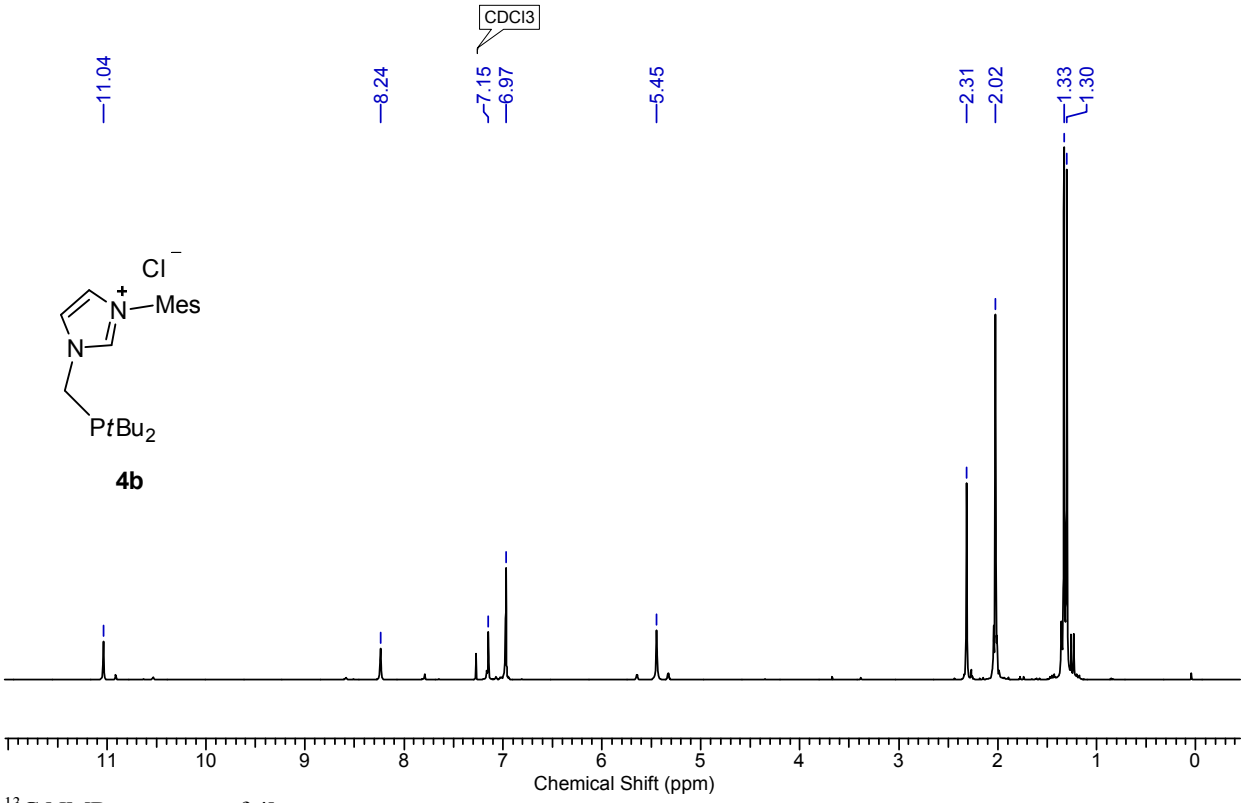

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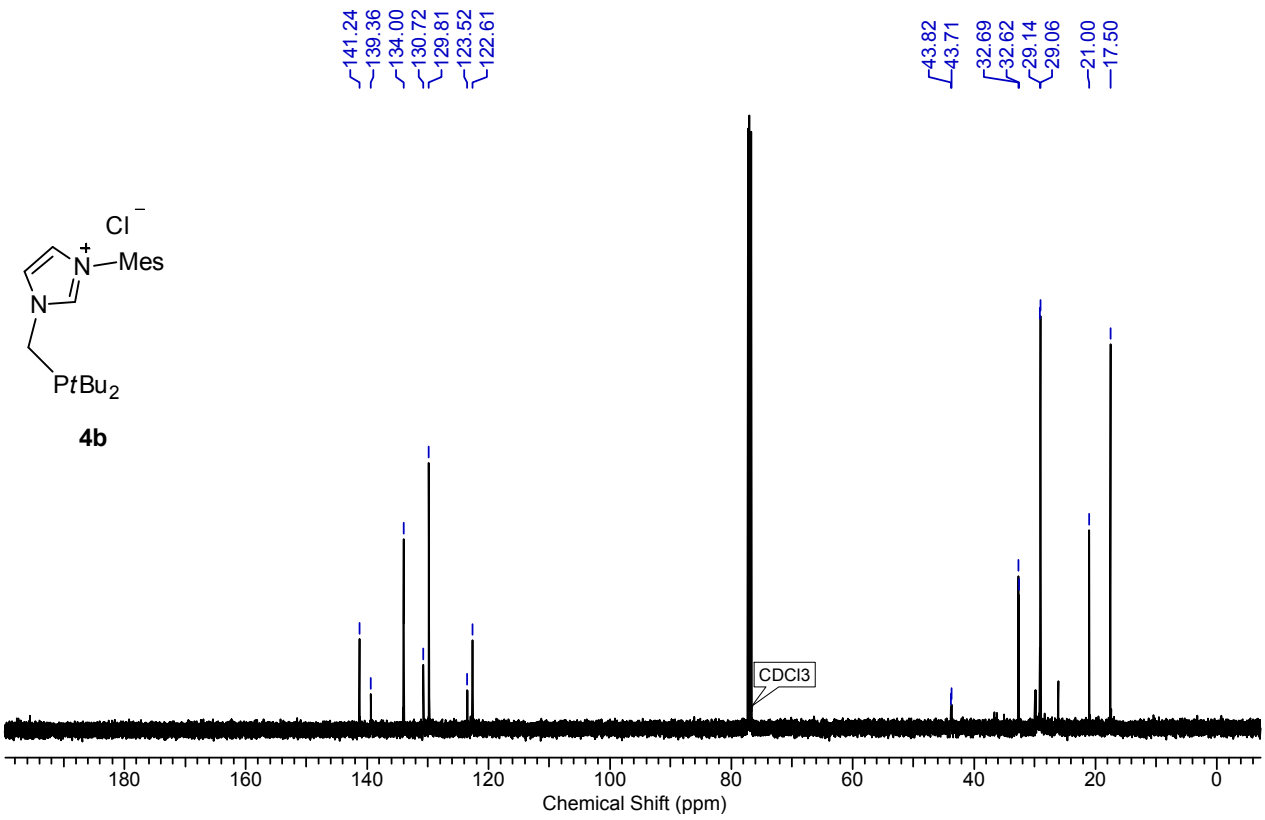
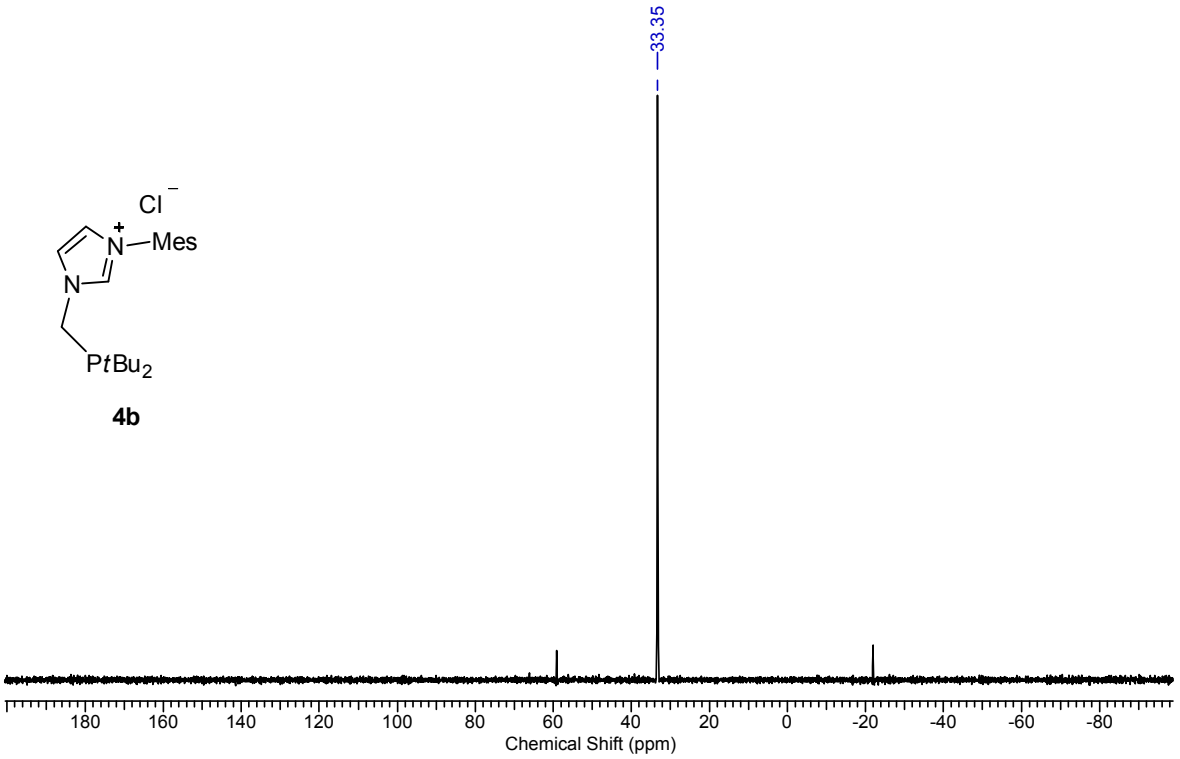
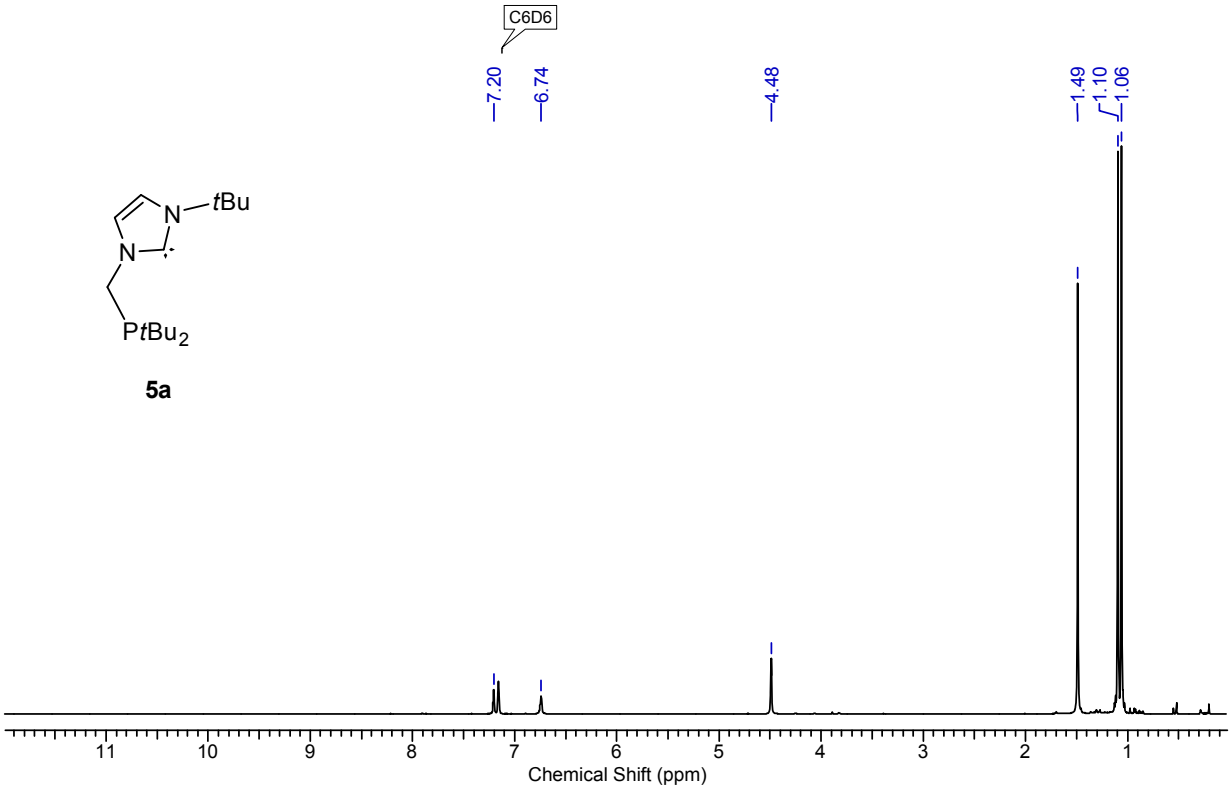


^{31}P NMR spectrum of **4b**



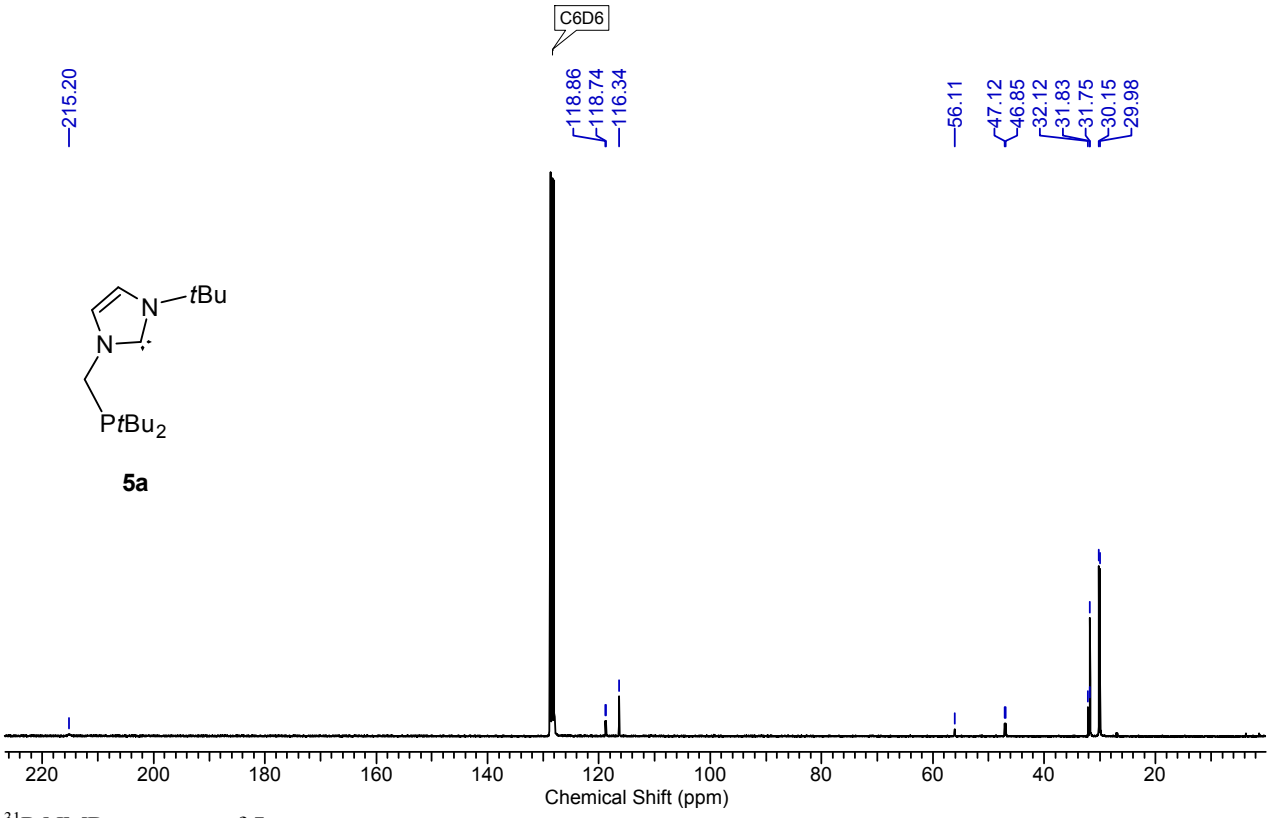
4b

^{1}H NMR spectrum of **5a**

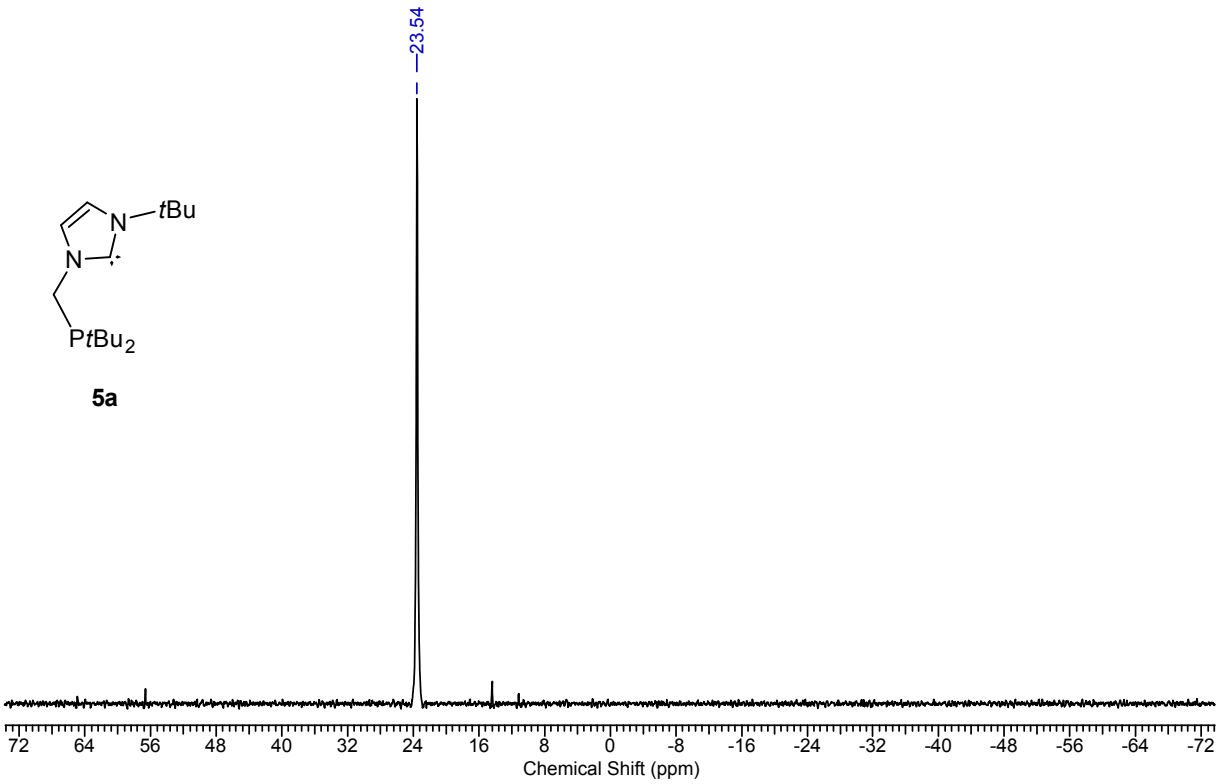


5a

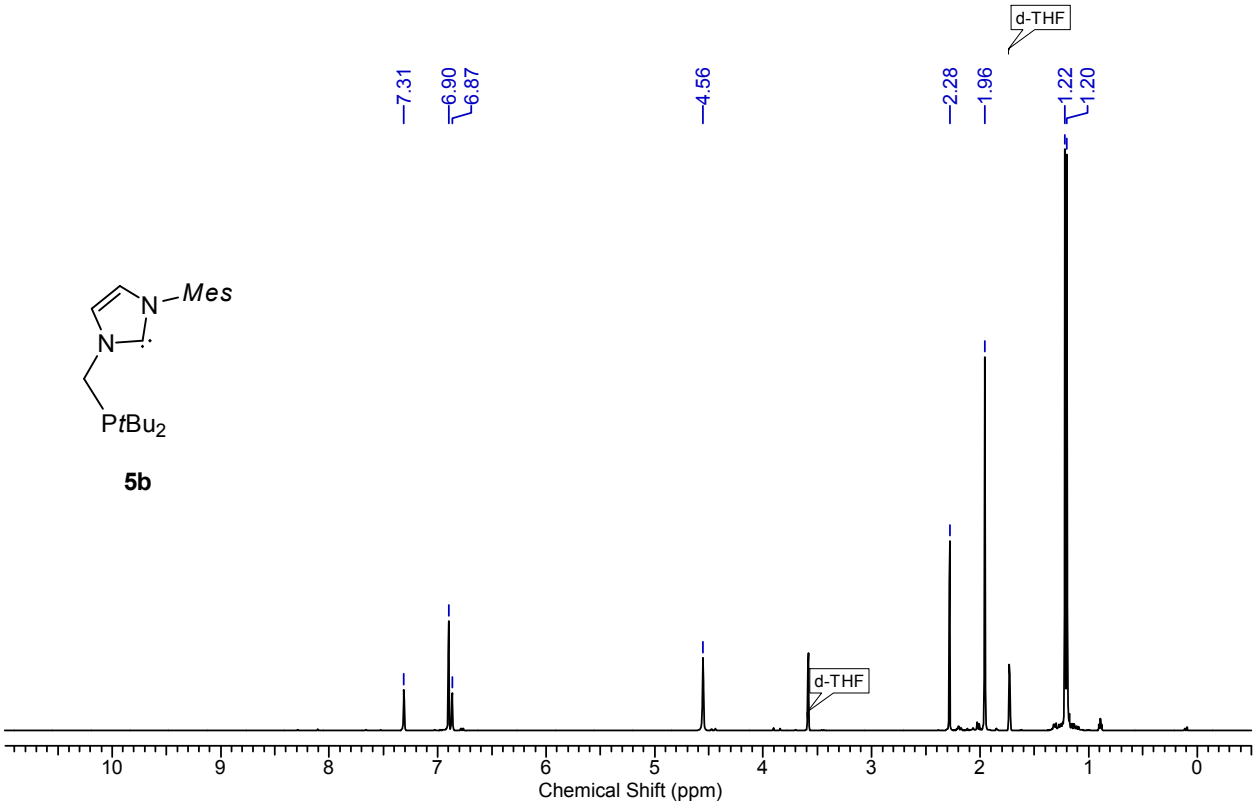
^{13}C NMR spectrum of **5a**



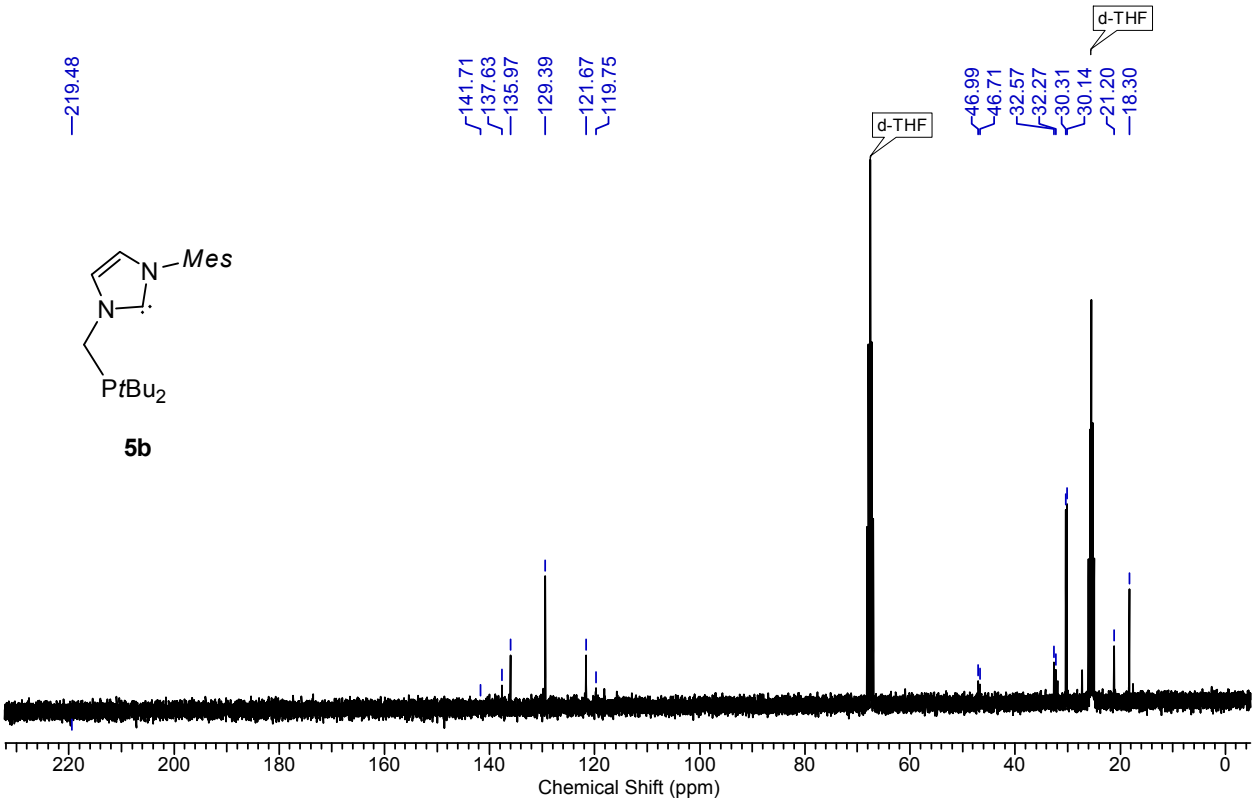
^{31}P NMR spectrum of **5a**



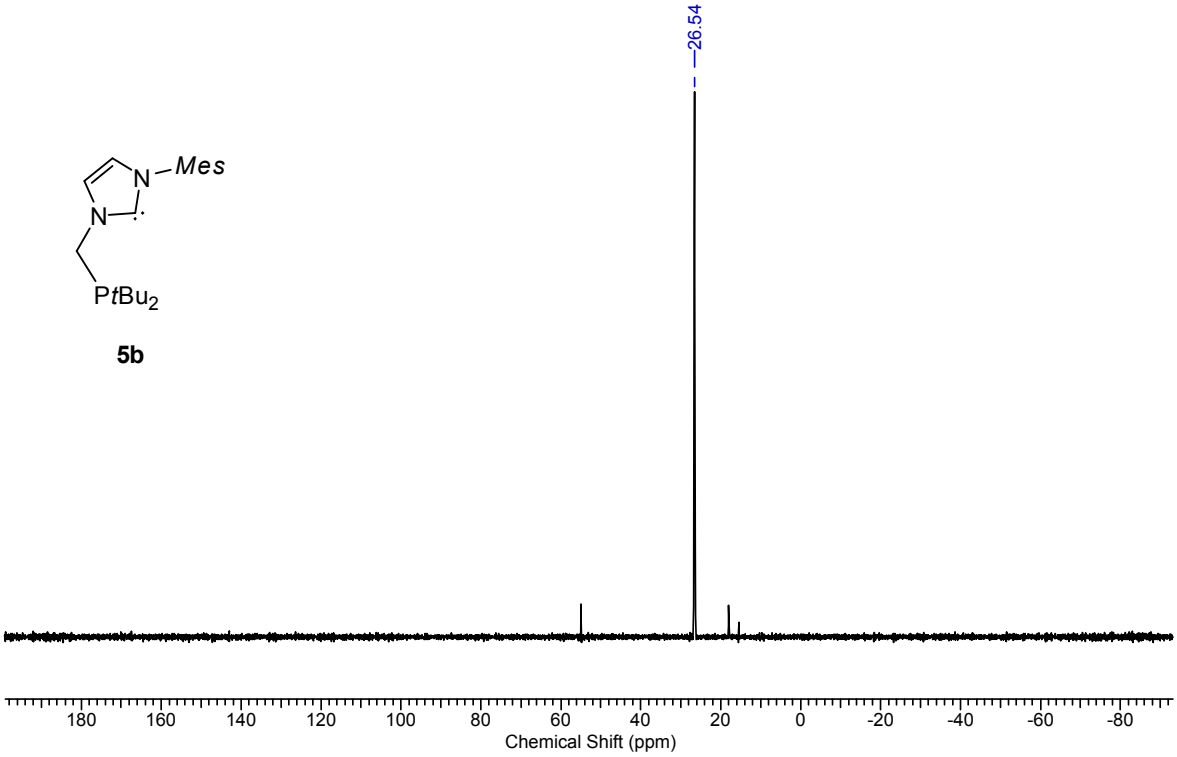
^{1}H NMR spectrum of **5b**



^{13}C NMR spectrum of **5b**

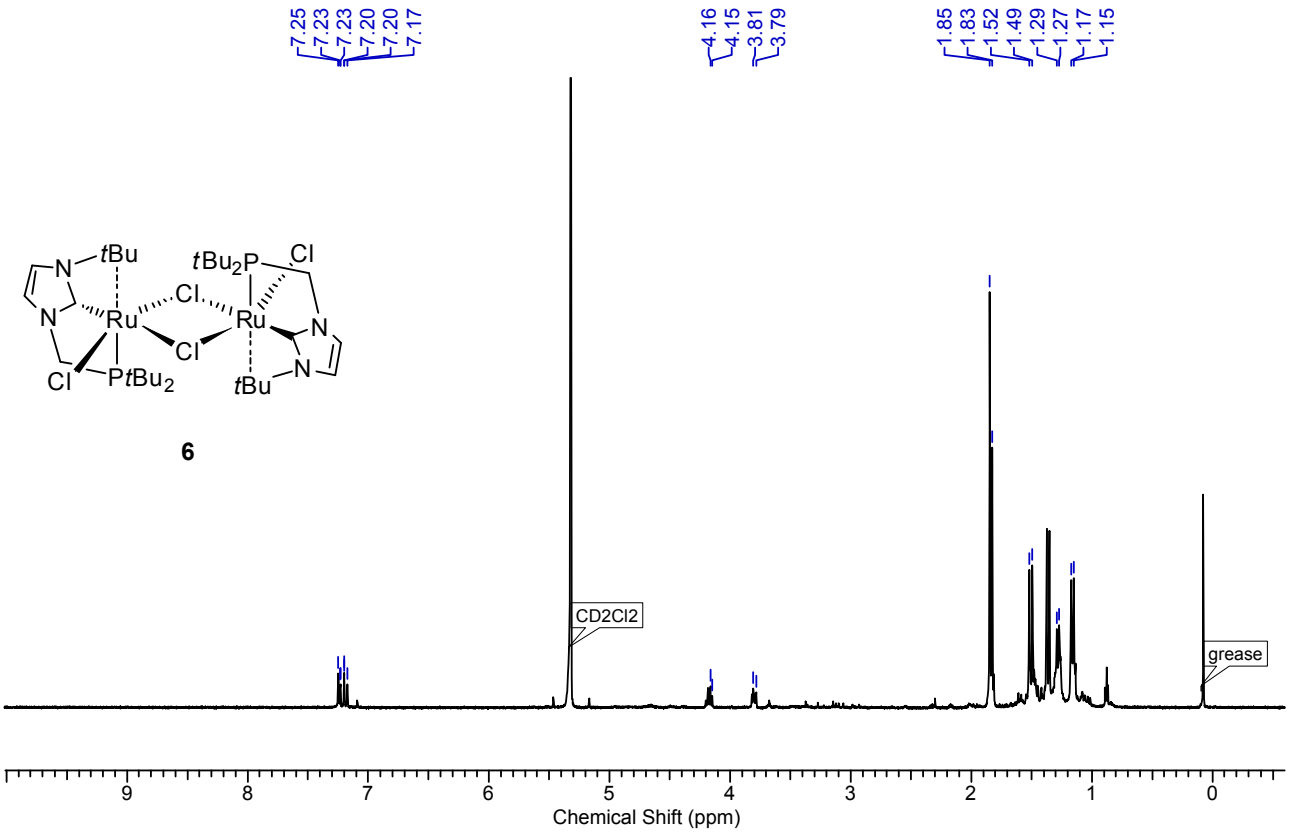


^{31}P NMR spectrum of **5b**



5b

^{1}H NMR spectrum of **6**



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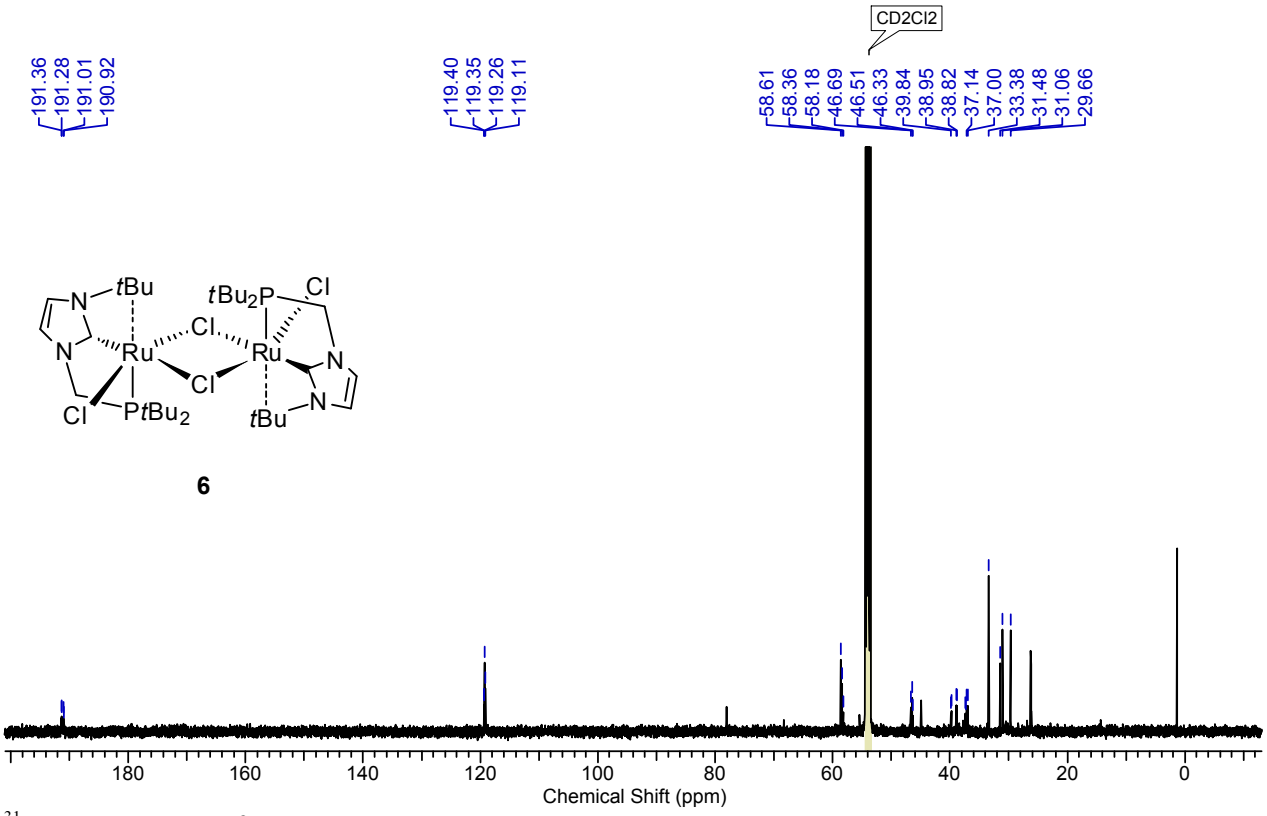
^{13}C NMR spectrum of **6**



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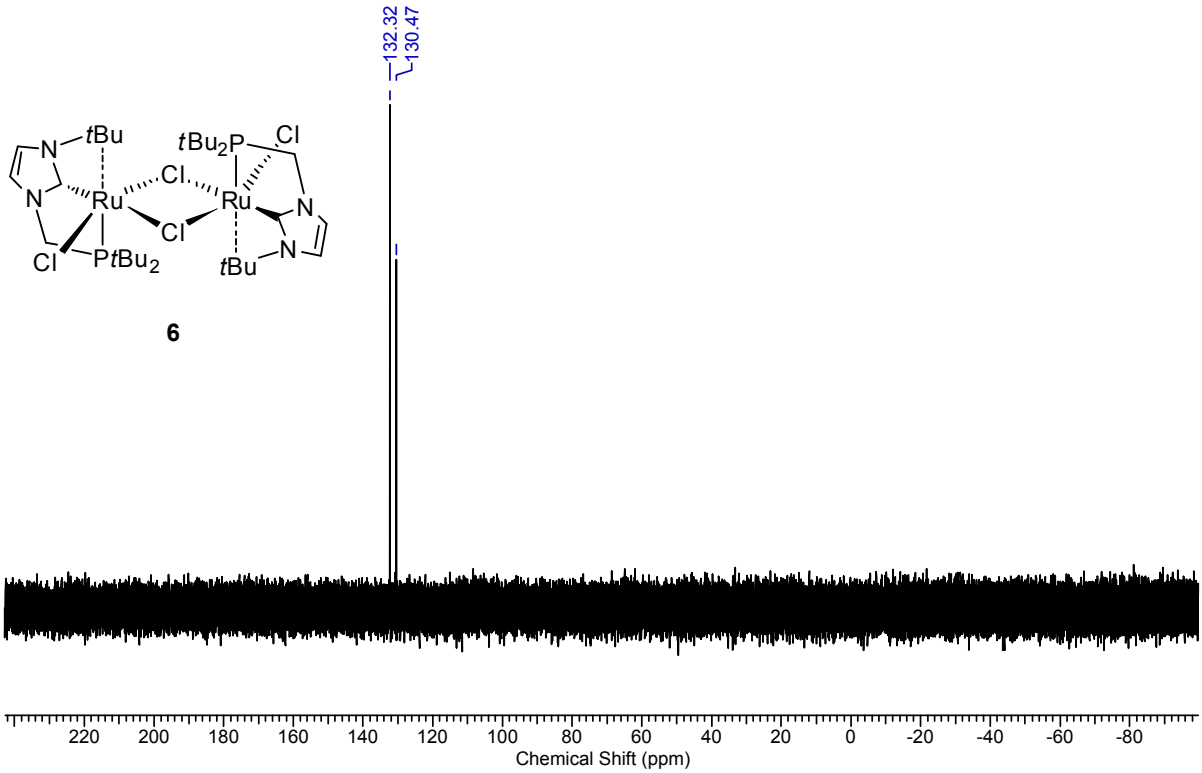
^{31}P NMR spectrum of **6**



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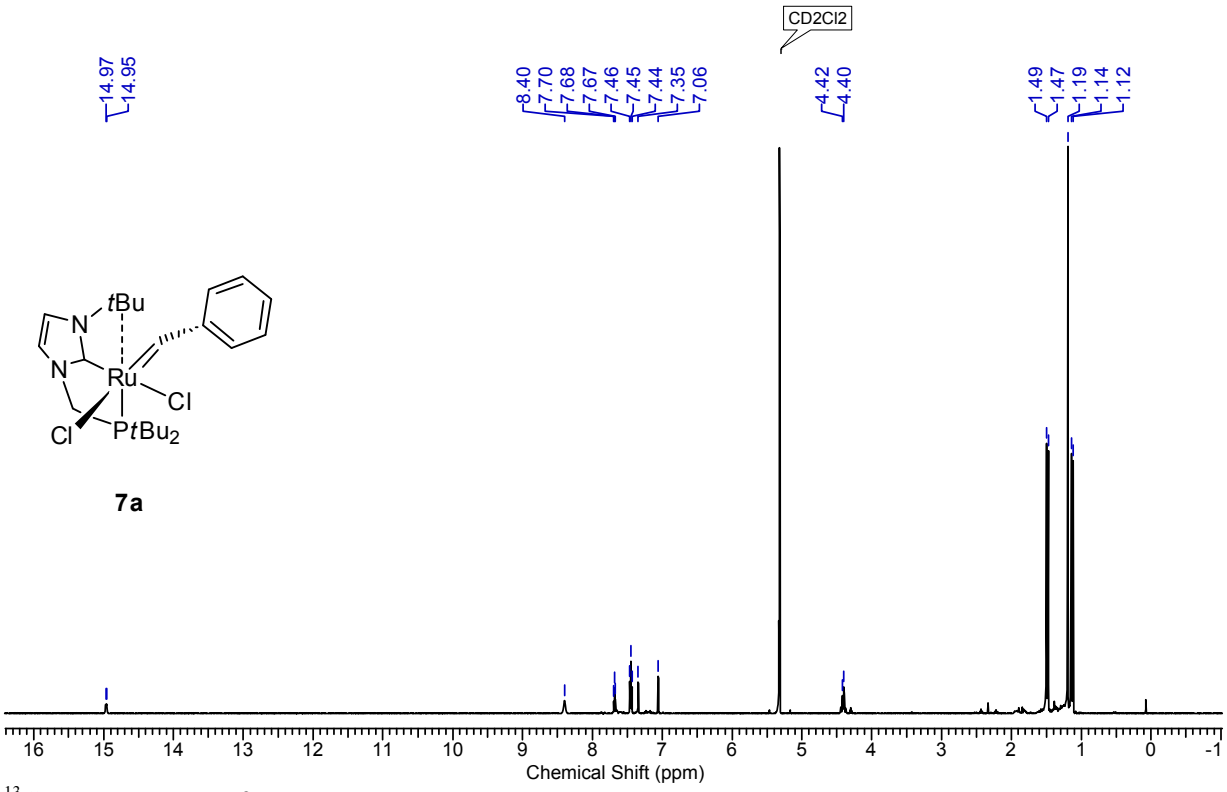
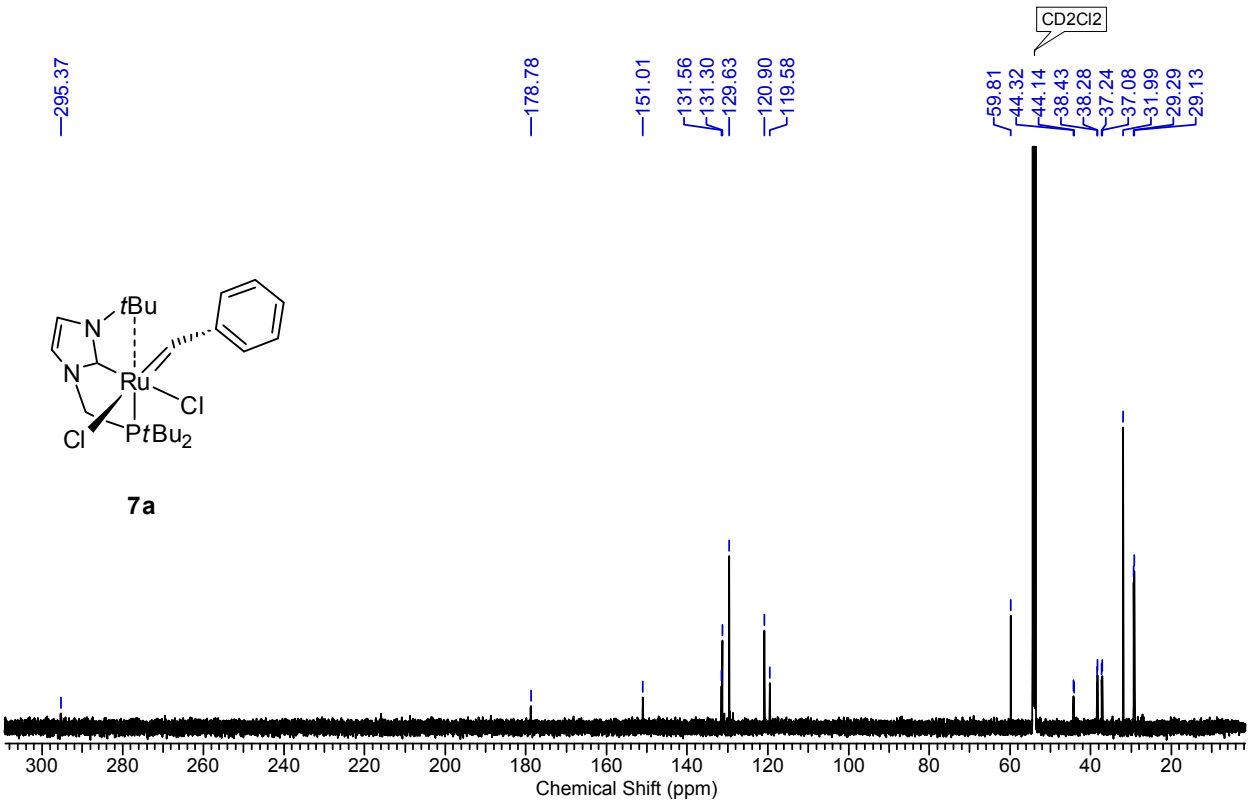
^{1}H NMR spectrum of **7a**



^{13}C NMR spectrum of **7a**



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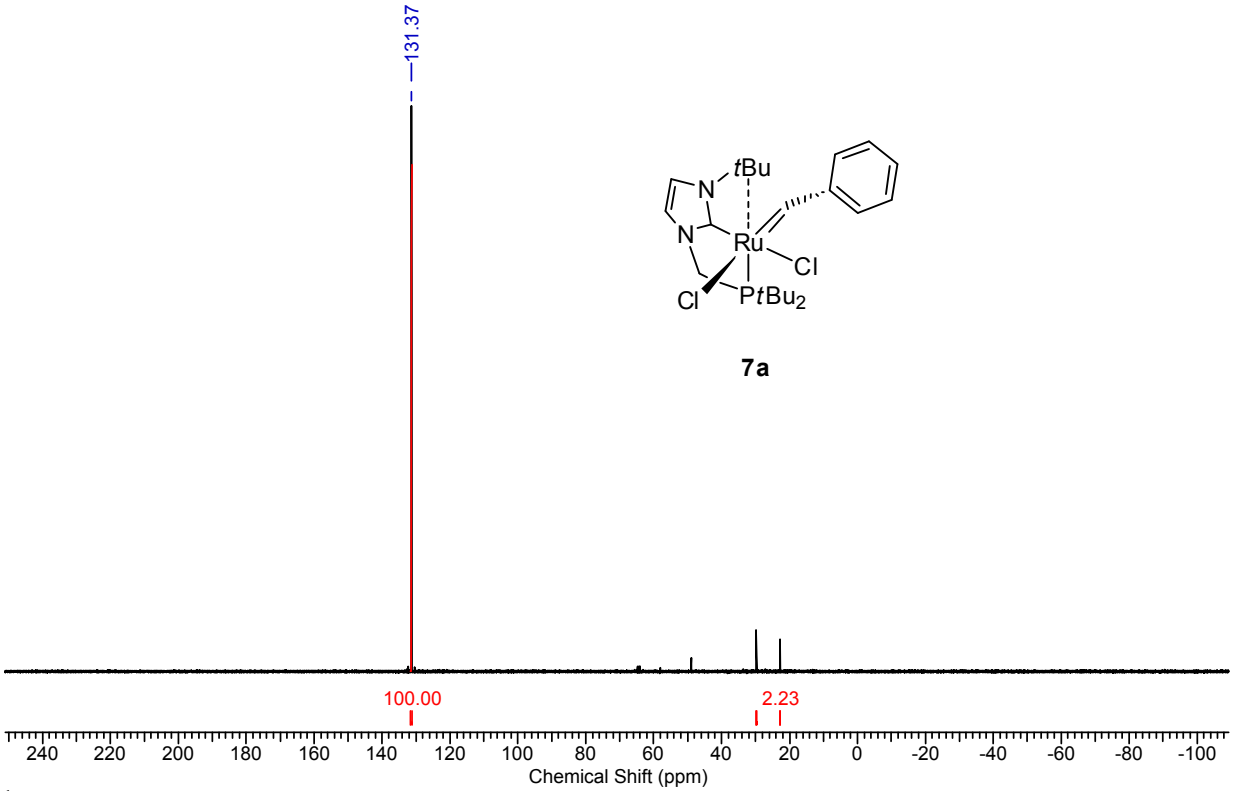
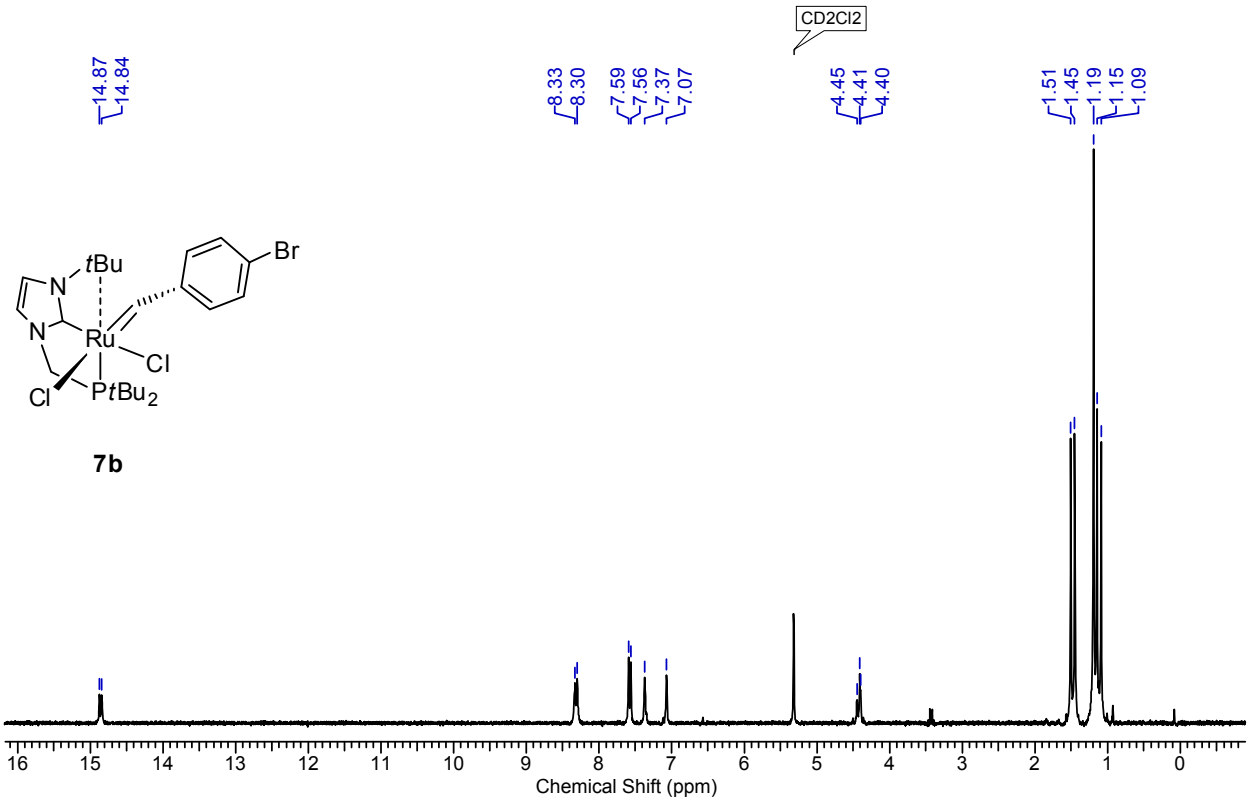


7a

^{1}H NMR spectrum of **7b**



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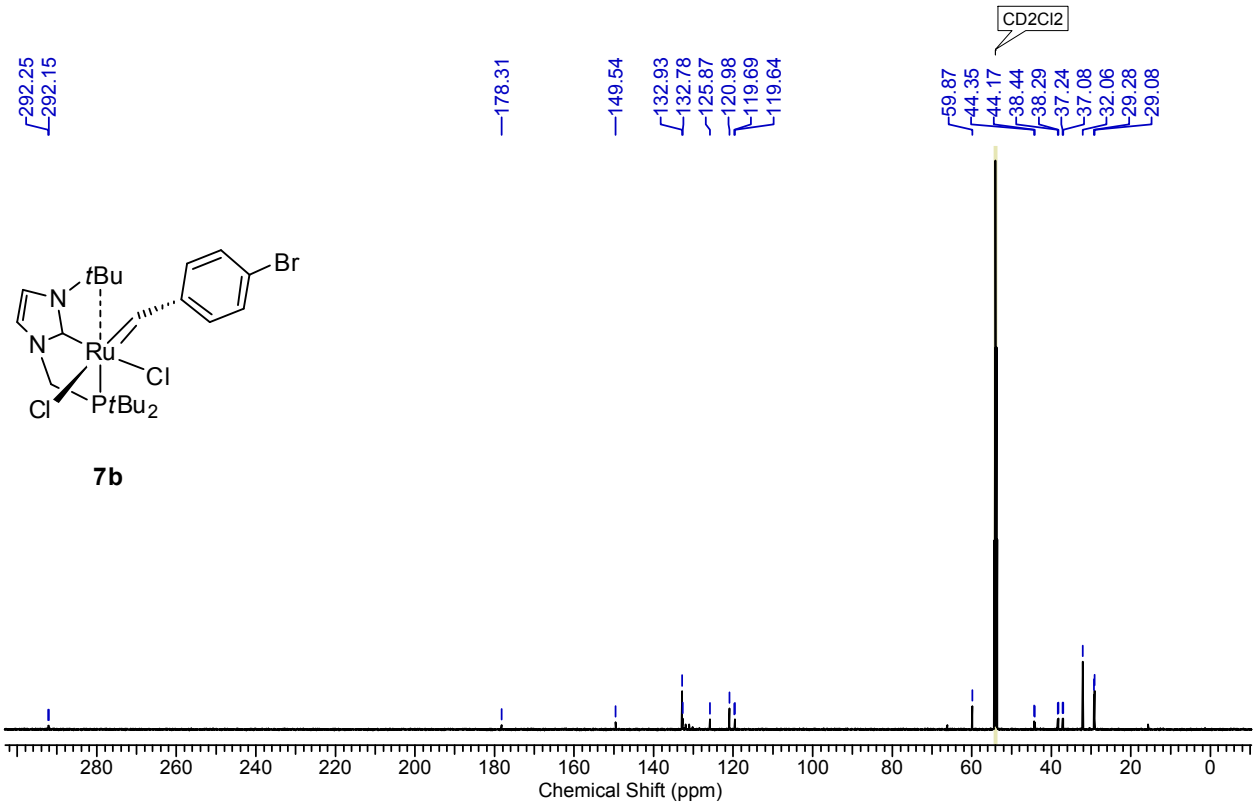
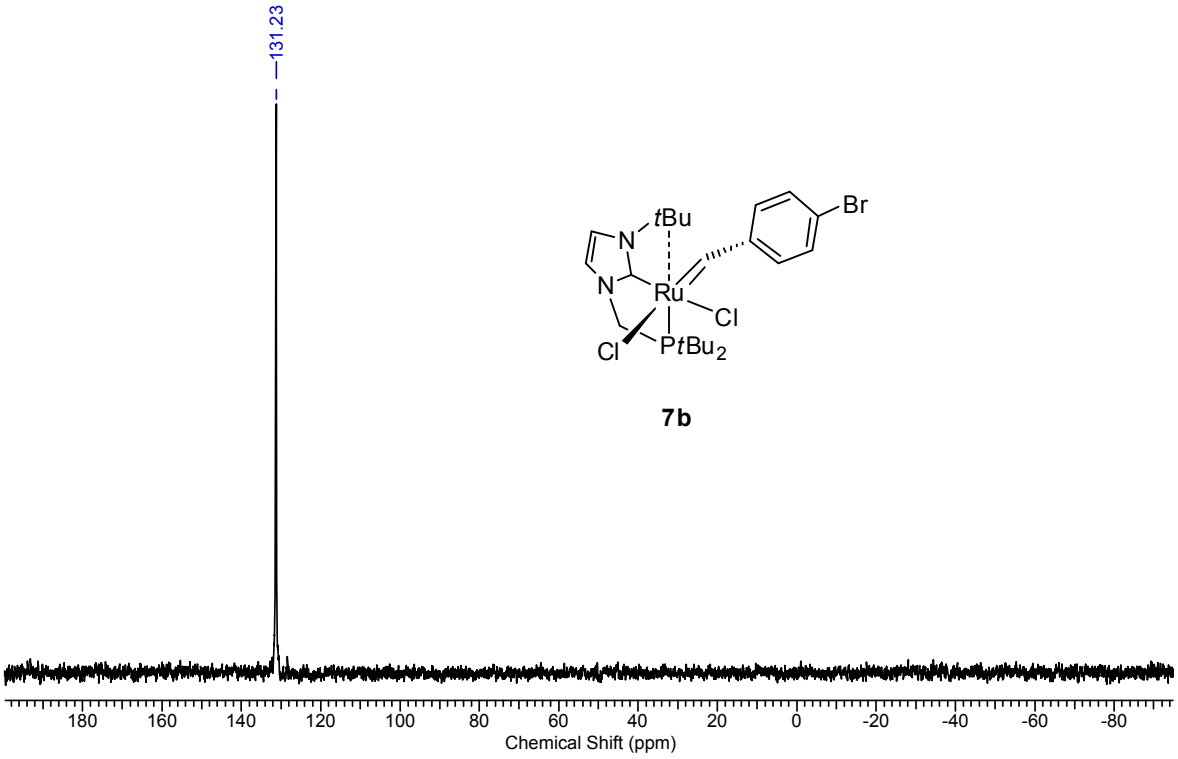
^{13}C NMR spectrum of **7b**



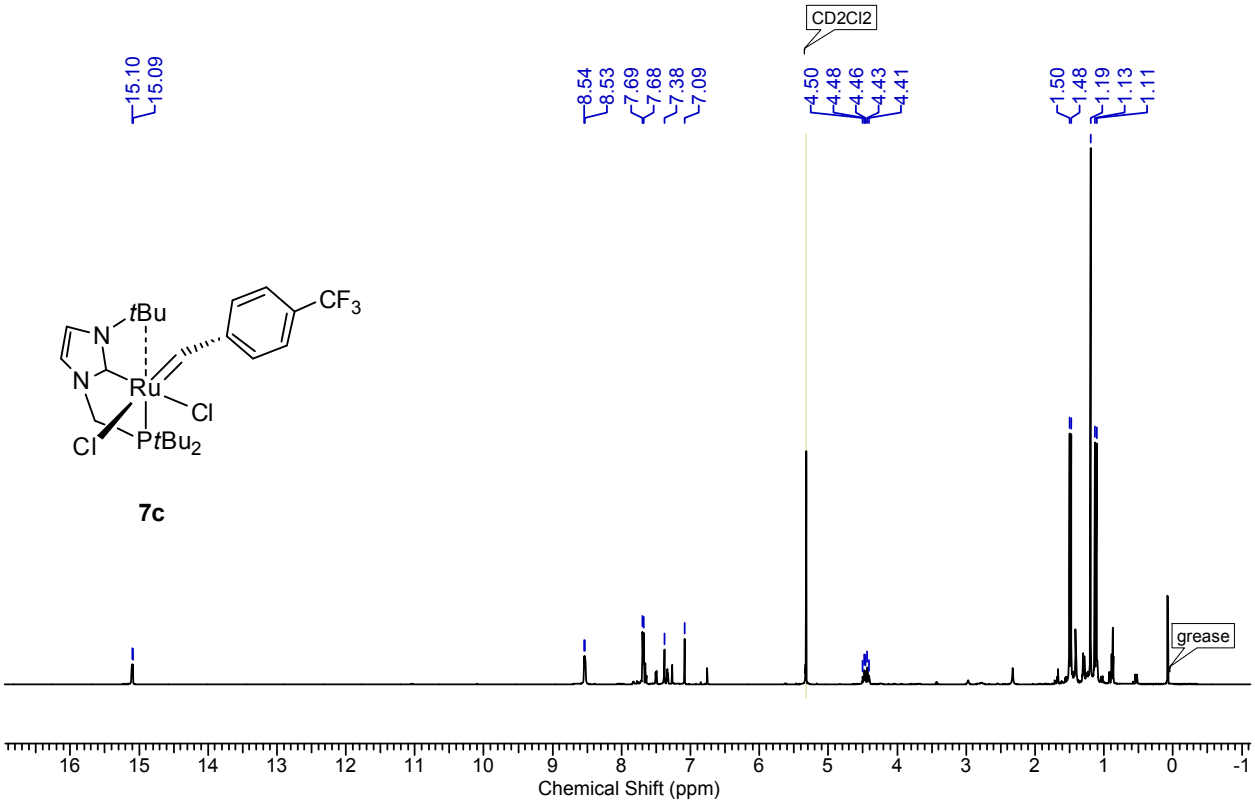
7b

^{31}P NMR spectrum of **7b**

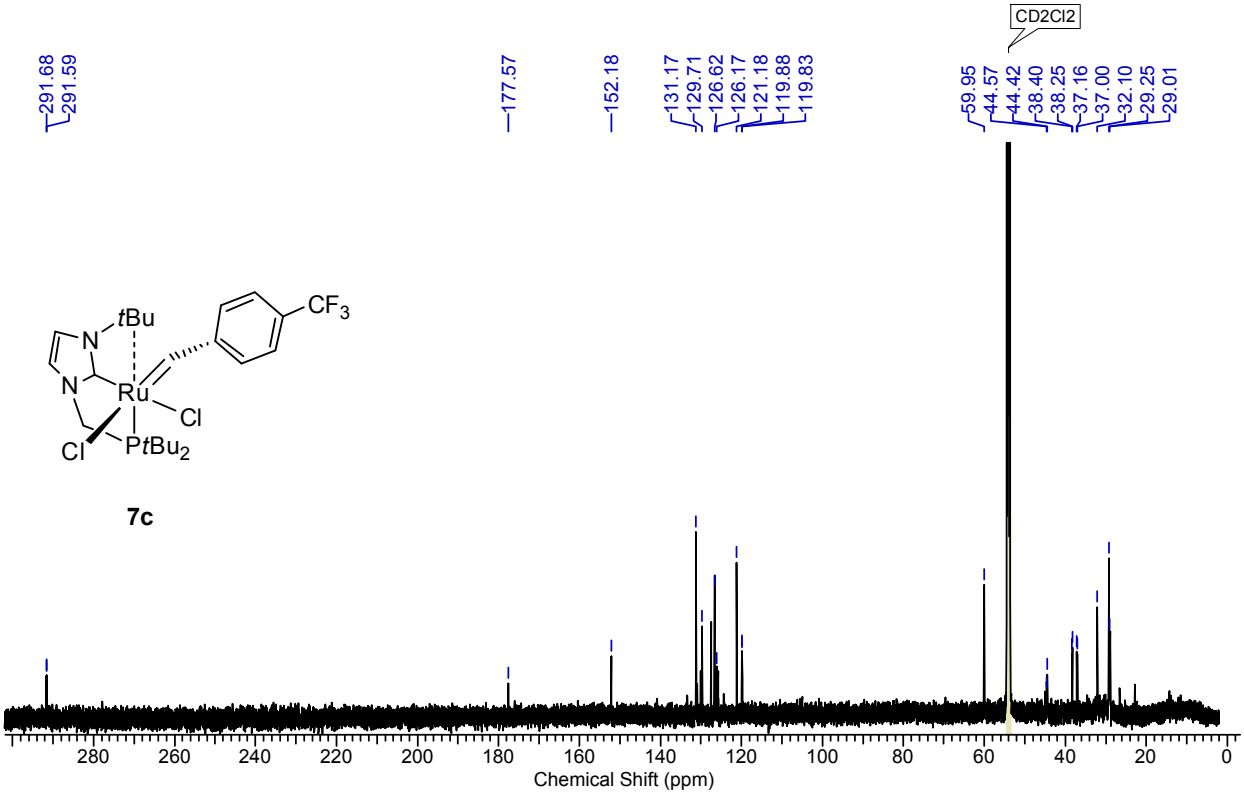


7b

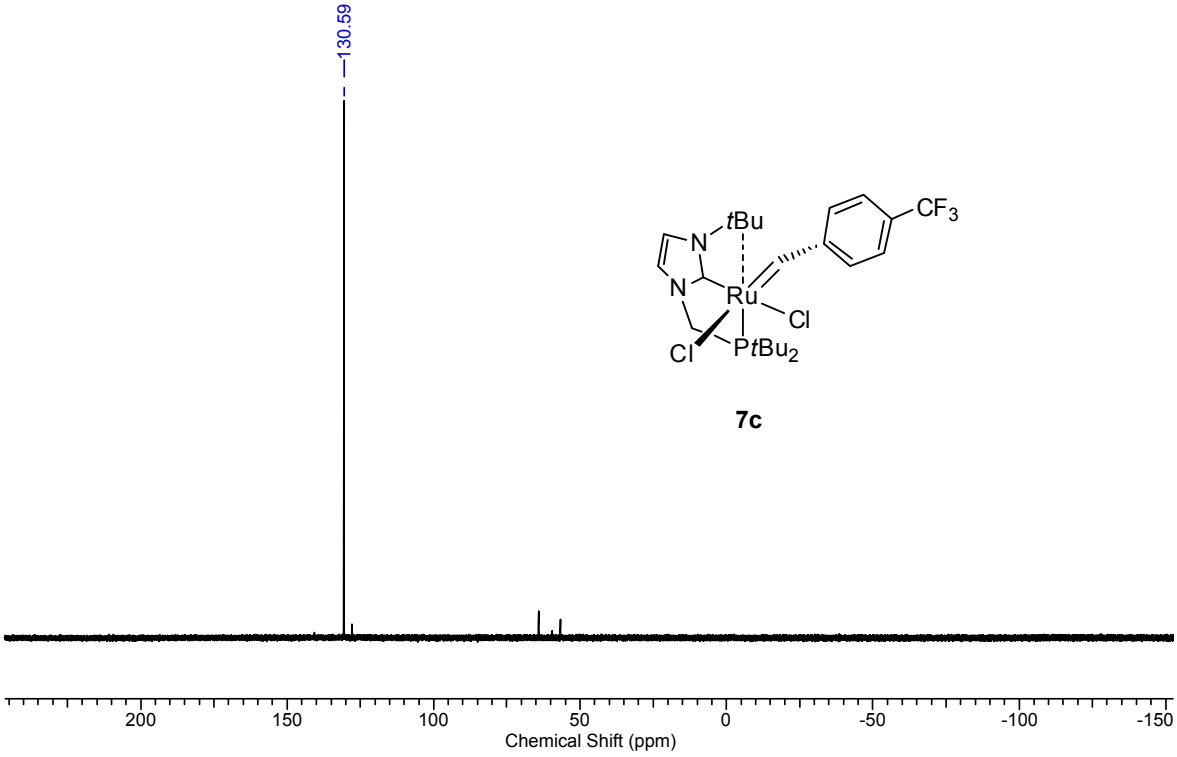
^{1}H NMR spectrum of **7c**



^{13}C NMR spectrum of **7c**

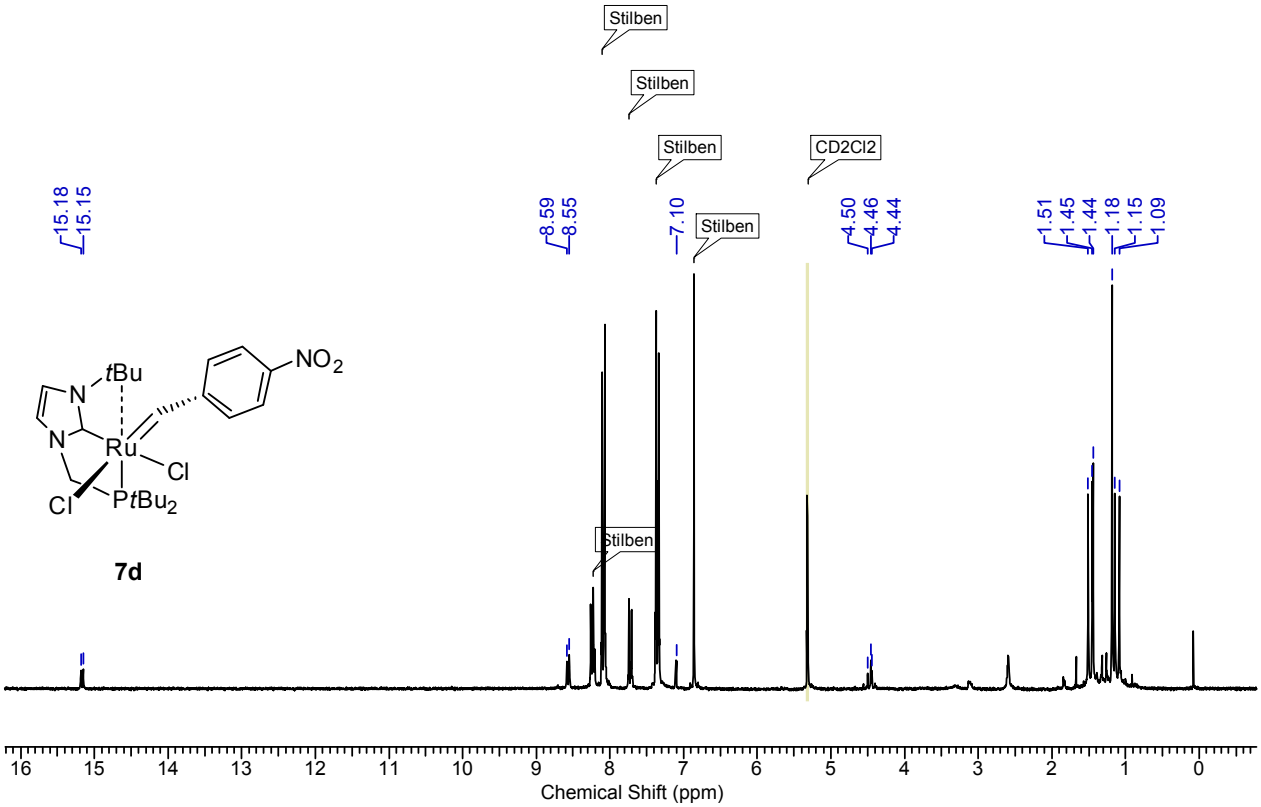


^{31}P NMR spectrum of **7c**



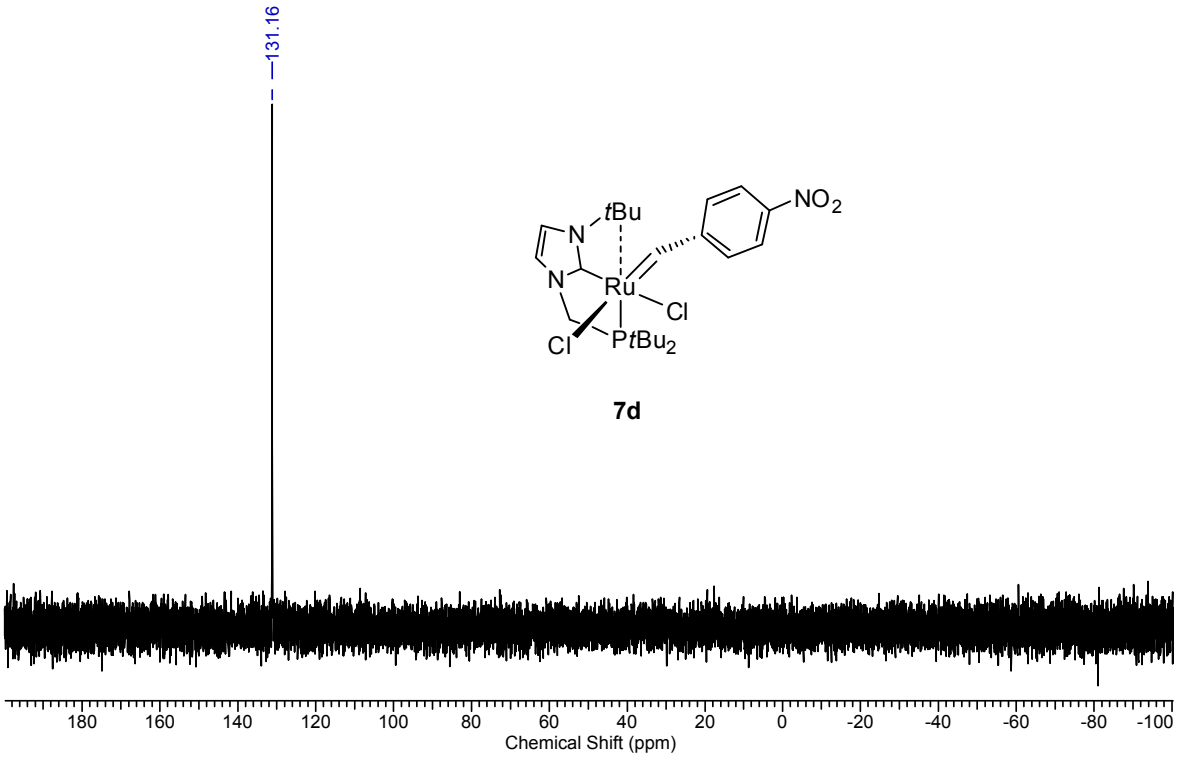
7c

^{1}H NMR spectrum of **7d**



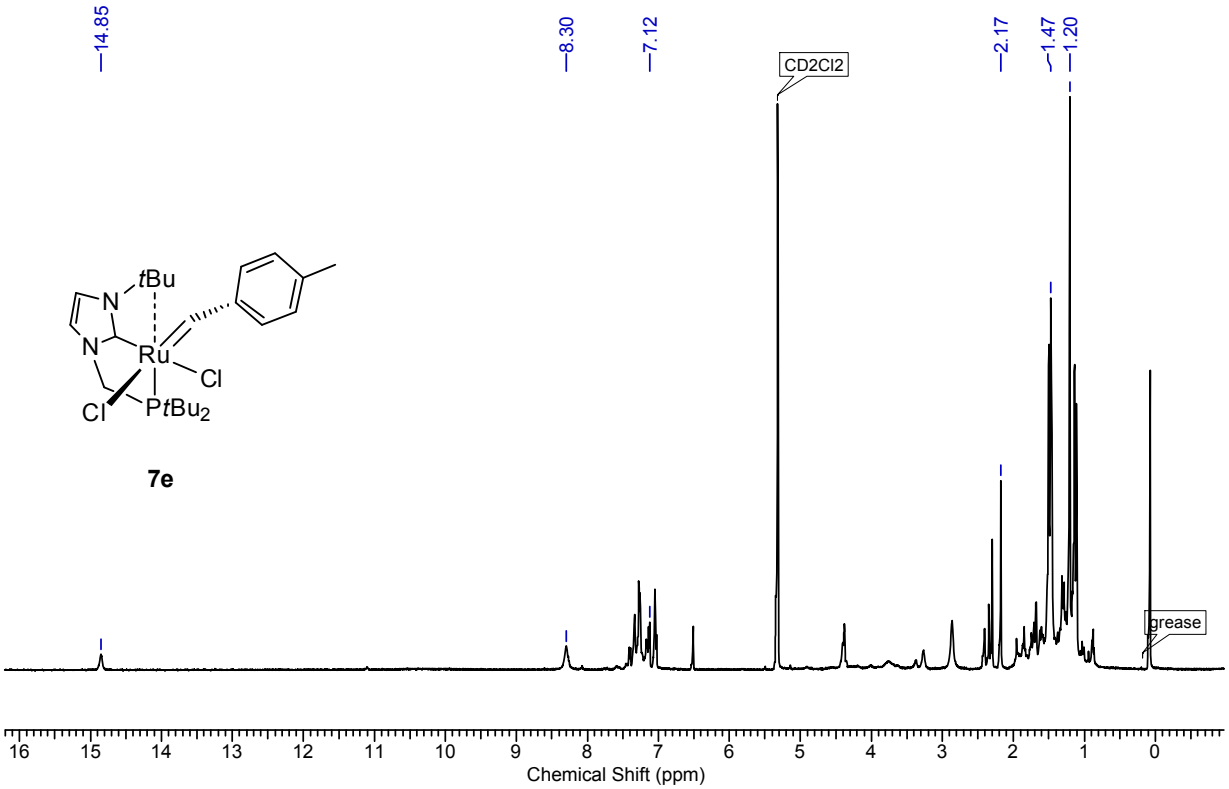
7d

^{31}P NMR spectrum of **7d**



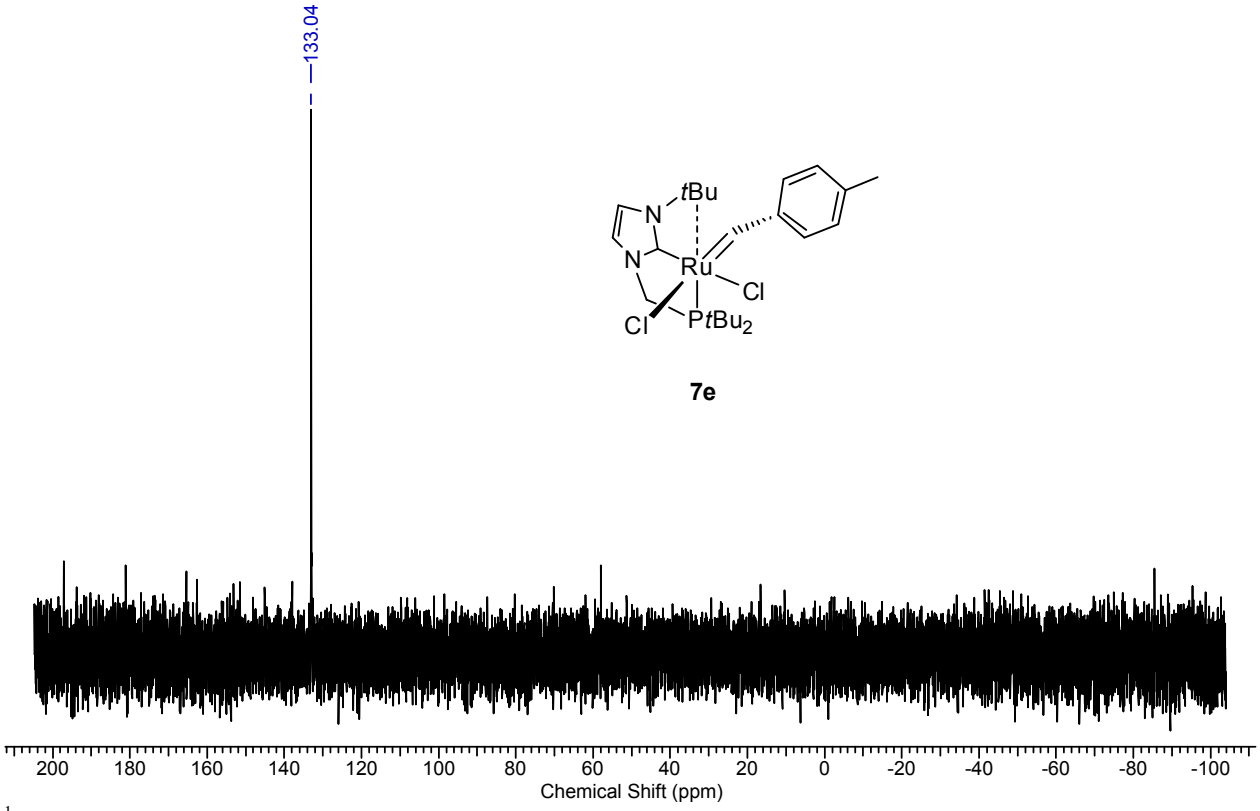
7d

^{1}H NMR spectrum of **7e**



7e

^{31}P NMR spectrum of **7e**



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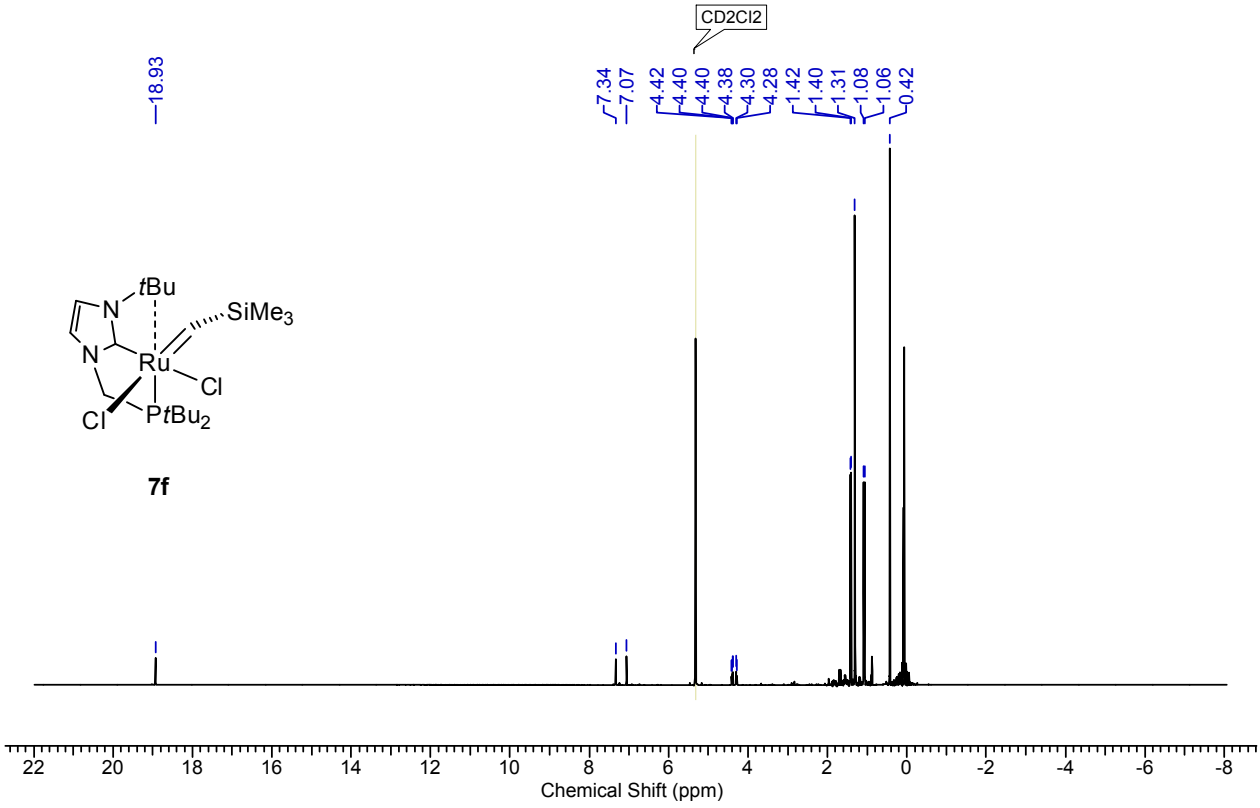
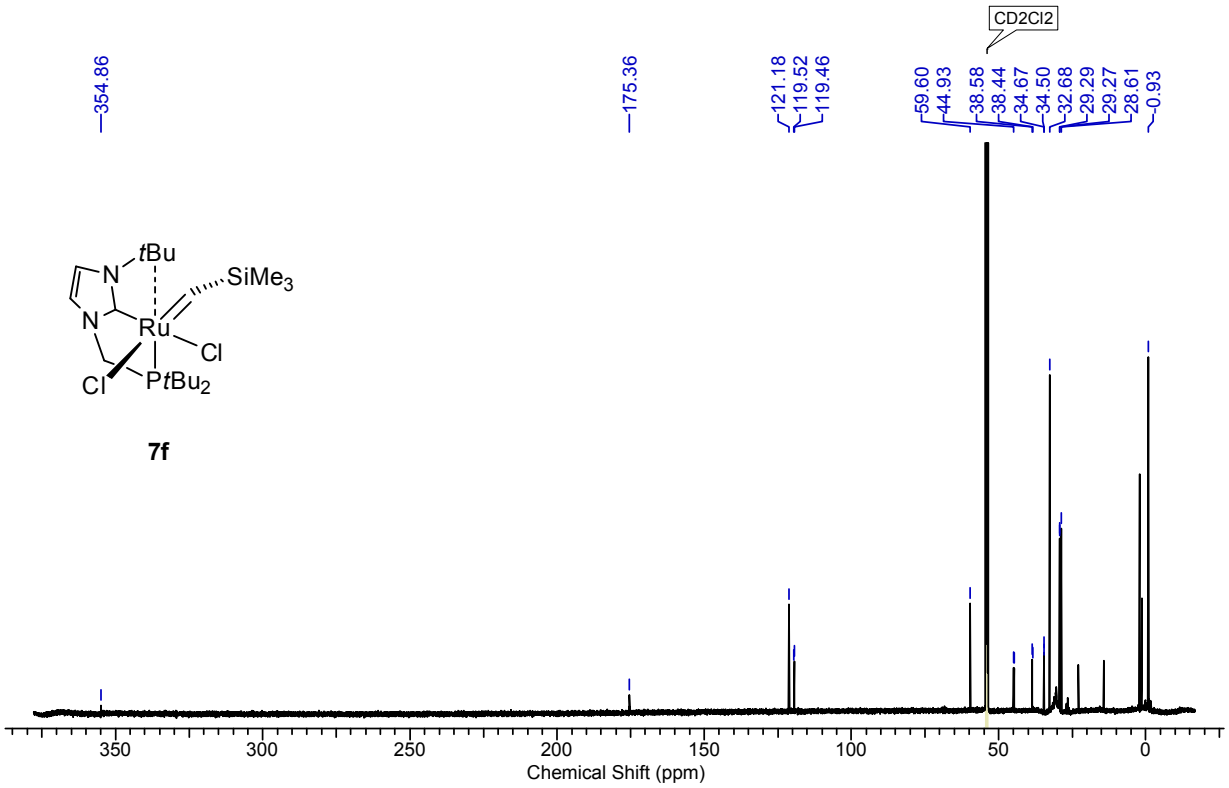
^{1}H NMR spectrum of **7f**



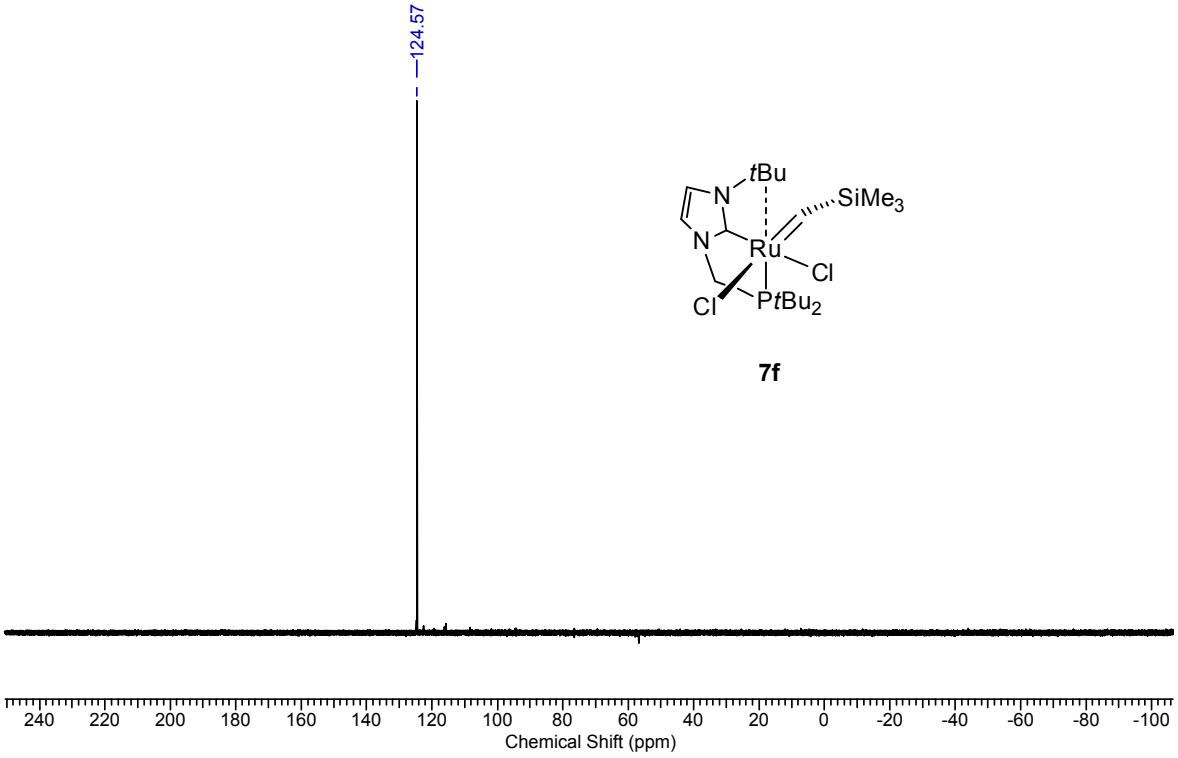
7f

^{13}C NMR spectrum of **7f**



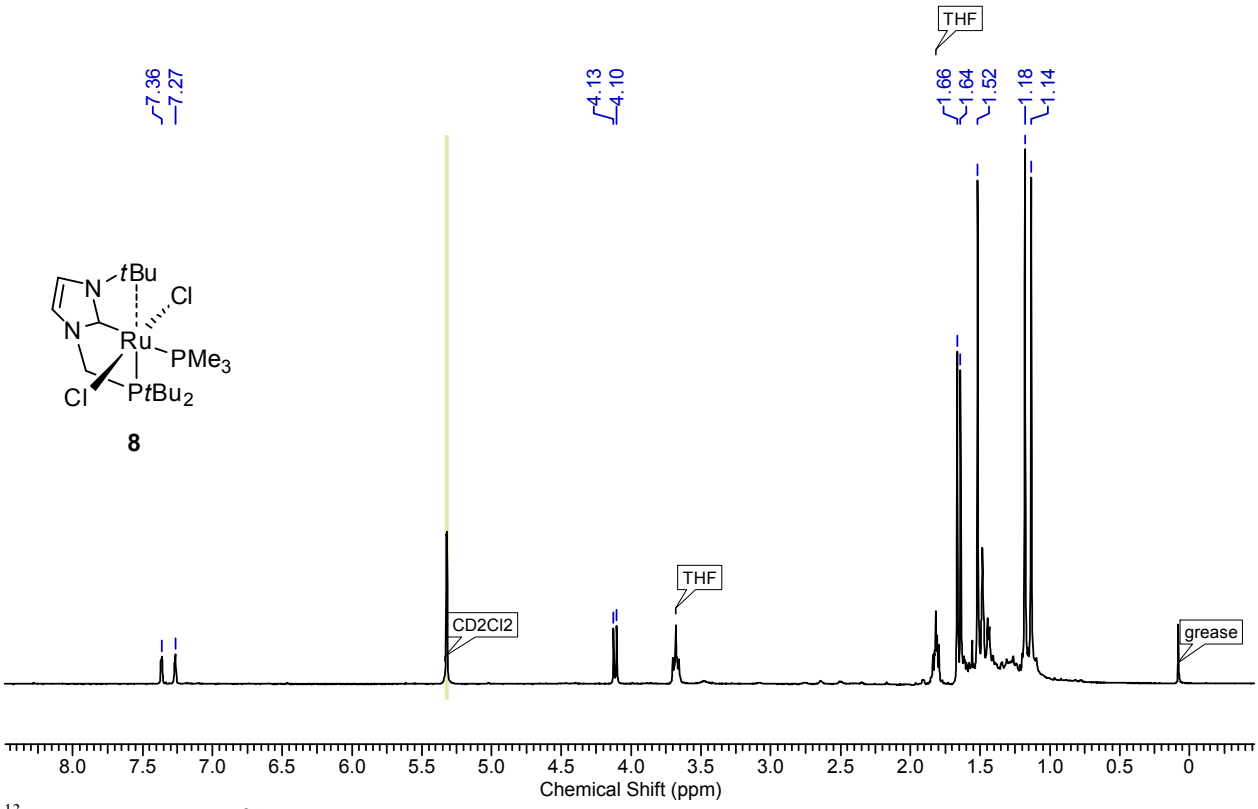
7f

^{31}P NMR spectrum of **7f**

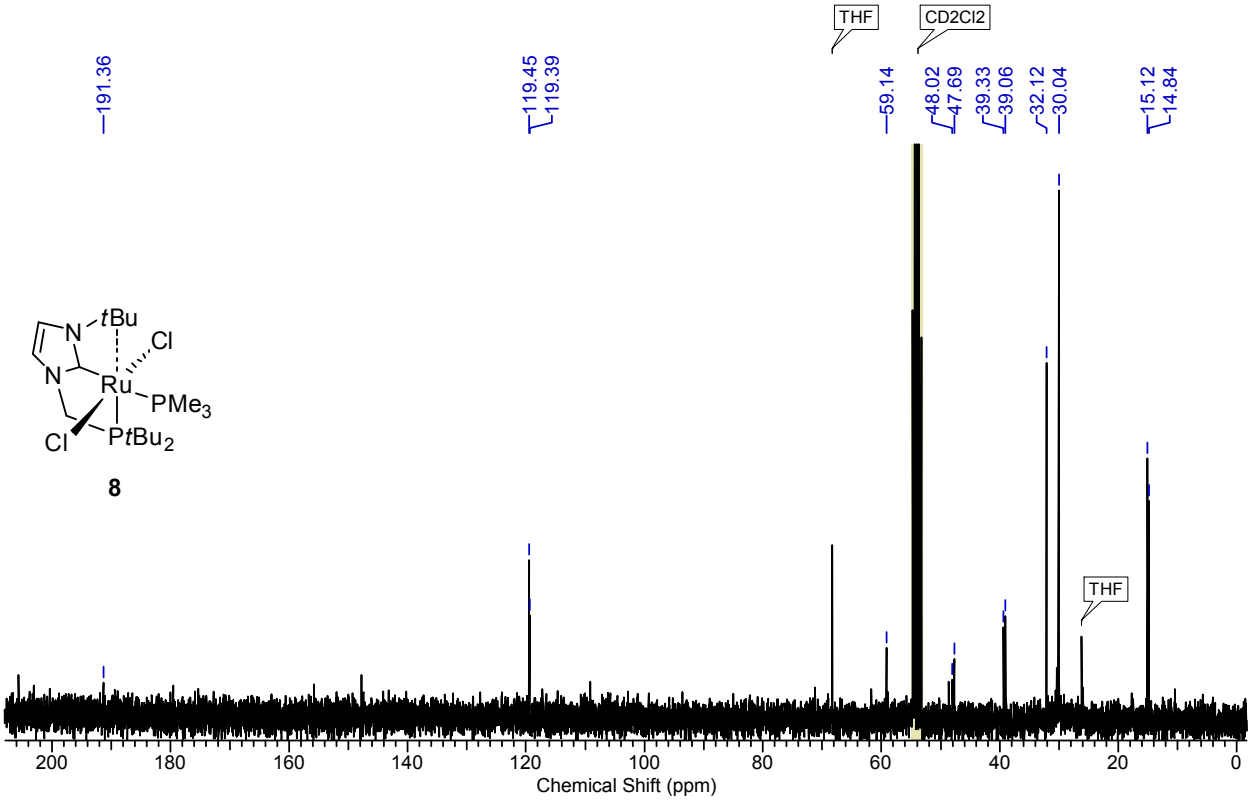


7f

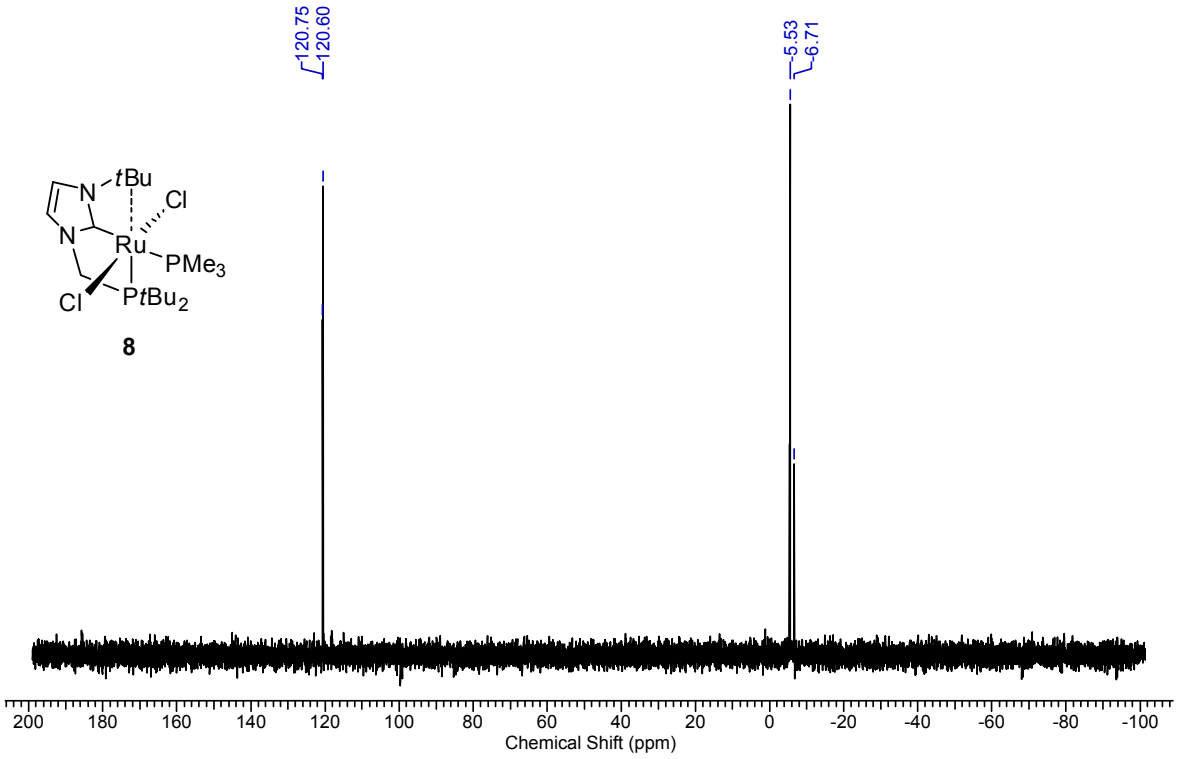
^{1}H NMR spectrum of **8**



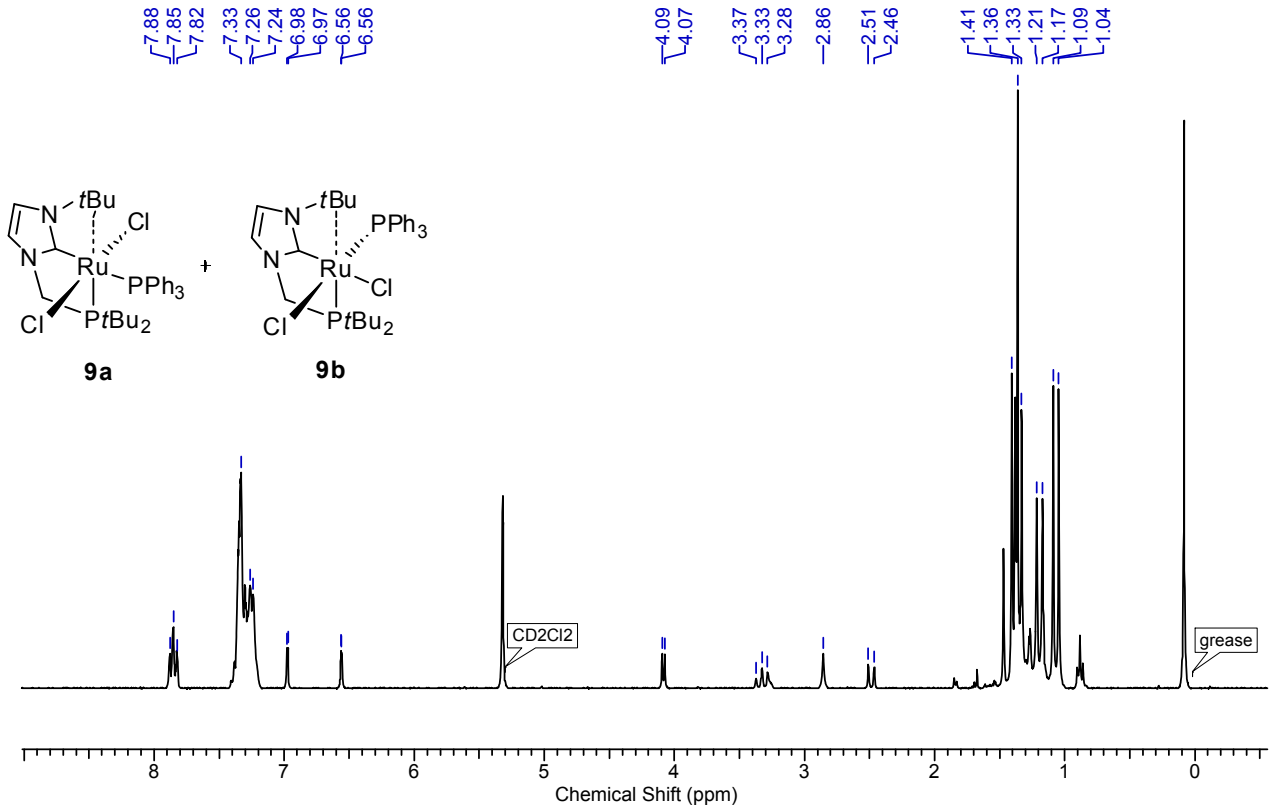
^{13}C NMR spectrum of **8**



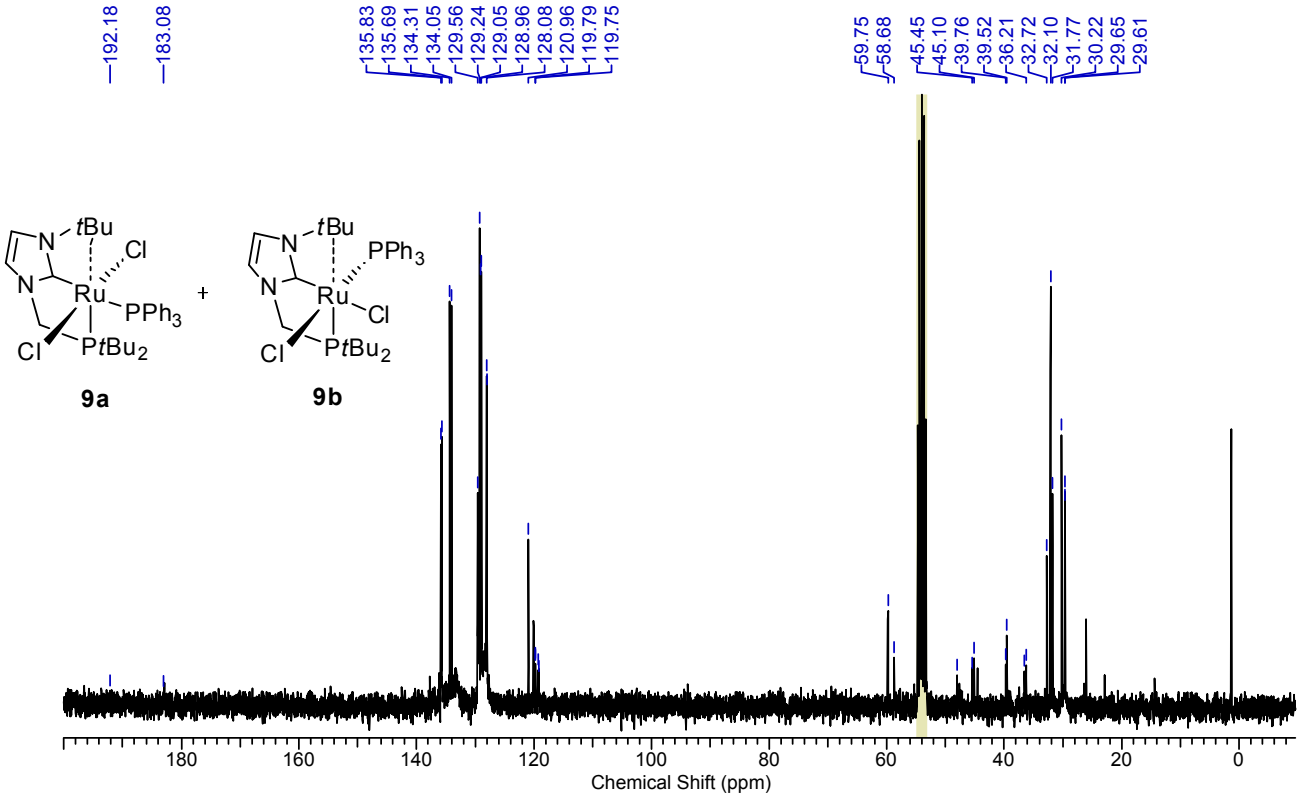
^{31}P NMR spectrum of **8**



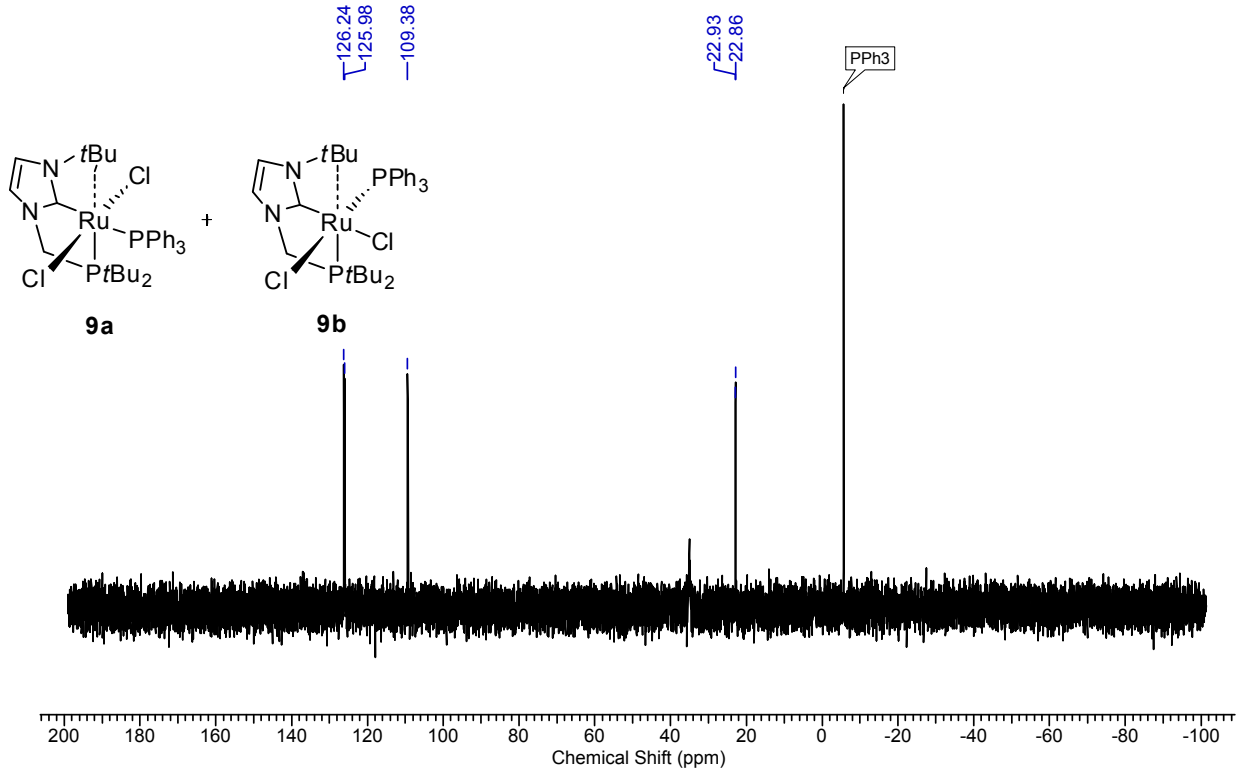
^{1}H NMR spectrum of **9a,b**



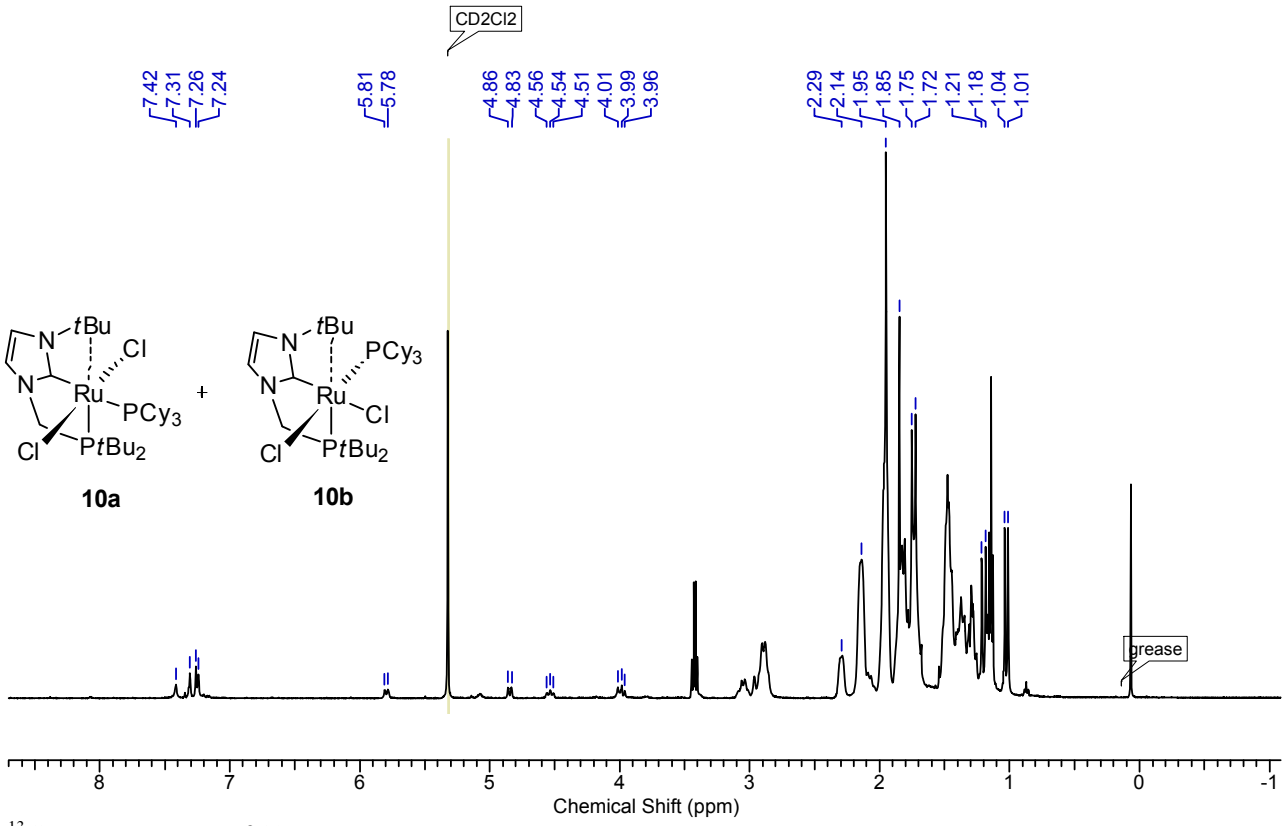
^{13}C NMR spectrum of **9a,b**



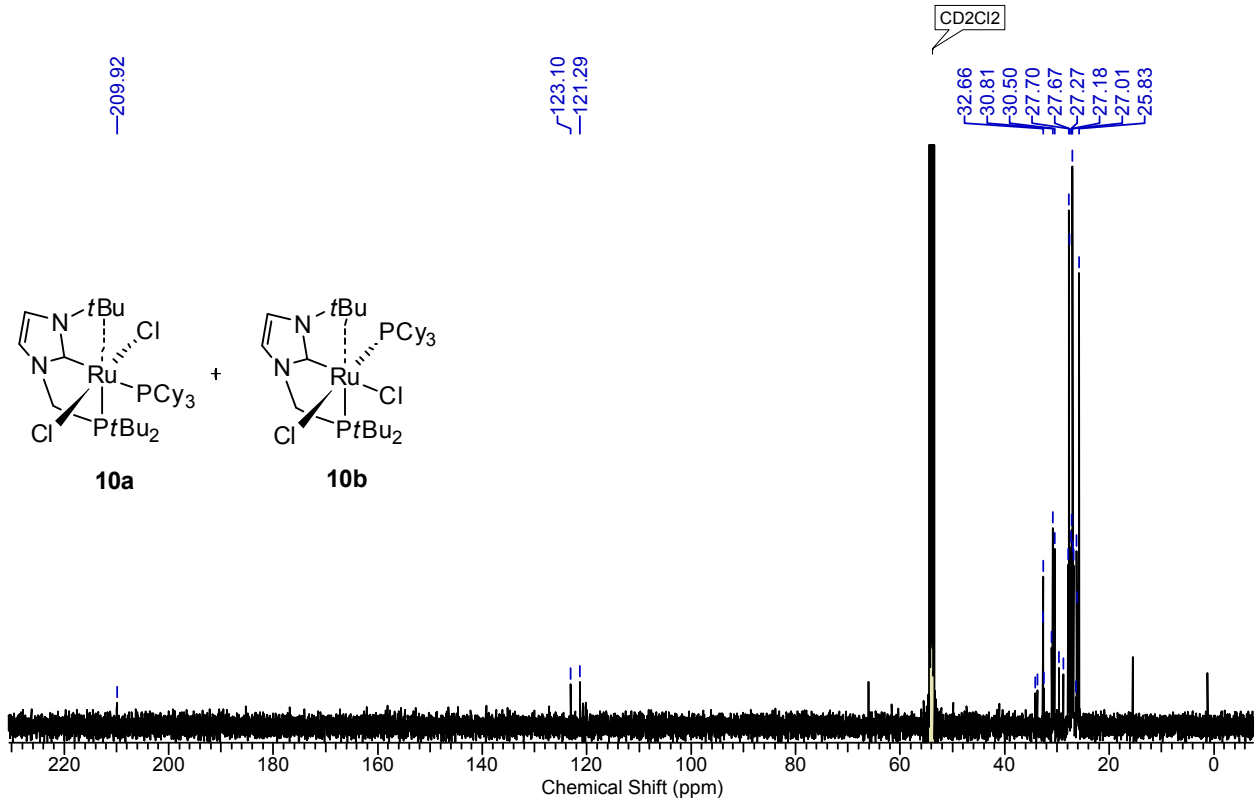
^{31}P NMR spectrum of **9a,b**



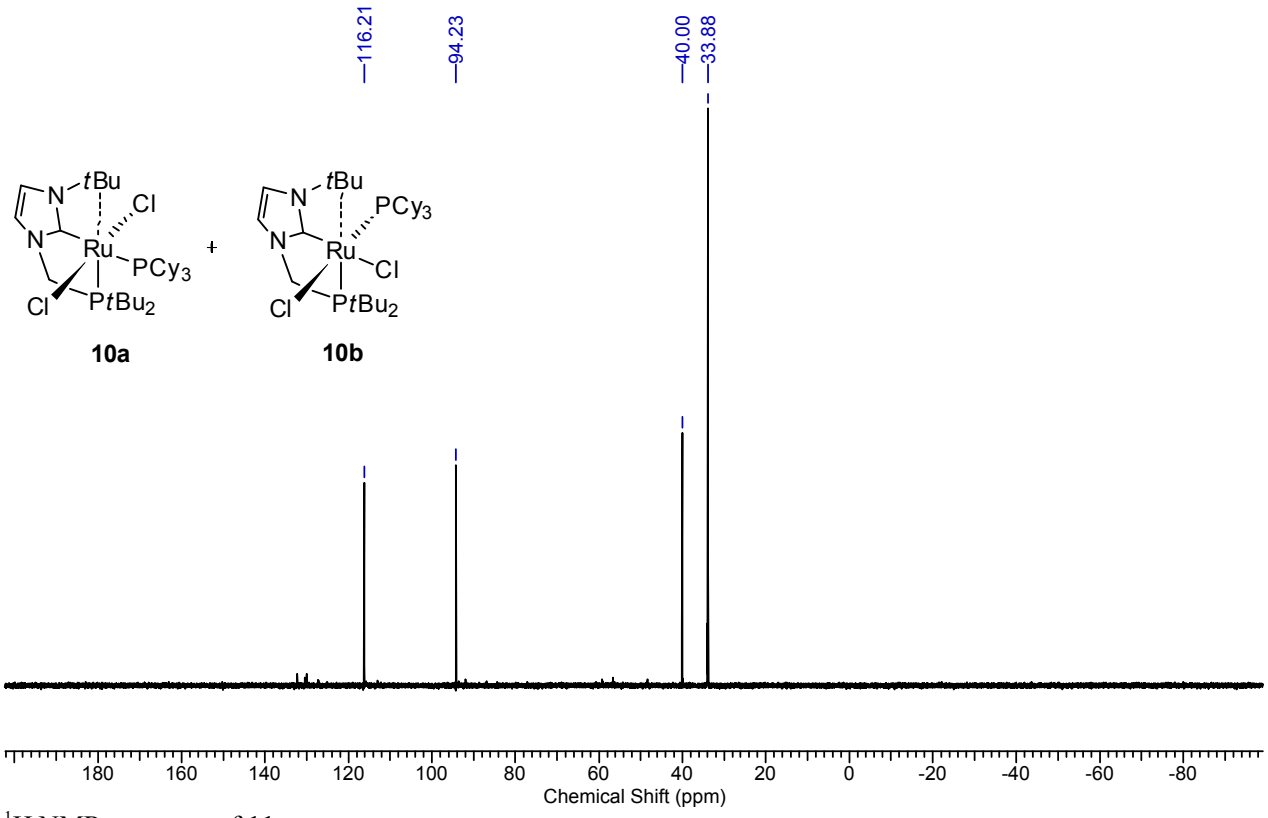
^{1}H NMR spectrum of **10a,b**



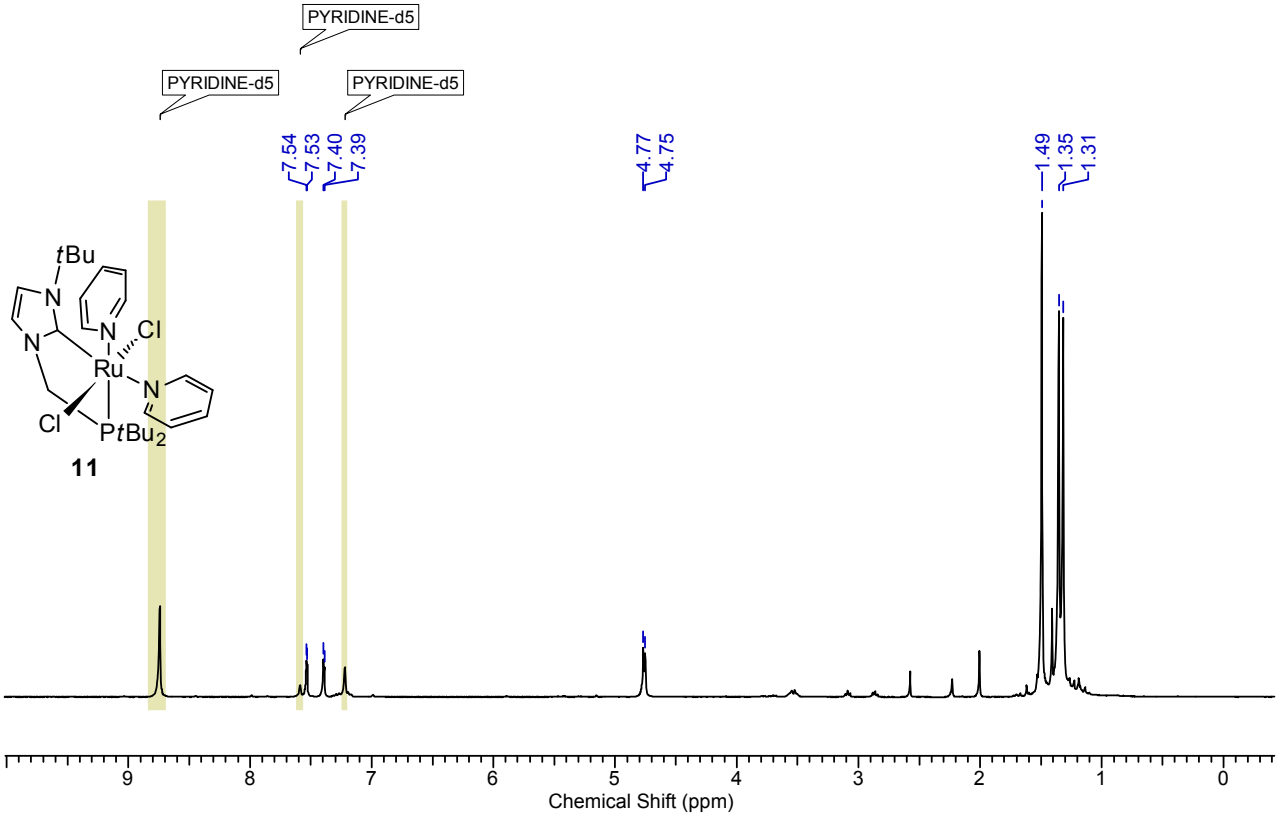
^{13}C NMR spectrum of **10a,b**



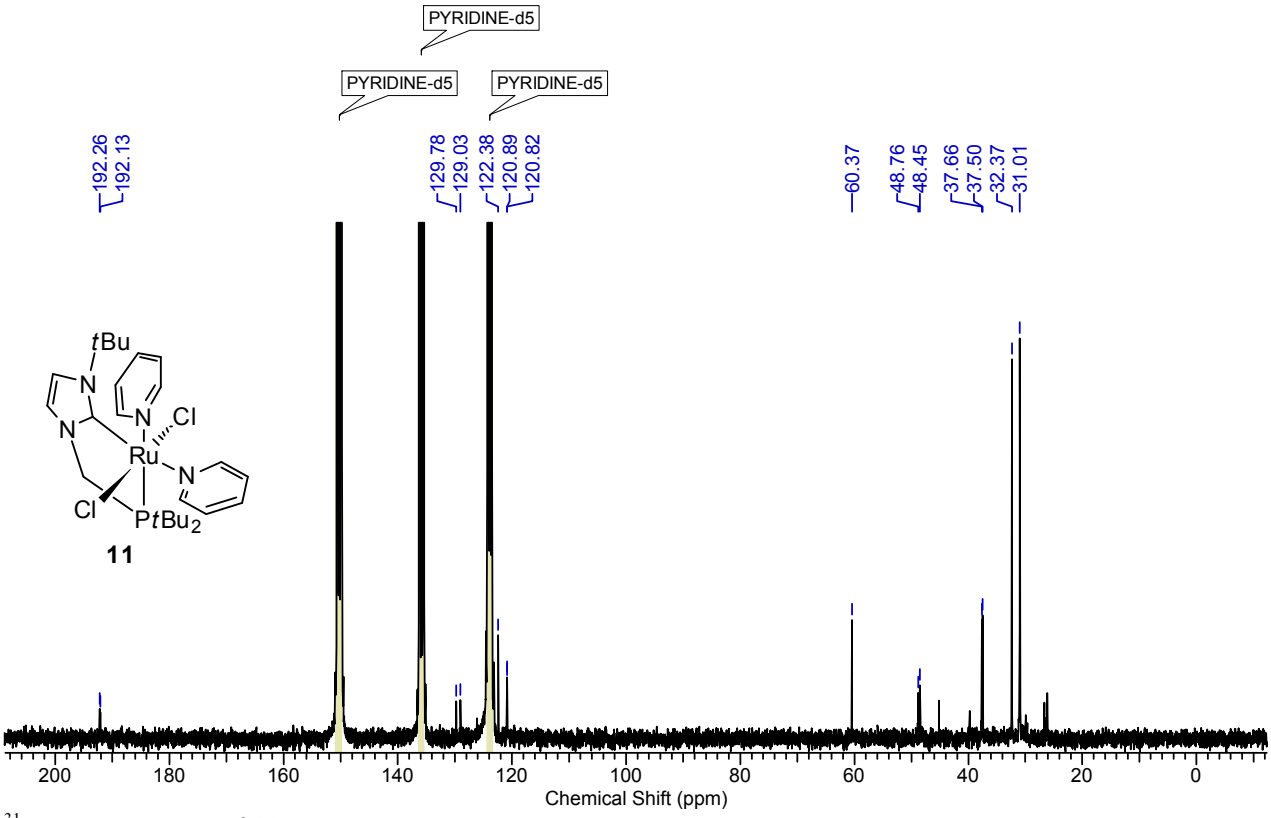
^{31}P NMR spectrum of **10a,b**



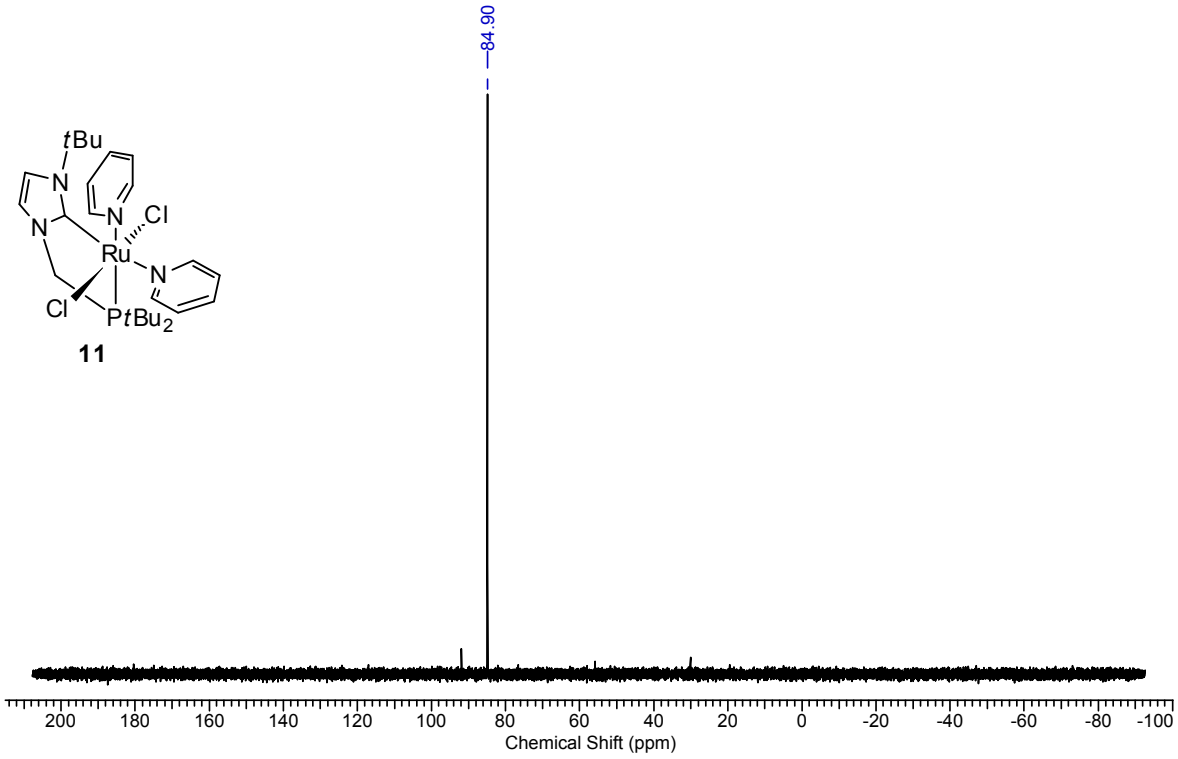
^{1}H NMR spectrum of **11**



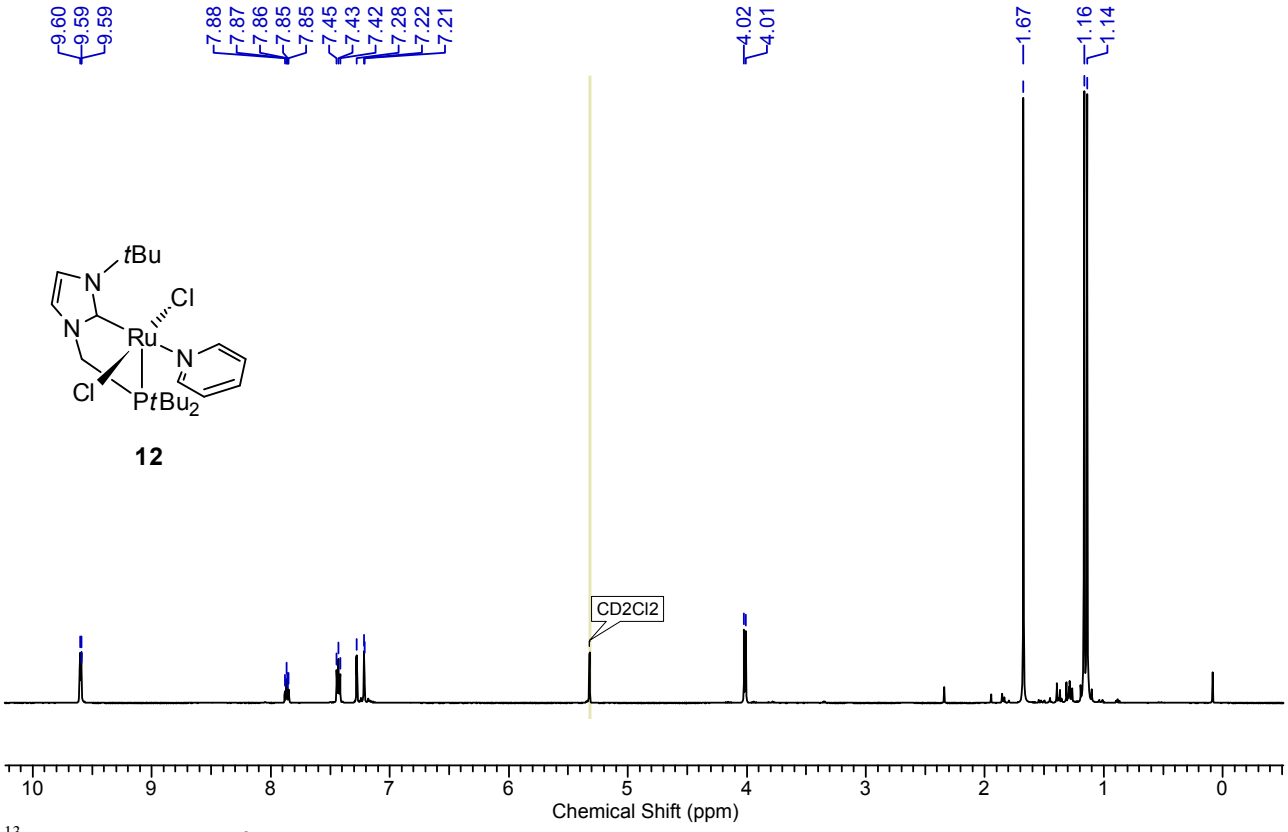
^{13}C NMR spectrum of **11**



^{31}P NMR spectrum of **11**

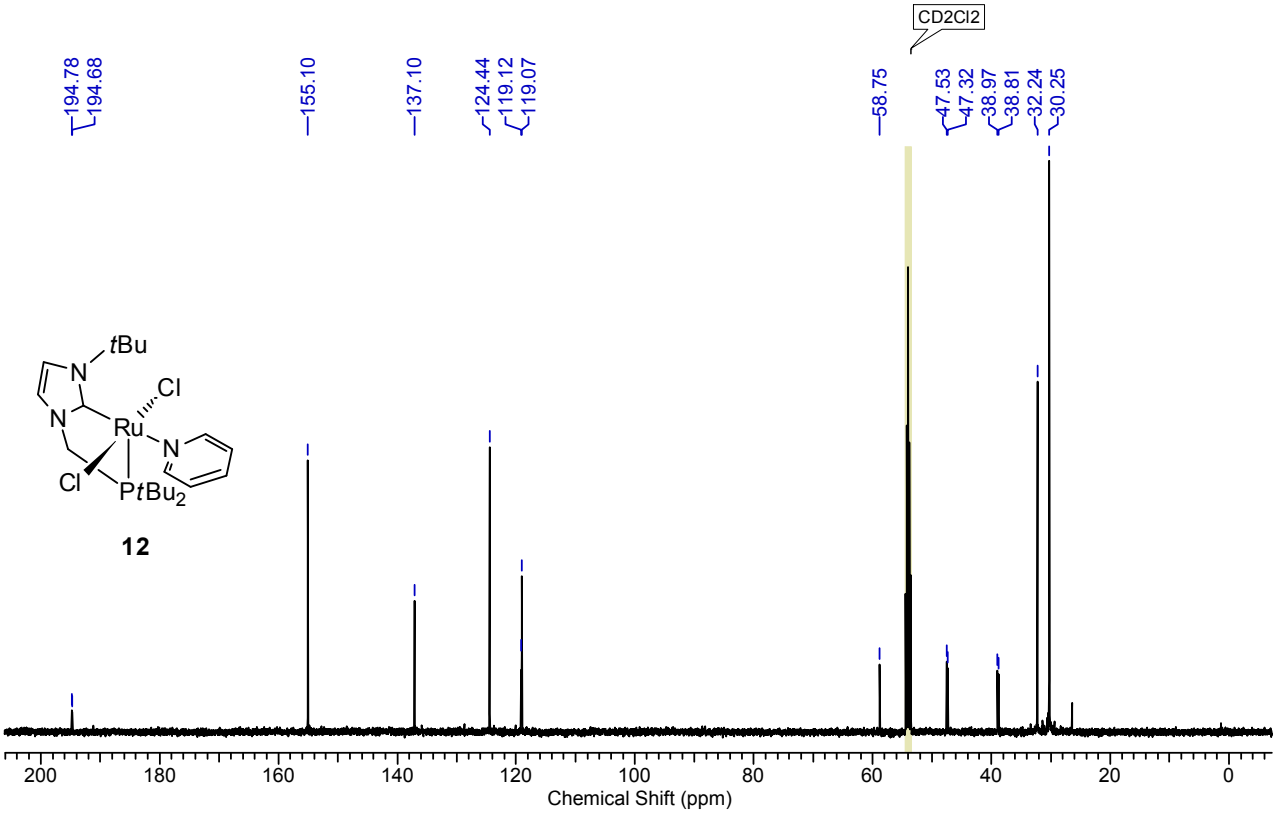


^{1}H NMR spectrum of **12**



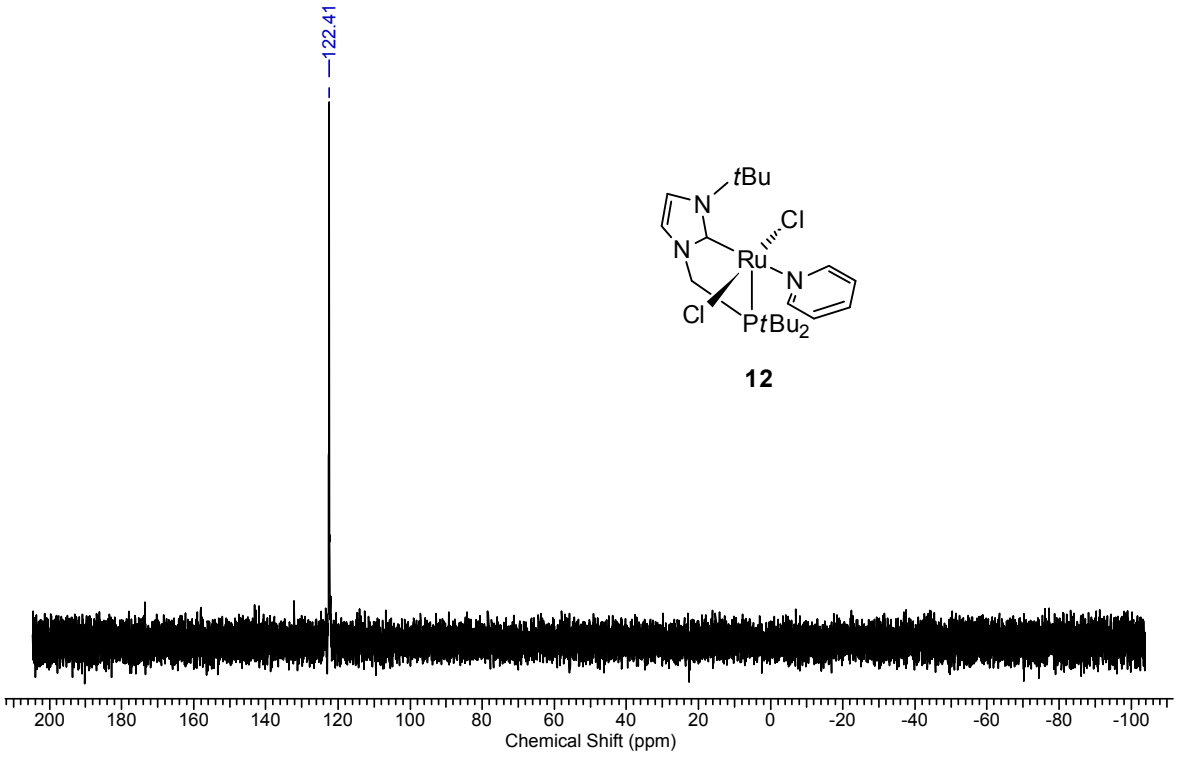
12

^{13}C NMR spectrum of **12**



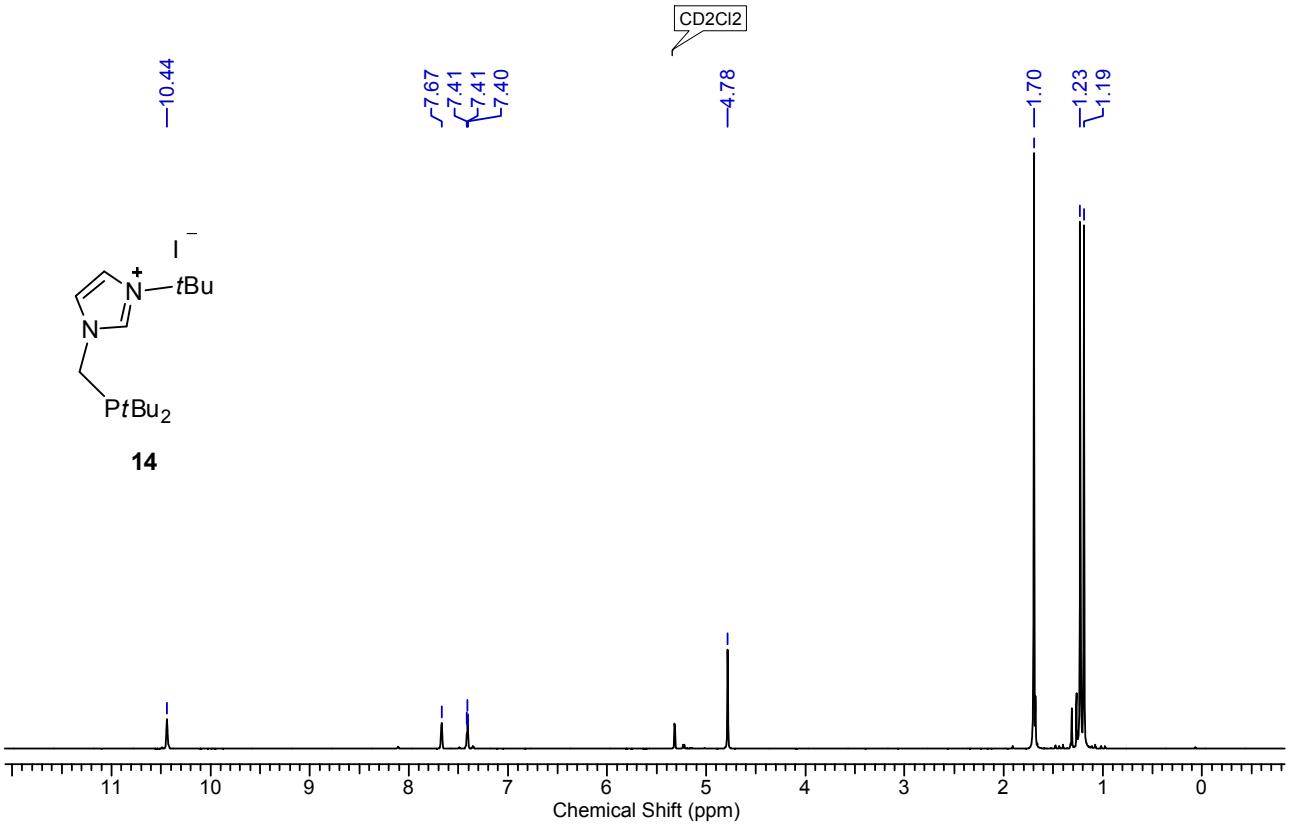
12

^{31}P NMR spectrum of **12**



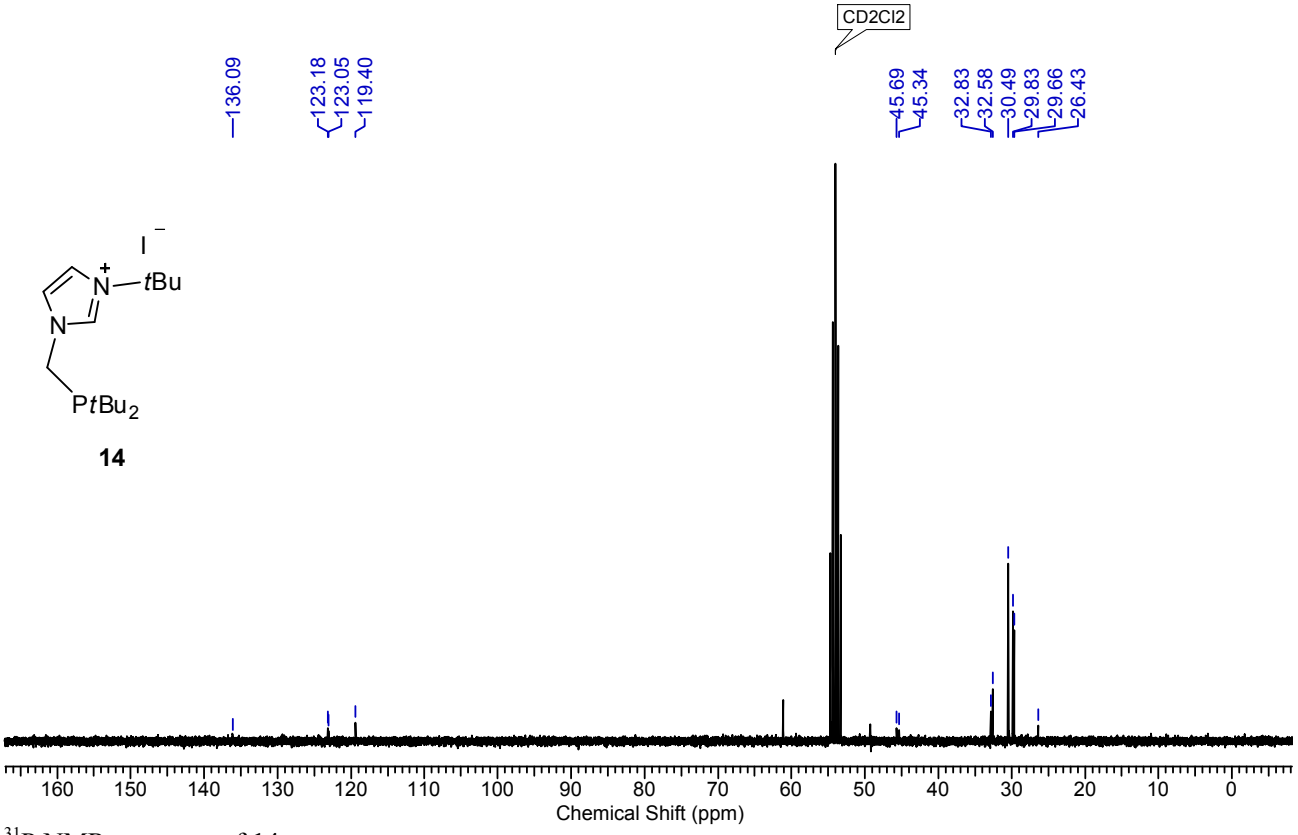
12

^{1}H NMR spectrum of **14**

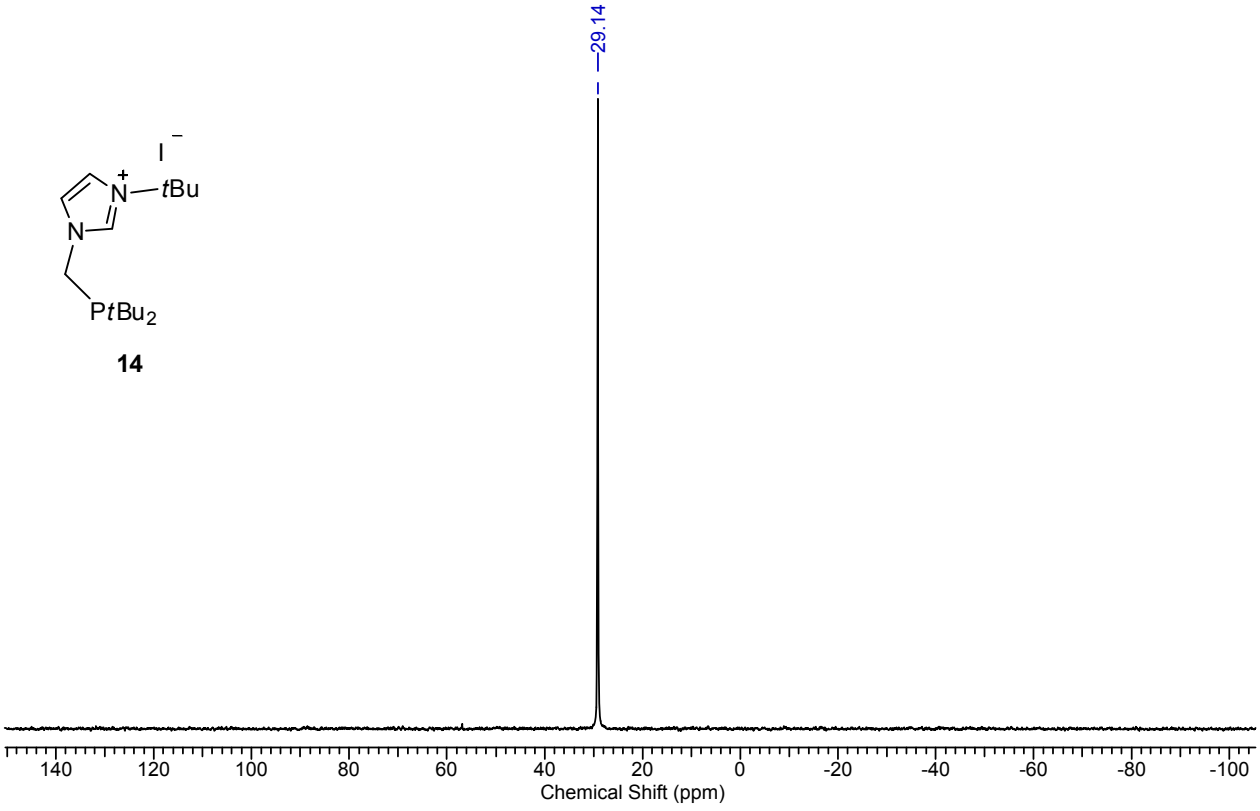


14

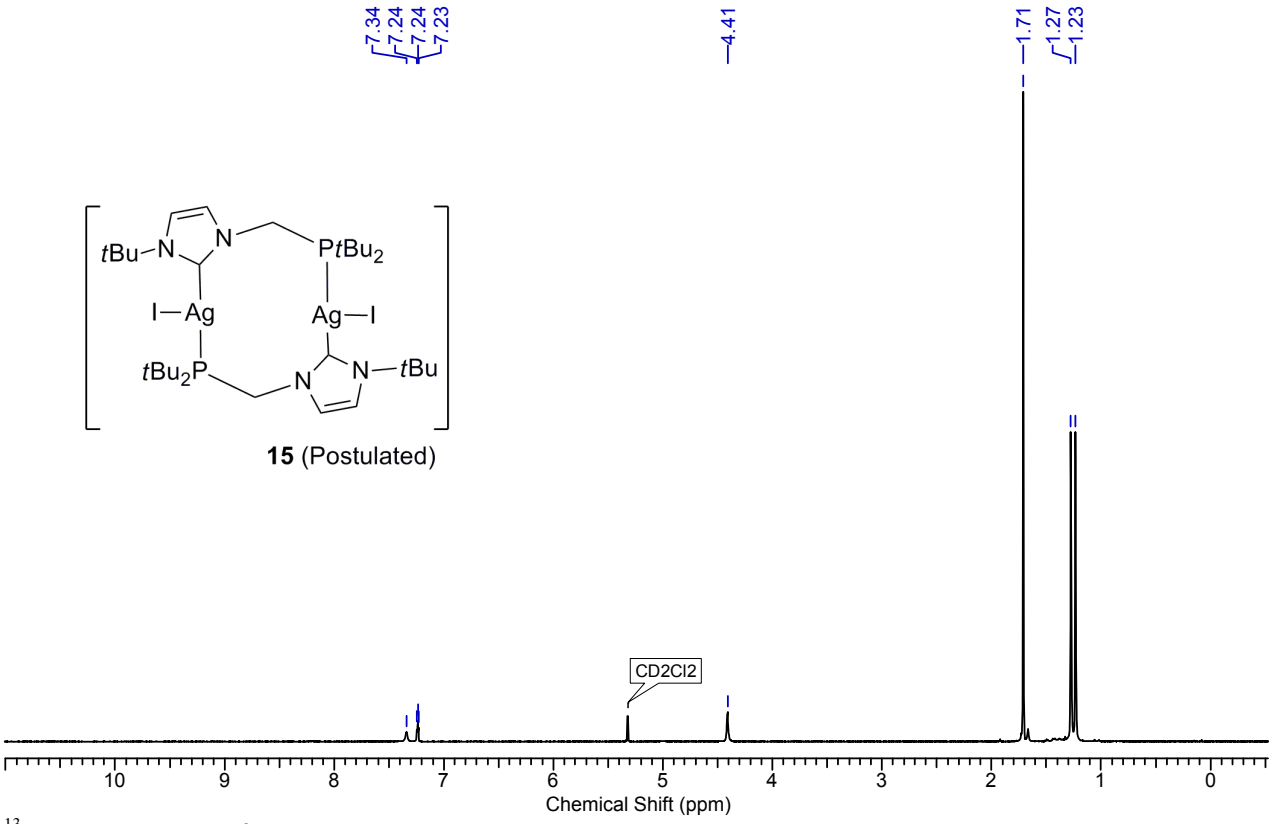
^{13}C NMR spectrum of **14**



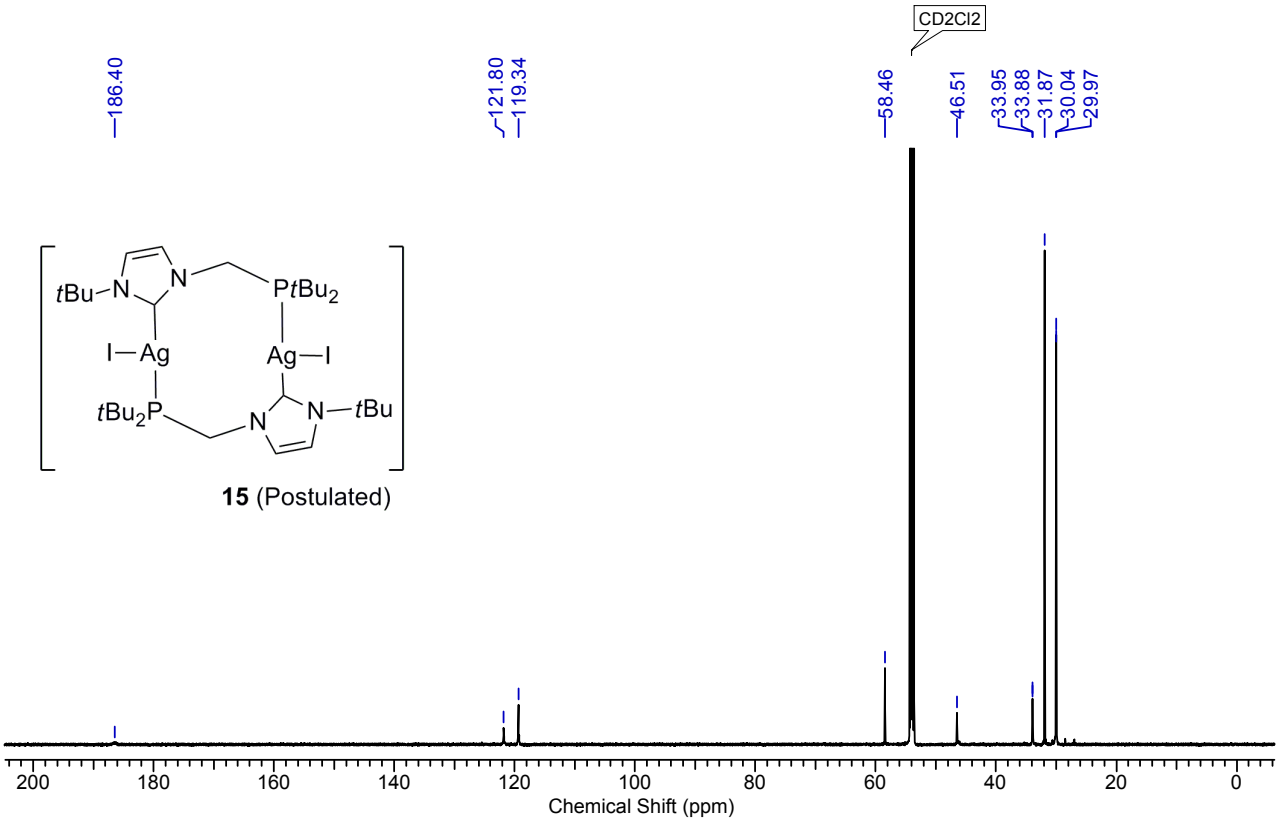
^{31}P NMR spectrum of **14**



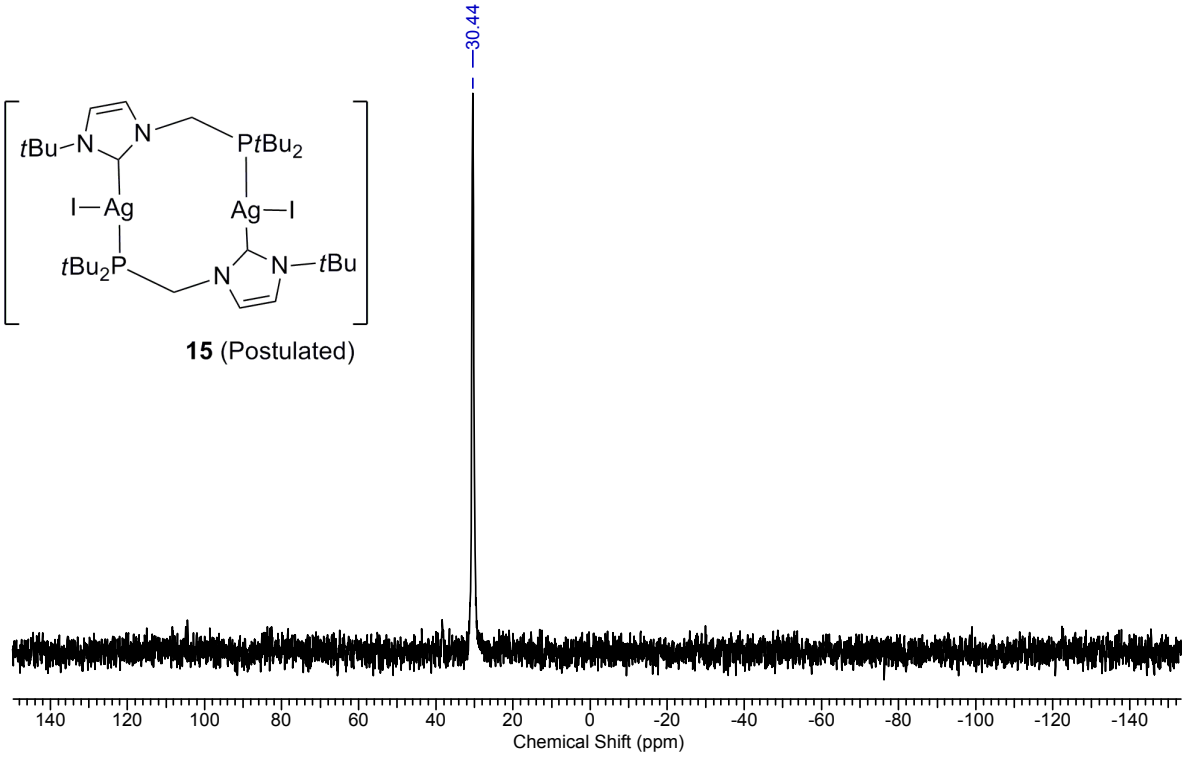
^{1}H NMR spectrum of **15**



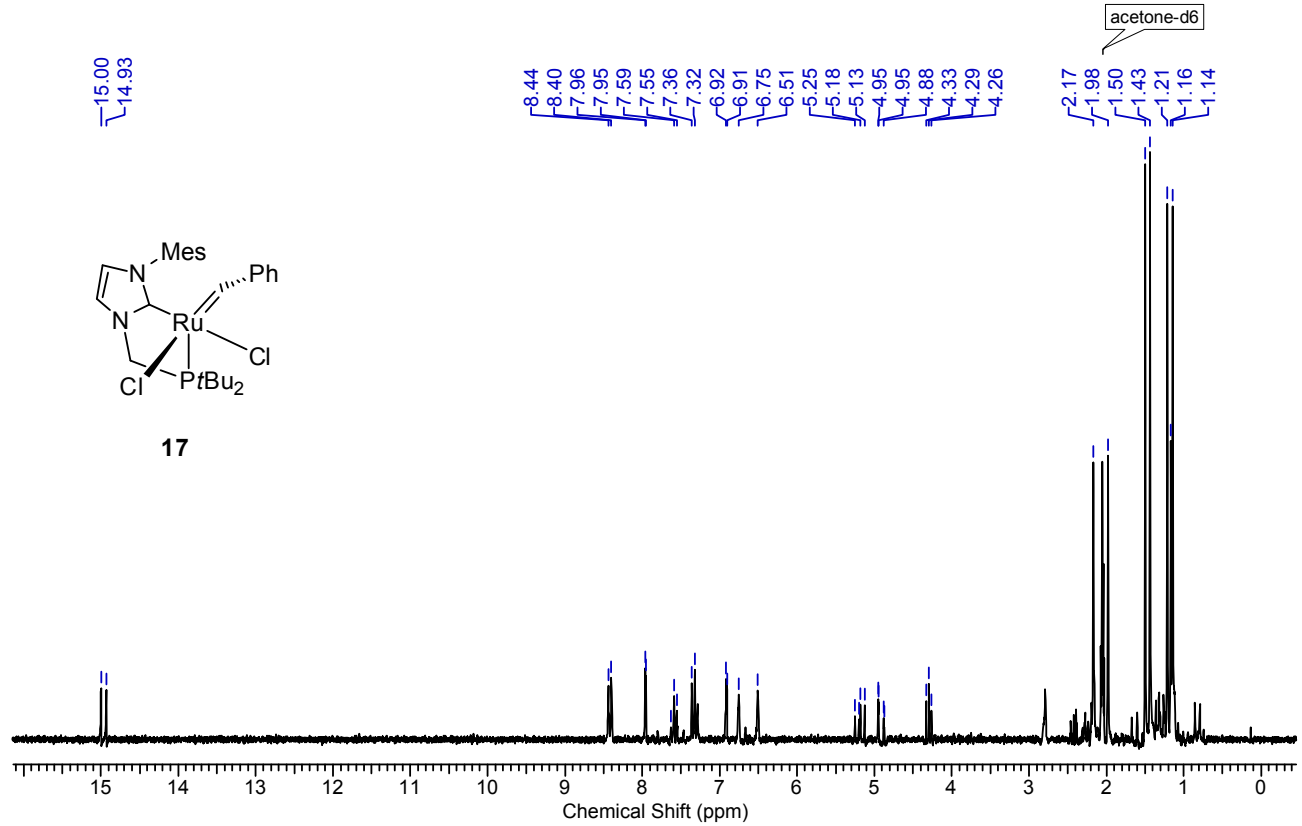
^{13}C NMR spectrum of **15**



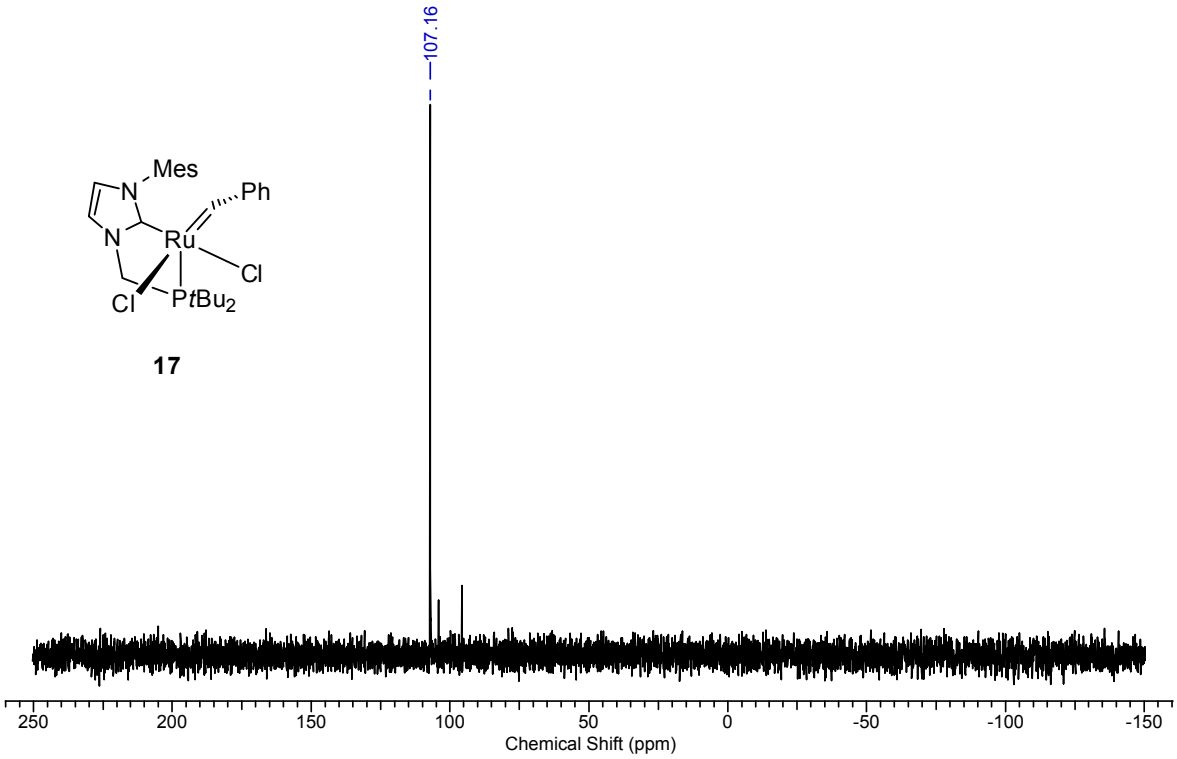
^{31}P NMR spectrum of **15**



^{1}H NMR spectrum of **17**

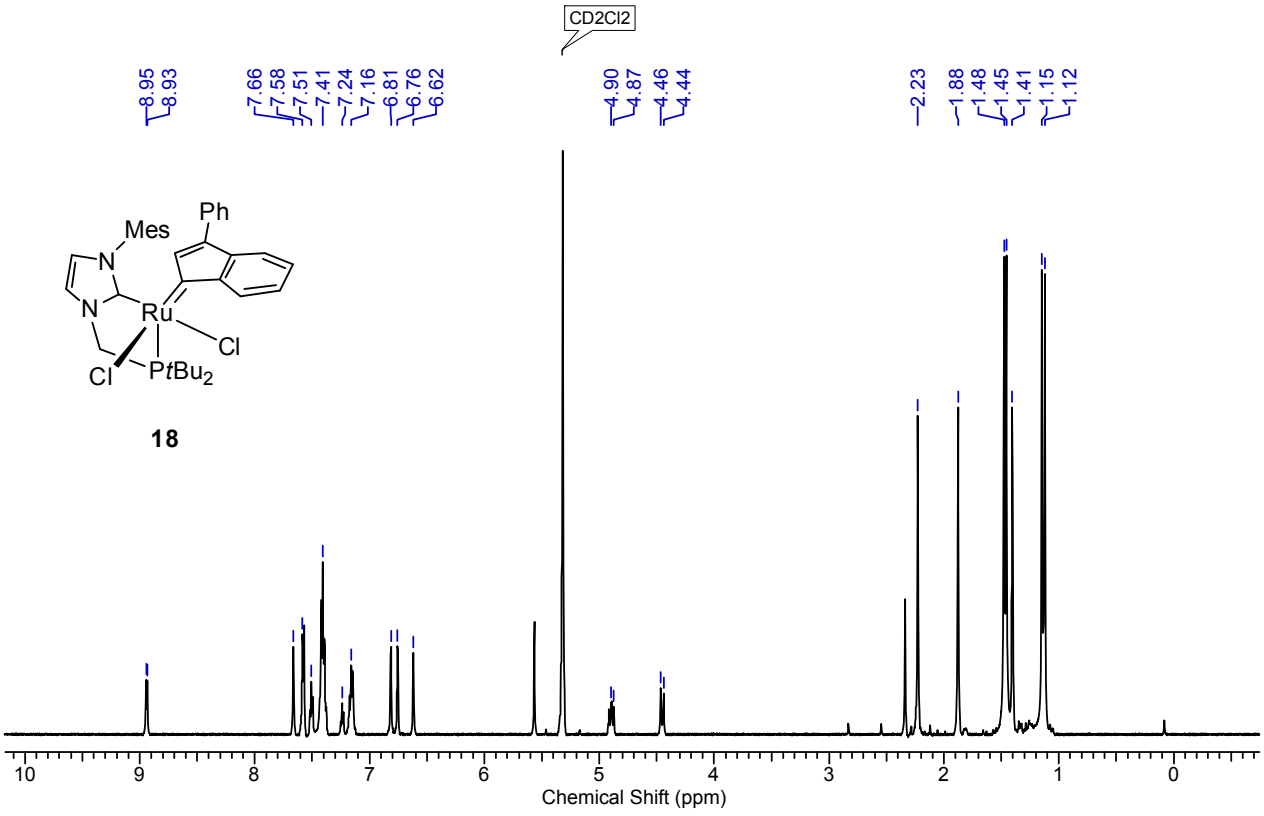


^{31}P NMR spectrum of **17**



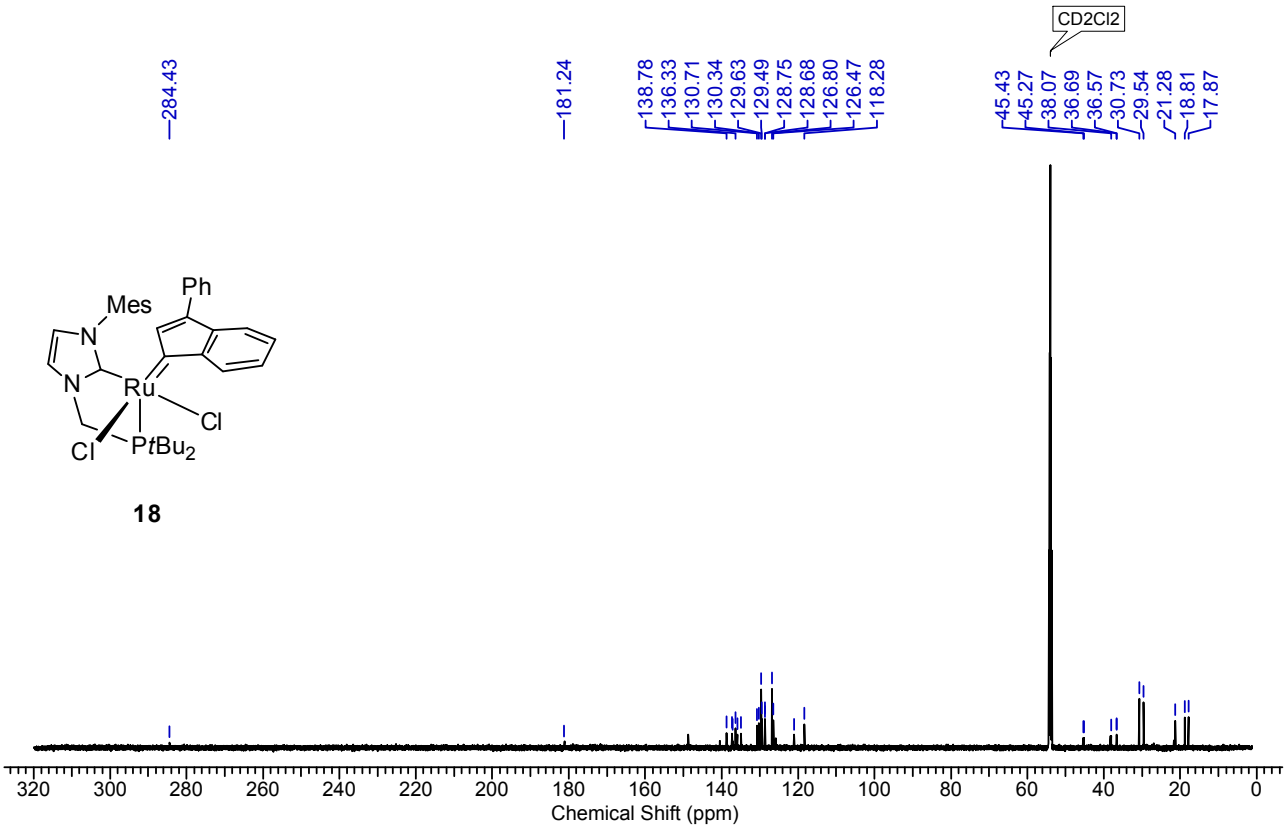
17

^{1}H NMR spectrum of **18**



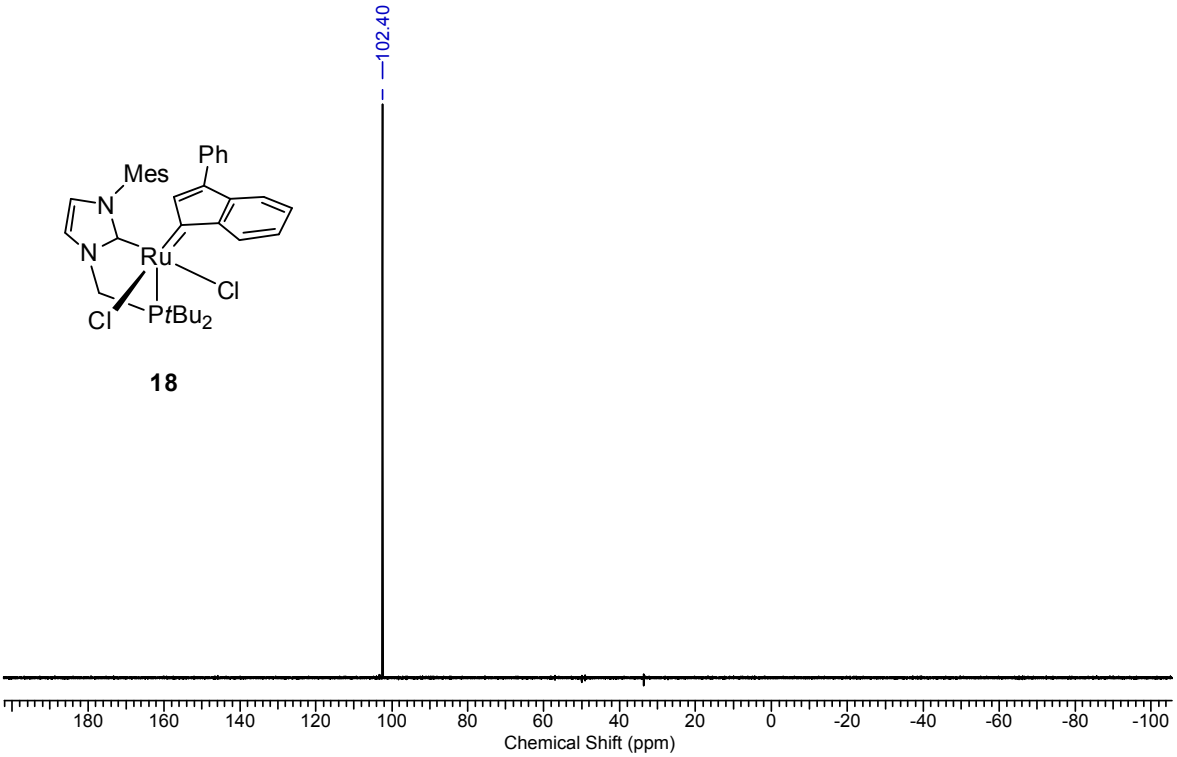
18

^{13}C NMR spectrum of **18**



18

^{31}P NMR spectrum of **18**



18

3. X-ray data

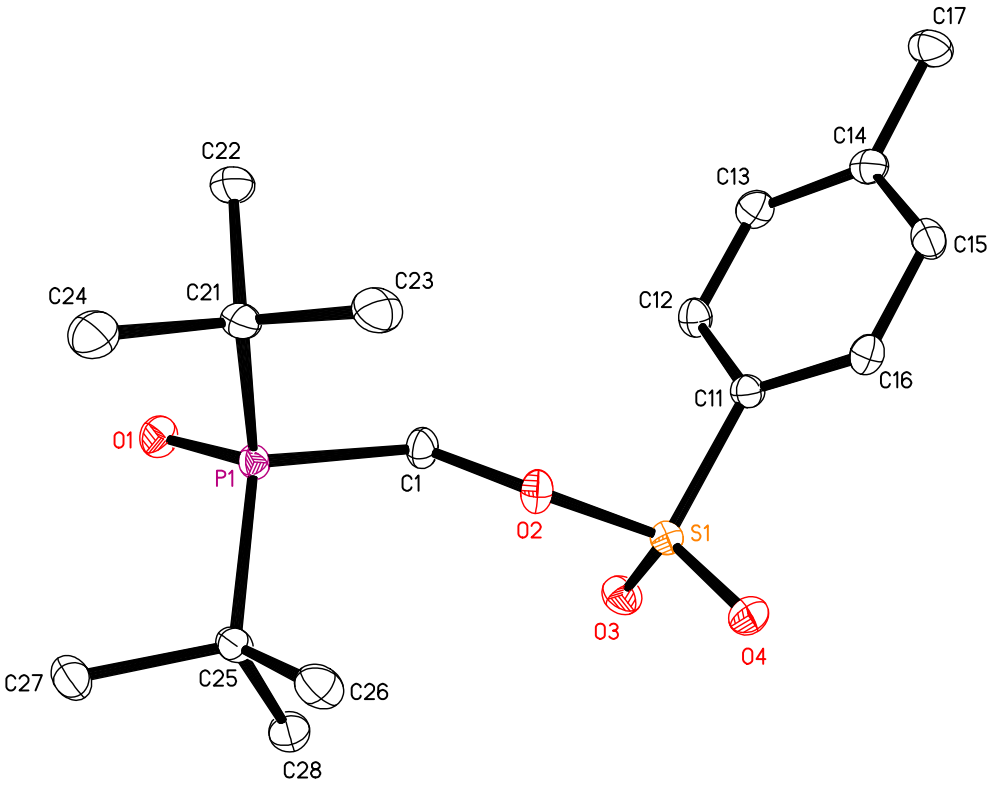


Table 1: Crystal data and structure refinement for **2**.

Identification code	ub4	
Empirical formula	$C_{16}H_{27}O_4PS$	
Formula weight	346.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Z	8	
Unit cell dimensions	a = 8.3785(7) Å	α = 90 deg.
	b = 12.2459(11) Å	β = 92.053(2) deg.
	c = 34.640(3) Å	γ = 90 deg.
Volume	3551.9(5) $Å^3$	
Density (calculated)	1.30 g/cm^3	
Absorption coefficient	0.29 mm^{-1}	
Crystal shape	prism	
Crystal size	0.48 x 0.23 x 0.20 mm^3	
Theta range for data collection	2.0 to 28.4 deg.	
Index ranges	$-11 \le h \le 11$, $-16 \le k \le 16$, $-46 \le l \le 45$	
Reflections collected	34959	
Independent reflections	8757 (R(int) = 0.0491)	
Observed reflections	7557 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.94 and 0.87	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	8757 / 0 / 613	
Goodness-of-fit on F^2	1.05	

Final R indices (I>2σ(I))	R1 = 0.039, wR2 = 0.096
Largest diff. peak and hole	0.54 and -0.38 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **2**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
S1	0.0723(1)	0.7631(1)	0.0029(1)	0.0124(1)
P1	0.4021(1)	0.9541(1)	0.0693(1)	0.0114(1)
O1	0.4575(1)	1.0663(1)	0.0588(1)	0.0166(2)
O2	0.2167(1)	0.7961(1)	0.0321(1)	0.0148(2)
O3	-0.0064(1)	0.8611(1)	-0.0099(1)	0.0178(2)
O4	-0.0123(1)	0.6818(1)	0.0236(1)	0.0168(2)
C1	0.3008(2)	0.8986(1)	0.0253(1)	0.0151(3)
C11	0.1653(2)	0.7012(1)	-0.0362(1)	0.0128(3)
C12	0.2431(2)	0.7663(1)	-0.0628(1)	0.0155(3)
C13	0.3188(2)	0.7161(1)	-0.0931(1)	0.0167(3)
C14	0.3160(2)	0.6026(1)	-0.0978(1)	0.0155(3)
C15	0.2344(2)	0.5398(1)	-0.0710(1)	0.0162(3)
C16	0.1599(2)	0.5884(1)	-0.0401(1)	0.0148(3)
C17	0.4002(2)	0.5496(1)	-0.1306(1)	0.0210(3)
C21	0.5726(2)	0.8631(1)	0.0811(1)	0.0148(3)
C22	0.6961(2)	0.8852(1)	0.0501(1)	0.0196(3)
C23	0.5300(2)	0.7408(1)	0.0803(1)	0.0205(3)
C24	0.6494(2)	0.8931(2)	0.1207(1)	0.0220(3)
C25	0.2523(2)	0.9603(1)	0.1073(1)	0.0130(3)
C26	0.2097(2)	0.8496(1)	0.1251(1)	0.0181(3)
C27	0.3162(2)	1.0386(1)	0.1393(1)	0.0178(3)
C28	0.0995(2)	1.0103(1)	0.0884(1)	0.0179(3)
C1A	0.7422(2)	0.0114(1)	0.2925(1)	0.0186(3)
S1A	0.9742(1)	0.0274(1)	0.3447(1)	0.0188(1)
P1A	0.6873(1)	0.0745(1)	0.2458(1)	0.0131(1)
O1A	0.5735(1)	-0.0023(1)	0.2258(1)	0.0216(2)
O2A	0.8390(1)	0.0828(1)	0.3174(1)	0.0190(2)
O3A	1.0456(1)	-0.0599(1)	0.3238(1)	0.0264(3)
O4A	1.0674(1)	0.1181(1)	0.3580(1)	0.0265(3)
C11A	0.8680(2)	-0.0281(1)	0.3829(1)	0.0160(3)
C12A	0.8393(2)	-0.1399(1)	0.3850(1)	0.0195(3)
C13A	0.7566(2)	-0.1803(1)	0.4160(1)	0.0200(3)
C14A	0.7019(2)	-0.1109(1)	0.4447(1)	0.0162(3)
C15A	0.7320(2)	0.0007(1)	0.4417(1)	0.0178(3)
C16A	0.8152(2)	0.0429(1)	0.4112(1)	0.0177(3)
C17A	0.6148(2)	-0.1557(2)	0.4785(1)	0.0226(3)
C21A	0.5916(2)	0.2072(1)	0.2558(1)	0.0183(3)
C22A	0.7086(2)	0.3002(1)	0.2660(1)	0.0240(3)
C23A	0.4877(2)	0.2382(2)	0.2199(1)	0.0264(4)
C24A	0.4797(2)	0.1890(2)	0.2897(1)	0.0277(4)
C25A	0.8748(2)	0.0853(1)	0.2193(1)	0.0179(3)
C26A	0.9197(2)	-0.0337(1)	0.2095(1)	0.0271(4)
C27A	1.0177(2)	0.1383(2)	0.2409(1)	0.0277(4)
C28A	0.8384(2)	0.1469(1)	0.1813(1)	0.0242(3)

Table 3:Hydrogen coordinates and isotropic displacement parameters (Å^2) for **2**.

Atom	x	y	z	U_{eq}
H1A	0.227(2)	0.9530(15)	0.0170(6)	0.024(5)
H1B	0.379(2)	0.8871(15)	0.0060(5)	0.022(5)
H12	0.2468(19)	0.8429(14)	-0.0605(5)	0.013(4)
H13	0.372(2)	0.7611(15)	-0.1102(5)	0.020(4)
H15	0.228(2)	0.4624(15)	-0.0739(5)	0.016(4)
H16	0.105(2)	0.5443(15)	-0.0228(6)	0.021(5)
H17A	0.514(3)	0.559(2)	-0.1288(8)	0.058(8)
H17B	0.358(3)	0.5756(19)	-0.1540(7)	0.045(6)
H17C	0.380(3)	0.473(2)	-0.1310(7)	0.051(7)
H22A	0.652(2)	0.8727(16)	0.0239(6)	0.028(5)
H22B	0.735(2)	0.9602(15)	0.0525(5)	0.021(5)
H22C	0.784(3)	0.8360(17)	0.0545(6)	0.032(5)
H23A	0.450(2)	0.7220(17)	0.0984(6)	0.031(5)
H23B	0.492(2)	0.7175(16)	0.0546(6)	0.026(5)
H23C	0.625(2)	0.6987(17)	0.0861(6)	0.032(5)
H24A	0.580(2)	0.8729(15)	0.1422(5)	0.020(4)
H24B	0.750(3)	0.855(2)	0.1230(7)	0.051(7)
H24C	0.672(2)	0.9689(18)	0.1219(6)	0.030(5)
H26A	0.172(2)	0.8028(15)	0.1064(6)	0.020(5)
H26B	0.123(2)	0.8612(16)	0.1437(6)	0.027(5)
H26C	0.298(2)	0.8170(15)	0.1402(5)	0.022(5)
H27A	0.401(2)	1.0099(16)	0.1555(6)	0.028(5)
H27B	0.228(2)	1.0569(15)	0.1568(6)	0.025(5)
H27C	0.356(2)	1.1060(17)	0.1282(6)	0.030(5)
H28A	0.121(2)	1.0816(16)	0.0750(6)	0.024(5)
H28B	0.049(2)	0.9634(15)	0.0693(6)	0.025(5)
H28C	0.023(2)	1.0221(16)	0.1097(6)	0.031(5)
H1C	0.804(2)	-0.0541(16)	0.2885(6)	0.027(5)
H1D	0.643(2)	-0.0085(15)	0.3056(5)	0.018(4)
H12A	0.874(2)	-0.1879(16)	0.3655(6)	0.025(5)
H13A	0.738(2)	-0.2535(17)	0.4173(6)	0.026(5)
H15A	0.696(2)	0.0500(16)	0.4613(6)	0.030(5)
H16A	0.836(2)	0.1206(16)	0.4092(5)	0.021(5)
H17D	0.511(3)	-0.116(2)	0.4813(7)	0.048(7)
H17E	0.683(3)	-0.1563(17)	0.5015(6)	0.035(5)
H17F	0.593(3)	-0.231(2)	0.4736(7)	0.047(7)
H22D	0.785(2)	0.2823(17)	0.2881(6)	0.030(5)
H22E	0.773(2)	0.3213(16)	0.2422(6)	0.026(5)
H22F	0.653(3)	0.3687(18)	0.2729(6)	0.037(6)
H23D	0.553(2)	0.2552(17)	0.1981(6)	0.029(5)
H23E	0.429(3)	0.301(2)	0.2271(7)	0.045(6)
H23F	0.418(3)	0.1841(18)	0.2122(6)	0.034(6)
H24D	0.418(2)	0.2557(18)	0.2919(6)	0.031(5)
H24E	0.411(3)	0.1286(19)	0.2839(7)	0.045(6)
H24F	0.542(2)	0.1771(17)	0.3146(6)	0.032(5)
H26D	0.835(3)	-0.0703(17)	0.1952(6)	0.034(6)
H26E	1.019(2)	-0.0301(16)	0.1940(6)	0.027(5)
H26F	0.947(3)	-0.0765(18)	0.2335(7)	0.036(6)
H27D	1.058(3)	0.0944(19)	0.2643(7)	0.044(6)
H27E	1.108(3)	0.1408(17)	0.2238(6)	0.035(6)
H27F	0.996(2)	0.2112(17)	0.2490(6)	0.030(5)
H28D	0.743(3)	0.1232(17)	0.1673(6)	0.031(5)
H28E	0.830(2)	0.2254(17)	0.1857(6)	0.029(5)
H28F	0.928(3)	0.1357(17)	0.1644(6)	0.036(6)

Table 4: Anisotropic displacement parameters ($Å^2$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 (h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S1	0.0126(2)	0.0123(2)	0.0125(2)	-0.0010(1)	0.0008(1)	-0.0005(1)
P1	0.0129(2)	0.0099(2)	0.0113(2)	-0.0008(1)	0.0015(1)	-0.0017(1)
O1	0.0188(5)	0.0125(5)	0.0187(5)	0.0015(4)	0.0024(4)	-0.0037(4)
O2	0.0174(5)	0.0135(5)	0.0134(5)	-0.0004(4)	-0.0016(4)	-0.0037(4)
O3	0.0185(5)	0.0158(5)	0.0191(5)	-0.0008(4)	-0.0001(4)	0.0038(4)
O4	0.0162(5)	0.0171(5)	0.0173(5)	0.0000(4)	0.0040(4)	-0.0033(4)
C1	0.0183(7)	0.0135(7)	0.0135(7)	-0.0006(5)	0.0017(5)	-0.0052(5)
C11	0.0121(6)	0.0153(6)	0.0109(6)	-0.0014(5)	-0.0001(5)	0.0003(5)
C12	0.0181(7)	0.0136(7)	0.0148(7)	0.0002(5)	0.0002(5)	-0.0017(5)
C13	0.0175(7)	0.0194(7)	0.0134(7)	0.0016(5)	0.0017(5)	-0.0021(6)
C14	0.0127(6)	0.0217(7)	0.0120(6)	-0.0023(5)	-0.0018(5)	0.0012(5)
C15	0.0179(7)	0.0137(7)	0.0168(7)	-0.0027(5)	-0.0013(5)	0.0007(5)
C16	0.0148(6)	0.0150(7)	0.0145(7)	0.0000(5)	-0.0011(5)	-0.0025(5)
C17	0.0196(7)	0.0273(9)	0.0164(8)	-0.0053(6)	0.0023(6)	0.0028(6)
C21	0.0138(6)	0.0137(6)	0.0170(7)	-0.0020(5)	0.0029(5)	0.0012(5)
C22	0.0158(7)	0.0197(8)	0.0237(8)	-0.0039(6)	0.0068(6)	-0.0017(6)
C23	0.0200(7)	0.0134(7)	0.0283(9)	-0.0001(6)	0.0047(6)	0.0021(6)
C24	0.0177(7)	0.0266(8)	0.0217(8)	-0.0020(6)	-0.0018(6)	0.0035(6)
C25	0.0150(6)	0.0118(6)	0.0124(6)	-0.0009(5)	0.0029(5)	0.0000(5)
C26	0.0241(7)	0.0148(7)	0.0160(7)	0.0014(6)	0.0065(6)	-0.0008(6)
C27	0.0202(7)	0.0170(7)	0.0163(7)	-0.0043(5)	0.0003(6)	0.0015(6)
C28	0.0152(7)	0.0186(7)	0.0199(7)	-0.0018(6)	-0.0005(6)	0.0016(6)
C1A	0.0200(7)	0.0191(7)	0.0166(7)	0.0024(6)	0.0000(6)	-0.0017(6)
S1A	0.0167(2)	0.0240(2)	0.0155(2)	0.0032(1)	-0.0008(1)	0.0016(1)
P1A	0.0139(2)	0.0131(2)	0.0124(2)	0.0000(1)	0.0001(1)	-0.0007(1)
O1A	0.0223(5)	0.0184(5)	0.0236(6)	-0.0013(4)	-0.0051(4)	-0.0048(4)
O2A	0.0215(5)	0.0187(5)	0.0165(5)	0.0016(4)	-0.0039(4)	0.0013(4)
O3A	0.0235(6)	0.0334(7)	0.0225(6)	0.0014(5)	0.0032(5)	0.0091(5)
O4A	0.0243(6)	0.0325(7)	0.0223(6)	0.0071(5)	-0.0026(5)	-0.0081(5)
C11A	0.0147(6)	0.0185(7)	0.0146(7)	0.0018(5)	-0.0017(5)	0.0018(5)
C12A	0.0227(7)	0.0164(7)	0.0191(7)	-0.0035(6)	-0.0014(6)	0.0040(6)
C13A	0.0233(7)	0.0116(7)	0.0250(8)	0.0014(6)	-0.0032(6)	0.0010(6)
C14A	0.0142(6)	0.0171(7)	0.0169(7)	0.0039(5)	-0.0038(5)	0.0006(5)
C15A	0.0212(7)	0.0158(7)	0.0163(7)	-0.0016(5)	-0.0010(6)	0.0028(6)
C16A	0.0221(7)	0.0118(7)	0.0191(7)	0.0012(5)	-0.0011(6)	-0.0003(5)
C17A	0.0196(7)	0.0268(9)	0.0211(8)	0.0074(6)	-0.0015(6)	-0.0017(6)
C21A	0.0183(7)	0.0179(7)	0.0186(7)	-0.0023(6)	0.0008(5)	0.0032(6)
C22A	0.0285(8)	0.0175(7)	0.0259(8)	-0.0055(6)	-0.0003(7)	0.0012(6)
C23A	0.0254(8)	0.0257(9)	0.0275(9)	-0.0003(7)	-0.0053(7)	0.0082(7)
C24A	0.0220(8)	0.0335(10)	0.0281(9)	-0.0040(7)	0.0080(7)	0.0052(7)
C25A	0.0190(7)	0.0200(7)	0.0150(7)	0.0001(5)	0.0046(5)	0.0011(6)
C26A	0.0316(9)	0.0228(8)	0.0275(9)	-0.0008(7)	0.0085(7)	0.0084(7)
C27A	0.0171(7)	0.0382(10)	0.0282(9)	-0.0028(8)	0.0064(6)	-0.0051(7)
C28A	0.0337(9)	0.0221(8)	0.0172(7)	0.0018(6)	0.0070(7)	0.0007(7)

Table 5: Bond lengths (Å) and angles (deg) for **2**.

S1-O4	1.4304(10)	P1-C21	1.8459(15)
S1-O3	1.4316(11)	P1-C25	1.8541(14)
S1-O2	1.6009(10)	O2-C1	1.4621(17)
S1-C11	1.7589(14)	C1-H1A	0.95(2)
P1-O1	1.4988(10)	C1-H1B	0.965(19)
P1-C1	1.8457(15)	C11-C16	1.389(2)

C11-C12	1.3981(19)	C21A-C22A	1.536(2)
C12-C13	1.388(2)	C21A-C23A	1.539(2)
C12-H12	0.942(17)	C21A-C24A	1.543(2)
C13-C14	1.399(2)	C22A-H22D	1.00(2)
C13-H13	0.931(19)	C22A-H22E	1.04(2)
C14-C15	1.400(2)	C22A-H22F	0.99(2)
C14-C17	1.508(2)	C23A-H23D	0.97(2)
C15-C16	1.392(2)	C23A-H23E	0.95(2)
C15-H15	0.955(18)	C23A-H23F	0.92(2)
C16-H16	0.936(19)	C24A-H24D	0.97(2)
C17-H17A	0.96(3)	C24A-H24E	0.95(2)
C17-H17B	0.93(3)	C24A-H24F	1.00(2)
C17-H17C	0.95(3)	C25A-C27A	1.534(2)
C21-C24	1.537(2)	C25A-C28A	1.538(2)
C21-C23	1.539(2)	C25A-C26A	1.546(2)
C21-C22	1.541(2)	C26A-H26D	0.96(2)
C22-H22A	0.98(2)	C26A-H26E	1.01(2)
C22-H22B	0.975(19)	C26A-H26F	1.00(2)
C22-H22C	0.96(2)	C27A-H27D	1.02(2)
C23-H23A	0.96(2)	C27A-H27E	0.98(2)
C23-H23B	0.98(2)	C27A-H27F	0.95(2)
C23-H23C	0.96(2)	C28A-H28D	0.96(2)
C24-H24A	0.995(19)	C28A-H28E	0.98(2)
C24-H24B	0.97(3)	C28A-H28F	0.98(2)
C24-H24C	0.95(2)		
C25-C26	1.537(2)	O4-S1-O3	120.53(6)
C25-C28	1.543(2)	O4-S1-O2	103.63(6)
C25-C27	1.544(2)	O3-S1-O2	108.23(6)
C26-H26A	0.915(19)	O4-S1-C11	109.15(6)
C26-H26B	1.00(2)	O3-S1-C11	109.56(6)
C26-H26C	0.974(19)	O2-S1-C11	104.45(6)
C27-H27A	0.95(2)	O1-P1-C1	105.97(6)
C27-H27B	1.00(2)	O1-P1-C21	111.29(6)
C27-H27C	0.97(2)	C1-P1-C21	106.85(7)
C28-H28A	1.01(2)	O1-P1-C25	110.94(6)
C28-H28B	0.96(2)	C1-P1-C25	107.37(7)
C28-H28C	1.00(2)	C21-P1-C25	113.95(6)
C1A-O2A	1.4539(18)	C1-O2-S1	118.25(9)
C1A-P1A	1.8376(16)	O2-C1-P1	113.19(9)
C1A-H1C	0.97(2)	O2-C1-H1A	109.7(11)
C1A-H1D	0.989(18)	P1-C1-H1A	105.6(12)
S1A-O4A	1.4250(13)	O2-C1-H1B	109.3(11)
S1A-O3A	1.4330(12)	P1-C1-H1B	108.7(11)
S1A-O2A	1.6000(11)	H1A-C1-H1B	110.3(16)
S1A-C11A	1.7579(15)	C16-C11-C12	121.09(13)
P1A-O1A	1.4911(11)	C16-C11-S1	119.35(11)
P1A-C21A	1.8514(15)	C12-C11-S1	119.56(11)
P1A-C25A	1.8532(15)	C13-C12-C11	118.91(13)
C11A-C12A	1.391(2)	C13-C12-H12	119.4(10)
C11A-C16A	1.394(2)	C11-C12-H12	121.7(10)
C12A-C13A	1.389(2)	C12-C13-C14	121.33(13)
C12A-H12A	0.95(2)	C12-C13-H13	117.2(11)
C13A-C14A	1.398(2)	C14-C13-H13	121.4(11)
C13A-H13A	0.91(2)	C13-C14-C15	118.41(13)
C14A-C15A	1.395(2)	C13-C14-C17	120.54(14)
C14A-C17A	1.506(2)	C15-C14-C17	121.05(14)
C15A-C16A	1.387(2)	C16-C15-C14	121.16(13)
C15A-H15A	0.97(2)	C16-C15-H15	118.5(11)
C16A-H16A	0.970(19)	C14-C15-H15	120.4(11)
C17A-H17D	1.00(2)	C11-C16-C15	119.07(13)
C17A-H17E	0.97(2)	C11-C16-H16	121.7(11)
C17A-H17F	0.96(2)	C15-C16-H16	119.2(11)

C14-C17-H17A	112.9(16)	O3A-S1A-O2A	108.52(7)
C14-C17-H17B	109.5(15)	O4A-S1A-C11A	110.12(7)
H17A-C17-H17B	112(2)	O3A-S1A-C11A	108.87(7)
C14-C17-H17C	110.1(15)	O2A-S1A-C11A	103.98(6)
H17A-C17-H17C	107(2)	O1A-P1A-C1A	106.22(7)
H17B-C17-H17C	105(2)	O1A-P1A-C21A	111.51(7)
C24-C21-C23	109.68(13)	C1A-P1A-C21A	107.49(7)
C24-C21-C22	107.97(12)	O1A-P1A-C25A	110.77(7)
C23-C21-C22	108.70(12)	C1A-P1A-C25A	106.07(7)
C24-C21-P1	110.43(10)	C21A-P1A-C25A	114.26(7)
C23-C21-P1	113.96(10)	C1A-O2A-S1A	117.56(9)
C22-C21-P1	105.85(10)	C12A-C11A-C16A	121.05(14)
C21-C22-H22A	112.1(11)	C12A-C11A-S1A	120.93(12)
C21-C22-H22B	109.5(11)	C16A-C11A-S1A	118.02(11)
H22A-C22-H22B	109.9(16)	C13A-C12A-C11A	118.98(14)
C21-C22-H22C	108.0(13)	C13A-C12A-H12A	120.2(12)
H22A-C22-H22C	107.9(17)	C11A-C12A-H12A	120.8(12)
H22B-C22-H22C	109.3(16)	C12A-C13A-C14A	121.18(14)
C21-C23-H23A	112.9(12)	C12A-C13A-H13A	118.7(13)
C21-C23-H23B	111.5(12)	C14A-C13A-H13A	120.1(13)
H23A-C23-H23B	108.2(17)	C15A-C14A-C13A	118.53(14)
C21-C23-H23C	109.2(12)	C15A-C14A-C17A	120.61(14)
H23A-C23-H23C	109.0(17)	C13A-C14A-C17A	120.85(14)
H23B-C23-H23C	105.7(16)	C16A-C15A-C14A	121.31(14)
C21-C24-H24A	111.7(11)	C16A-C15A-H15A	118.9(12)
C21-C24-H24B	107.2(15)	C14A-C15A-H15A	119.8(12)
H24A-C24-H24B	110.5(18)	C15A-C16A-C11A	118.95(13)
C21-C24-H24C	110.5(13)	C15A-C16A-H16A	121.1(11)
H24A-C24-H24C	109.2(16)	C11A-C16A-H16A	120.0(11)
H24B-C24-H24C	107.5(19)	C14A-C17A-H17D	110.0(14)
C26-C25-C28	108.59(12)	C14A-C17A-H17E	110.8(13)
C26-C25-C27	109.86(12)	H17D-C17A-H17E	114.6(18)
C28-C25-C27	108.62(12)	C14A-C17A-H17F	108.0(14)
C26-C25-P1	114.92(10)	H17D-C17A-H17F	109(2)
C28-C25-P1	106.68(10)	H17E-C17A-H17F	104.2(19)
C27-C25-P1	107.98(10)	C22A-C21A-C23A	109.99(14)
C25-C26-H26A	110.3(12)	C22A-C21A-C24A	109.38(13)
C25-C26-H26B	108.5(11)	C23A-C21A-C24A	107.96(14)
H26A-C26-H26B	107.9(16)	C22A-C21A-P1A	114.64(11)
C25-C26-H26C	113.2(11)	C23A-C21A-P1A	107.52(11)
H26A-C26-H26C	111.2(16)	C24A-C21A-P1A	107.13(11)
H26B-C26-H26C	105.3(15)	C21A-C22A-H22D	113.5(12)
C25-C27-H27A	115.1(12)	C21A-C22A-H22E	110.4(11)
C25-C27-H27B	109.2(11)	H22D-C22A-H22E	108.8(16)
H27A-C27-H27B	105.8(16)	C21A-C22A-H22F	112.2(13)
C25-C27-H27C	111.0(12)	H22D-C22A-H22F	107.3(17)
H27A-C27-H27C	106.7(17)	H22E-C22A-H22F	104.2(16)
H27B-C27-H27C	108.6(16)	C21A-C23A-H23D	111.2(12)
C25-C28-H28A	112.2(11)	C21A-C23A-H23E	105.7(15)
C25-C28-H28B	113.3(11)	H23D-C23A-H23E	110.1(18)
H28A-C28-H28B	106.3(16)	C21A-C23A-H23F	113.2(14)
C25-C28-H28C	106.7(12)	H23D-C23A-H23F	107.7(18)
H28A-C28-H28C	110.1(16)	H23E-C23A-H23F	109.0(19)
H28B-C28-H28C	108.2(16)	C21A-C24A-H24D	106.0(12)
O2A-C1A-P1A	112.70(10)	C21A-C24A-H24E	109.3(14)
O2A-C1A-H1C	107.2(12)	H24D-C24A-H24E	110.7(18)
P1A-C1A-H1C	109.8(12)	C21A-C24A-H24F	111.2(12)
O2A-C1A-H1D	109.6(11)	H24D-C24A-H24F	108.4(17)
P1A-C1A-H1D	108.6(11)	H24E-C24A-H24F	111.1(18)
H1C-C1A-H1D	108.8(15)	C27A-C25A-C28A	109.81(14)
O4A-S1A-O3A	120.72(8)	C27A-C25A-C26A	108.35(14)
O4A-S1A-O2A	103.23(7)	C28A-C25A-C26A	108.50(13)

C27A-C25A-P1A	116.62(11)
C28A-C25A-P1A	108.26(11)
C26A-C25A-P1A	104.97(11)
C25A-C26A-H26D	111.9(13)
C25A-C26A-H26E	106.7(11)
H26D-C26A-H26E	110.7(17)
C25A-C26A-H26F	111.2(13)
H26D-C26A-H26F	109.2(18)
H26E-C26A-H26F	107.0(17)
C25A-C27A-H27D	113.3(13)
C25A-C27A-H27E	108.8(13)
H27D-C27A-H27E	104.8(18)
C25A-C27A-H27F	112.9(13)
H27D-C27A-H27F	108.7(18)
H27E-C27A-H27F	107.8(17)
C25A-C28A-H28D	114.7(13)
C25A-C28A-H28E	111.1(12)
H28D-C28A-H28E	108.4(17)
C25A-C28A-H28F	108.0(13)
H28D-C28A-H28F	107.3(17)
H28E-C28A-H28F	106.9(17)

Crystal data for 3a:

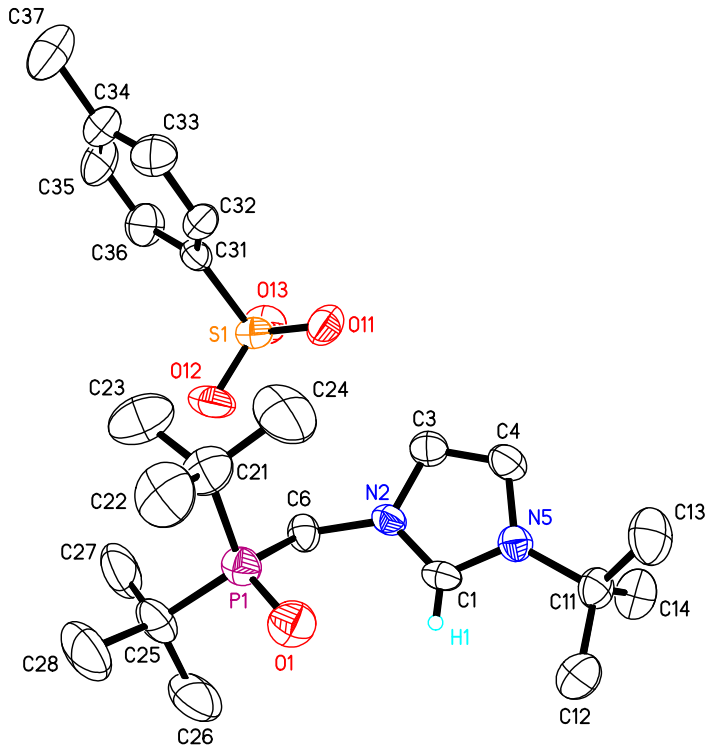


Table 1: Crystal data and structure refinement for **3a**.

Identification code	ub7	
Empirical formula	$C_{25}H_{43}Cl_4N_2O_4PS$	
Formula weight	640.44	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Z	4	
Unit cell dimensions	a = 13.9930(2) Å	α = 90 deg.
	b = 8.8988(2) Å	β = 91.122(1) deg.
	c = 26.3816(7) Å	γ = 90 deg.
Volume	3284.43(12) $Å^3$	
Density (calculated)	1.29 g/cm^3	
Absorption coefficient	0.50 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.52 x 0.12 x 0.08 mm^3	
Theta range for data collection	1.5 to 20.8 deg.	
Index ranges	$-13\le h\le 13$, $-8\le k\le 8$, $-26\le l\le 26$	
Reflections collected	17898	
Independent reflections	3428 (R(int) = 0.0733)	
Observed reflections	2413 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.78	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3428 / 0 / 349	
Goodness-of-fit on F^2	1.02	
Final R indices ($I>2\sigma(I)$)	R1 = 0.086, wR2 = 0.230	

Largest diff. peak and hole	0.64 and -0.69 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **3a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
P1	1.0034(1)	0.8100(2)	0.2574(1)	0.0395(7)
O1	1.0393(4)	0.8272(6)	0.3102(2)	0.0539(16)
S1	0.7736(1)	0.4954(2)	0.1331(1)	0.0391(7)
O11	0.7900(4)	0.4003(6)	0.1770(2)	0.0508(15)
O12	0.8086(4)	0.6479(6)	0.1410(2)	0.0576(16)
O13	0.6752(3)	0.4896(6)	0.1146(2)	0.0532(15)
C1	0.8722(5)	0.6494(11)	0.3468(3)	0.036(2)
H1	0.886(4)	0.723(7)	0.361(2)	0.005(19)
N2	0.8672(4)	0.6222(6)	0.2979(2)	0.0318(15)
C3	0.8446(5)	0.4746(8)	0.2916(3)	0.039(2)
C4	0.8356(5)	0.4150(9)	0.3382(3)	0.042(2)
N5	0.8539(4)	0.5268(7)	0.3728(2)	0.0348(15)
C6	0.8813(5)	0.7316(8)	0.2573(3)	0.0352(19)
C11	0.8441(5)	0.5123(9)	0.4290(3)	0.041(2)
C12	0.8890(7)	0.6501(10)	0.4542(3)	0.061(2)
C13	0.8965(7)	0.3706(11)	0.4457(3)	0.067(3)
C14	0.7379(6)	0.5019(11)	0.4400(3)	0.063(3)
C21	1.0803(6)	0.6811(11)	0.2225(3)	0.060(2)
C22	1.1855(6)	0.7241(12)	0.2309(4)	0.082(3)
C23	1.0605(7)	0.6808(13)	0.1640(4)	0.086(3)
C24	1.0659(8)	0.5234(11)	0.2425(5)	0.105(4)
C25	0.9846(6)	0.9925(9)	0.2254(3)	0.053(2)
C26	0.9260(7)	1.0899(10)	0.2620(4)	0.080(3)
C27	0.9272(7)	0.9809(11)	0.1751(4)	0.079(3)
C28	1.0805(7)	1.0732(12)	0.2170(4)	0.088(3)
C31	0.8434(5)	0.4192(8)	0.0847(3)	0.0340(18)
C32	0.9273(6)	0.3466(9)	0.0963(3)	0.044(2)
C33	0.9825(6)	0.2837(10)	0.0589(4)	0.058(2)
C34	0.9557(7)	0.2957(10)	0.0091(4)	0.060(3)
C35	0.8731(8)	0.3689(11)	-0.0031(3)	0.070(3)
C36	0.8169(7)	0.4315(10)	0.0342(3)	0.057(2)
C37	1.0150(9)	0.2251(14)	-0.0322(4)	0.106(4)
C41	1.3080(11)	1.234(2)	0.1022(7)	0.185(9)
Cl1	1.2714(7)	1.0449(7)	0.0958(2)	0.267(4)
Cl2	1.2192(3)	1.3383(6)	0.1248(2)	0.172(2)
C42	1.0475(11)	0.061(2)	0.3962(6)	0.154(7)
Cl3	1.1214(4)	0.2091(9)	0.3819(3)	0.253(4)
Cl4	1.0713(5)	0.0109(9)	0.4585(3)	0.253(3)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **3a**.

Atom	x	y	z	U_{eq}
H1	0.886(4)	0.723(7)	0.361(2)	0.005(19)
H3	0.8367	0.4233	0.2602	0.047
H4	0.8195	0.3138	0.3457	0.050

H6A	0.8349	0.8148	0.2611	0.042
H6B	0.8680	0.6826	0.2243	0.042
H12A	0.9567	0.6558	0.4455	0.091
H12B	0.8833	0.6422	0.4910	0.091
H12C	0.8560	0.7408	0.4421	0.091
H13A	0.8640	0.2825	0.4312	0.101
H13B	0.8968	0.3638	0.4828	0.101
H13C	0.9624	0.3741	0.4339	0.101
H14A	0.7059	0.5943	0.4287	0.094
H14B	0.7294	0.4890	0.4765	0.094
H14C	0.7102	0.4158	0.4219	0.094
H22A	1.2002	0.7283	0.2674	0.123
H22B	1.1974	0.8226	0.2157	0.123
H22C	1.2263	0.6487	0.2151	0.123
H23A	1.0968	0.5995	0.1484	0.129
H23B	1.0802	0.7773	0.1497	0.129
H23C	0.9920	0.6655	0.1573	0.129
H24A	1.0012	0.4890	0.2334	0.157
H24B	1.0742	0.5232	0.2794	0.157
H24C	1.1129	0.4559	0.2275	0.157
H26A	0.9285	1.1952	0.2512	0.120
H26B	0.9529	1.0806	0.2964	0.120
H26C	0.8594	1.0557	0.2615	0.120
H27A	0.8730	0.9126	0.1794	0.118
H27B	0.9686	0.9420	0.1486	0.118
H27C	0.9035	1.0806	0.1653	0.118
H28A	1.1161	1.0202	0.1908	0.131
H28B	1.1180	1.0740	0.2487	0.131
H28C	1.0682	1.1768	0.2060	0.131
H32	0.9480	0.3394	0.1307	0.053
H33	1.0395	0.2315	0.0680	0.070
H35	0.8536	0.3774	-0.0376	0.083
H36	0.7597	0.4831	0.0249	0.068
H37A	0.9916	0.1233	-0.0392	0.159
H37B	1.0821	0.2206	-0.0209	0.159
H37C	1.0096	0.2859	-0.0631	0.159
H41A	1.3641	1.2396	0.1256	0.222
H41B	1.3271	1.2732	0.0688	0.222
H42A	1.0598	-0.0248	0.3734	0.185
H42B	0.9797	0.0913	0.3919	0.185

Table 4: Anisotropic displacement parameters ($Å^2$) for **3a**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	0.0327(12)	0.0398(13)	0.0459(14)	-0.0022(10)	0.0010(9)	-0.0027(10)
O1	0.046(3)	0.063(4)	0.052(4)	-0.005(3)	-0.007(3)	-0.009(3)
S1	0.0409(13)	0.0358(13)	0.0407(12)	-0.0058(10)	0.0016(9)	0.0020(10)
O11	0.058(4)	0.058(4)	0.036(3)	0.002(3)	0.007(3)	0.008(3)
O12	0.058(4)	0.035(3)	0.080(4)	-0.018(3)	0.010(3)	-0.002(3)
O13	0.039(3)	0.057(4)	0.063(4)	-0.006(3)	-0.003(3)	0.003(3)
C1	0.038(5)	0.026(5)	0.045(6)	-0.008(5)	0.000(4)	-0.004(4)
N2	0.034(4)	0.026(4)	0.036(4)	-0.003(3)	0.000(3)	-0.005(3)
C3	0.040(5)	0.038(5)	0.039(5)	-0.004(4)	-0.004(4)	-0.006(4)
C4	0.046(5)	0.031(5)	0.048(6)	-0.001(4)	-0.001(4)	-0.007(4)
N5	0.038(4)	0.032(4)	0.034(4)	0.003(4)	-0.003(3)	0.003(3)

C6	0.034(4)	0.034(4)	0.037(4)	0.008(4)	0.003(3)	0.004(4)
C11	0.046(5)	0.043(5)	0.033(5)	0.006(4)	-0.007(4)	0.001(4)
C12	0.076(6)	0.064(6)	0.042(5)	-0.002(5)	-0.006(4)	-0.002(5)
C13	0.074(6)	0.070(7)	0.057(6)	0.022(5)	-0.010(5)	0.011(5)
C14	0.063(6)	0.074(6)	0.052(5)	0.007(5)	0.003(4)	-0.001(5)
C21	0.044(5)	0.071(7)	0.064(6)	-0.007(5)	0.005(4)	0.008(5)
C22	0.040(6)	0.098(8)	0.108(8)	0.001(7)	0.016(5)	0.009(6)
C23	0.071(7)	0.104(9)	0.083(8)	-0.028(7)	0.003(6)	0.021(6)
C24	0.087(8)	0.060(7)	0.170(12)	0.006(7)	0.060(8)	0.029(6)
C25	0.051(5)	0.041(5)	0.067(6)	0.005(4)	-0.003(4)	-0.020(5)
C26	0.091(8)	0.038(6)	0.111(9)	0.003(6)	0.012(6)	0.006(5)
C27	0.105(8)	0.055(6)	0.075(7)	0.030(5)	-0.005(6)	-0.018(6)
C28	0.074(7)	0.064(7)	0.125(9)	0.008(6)	0.019(6)	-0.031(6)
C31	0.043(5)	0.026(4)	0.034(5)	0.003(3)	-0.002(4)	0.000(4)
C32	0.055(5)	0.043(5)	0.034(5)	-0.001(4)	0.009(4)	0.005(4)
C33	0.057(6)	0.054(6)	0.064(7)	-0.002(5)	0.006(5)	0.011(5)
C34	0.076(7)	0.056(6)	0.051(6)	-0.002(5)	0.027(5)	0.004(5)
C35	0.107(8)	0.079(7)	0.022(5)	0.005(5)	0.006(5)	-0.007(7)
C36	0.077(6)	0.058(6)	0.035(5)	0.009(4)	-0.008(5)	0.006(5)
C37	0.123(10)	0.115(10)	0.082(8)	-0.013(7)	0.058(7)	-0.008(8)
C41	0.127(12)	0.212(19)	0.218(19)	-0.148(16)	0.011(12)	0.017(13)
Cl1	0.482(12)	0.137(4)	0.185(5)	-0.047(4)	0.081(6)	-0.015(6)
Cl2	0.116(3)	0.161(4)	0.238(6)	0.002(4)	-0.007(3)	0.027(3)
C42	0.124(12)	0.198(17)	0.139(13)	-0.098(12)	-0.028(10)	-0.021(12)
Cl3	0.160(5)	0.307(8)	0.297(8)	-0.165(7)	0.087(5)	-0.098(5)
Cl4	0.254(7)	0.286(8)	0.217(6)	-0.114(6)	-0.055(5)	-0.010(6)

Table 5: Bond lengths (Å) and angles (deg) for **3a**.

P1-O1	1.480(5)	C35-C36	1.389(13)
P1-C21	1.832(9)	C41-Cl2	1.672(14)
P1-C6	1.846(7)	C41-Cl1	1.765(18)
P1-C25	1.847(8)	C42-Cl3	1.721(18)
S1-O11	1.449(5)	C42-Cl4	1.729(17)
S1-O13	1.452(5)	O1-P1-C21	110.2(4)
S1-O12	1.457(5)	O1-P1-C6	109.7(3)
S1-C31	1.758(7)	C21-P1-C6	108.4(4)
C1-N2	1.314(10)	O1-P1-C25	112.5(4)
C1-N5	1.316(9)	C21-P1-C25	113.6(4)
N2-C3	1.360(9)	C6-P1-C25	102.0(3)
N2-C6	1.464(9)	O11-S1-O13	112.4(3)
C3-C4	1.347(10)	O11-S1-O12	112.4(3)
C4-N5	1.371(9)	O13-S1-O12	113.3(3)
N5-C11	1.497(9)	O11-S1-C31	105.8(3)
C11-C13	1.520(11)	O13-S1-C31	106.3(3)
C11-C14	1.522(11)	O12-S1-C31	105.8(3)
C11-C12	1.525(11)	N2-C1-N5	110.5(8)
C21-C24	1.514(13)	C1-N2-C3	107.9(6)
C21-C22	1.534(12)	C1-N2-C6	126.2(6)
C21-C23	1.563(13)	C3-N2-C6	125.9(6)
C25-C27	1.541(12)	C4-C3-N2	107.1(6)
C25-C28	1.542(12)	C3-C4-N5	107.6(7)
C25-C26	1.544(12)	C1-N5-C4	106.9(7)
C31-C32	1.369(10)	C1-N5-C11	127.5(7)
C31-C36	1.381(10)	C4-N5-C11	125.3(6)
C32-C33	1.383(11)	N2-C6-P1	112.9(5)
C33-C34	1.364(12)	N5-C11-C13	107.8(6)
C34-C35	1.359(13)	N5-C11-C14	107.6(6)
C34-C37	1.517(13)	C13-C11-C14	111.2(7)

N5-C11-C12	108.5(6)
C13-C11-C12	110.4(6)
C14-C11-C12	111.2(7)
C24-C21-C22	108.3(8)
C24-C21-C23	108.6(9)
C22-C21-C23	107.1(8)
C24-C21-P1	108.8(6)
C22-C21-P1	110.1(6)
C23-C21-P1	113.7(6)
C27-C25-C28	110.3(8)
C27-C25-C26	107.6(8)
C28-C25-C26	107.6(7)
C27-C25-P1	113.7(6)
C28-C25-P1	111.0(6)
C26-C25-P1	106.3(6)
C32-C31-C36	117.8(7)
C32-C31-S1	120.4(5)
C36-C31-S1	121.8(6)
C31-C32-C33	121.3(7)
C34-C33-C32	120.6(8)
C35-C34-C33	118.7(8)
C35-C34-C37	120.2(10)
C33-C34-C37	121.0(10)
C34-C35-C36	121.1(8)
C31-C36-C35	120.4(8)
Cl2-C41-Cl1	110.3(10)
Cl3-C42-Cl4	107.5(7)

Crystal data for 3b:

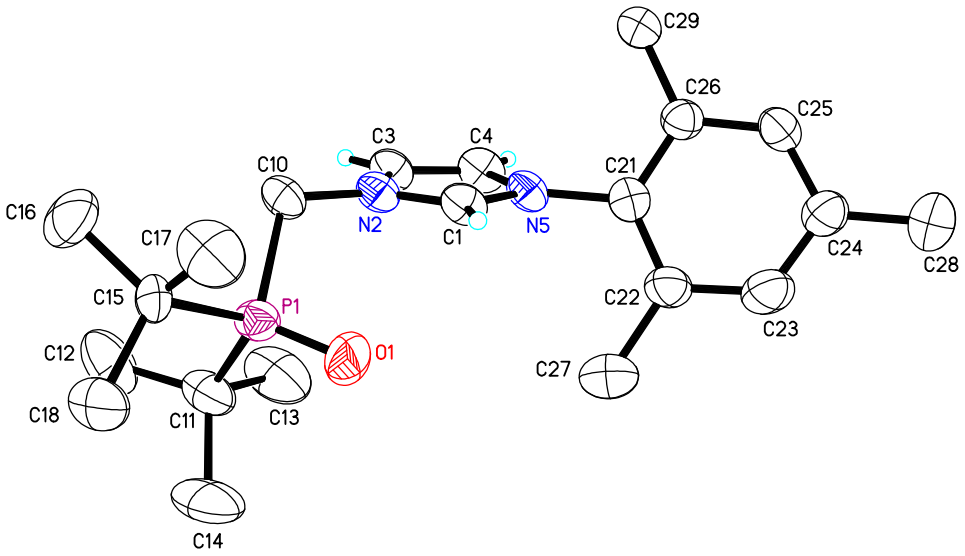


Table 1: Crystal data and structure refinement for **3b**.

Identification code	pn1	
Empirical formula	$C_{29}H_{42}Cl_3N_2O_4PS$	
Formula weight	652.03	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	$P\bar{1}$	
Z	2	
Unit cell dimensions	a = 8.5358(2) Å	α =101.698(1) deg.
	b = 13.0227(3) Å	β = 98.601(1) deg.
	c = 15.8524(4) Å	γ = 91.077(1) deg.
Volume	1703.94(7) $Å^3$	
Density (calculated)	1.27 g/cm^3	
Absorption coefficient	0.41 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.17 x 0.11 x 0.05 mm^3	
Crystal colour	colorless	
Theta range for data collection	1.9 to 20.8 deg.	
Index ranges	$-8\le h\le 8$, $-13\le k\le 13$, $-15\le l\le 15$	
Reflections collected	9487	
Independent reflections	3568 (R(int) = 0.0683)	
Observed reflections	2286 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.98 and 0.93	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3568 / 205 / 415	
Goodness-of-fit on F^2	1.03	
Final R indices ($I>2\sigma(I)$)	R1 = 0.068, wR2 = 0.131	
Largest diff. peak and hole	0.47 and -0.35 $eÅ^{-3}$	

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **3b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
O1	0.3419(6)	0.8649(4)	0.1964(3)	0.0733(17)
C1	0.5674(8)	0.8025(5)	0.3392(4)	0.0369(16)
N2	0.5668(6)	0.9047(4)	0.3712(3)	0.0350(13)
C3	0.7146(7)	0.9382(5)	0.4170(4)	0.0384(17)
C4	0.8066(7)	0.8546(5)	0.4108(4)	0.0394(17)
N5	0.7116(6)	0.7705(4)	0.3617(3)	0.0351(13)
C10	0.4285(7)	0.9690(5)	0.3631(4)	0.0369(16)
P1	0.3472(2)	0.9713(1)	0.2491(1)	0.0367(5)
C11	0.4626(11)	1.0769(8)	0.2168(6)	0.054(3)
C12	0.4336(13)	1.1900(7)	0.2622(7)	0.074(4)
C13	0.6389(11)	1.0590(11)	0.2437(9)	0.079(4)
C14	0.424(2)	1.0633(17)	0.1172(8)	0.080(9)
C15	0.1390(11)	1.0070(9)	0.2535(6)	0.041(3)
C16	0.1145(12)	1.0917(9)	0.3330(6)	0.064(3)
C17	0.0495(11)	0.9048(8)	0.2592(7)	0.067(3)
C18	0.0651(17)	1.0383(15)	0.1686(9)	0.059(8)
C21	0.7605(7)	0.6631(5)	0.3376(4)	0.0365(16)
C22	0.7612(8)	0.6203(5)	0.2507(4)	0.0447(18)
C23	0.8122(8)	0.5183(6)	0.2317(5)	0.055(2)
C24	0.8615(8)	0.4611(5)	0.2954(5)	0.0474(18)
C25	0.8566(7)	0.5091(5)	0.3807(4)	0.0421(17)
C26	0.8064(7)	0.6104(5)	0.4048(4)	0.0376(17)
C27	0.7128(9)	0.6791(6)	0.1783(4)	0.070(2)
C28	0.9200(9)	0.3525(5)	0.2723(5)	0.069(2)
C29	0.8069(8)	0.6585(5)	0.4996(4)	0.0450(18)
S1	0.2838(2)	0.7576(1)	0.4947(1)	0.0428(5)
O11	0.2398(7)	0.7100(4)	0.5621(3)	0.0857(19)
O12	0.1682(5)	0.8289(3)	0.4646(4)	0.0721(16)
O13	0.4408(5)	0.8089(3)	0.5151(3)	0.0500(12)
C31	0.2910(7)	0.6560(5)	0.4038(4)	0.0355(16)
C32	0.3957(8)	0.5777(5)	0.4112(5)	0.052(2)
C33	0.4122(9)	0.5021(6)	0.3373(6)	0.072(2)
C34	0.3260(11)	0.5033(8)	0.2564(6)	0.081(3)
C35	0.2214(10)	0.5805(8)	0.2514(5)	0.083(3)
C36	0.2023(8)	0.6569(6)	0.3236(5)	0.057(2)
C37	0.3524(12)	0.4237(8)	0.1753(7)	0.149(5)
C41	0.2137(10)	0.7259(7)	0.0258(6)	0.075(4)
Cl1	0.3793(5)	0.6787(4)	-0.0161(2)	0.161(3)
Cl2	0.0676(6)	0.6296(4)	0.0138(3)	0.147(2)
Cl3	0.1442(6)	0.8197(3)	-0.0347(2)	0.137(2)
C41B	0.226(3)	0.711(2)	0.039(2)	0.22(5)
Cl1B	0.022(3)	0.713(2)	0.0138(19)	0.242(14)
Cl2B	0.286(2)	0.7677(13)	-0.0419(10)	0.136(6)
Cl3B	0.296(2)	0.5862(13)	0.0251(11)	0.147(7)
C11B	0.5005(17)	1.0209(12)	0.1952(10)	0.034(6)
C12B	0.6125(19)	0.9339(12)	0.1660(11)	0.037(6)
C13B	0.601(3)	1.1117(15)	0.2576(16)	0.061(9)
C14B	0.424(4)	1.060(3)	0.1139(15)	0.055(16)
C15B	0.1715(18)	1.0470(13)	0.2643(13)	0.037(9)
C16B	0.220(3)	1.1623(12)	0.3055(14)	0.065(7)
C17B	0.081(2)	0.9966(17)	0.3240(14)	0.057(7)
C18B	0.061(4)	1.039(3)	0.1769(18)	0.08(2)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **3b**.

Atom	x	y	z	U_{eq}
H1	0.4796	0.7594	0.3057	0.044
H3	0.7464	1.0077	0.4475	0.046
H4	0.9150	0.8540	0.4354	0.047
H10A	0.4591	1.0418	0.3951	0.044
H10B	0.3447	0.9415	0.3907	0.044
H12A	0.3221	1.2047	0.2464	0.112
H12B	0.5017	1.2397	0.2435	0.112
H12C	0.4587	1.1972	0.3256	0.112
H13A	0.6627	1.0684	0.3073	0.119
H13B	0.7044	1.1095	0.2244	0.119
H13C	0.6619	0.9874	0.2166	0.119
H14A	0.3114	1.0746	0.1006	0.120
H14B	0.4472	0.9921	0.0894	0.120
H14C	0.4887	1.1145	0.0981	0.120
H16A	0.1638	1.0712	0.3866	0.096
H16B	0.0007	1.0990	0.3339	0.096
H16C	0.1635	1.1589	0.3289	0.096
H17A	0.0930	0.8830	0.3132	0.101
H17B	0.0620	0.8494	0.2091	0.101
H17C	-0.0635	0.9174	0.2589	0.101
H18A	0.0813	0.9835	0.1187	0.088
H18B	0.1156	1.1048	0.1643	0.088
H18C	-0.0488	1.0464	0.1684	0.088
H23	0.8135	0.4862	0.1724	0.066
H25	0.8891	0.4713	0.4251	0.050
H27A	0.5969	0.6812	0.1674	0.104
H27B	0.7502	0.6431	0.1251	0.104
H27C	0.7599	0.7509	0.1957	0.104
H28A	1.0362	0.3563	0.2800	0.103
H28B	0.8774	0.3211	0.2115	0.103
H28C	0.8845	0.3094	0.3105	0.103
H29A	0.8051	0.6027	0.5327	0.067
H29B	0.7131	0.7000	0.5056	0.067
H29C	0.9029	0.7042	0.5221	0.067
H32	0.4561	0.5753	0.4661	0.063
H33	0.4845	0.4484	0.3427	0.087
H35	0.1595	0.5820	0.1966	0.100
H36	0.1284	0.7096	0.3180	0.069
H37A	0.2496	0.3953	0.1415	0.223
H37B	0.4133	0.3664	0.1930	0.223
H37C	0.4113	0.4583	0.1394	0.223
H41	0.2435	0.7601	0.0888	0.090
H41B	0.2663	0.7536	0.0986	0.260
H12D	0.5510	0.8752	0.1252	0.056
H12E	0.6651	0.9094	0.2170	0.056
H12F	0.6925	0.9619	0.1371	0.056
H13D	0.6513	1.0874	0.3092	0.092
H13E	0.5327	1.1693	0.2753	0.092
H13F	0.6827	1.1364	0.2281	0.092
H14D	0.3591	1.0018	0.0736	0.082
H14E	0.5065	1.0838	0.0849	0.082
H14F	0.3558	1.1175	0.1313	0.082
H16D	0.2908	1.1666	0.3610	0.097
H16E	0.1254	1.2012	0.3159	0.097
H16F	0.2757	1.1929	0.2658	0.097
H17D	0.0501	0.9233	0.2961	0.085

H17E	-0.0149	1.0351	0.3336	0.085
H17F	0.1487	0.9995	0.3800	0.085
H18D	0.0326	0.9653	0.1504	0.121
H18E	0.1154	1.0712	0.1377	0.121
H18F	-0.0355	1.0764	0.1871	0.121

Table 4: Anisotropic displacement parameters ($Å^2$) for **3b**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{12}
O1	0.119(5)	0.055(4)	0.035(3)	-0.007(3)	-0.005(3)	0.039(3)	
C1	0.038(5)	0.036(5)	0.034(4)	0.010(4)	-0.004(3)	-0.007(3)	
N2	0.034(4)	0.038(4)	0.033(3)	0.011(3)	-0.001(3)	0.000(3)	
C3	0.038(4)	0.038(4)	0.037(4)	0.010(3)	-0.005(3)	-0.004(4)	
C4	0.030(4)	0.042(5)	0.042(4)	0.009(4)	-0.007(3)	-0.011(4)	
N5	0.033(3)	0.037(4)	0.036(3)	0.013(3)	-0.002(3)	0.001(3)	
C10	0.032(4)	0.042(4)	0.038(4)	0.016(3)	-0.001(3)	0.003(3)	
P1	0.0330(11)	0.0457(12)	0.0327(10)	0.0111(9)	0.0044(8)	0.0049(8)	
C11	0.054(6)	0.064(7)	0.050(7)	0.030(6)	0.008(6)	0.005(7)	
C12	0.081(9)	0.050(7)	0.095(9)	0.035(6)	-0.002(7)	-0.005(6)	
C13	0.047(7)	0.116(12)	0.096(10)	0.061(10)	0.025(6)	0.006(7)	
C14	0.083(13)	0.118(16)	0.057(7)	0.050(7)	0.025(6)	0.005(8)	
C15	0.044(7)	0.042(7)	0.040(6)	0.010(6)	0.007(6)	0.022(5)	
C16	0.048(7)	0.087(8)	0.055(6)	0.004(6)	0.015(6)	0.026(6)	
C17	0.043(7)	0.082(8)	0.085(9)	0.034(7)	0.014(6)	0.001(6)	
C18	0.028(9)	0.103(15)	0.054(7)	0.032(8)	0.008(5)	0.021(6)	
C21	0.032(4)	0.036(5)	0.042(5)	0.009(4)	0.005(3)	0.000(3)	
C22	0.056(5)	0.043(5)	0.033(5)	0.008(4)	0.001(3)	-0.002(4)	
C23	0.070(5)	0.055(6)	0.036(5)	0.002(4)	0.005(4)	-0.004(4)	
C24	0.054(5)	0.045(5)	0.041(5)	0.004(4)	0.007(4)	0.000(4)	
C25	0.046(4)	0.039(5)	0.043(5)	0.015(4)	0.003(3)	0.003(3)	
C26	0.039(4)	0.038(5)	0.036(4)	0.008(4)	0.007(3)	-0.001(3)	
C27	0.094(6)	0.075(6)	0.040(5)	0.013(4)	0.009(4)	0.010(5)	
C28	0.087(6)	0.048(5)	0.068(6)	0.003(4)	0.017(5)	0.009(4)	
C29	0.055(5)	0.044(4)	0.039(4)	0.013(4)	0.007(3)	0.007(3)	
S1	0.0439(12)	0.0336(11)	0.0522(12)	0.0091(10)	0.0112(9)	0.0014(9)	
O11	0.151(5)	0.055(3)	0.059(3)	0.010(3)	0.048(4)	-0.030(3)	
O12	0.047(3)	0.045(3)	0.114(4)	0.001(3)	-0.002(3)	0.020(2)	
O13	0.044(3)	0.047(3)	0.054(3)	0.001(2)	0.004(2)	-0.004(2)	
C31	0.024(4)	0.036(4)	0.046(5)	0.010(3)	0.001(3)	0.003(3)	
C32	0.054(5)	0.036(5)	0.064(5)	0.006(4)	0.006(4)	0.007(4)	
C33	0.052(5)	0.054(6)	0.105(8)	-0.004(6)	0.020(5)	0.015(4)	
C34	0.056(6)	0.088(8)	0.082(7)	-0.028(6)	0.022(6)	-0.022(5)	
C35	0.061(6)	0.124(9)	0.052(6)	-0.003(6)	0.003(5)	-0.011(6)	
C36	0.048(5)	0.077(6)	0.047(5)	0.011(5)	0.008(4)	0.010(4)	
C37	0.134(10)	0.145(10)	0.128(9)	-0.091(8)	0.065(8)	-0.033(8)	
C41	0.105(8)	0.091(8)	0.020(5)	-0.001(5)	0.003(5)	0.000(5)	
Cl1	0.111(3)	0.226(6)	0.096(3)	-0.065(3)	-0.010(2)	0.043(3)	
Cl2	0.165(4)	0.172(5)	0.103(3)	0.042(3)	0.008(3)	-0.066(3)	
Cl3	0.235(5)	0.101(3)	0.062(2)	0.0164(19)	-0.023(2)	0.029(3)	

Table 5: Bond lengths (Å) and angles (deg) for **3b**.

O1-P1	1.462(5)	S1-O11	1.431(5)
C1-N2	1.325(7)	S1-O13	1.448(4)
C1-N5	1.328(7)	S1-O12	1.462(5)
C1-H1	0.9500	S1-C31	1.758(6)
N2-C3	1.373(7)	C31-C32	1.380(8)
N2-C10	1.465(7)	C31-C36	1.380(8)
C3-C4	1.350(8)	C32-C33	1.396(10)
C3-H3	0.9500	C32-H32	0.9500
C4-N5	1.377(7)	C33-C34	1.383(11)
C4-H4	0.9500	C33-H33	0.9500
N5-C21	1.459(7)	C34-C35	1.364(11)
C10-P1	1.841(6)	C34-C37	1.527(11)
C10-H10A	0.9900	C35-C36	1.389(10)
C10-H10B	0.9900	C35-H35	0.9500
P1-C15B	1.829(14)	C36-H36	0.9500
P1-C11B	1.841(13)	C37-H37A	0.9800
P1-C15	1.853(8)	C37-H37B	0.9800
P1-C11	1.874(9)	C37-H37C	0.9800
C11-C14	1.537(11)	C41-Cl2	1.714(9)
C11-C13	1.537(10)	C41-Cl1	1.722(9)
C11-C12	1.544(11)	C41-Cl3	1.759(10)
C12-H12A	0.9800	C41-H41	1.0000
C12-H12B	0.9800	C41B-Cl3B	1.725(17)
C12-H12C	0.9800	C41B-Cl1B	1.730(17)
C13-H13A	0.9800	C41B-Cl2B	1.737(17)
C13-H13B	0.9800	C41B-H41B	1.0000
C13-H13C	0.9800	C11B-C13B	1.530(14)
C14-H14A	0.9800	C11B-C14B	1.540(14)
C14-H14B	0.9800	C11B-C12B	1.540(13)
C14-H14C	0.9800	C12B-H12D	0.9800
C15-C18	1.535(10)	C12B-H12E	0.9800
C15-C16	1.540(10)	C12B-H12F	0.9800
C15-C17	1.547(11)	C13B-H13D	0.9800
C16-H16A	0.9800	C13B-H13E	0.9800
C16-H16B	0.9800	C13B-H13F	0.9800
C16-H16C	0.9800	C14B-H14D	0.9800
C17-H17A	0.9800	C14B-H14E	0.9800
C17-H17B	0.9800	C14B-H14F	0.9800
C17-H17C	0.9800	C15B-C16B	1.534(13)
C18-H18A	0.9800	C15B-C18B	1.539(14)
C18-H18B	0.9800	C15B-C17B	1.542(14)
C18-H18C	0.9800	C16B-H16D	0.9800
C21-C22	1.378(8)	C16B-H16E	0.9800
C21-C26	1.394(8)	C16B-H16F	0.9800
C22-C23	1.394(9)	C17B-H17D	0.9800
C22-C27	1.516(9)	C17B-H17E	0.9800
C23-C24	1.393(9)	C17B-H17F	0.9800
C23-H23	0.9500	C18B-H18D	0.9800
C24-C25	1.376(8)	C18B-H18E	0.9800
C24-C28	1.501(9)	C18B-H18F	0.9800
C25-C26	1.392(8)	N2-C1-N5	108.4(5)
C25-H25	0.9500	N2-C1-H1	125.8
C26-C29	1.505(8)	N5-C1-H1	125.8
C27-H27A	0.9800	C1-N2-C3	108.4(5)
C27-H27B	0.9800	C1-N2-C10	125.3(5)
C27-H27C	0.9800	C3-N2-C10	126.2(6)
C28-H28A	0.9800	C4-C3-N2	107.8(6)
C28-H28B	0.9800	C4-C3-H3	126.1
C28-H28C	0.9800	N2-C3-H3	126.1
C29-H29A	0.9800	C3-C4-N5	106.2(5)
C29-H29B	0.9800	C3-C4-H4	126.9
C29-H29C	0.9800	N5-C4-H4	126.9

C1-N5-C4	109.2(5)	H17A-C17-H17B	109.5
C1-N5-C21	125.0(5)	C15-C17-H17C	109.5
C4-N5-C21	125.8(5)	H17A-C17-H17C	109.5
N2-C10-P1	113.2(4)	H17B-C17-H17C	109.5
N2-C10-H10A	108.9	C15-C18-H18A	109.5
P1-C10-H10A	108.9	C15-C18-H18B	109.5
N2-C10-H10B	108.9	H18A-C18-H18B	109.5
P1-C10-H10B	108.9	C15-C18-H18C	109.5
H10A-C10-H10B	107.7	H18A-C18-H18C	109.5
O1-P1-C15B	123.8(6)	H18B-C18-H18C	109.5
O1-P1-C11B	93.8(5)	C22-C21-C26	123.9(6)
C15B-P1-C11B	119.1(7)	C22-C21-N5	118.7(6)
O1-P1-C10	109.1(3)	C26-C21-N5	117.4(6)
C15B-P1-C10	100.8(7)	C21-C22-C23	116.2(6)
C11B-P1-C10	110.2(5)	C21-C22-C27	123.3(6)
O1-P1-C15	107.0(4)	C23-C22-C27	120.5(6)
C15B-P1-C15	17.7(6)	C24-C23-C22	123.2(6)
C11B-P1-C15	131.1(6)	C24-C23-H23	118.4
C10-P1-C15	104.0(3)	C22-C23-H23	118.4
O1-P1-C11	118.0(4)	C25-C24-C23	117.1(6)
C15B-P1-C11	95.7(6)	C25-C24-C28	121.4(6)
C11B-P1-C11	25.9(5)	C23-C24-C28	121.5(6)
C10-P1-C11	107.2(4)	C24-C25-C26	123.1(6)
C15-P1-C11	110.7(4)	C24-C25-H25	118.5
C14-C11-C13	110.0(10)	C26-C25-H25	118.5
C14-C11-C12	110.6(10)	C25-C26-C21	116.5(6)
C13-C11-C12	106.9(9)	C25-C26-C29	120.1(6)
C14-C11-P1	107.8(9)	C21-C26-C29	123.4(6)
C13-C11-P1	106.5(7)	C22-C27-H27A	109.5
C12-C11-P1	114.9(7)	C22-C27-H27B	109.5
C11-C12-H12A	109.5	H27A-C27-H27B	109.5
C11-C12-H12B	109.5	C22-C27-H27C	109.5
H12A-C12-H12B	109.5	H27A-C27-H27C	109.5
C11-C12-H12C	109.5	H27B-C27-H27C	109.5
H12A-C12-H12C	109.5	C24-C28-H28A	109.5
H12B-C12-H12C	109.5	C24-C28-H28B	109.5
C11-C13-H13A	109.5	H28A-C28-H28B	109.5
C11-C13-H13B	109.5	C24-C28-H28C	109.5
H13A-C13-H13B	109.5	H28A-C28-H28C	109.5
C11-C13-H13C	109.5	H28B-C28-H28C	109.5
H13A-C13-H13C	109.5	C26-C29-H29A	109.5
H13B-C13-H13C	109.5	C26-C29-H29B	109.5
C11-C14-H14A	109.5	H29A-C29-H29B	109.5
C11-C14-H14B	109.5	C26-C29-H29C	109.5
H14A-C14-H14B	109.5	H29A-C29-H29C	109.5
C11-C14-H14C	109.5	H29B-C29-H29C	109.5
H14A-C14-H14C	109.5	O11-S1-O13	114.3(3)
H14B-C14-H14C	109.5	O11-S1-O12	114.0(3)
C18-C15-C16	110.4(10)	O13-S1-O12	109.9(3)
C18-C15-C17	107.3(10)	O11-S1-C31	107.0(3)
C16-C15-C17	107.5(8)	O13-S1-C31	105.2(3)
C18-C15-P1	110.7(8)	O12-S1-C31	105.6(3)
C16-C15-P1	115.2(7)	C32-C31-C36	119.3(6)
C17-C15-P1	105.2(6)	C32-C31-S1	119.2(5)
C15-C16-H16A	109.5	C36-C31-S1	121.4(5)
C15-C16-H16B	109.5	C31-C32-C33	119.5(7)
H16A-C16-H16B	109.5	C31-C32-H32	120.3
C15-C16-H16C	109.5	C33-C32-H32	120.3
H16A-C16-H16C	109.5	C34-C33-C32	121.7(7)
H16B-C16-H16C	109.5	C34-C33-H33	119.1
C15-C17-H17A	109.5	C32-C33-H33	119.1
C15-C17-H17B	109.5	C35-C34-C33	117.5(8)

C35-C34-C37	121.5(10)
C33-C34-C37	121.0(10)
C34-C35-C36	122.1(8)
C34-C35-H35	118.9
C36-C35-H35	118.9
C31-C36-C35	119.9(7)
C31-C36-H36	120.1
C35-C36-H36	120.1
C34-C37-H37A	109.5
C34-C37-H37B	109.5
H37A-C37-H37B	109.5
C34-C37-H37C	109.5
H37A-C37-H37C	109.5
H37B-C37-H37C	109.5
Cl2-C41-Cl1	112.4(6)
Cl2-C41-Cl3	109.1(5)
Cl1-C41-Cl3	105.4(5)
Cl2-C41-H41	109.9
Cl1-C41-H41	109.9
Cl3-C41-H41	109.9
Cl3B-C41B-Cl1B	113.6(19)
Cl3B-C41B-Cl2B	106.8(16)
Cl1B-C41B-Cl2B	101.0(16)
Cl3B-C41B-H41B	111.6
Cl1B-C41B-H41B	111.6
Cl2B-C41B-H41B	111.6
C13B-C11B-C14B	109.0(15)
C13B-C11B-C12B	107.9(13)
C14B-C11B-C12B	108.0(15)
C13B-C11B-P1	110.6(13)
C14B-C11B-P1	110.4(15)
C12B-C11B-P1	110.8(10)
C11B-C12B-H12D	109.5
C11B-C12B-H12E	109.5
H12D-C12B-H12E	109.5
C11B-C12B-H12F	109.5
H12D-C12B-H12F	109.5
H12E-C12B-H12F	109.5
C11B-C13B-H13D	109.5
C11B-C13B-H13E	109.5
H13D-C13B-H13E	109.5
C11B-C13B-H13F	109.5
H13D-C13B-H13F	109.5
H13E-C13B-H13F	109.5
C11B-C14B-H14D	109.5
C11B-C14B-H14E	109.5
H14D-C14B-H14E	109.5
C11B-C14B-H14F	109.5
H14D-C14B-H14F	109.5
H14E-C14B-H14F	109.5
C16B-C15B-C18B	109.9(17)
C16B-C15B-C17B	111.0(14)
C18B-C15B-C17B	107.6(16)
C16B-C15B-P1	110.4(12)
C18B-C15B-P1	110.9(17)
C17B-C15B-P1	107.0(12)
C15B-C16B-H16D	109.5
C15B-C16B-H16E	109.5
H16D-C16B-H16E	109.5
C15B-C16B-H16F	109.5
H16D-C16B-H16F	109.5
H16E-C16B-H16F	109.5
C15B-C17B-H17D	109.5
C15B-C17B-H17E	109.5
H17D-C17B-H17E	109.5
C15B-C17B-H17F	109.5
H17D-C17B-H17F	109.5
H17E-C17B-H17F	109.5
C15B-C18B-H18D	109.5
C15B-C18B-H18E	109.5
H18D-C18B-H18E	109.5
C15B-C18B-H18F	109.5
H18D-C18B-H18F	109.5
H18E-C18B-H18F	109.5

Crystal data for 4a:

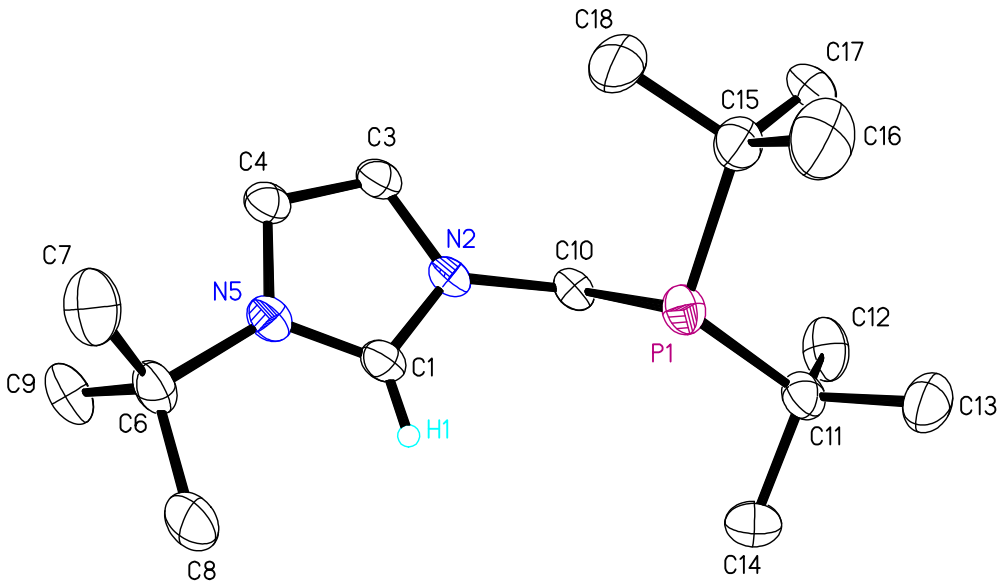


Table 1: Crystal data and structure refinement for **4a**.

Identification code	ub8		
Empirical formula	$C_{16}H_{32}Cl_{0.50}N_2O_3PS$		
Formula weight	381.19		
Temperature	100(2) K		
Wavelength	0.71073 Å		
Crystal system	triclinic		
Space group	$P\bar{1}$		
Z	2		
Unit cell dimensions	a = 8.8210(10) Å	α =	79.030(2) deg.
	b = 11.2465(13) Å	β =	72.245(2) deg.
	c = 13.8864(16) Å	γ =	87.263(2) deg.
Volume	1287.9(3) $Å^3$		
Density (calculated)	0.98 g/cm^3		
Absorption coefficient	0.25 mm^{-1}		
Crystal shape	polyhedron		
Crystal size	0.21 x 0.18 x 0.17 mm^3		
Theta range for data collection	2.2 to 28.3 deg.		
Index ranges	$-11 \le h \le 11$, $-14 \le k \le 14$, $-18 \le l \le 18$		
Reflections collected	13037		
Independent reflections	6243 (R(int) = 0.0232)		
Observed reflections	5400 ($I > 2\sigma(I)$)		
Absorption correction	Semi-empirical from equivalents		
Max. and min. transmission	0.96 and 0.95		
Refinement method	Full-matrix least-squares on F^2		
Data/restraints/parameters	6243 / 0 / 294		
Goodness-of-fit on F^2	1.11		
Final R indices ($I > 2\sigma(I)$)	R1 = 0.066, wR2 = 0.181		
Largest diff. peak and hole	0.60 and -0.30 $eÅ^{-3}$		

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for ub8. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
P1	0.3158(1)	0.6531(1)	0.2288(1)	0.0252(2)
O11	0.358(2)	0.7601(19)	0.2124(16)	0.041(7)
C1	0.5827(3)	0.7465(2)	0.0010(2)	0.0247(5)
H1	0.501(3)	0.790(3)	-0.006(2)	0.027(7)
N2	0.5727(2)	0.6356(2)	0.0573(1)	0.0221(4)
C3	0.7250(3)	0.5902(2)	0.0431(2)	0.0253(5)
C4	0.8258(3)	0.6773(2)	-0.0225(2)	0.0256(5)
N5	0.7346(2)	0.7742(2)	-0.0480(2)	0.0247(4)
C6	0.8007(3)	0.8884(2)	-0.1220(2)	0.0301(5)
C7	0.9160(4)	0.9438(3)	-0.0786(2)	0.0427(7)
C8	0.6663(4)	0.9741(3)	-0.1310(3)	0.0506(8)
C9	0.8868(4)	0.8528(2)	-0.2255(2)	0.0376(6)
C10	0.4237(3)	0.5723(2)	0.1226(2)	0.0229(4)
C11	0.1062(3)	0.6023(2)	0.2508(2)	0.0286(5)
C12	0.0820(4)	0.4683(3)	0.2510(2)	0.0401(6)
C13	-0.0005(3)	0.6351(3)	0.3514(2)	0.0390(6)
C14	0.0555(4)	0.6790(4)	0.1612(2)	0.0507(8)
C15	0.3916(3)	0.5792(3)	0.3385(2)	0.0403(7)
C16	0.3378(4)	0.6576(4)	0.4215(3)	0.0628(11)
C17	0.3416(4)	0.4480(3)	0.3861(2)	0.0496(8)
C18	0.5740(4)	0.5855(4)	0.2971(2)	0.0578(10)
S1	1.3254(1)	0.7648(1)	-0.1572(1)	0.0271(2)
O1	1.4836(2)	0.7131(2)	-0.1846(2)	0.0346(5)
O2	1.2000(3)	0.6758(2)	-0.1384(2)	0.0379(5)
O3	1.2982(2)	0.8343(2)	-0.0752(2)	0.0341(5)
C21	1.3129(3)	0.8704(2)	-0.2675(2)	0.0273(5)
C22	1.3131(3)	0.9939(3)	-0.2687(2)	0.0335(6)
C23	1.2963(4)	1.0749(3)	-0.3538(2)	0.0415(7)
C24	1.2788(4)	1.0335(3)	-0.4381(2)	0.0435(8)
C25	1.2819(4)	0.9085(3)	-0.4360(2)	0.0445(8)
C26	1.2992(4)	0.8276(3)	-0.3517(2)	0.0384(7)
C27	1.2578(6)	1.1207(4)	-0.5313(3)	0.0694(13)
Cl1	1.2896(9)	0.7079(8)	-0.1151(6)	0.027(2)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **4a**.

Atom	x	y	z	U_{eq}
H1	0.501(3)	0.790(3)	-0.006(2)	0.027(7)
H3	0.7533	0.5128	0.0736	0.030
H4	0.9386	0.6727	-0.0465	0.031
H7A	0.8575	0.9635	-0.0113	0.064
H7B	0.9643	1.0178	-0.1258	0.064
H7C	0.9996	0.8855	-0.0709	0.064
H8A	0.5936	0.9365	-0.1578	0.076
H8B	0.7099	1.0495	-0.1779	0.076
H8C	0.6082	0.9918	-0.0630	0.076
H9A	0.9723	0.7964	-0.2180	0.056
H9B	0.9321	0.9254	-0.2760	0.056
H9C	0.8112	0.8137	-0.2491	0.056

H10A	0.4484	0.4892	0.1524	0.027
H10B	0.3540	0.5659	0.0798	0.027
H12A	0.1019	0.4187	0.3120	0.060
H12B	0.1562	0.4457	0.1888	0.060
H12C	-0.0276	0.4548	0.2523	0.060
H13A	-0.1123	0.6232	0.3568	0.058
H13B	0.0179	0.7201	0.3523	0.058
H13C	0.0245	0.5832	0.4096	0.058
H14A	-0.0561	0.6613	0.1700	0.076
H14B	0.1227	0.6593	0.0959	0.076
H14C	0.0679	0.7652	0.1611	0.076
H16A	0.2213	0.6565	0.4480	0.094
H16B	0.3757	0.7411	0.3919	0.094
H16C	0.3820	0.6255	0.4779	0.094
H17A	0.3965	0.4174	0.4373	0.074
H17B	0.3700	0.3988	0.3321	0.074
H17C	0.2263	0.4435	0.4194	0.074
H18A	0.6186	0.5669	0.3548	0.087
H18B	0.6078	0.6672	0.2585	0.087
H18C	0.6120	0.5265	0.2516	0.087
H22	1.3248	1.0231	-0.2115	0.040
H23	1.2966	1.1595	-0.3544	0.050
H25	1.2719	0.8788	-0.4935	0.053
H26	1.3017	0.7430	-0.3515	0.046

Table 4: Anisotropic displacement parameters ($Å^2$) for ub8. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	0.0278(3)	0.0267(3)	0.0213(3)	-0.0064(2)	-0.0059(2)	-0.0025(2)
C1	0.0298(12)	0.0208(10)	0.0224(10)	-0.0005(8)	-0.0083(9)	0.0019(9)
N2	0.0282(10)	0.0206(9)	0.0172(8)	-0.0013(7)	-0.0079(7)	-0.0002(7)
C3	0.0306(12)	0.0257(11)	0.0199(10)	-0.0026(8)	-0.0094(9)	0.0037(9)
C4	0.0297(12)	0.0280(11)	0.0198(10)	-0.0041(8)	-0.0091(9)	0.0033(9)
N5	0.0308(10)	0.0201(9)	0.0222(9)	-0.0026(7)	-0.0072(8)	-0.0001(7)
C6	0.0346(13)	0.0219(11)	0.0279(12)	0.0026(9)	-0.0044(10)	-0.0042(9)
C7	0.0481(17)	0.0342(14)	0.0430(15)	-0.0121(12)	-0.0047(13)	-0.0116(12)
C8	0.0449(17)	0.0267(13)	0.061(2)	0.0157(13)	-0.0026(14)	0.0022(12)
C9	0.0507(16)	0.0325(13)	0.0234(12)	0.0008(10)	-0.0044(11)	-0.0077(12)
C10	0.0289(11)	0.0201(10)	0.0190(9)	-0.0007(8)	-0.0075(8)	-0.0027(8)
C11	0.0289(12)	0.0358(13)	0.0210(10)	-0.0030(9)	-0.0083(9)	-0.0040(10)
C12	0.0408(15)	0.0437(15)	0.0339(13)	-0.0108(12)	-0.0041(11)	-0.0150(12)
C13	0.0307(13)	0.0513(17)	0.0343(14)	-0.0144(12)	-0.0054(11)	0.0033(12)
C14	0.0369(15)	0.072(2)	0.0398(16)	0.0071(15)	-0.0178(13)	0.0081(14)
C15	0.0290(13)	0.075(2)	0.0203(11)	-0.0145(12)	-0.0092(10)	0.0024(13)
C16	0.0465(18)	0.118(3)	0.0358(16)	-0.040(2)	-0.0134(14)	-0.0024(19)
C17	0.0438(16)	0.073(2)	0.0226(12)	0.0081(13)	-0.0082(11)	0.0146(15)
C18	0.0309(15)	0.120(3)	0.0282(14)	-0.0186(17)	-0.0147(12)	0.0015(17)
S1	0.0261(3)	0.0246(4)	0.0269(3)	0.0021(3)	-0.0073(3)	0.0044(3)
O1	0.0316(10)	0.0295(10)	0.0403(11)	-0.0033(8)	-0.0103(8)	0.0081(8)
O2	0.0358(11)	0.0292(10)	0.0435(12)	0.0081(9)	-0.0133(9)	-0.0006(8)
O3	0.0356(11)	0.0383(11)	0.0252(9)	-0.0018(8)	-0.0084(8)	0.0111(8)
C21	0.0272(12)	0.0278(12)	0.0206(11)	0.0019(9)	-0.0025(9)	0.0036(10)
C22	0.0364(15)	0.0287(13)	0.0316(14)	0.0009(11)	-0.0092(11)	0.0024(11)
C23	0.0447(17)	0.0266(14)	0.0389(16)	0.0108(12)	-0.0026(13)	0.0039(12)
C24	0.0420(17)	0.0476(18)	0.0278(14)	0.0089(13)	-0.0022(12)	0.0085(14)

C25	0.056(2)	0.0534(19)	0.0197(13)	-0.0080(12)	-0.0062(12)	0.0117(15)
C26	0.0485(17)	0.0363(15)	0.0264(13)	-0.0055(11)	-0.0068(12)	0.0089(13)
C27	0.078(3)	0.077(3)	0.0329(18)	0.0213(18)	-0.0088(18)	0.019(2)

Table 5: Bond lengths (Å) and angles (deg) for **4a**.

P1-O11	1.24(2)	C13-C11-C12	109.5(2)
P1-C10	1.865(2)	C13-C11-C14	108.2(2)
P1-C11	1.879(3)	C12-C11-C14	108.4(2)
P1-C15	1.882(3)	C13-C11-P1	109.14(17)
C1-N5	1.326(3)	C12-C11-P1	116.59(19)
C1-N2	1.332(3)	C14-C11-P1	104.65(18)
N2-C3	1.384(3)	C17-C15-C16	109.5(3)
N2-C10	1.474(3)	C17-C15-C18	108.3(3)
C3-C4	1.353(3)	C16-C15-C18	108.1(3)
C4-N5	1.380(3)	C17-C15-P1	117.1(2)
N5-C6	1.500(3)	C16-C15-P1	107.0(2)
C6-C8	1.512(4)	C18-C15-P1	106.53(19)
C6-C9	1.525(4)	O1-S1-O3	113.23(12)
C6-C7	1.537(4)	O1-S1-O2	112.55(13)
C11-C13	1.528(3)	O3-S1-O2	113.09(13)
C11-C12	1.531(4)	O1-S1-C21	106.48(12)
C11-C14	1.544(4)	O3-S1-C21	105.76(12)
C15-C17	1.524(5)	O2-S1-C21	104.88(13)
C15-C16	1.532(4)	C22-C21-C26	120.2(2)
C15-C18	1.534(4)	C22-C21-S1	120.7(2)
S1-O1	1.454(2)	C26-C21-S1	119.1(2)
S1-O3	1.455(2)	C21-C22-C23	119.9(3)
S1-O2	1.457(2)	C24-C23-C22	120.7(3)
S1-C21	1.780(3)	C23-C24-C25	118.4(3)
C21-C22	1.385(4)	C23-C24-C27	121.5(3)
C21-C26	1.385(4)	C25-C24-C27	120.0(3)
C22-C23	1.391(4)	C26-C25-C24	121.1(3)
C23-C24	1.390(5)	C25-C26-C21	119.7(3)
C24-C25	1.399(5)		
C24-C27	1.523(4)		
C25-C26	1.383(4)		
O11-P1-C10	112.9(10)		
O11-P1-C11	124.2(10)		
C10-P1-C11	99.98(11)		
O11-P1-C15	104.0(10)		
C10-P1-C15	103.35(12)		
C11-P1-C15	110.73(12)		
N5-C1-N2	109.0(2)		
C1-N2-C3	108.42(19)		
C1-N2-C10	125.3(2)		
C3-N2-C10	126.23(19)		
C4-C3-N2	106.8(2)		
C3-C4-N5	107.3(2)		
C1-N5-C4	108.50(19)		
C1-N5-C6	127.2(2)		
C4-N5-C6	124.2(2)		
N5-C6-C8	109.5(2)		
N5-C6-C9	107.14(19)		
C8-C6-C9	110.6(2)		
N5-C6-C7	106.8(2)		
C8-C6-C7	110.9(2)		
C9-C6-C7	111.6(2)		
N2-C10-P1	111.81(14)		

Crystal data for 5a:

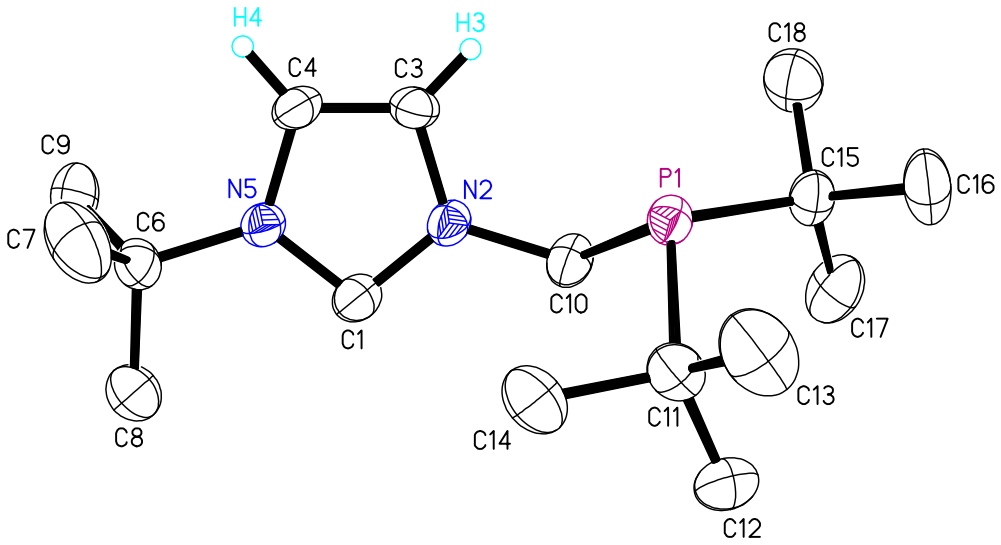


Table 1: Crystal data and structure refinement for **5a**.

Identification code	ub10	
Empirical formula	$C_{16}H_{31}N_2P$	
Formula weight	282.40	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Z	4	
Unit cell dimensions	a = 12.4480(1) Å	α = 90 deg.
	b = 14.2069(3) Å	β =116.665(1) deg.
	c = 11.5696(2) Å	γ = 90 deg.
Volume	1828.45(5) $Å^3$	
Density (calculated)	1.03 g/cm^3	
Absorption coefficient	0.14 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.38 x 0.2 x 0.2 mm^3	
Theta range for data collection	1.8 to 25.4 deg.	
Index ranges	$-14\le h\le 14$, $-17\le k\le 17$, $-13\le l\le 13$	
Reflections collected	15701	
Independent reflections	3332 (R(int) = 0.0621)	
Observed reflections	2334 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	3332 / 0 / 189	
Goodness-of-fit on F^2	1.02	
Final R indices ($I>2\sigma(I)$)	R1 = 0.042, wR2 = 0.082	
Largest diff. peak and hole	0.16 and -0.23 $eÅ^{-3}$	

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **5a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

x	y	z	U_{eq}	
P1	0.7218(1)	0.1218(1)	0.3426(1)	0.0282(2)
C1	1.0362(2)	0.2375(2)	0.5004(2)	0.0329(5)
N2	0.9606(1)	0.1680(1)	0.5013(1)	0.0297(4)
C3	0.9600(2)	0.1592(2)	0.6204(2)	0.0322(5)
H3	0.9117(16)	0.1146(13)	0.6314(17)	0.029(5)
C4	1.0361(2)	0.2232(2)	0.6979(2)	0.0317(5)
H4	1.0564(16)	0.2389(13)	0.7826(19)	0.031(5)
N5	1.0822(1)	0.2707(1)	0.6244(1)	0.0282(4)
C6	1.1633(2)	0.3534(1)	0.6732(2)	0.0347(5)
C7	1.0949(2)	0.4322(2)	0.7008(3)	0.0640(8)
C8	1.2015(2)	0.3848(2)	0.5714(2)	0.0528(6)
C9	1.2741(2)	0.3259(2)	0.7970(2)	0.0546(7)
C10	0.8856(2)	0.1121(2)	0.3873(2)	0.0344(5)
C11	0.6698(2)	0.2141(1)	0.2121(2)	0.0373(5)
C12	0.6841(2)	0.1928(2)	0.0904(2)	0.0534(7)
C13	0.5370(2)	0.2372(2)	0.1748(3)	0.0637(8)
C14	0.7437(2)	0.3031(2)	0.2768(2)	0.0492(6)
C15	0.6712(2)	0.0010(1)	0.2723(2)	0.0349(5)
C16	0.5333(2)	-0.0014(2)	0.2023(2)	0.0534(7)
C17	0.7207(2)	-0.0368(2)	0.1806(2)	0.0532(7)
C18	0.7124(2)	-0.0639(2)	0.3901(2)	0.0553(7)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **5a**.

Atom	x	y	z	U_{eq}
H3	0.9117(16)	0.1146(13)	0.6314(17)	0.029(5)
H4	1.0564(16)	0.2389(13)	0.7826(19)	0.031(5)
H7A	1.0216	0.4467	0.6219	0.096
H7B	1.1457	0.4885	0.7294	0.096
H7C	1.0735	0.4121	0.7688	0.096
H8A	1.2444	0.3333	0.5536	0.079
H8B	1.2546	0.4396	0.6033	0.079
H8C	1.1302	0.4016	0.4917	0.079
H9A	1.2492	0.3056	0.8623	0.082
H9B	1.3279	0.3803	0.8297	0.082
H9C	1.3163	0.2743	0.7785	0.082
H10A	0.9101	0.0453	0.4043	0.041
H10B	0.8992	0.1333	0.3134	0.041
H12A	0.6674	0.2498	0.0373	0.080
H12B	0.6276	0.1431	0.0408	0.080
H12C	0.7665	0.1718	0.1149	0.080
H13A	0.5127	0.2932	0.1194	0.096
H13B	0.5278	0.2492	0.2533	0.096
H13C	0.4863	0.1838	0.1279	0.096
H14A	0.8283	0.2923	0.2983	0.074
H14B	0.7365	0.3170	0.3560	0.074
H14C	0.7131	0.3565	0.2171	0.074
H16A	0.5048	0.0340	0.1211	0.080
H16B	0.5012	0.0272	0.2574	0.080
H16C	0.5059	-0.0668	0.1835	0.080
H17A	0.8087	-0.0377	0.2259	0.080
H17B	0.6941	0.0041	0.1045	0.080
H17C	0.6907	-0.1008	0.1533	0.080

H18A	0.6832	-0.1279	0.3616	0.083
H18B	0.6799	-0.0410	0.4481	0.083
H18C	0.8004	-0.0642	0.4362	0.083

Table 4: Anisotropic displacement parameters ($Å^2$) for **5a**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	0.0244(3)	0.0323(3)	0.0282(3)	-0.0041(2)	0.0121(2)	-0.0010(2)
C1	0.0248(10)	0.0466(13)	0.0277(11)	-0.0017(10)	0.0122(9)	-0.0008(10)
N2	0.0242(8)	0.0403(10)	0.0249(9)	-0.0049(8)	0.0113(7)	-0.0039(8)
C3	0.0281(11)	0.0412(13)	0.0286(12)	0.0047(10)	0.0140(9)	-0.0038(10)
C4	0.0292(11)	0.0437(13)	0.0219(11)	0.0000(10)	0.0111(9)	-0.0002(10)
N5	0.0244(8)	0.0355(10)	0.0245(9)	-0.0010(7)	0.0107(7)	-0.0031(7)
C6	0.0332(11)	0.0363(13)	0.0377(12)	-0.0053(10)	0.0187(10)	-0.0068(9)
C7	0.0673(18)	0.0407(15)	0.100(2)	-0.0115(15)	0.0523(17)	-0.0068(13)
C8	0.0473(14)	0.0646(17)	0.0500(15)	-0.0044(13)	0.0250(12)	-0.0224(13)
C9	0.0444(14)	0.0610(17)	0.0441(14)	-0.0093(12)	0.0070(11)	-0.0178(12)
C10	0.0276(10)	0.0437(13)	0.0317(11)	-0.0081(10)	0.0130(9)	-0.0008(10)
C11	0.0327(12)	0.0344(12)	0.0429(13)	0.0054(10)	0.0154(10)	0.0030(10)
C12	0.0649(16)	0.0532(16)	0.0351(13)	0.0089(11)	0.0162(12)	-0.0064(13)
C13	0.0399(14)	0.0515(16)	0.089(2)	0.0196(15)	0.0191(14)	0.0117(12)
C14	0.0539(15)	0.0328(13)	0.0628(16)	0.0022(12)	0.0278(13)	-0.0023(11)
C15	0.0344(11)	0.0295(11)	0.0333(12)	-0.0020(10)	0.0084(10)	-0.0020(9)
C16	0.0397(13)	0.0467(15)	0.0580(16)	-0.0068(12)	0.0079(12)	-0.0139(11)
C17	0.0647(16)	0.0392(14)	0.0466(14)	-0.0118(12)	0.0168(12)	0.0067(12)
C18	0.0592(16)	0.0424(15)	0.0532(15)	0.0085(12)	0.0153(13)	-0.0038(12)

Table 5: Bond lengths (Å) and angles (deg) for **5a**.

P1-C10	1.8693(18)	C1-N2-C3	112.52(16)
P1-C11	1.882(2)	C1-N2-C10	123.27(16)
P1-C15	1.882(2)	C3-N2-C10	124.17(16)
C1-N2	1.367(2)	C4-C3-N2	106.77(18)
C1-N5	1.368(2)	C3-C4-N5	106.49(18)
N2-C3	1.387(2)	C1-N5-C4	112.27(16)
N2-C10	1.462(2)	C1-N5-C6	124.39(16)
C3-C4	1.328(3)	C4-N5-C6	123.12(16)
C4-N5	1.394(2)	N5-C6-C8	109.43(16)
N5-C6	1.486(2)	N5-C6-C7	108.18(16)
C6-C8	1.521(3)	C8-C6-C7	110.21(19)
C6-C7	1.524(3)	N5-C6-C9	109.13(17)
C6-C9	1.528(3)	C8-C6-C9	109.66(18)
C11-C12	1.527(3)	C7-C6-C9	110.20(19)
C11-C13	1.544(3)	N2-C10-P1	112.67(13)
C11-C14	1.545(3)	C12-C11-C13	109.73(19)
C15-C18	1.531(3)	C12-C11-C14	108.58(18)
C15-C16	1.534(3)	C13-C11-C14	106.98(18)
C15-C17	1.543(3)	C12-C11-P1	117.42(15)
C10-P1-C11	102.31(9)	C13-C11-P1	108.18(15)
C10-P1-C15	99.50(9)	C14-C11-P1	105.43(14)
C11-P1-C15	111.16(9)	C18-C15-C16	107.78(18)
N2-C1-N5	101.94(15)	C18-C15-C17	108.96(18)

C16-C15-C17	109.06(18)
C18-C15-P1	104.51(14)
C16-C15-P1	109.07(15)
C17-C15-P1	117.05(15)

Crystal data for 6:

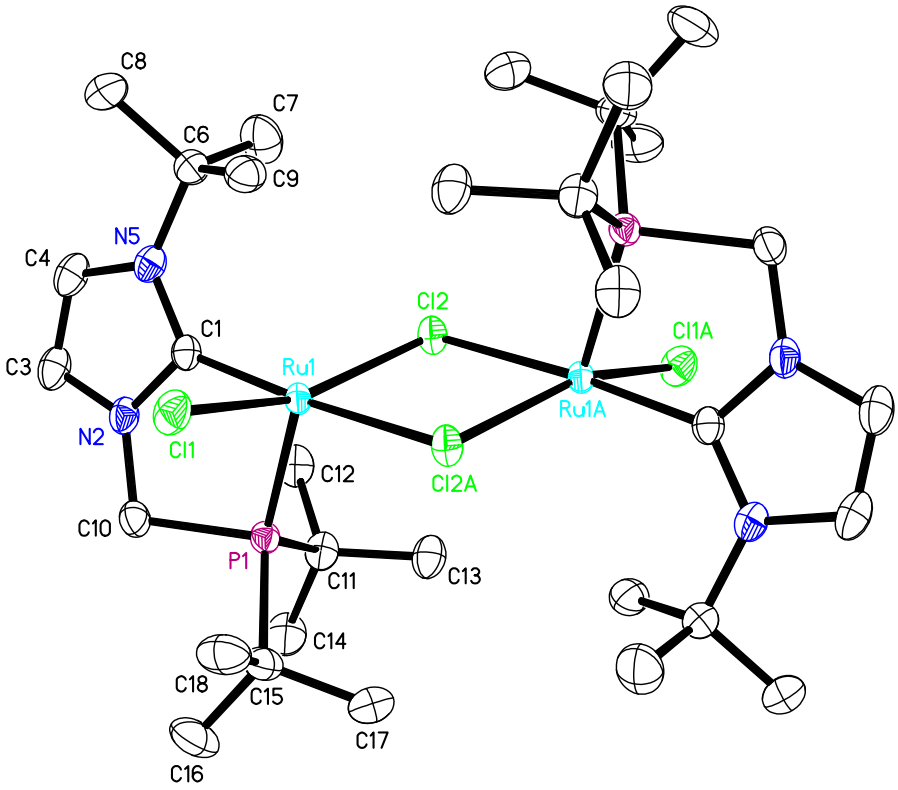


Table 1: Crystal data and structure refinement for **6**.

Identification code	msi19	
Empirical formula	$C_{34}H_{66}Cl_8N_4P_2Ru_2$	
Formula weight	1078.59	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	2	
Unit cell dimensions	a = 11.8023(1) Å	α = 90 deg.
	b = 18.0801(1) Å	β =116.582(1) deg.
	c = 12.1946(1) Å	γ = 90 deg.
Volume	2327.10(3) $Å^3$	
Density (calculated)	1.54 g/cm^3	
Absorption coefficient	1.21 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.30 x 0.19 x 0.17 mm^3	
Crystal colour	brown	
Theta range for data collection	2.0 to 27.4 deg.	
Index ranges	$-15\le h\le 15$, $-23\le k\le 22$, $-15\le l\le 15$	
Reflections collected	22349	
Independent reflections	5300 (R(int) = 0.0315)	
Observed reflections	4831 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.82 and 0.71	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5300 / 0 / 246	

Goodness-of-fit on F^2	1.06
Final R indices ($I>2\sigma(I)$)	R1 = 0.023, wR2 = 0.056
Largest diff. peak and hole	0.50 and -0.41 $eÅ^{-3}$

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **6**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.4912(1)	0.1001(1)	0.0376(1)	0.0165(1)
Cl1	0.5835(1)	0.1578(1)	0.2334(1)	0.0292(1)
Cl2	0.4776(1)	0.0260(1)	-0.1350(1)	0.0227(1)
P1	0.2900(1)	0.1257(1)	-0.0147(1)	0.0191(1)
C1	0.4877(2)	0.2006(1)	-0.0272(2)	0.0207(3)
N2	0.3932(1)	0.2497(1)	-0.0438(1)	0.0233(3)
C3	0.4132(2)	0.3178(1)	-0.0848(2)	0.0292(4)
C4	0.5218(2)	0.3111(1)	-0.0958(2)	0.0307(4)
N5	0.5696(2)	0.2399(1)	-0.0557(1)	0.0235(3)
C6	0.6908(2)	0.2115(1)	-0.0505(2)	0.0274(4)
C7	0.6642(3)	0.1806(1)	-0.1765(2)	0.0425(5)
C8	0.7871(2)	0.2750(1)	-0.0138(3)	0.0420(6)
C9	0.7436(2)	0.1516(1)	0.0478(2)	0.0294(4)
H9A	0.688(2)	0.1089(14)	0.026(2)	0.037(7)
H9B	0.755(2)	0.1679(13)	0.125(2)	0.034(6)
H9C	0.827(2)	0.1377(14)	0.060(2)	0.039(7)
C10	0.2926(2)	0.2290(1)	-0.0119(2)	0.0248(4)
C11	0.1691(2)	0.1056(1)	-0.1793(2)	0.0256(4)
C12	0.2151(2)	0.1461(1)	-0.2634(2)	0.0301(4)
C13	0.1604(2)	0.0222(1)	-0.2083(2)	0.0310(4)
C14	0.0344(2)	0.1344(1)	-0.2125(2)	0.0361(5)
C15	0.2193(2)	0.1016(1)	0.0938(2)	0.0278(4)
C16	0.1084(2)	0.1524(1)	0.0782(2)	0.0430(6)
C17	0.1758(2)	0.0204(1)	0.0750(2)	0.0388(5)
C18	0.3212(2)	0.1087(1)	0.2264(2)	0.0385(5)
C31	0.6565(3)	0.0232(2)	0.4649(2)	0.0502(6)
Cl3	0.6273(1)	0.0875(1)	0.5568(1)	0.0773(2)
Cl4	0.8163(1)	-0.0044(1)	0.5322(1)	0.0665(2)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **6**.

Atom	x	y	z	U_{eq}
H3	0.3611	0.3605	-0.1018	0.035
H4	0.5589	0.3478	-0.1253	0.037
H7A	0.6042	0.1394	-0.1970	0.064
H7B	0.7435	0.1631	-0.1749	0.064
H7C	0.6278	0.2196	-0.2384	0.064
H8A	0.7566	0.3131	-0.0778	0.063
H8B	0.8688	0.2560	-0.0042	0.063
H8C	0.7974	0.2964	0.0639	0.063
H9A	0.688(2)	0.1089(14)	0.026(2)	0.037(7)
H9B	0.755(2)	0.1679(13)	0.125(2)	0.034(6)
H9C	0.827(2)	0.1377(14)	0.060(2)	0.039(7)
H10A	0.2103	0.2493	-0.0722	0.030
H10B	0.3107	0.2477	0.0706	0.030

H12A	0.3026	0.1316	-0.2415	0.045
H12B	0.2113	0.1996	-0.2530	0.045
H12C	0.1606	0.1328	-0.3490	0.045
H13A	0.1119	0.0148	-0.2969	0.047
H13B	0.1180	-0.0031	-0.1658	0.047
H13C	0.2459	0.0020	-0.1805	0.047
H14A	0.0390	0.1864	-0.1880	0.054
H14B	-0.0030	0.1051	-0.1694	0.054
H14C	-0.0184	0.1301	-0.3012	0.054
H16A	0.0376	0.1448	-0.0032	0.065
H16B	0.1359	0.2042	0.0867	0.065
H16C	0.0811	0.1407	0.1412	0.065
H17A	0.1501	0.0061	0.1381	0.058
H17B	0.2457	-0.0113	0.0811	0.058
H17C	0.1039	0.0146	-0.0063	0.058
H18A	0.3527	0.1596	0.2420	0.058
H18B	0.3913	0.0750	0.2401	0.058
H18C	0.2849	0.0959	0.2822	0.058
H31A	0.6343	0.0454	0.3836	0.060
H31B	0.6020	-0.0208	0.4524	0.060

Table 4: Anisotropic displacement parameters ($Å^2$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0162(1)	0.0138(1)	0.0175(1)	-0.0012(1)	0.0059(1)	0.0006(1)
Cl1	0.0306(2)	0.0287(2)	0.0244(2)	-0.0077(2)	0.0087(2)	-0.0077(2)
Cl2	0.0292(2)	0.0172(2)	0.0209(2)	-0.0002(2)	0.0103(2)	0.0020(2)
P1	0.0167(2)	0.0176(2)	0.0209(2)	-0.0011(2)	0.0066(2)	0.0010(2)
C1	0.0221(8)	0.0185(8)	0.0189(8)	-0.0023(6)	0.0069(7)	-0.0007(7)
N2	0.0233(8)	0.0156(7)	0.0275(8)	0.0006(6)	0.0083(7)	0.0018(6)
C3	0.0278(10)	0.0189(9)	0.0308(10)	0.0023(7)	0.0041(8)	0.0012(7)
C4	0.0352(11)	0.0201(9)	0.0313(10)	0.0054(8)	0.0100(9)	-0.0029(8)
N5	0.0258(8)	0.0188(7)	0.0244(8)	0.0024(6)	0.0099(7)	-0.0010(6)
C6	0.0313(10)	0.0226(9)	0.0342(10)	0.0004(8)	0.0199(9)	-0.0010(8)
C7	0.0623(16)	0.0377(13)	0.0386(12)	0.0003(10)	0.0326(12)	0.0025(11)
C8	0.0380(12)	0.0318(12)	0.0666(16)	-0.0020(11)	0.0327(12)	-0.0075(9)
C9	0.0250(10)	0.0290(11)	0.0346(11)	0.0044(8)	0.0136(9)	0.0028(8)
C10	0.0219(9)	0.0200(9)	0.0301(10)	-0.0025(7)	0.0096(8)	0.0028(7)
C11	0.0217(9)	0.0237(9)	0.0236(9)	0.0005(7)	0.0032(7)	0.0011(7)
C12	0.0312(10)	0.0293(10)	0.0217(9)	0.0014(8)	0.0046(8)	0.0024(8)
C13	0.0299(10)	0.0256(10)	0.0287(10)	-0.0036(8)	0.0052(8)	-0.0028(8)
C14	0.0212(10)	0.0357(12)	0.0396(12)	-0.0014(9)	0.0029(9)	0.0026(8)
C15	0.0231(9)	0.0319(11)	0.0318(10)	-0.0022(8)	0.0154(8)	0.0005(8)
C16	0.0371(12)	0.0486(14)	0.0533(15)	-0.0004(11)	0.0292(11)	0.0118(10)
C17	0.0390(12)	0.0377(12)	0.0494(13)	-0.0011(10)	0.0286(11)	-0.0076(10)
C18	0.0359(12)	0.0555(15)	0.0290(11)	-0.0035(10)	0.0189(10)	-0.0052(10)
C31	0.0555(16)	0.0502(15)	0.0391(13)	-0.0066(11)	0.0161(12)	-0.0073(12)
Cl3	0.0946(7)	0.0776(6)	0.0736(5)	-0.0206(4)	0.0499(5)	-0.0019(5)
Cl4	0.0609(4)	0.0556(4)	0.0717(5)	0.0025(4)	0.0197(4)	0.0059(3)

Table 5: Bond lengths (Å) and angles (deg) for **6**.

Ru1-C1	1.9757(18)	Ru1-P1	2.2153(5)

Ru1-Cl1	2.3763(5)
Ru1-Cl2	2.4382(4)
Ru1-Cl2#1	2.5201(4)
Cl2-Ru1#1	2.5201(4)
P1-C10	1.8681(19)
P1-C15	1.904(2)
P1-C11	1.9060(19)
C1-N5	1.363(2)
C1-N2	1.368(2)
N2-C3	1.389(2)
N2-C10	1.454(2)
C3-C4	1.352(3)
C4-N5	1.403(2)
N5-C6	1.494(2)
C6-C9	1.525(3)
C6-C7	1.530(3)
C6-C8	1.535(3)
C11-C13	1.540(3)
C11-C12	1.543(3)
C11-C14	1.546(3)
C15-C18	1.529(3)
C15-C17	1.539(3)
C15-C16	1.539(3)
C31-Cl3	1.753(3)
C31-Cl4	1.759(3)
C1-Ru1-P1	82.20(5)
C1-Ru1-Cl1	85.16(5)
P1-Ru1-Cl1	98.523(18)
C1-Ru1-Cl2	100.27(5)
P1-Ru1-Cl2	102.599(16)
Cl1-Ru1-Cl2	158.705(17)
C1-Ru1-Cl2#1	173.47(5)
P1-Ru1-Cl2#1	103.692(17)
Cl1-Ru1-Cl2#1	91.130(16)
Cl2-Ru1-Cl2#1	81.337(15)
Ru1-Cl2-Ru1#1	98.663(15)
C10-P1-C15	102.97(9)
C10-P1-C11	102.05(8)
C15-P1-C11	109.52(9)
C10-P1-Ru1	101.36(6)
C15-P1-Ru1	119.92(6)
C11-P1-Ru1	117.66(6)
N5-C1-N2	104.40(15)
N5-C1-Ru1	133.68(14)
N2-C1-Ru1	121.74(13)
C1-N2-C3	111.72(16)
C1-N2-C10	120.19(15)
C3-N2-C10	127.98(16)
C4-C3-N2	106.10(17)
C3-C4-N5	107.40(17)
C1-N5-C4	110.26(16)
C1-N5-C6	125.78(15)
C4-N5-C6	123.93(16)
N5-C6-C9	108.95(15)
N5-C6-C7	108.68(17)
C9-C6-C7	110.99(18)
N5-C6-C8	109.01(16)
C9-C6-C8	108.20(18)
C7-C6-C8	110.96(18)
N2-C10-P1	105.16(12)
C13-C11-C12	108.62(17)
C13-C11-C14	108.37(16)
C12-C11-C14	107.00(16)
C13-C11-P1	111.70(13)
C12-C11-P1	106.79(13)
C14-C11-P1	114.14(14)
C18-C15-C17	106.82(18)
C18-C15-C16	107.71(18)
C17-C15-C16	110.07(18)
C18-C15-P1	109.52(14)
C17-C15-P1	109.55(14)
C16-C15-P1	112.96(15)
Cl3-C31-Cl4	111.52(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z

Crystal data for 7a:

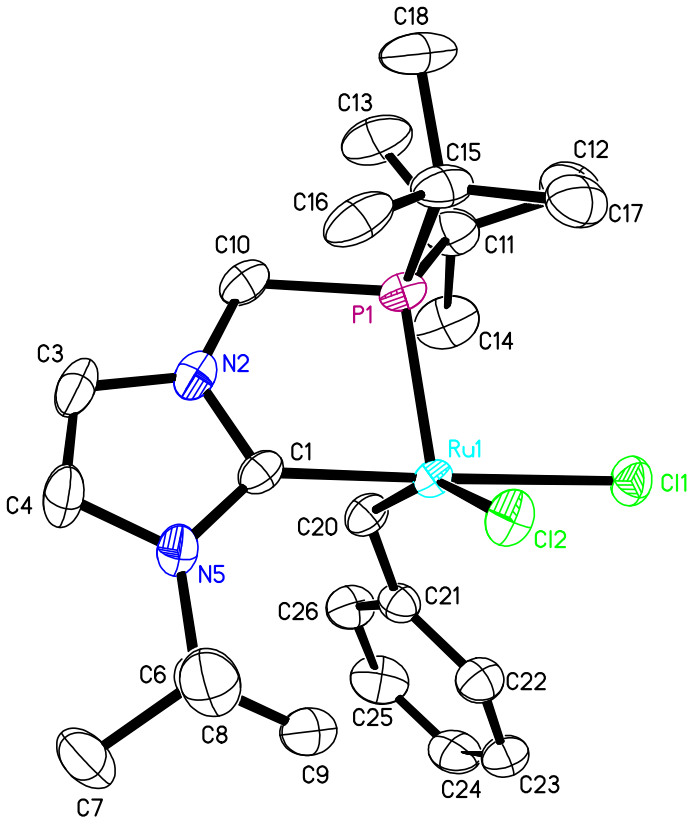


Table 1: Crystal data and structure refinement for **7a**.

Identification code	hi6	
Empirical formula	$C_{24}H_{39}Cl_4N_2PRu$	
Formula weight	629.41	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	trigonal	
Space group	$P3_121$	
Z	6	
Unit cell dimensions	a = 12.4946(11) Å	α = 90 deg.
	b = 12.4946(11) Å	β = 90 deg.
	c = 31.855(4) Å	γ = 120 deg.
Volume	4306.8(7) $Å^3$	
Density (calculated)	1.46 g/cm^3	
Absorption coefficient	0.99 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.18 x 0.09 x 0.08 mm^3	
Crystal colour	dark orange	
Theta range for data collection	1.9 to 28.4 deg.	
Index ranges	$-16 \le h \le 16$, $-16 \le k \le 16$, $-42 \le l \le 42$	
Reflections collected	45832	
Independent reflections	7137 (R(int) = 0.0615)	
Observed reflections	6633 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.93 and 0.84
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7137 / 0 / 289
Goodness-of-fit on F^2	1.10
Final R indices ($I>2\sigma(I)$)	R1 = 0.035, wR2 = 0.072
Absolute structure parameter	0.07(3)
Largest diff. peak and hole	0.73 and -0.37 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **7a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.6338(1)	0.4378(1)	0.7633(1)	0.0198(1)
P1	0.7747(1)	0.6364(1)	0.7688(1)	0.0253(2)
Cl1	0.4599(1)	0.4573(1)	0.7879(1)	0.0306(2)
Cl2	0.5355(1)	0.3877(1)	0.6927(1)	0.0297(2)
C1	0.7816(3)	0.4259(3)	0.7426(1)	0.0243(6)
N2	0.8986(2)	0.5232(2)	0.7481(1)	0.0283(6)
C3	0.9871(3)	0.4967(4)	0.7337(1)	0.0379(8)
C4	0.9261(3)	0.3812(4)	0.7196(1)	0.0396(8)
N5	0.8004(2)	0.3360(2)	0.7254(1)	0.0287(6)
C6	0.7048(3)	0.2062(3)	0.7135(1)	0.0324(7)
C7	0.7565(4)	0.1195(4)	0.7237(1)	0.0495(10)
C8	0.6800(4)	0.2048(4)	0.6667(1)	0.0453(9)
C9	0.5881(3)	0.1635(3)	0.7397(1)	0.0453(9)
C10	0.9225(3)	0.6345(3)	0.7700(1)	0.0313(7)
C11	0.7836(3)	0.7292(3)	0.8168(1)	0.0380(8)
C12	0.6965(4)	0.7816(4)	0.8127(1)	0.0586(11)
C13	0.9174(4)	0.8334(3)	0.8252(1)	0.0529(10)
C14	0.7420(4)	0.6433(4)	0.8555(1)	0.0475(10)
C15	0.7857(3)	0.7251(3)	0.7194(1)	0.0354(8)
C16	0.8219(3)	0.6666(3)	0.6833(1)	0.0415(9)
C17	0.6610(4)	0.7135(3)	0.7088(1)	0.0433(9)
C18	0.8855(4)	0.8631(3)	0.7219(1)	0.0517(10)
C20	0.6828(3)	0.4049(3)	0.8153(1)	0.0265(6)
C21	0.6021(3)	0.3136(3)	0.8463(1)	0.0264(7)
C22	0.4765(3)	0.2330(3)	0.8397(1)	0.0324(7)
C23	0.4040(3)	0.1493(3)	0.8703(1)	0.0378(8)
C24	0.4556(3)	0.1478(3)	0.9085(1)	0.0399(8)
C25	0.5801(4)	0.2263(3)	0.9158(1)	0.0426(9)
C26	0.6531(3)	0.3083(3)	0.8849(1)	0.0344(8)
C31	1.2381(3)	0.2245(3)	0.7256(1)	0.0430(9)
Cl3	1.0863(1)	0.1823(1)	0.7113(1)	0.0435(2)
Cl4	1.2441(1)	0.1004(1)	0.7489(1)	0.0509(2)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **7a**.

Atom	x	y	z	U_{eq}
H3	1.0741	0.5503	0.7339	0.045
H4	0.9622	0.3371	0.7075	0.048
H7A	0.8315	0.1444	0.7072	0.074

H7B	0.6945	0.0342	0.7166	0.074
H7C	0.7762	0.1249	0.7536	0.074
H8A	0.7572	0.2325	0.6512	0.068
H8B	0.6477	0.2603	0.6608	0.068
H8C	0.6193	0.1206	0.6580	0.068
H9A	0.6082	0.1652	0.7696	0.068
H9B	0.5263	0.0791	0.7317	0.068
H9C	0.5548	0.2187	0.7348	0.068
H10A	0.9887	0.7084	0.7557	0.038
H10B	0.9481	0.6332	0.7993	0.038
H12A	0.6122	0.7139	0.8075	0.088
H12B	0.7233	0.8401	0.7893	0.088
H12C	0.6982	0.8242	0.8387	0.088
H13A	0.9714	0.7978	0.8279	0.079
H13B	0.9201	0.8765	0.8512	0.079
H13C	0.9457	0.8921	0.8017	0.079
H14A	0.6573	0.5754	0.8513	0.071
H14B	0.7450	0.6904	0.8805	0.071
H14C	0.7973	0.6097	0.8594	0.071
H16A	0.7605	0.5785	0.6811	0.062
H16B	0.9033	0.6762	0.6891	0.062
H16C	0.8249	0.7080	0.6568	0.062
H17A	0.5975	0.6260	0.7073	0.065
H17B	0.6666	0.7531	0.6817	0.065
H17C	0.6388	0.7542	0.7307	0.065
H18A	0.8646	0.9028	0.7445	0.078
H18B	0.8892	0.9035	0.6951	0.078
H18C	0.9660	0.8706	0.7277	0.078
H20	0.7681	0.4521	0.8221	0.032
H22	0.4401	0.2356	0.8138	0.039
H23	0.3190	0.0931	0.8651	0.045
H24	0.4053	0.0925	0.9299	0.048
H25	0.6154	0.2240	0.9419	0.051
H26	0.7388	0.3615	0.8900	0.041
H31A	1.2915	0.2521	0.7004	0.052
H31B	1.2702	0.2945	0.7456	0.052

Table 4: Anisotropic displacement parameters ($Å^2$) for **7a**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0176(1)	0.0200(1)	0.0186(1)	0.0002(1)	0.0007(1)	0.0069(1)
P1	0.0240(4)	0.0214(4)	0.0233(4)	-0.0001(3)	-0.0002(3)	0.0060(3)
Cl1	0.0266(4)	0.0348(4)	0.0325(4)	-0.0035(3)	0.0031(3)	0.0170(3)
Cl2	0.0265(4)	0.0380(4)	0.0232(3)	-0.0037(3)	-0.0019(3)	0.0151(3)
C1	0.0206(15)	0.0262(16)	0.0208(14)	0.0026(12)	0.0002(11)	0.0077(13)
N2	0.0211(13)	0.0336(14)	0.0273(13)	0.0023(11)	0.0009(10)	0.0115(11)
C3	0.0206(16)	0.049(2)	0.042(2)	0.0074(17)	0.0065(15)	0.0156(16)
C4	0.0278(17)	0.051(2)	0.045(2)	-0.0019(18)	0.0068(15)	0.0235(18)
N5	0.0237(13)	0.0342(15)	0.0300(13)	-0.0017(10)	0.0013(10)	0.0160(12)
C6	0.0321(18)	0.0302(17)	0.0397(18)	-0.0055(14)	-0.0031(14)	0.0192(15)
C7	0.061(3)	0.042(2)	0.061(3)	-0.0050(19)	-0.005(2)	0.037(2)
C8	0.048(2)	0.050(2)	0.044(2)	-0.0137(18)	-0.0110(18)	0.029(2)
C9	0.037(2)	0.0294(19)	0.063(2)	-0.0019(18)	0.0070(19)	0.0121(16)
C10	0.0225(16)	0.0305(16)	0.0306(16)	-0.0007(13)	-0.0030(13)	0.0056(14)
C11	0.042(2)	0.0313(17)	0.0350(18)	-0.0104(15)	-0.0021(16)	0.0145(17)

C12	0.072(3)	0.048(2)	0.064(3)	-0.018(2)	-0.001(2)	0.035(2)
C13	0.051(2)	0.035(2)	0.046(2)	-0.0163(18)	-0.0058(19)	0.0013(17)
C14	0.056(2)	0.045(2)	0.0276(17)	-0.0142(16)	0.0037(17)	0.0146(19)
C15	0.0378(19)	0.0283(17)	0.0286(16)	0.0103(13)	-0.0023(15)	0.0078(15)
C16	0.0324(19)	0.043(2)	0.0259(16)	0.0108(15)	0.0026(14)	0.0017(16)
C17	0.047(2)	0.0355(19)	0.044(2)	0.0056(16)	-0.0119(18)	0.0184(17)
C18	0.053(2)	0.0269(18)	0.051(2)	0.0106(17)	-0.0060(19)	0.0016(17)
C20	0.0232(15)	0.0290(16)	0.0229(14)	0.0018(12)	0.0004(12)	0.0096(12)
C21	0.0301(17)	0.0245(15)	0.0253(15)	0.0029(12)	0.0026(12)	0.0143(13)
C22	0.0347(18)	0.0323(17)	0.0279(16)	0.0059(13)	0.0008(14)	0.0151(15)
C23	0.0319(18)	0.0287(18)	0.048(2)	0.0086(15)	0.0090(15)	0.0112(15)
C24	0.050(2)	0.0321(18)	0.0359(18)	0.0128(16)	0.0180(16)	0.0189(17)
C25	0.060(2)	0.042(2)	0.0238(15)	0.0084(14)	-0.0012(16)	0.024(2)
C26	0.0365(18)	0.0334(18)	0.0293(16)	0.0037(14)	-0.0044(14)	0.0145(15)
C31	0.0310(18)	0.037(2)	0.057(2)	0.0058(17)	-0.0087(17)	0.0136(16)
Cl3	0.0310(4)	0.0444(5)	0.0534(5)	-0.0019(4)	-0.0105(4)	0.0177(4)
Cl4	0.0562(6)	0.0477(6)	0.0585(6)	0.0030(5)	-0.0104(5)	0.0331(5)

Table 5: Bond lengths (Å) and angles (deg) for **7a**.

Ru1-C20	1.883(3)	C13-H13C	0.9800
Ru1-C1	2.035(3)	C14-H14A	0.9800
Ru1-P1	2.2175(8)	C14-H14B	0.9800
Ru1-Cl1	2.4339(8)	C14-H14C	0.9800
Ru1-Cl2	2.4864(8)	C15-C17	1.529(5)
P1-C10	1.858(3)	C15-C18	1.544(5)
P1-C15	1.890(3)	C15-C16	1.546(5)
P1-C11	1.891(3)	C16-H16A	0.9800
C1-N2	1.367(4)	C16-H16B	0.9800
C1-N5	1.371(4)	C16-H16C	0.9800
N2-C3	1.381(4)	C17-H17A	0.9800
N2-C10	1.447(4)	C17-H17B	0.9800
C3-C4	1.329(5)	C17-H17C	0.9800
C3-H3	0.9500	C18-H18A	0.9800
C4-N5	1.390(4)	C18-H18B	0.9800
C4-H4	0.9500	C18-H18C	0.9800
N5-C6	1.504(4)	C20-C21	1.464(4)
C6-C8	1.521(5)	C20-H20	0.9500
C6-C9	1.526(5)	C21-C22	1.393(4)
C6-C7	1.549(4)	C21-C26	1.402(4)
C7-H7A	0.9800	C22-C23	1.386(4)
C7-H7B	0.9800	C22-H22	0.9500
C7-H7C	0.9800	C23-C24	1.380(5)
C8-H8A	0.9800	C23-H23	0.9500
C8-H8B	0.9800	C24-C25	1.382(5)
C8-H8C	0.9800	C24-H24	0.9500
C9-H9A	0.9800	C25-C26	1.382(4)
C9-H9B	0.9800	C25-H25	0.9500
C9-H9C	0.9800	C26-H26	0.9500
C10-H10A	0.9900	C31-Cl4	1.753(4)
C10-H10B	0.9900	C31-Cl3	1.756(4)
C11-C12	1.529(6)	C31-H31A	0.9900
C11-C14	1.544(5)	C31-H31B	0.9900
C11-C13	1.544(5)	C20-Ru1-C1	82.09(12)
C12-H12A	0.9800	C20-Ru1-P1	90.67(10)
C12-H12B	0.9800	C1-Ru1-P1	82.27(9)
C12-H12C	0.9800	C20-Ru1-Cl1	98.19(9)
C13-H13A	0.9800	C1-Ru1-Cl1	178.70(9)
C13-H13B	0.9800	P1-Ru1-Cl1	96.46(3)

C20-Ru1-Cl2	156.14(10)	C11-C12-H12B	109.5
C1-Ru1-Cl2	92.35(8)	H12A-C12-H12B	109.5
P1-Ru1-Cl2	111.66(3)	C11-C12-H12C	109.5
Cl1-Ru1-Cl2	87.89(3)	H12A-C12-H12C	109.5
C10-P1-C15	104.09(16)	H12B-C12-H12C	109.5
C10-P1-C11	103.73(16)	C11-C13-H13A	109.5
C15-P1-C11	110.47(16)	C11-C13-H13B	109.5
C10-P1-Ru1	103.05(11)	H13A-C13-H13B	109.5
C15-P1-Ru1	111.99(11)	C11-C13-H13C	109.5
C11-P1-Ru1	121.36(12)	H13A-C13-H13C	109.5
N2-C1-N5	103.6(3)	H13B-C13-H13C	109.5
N2-C1-Ru1	119.9(2)	C11-C14-H14A	109.5
N5-C1-Ru1	136.3(2)	C11-C14-H14B	109.5
C1-N2-C3	111.9(3)	H14A-C14-H14B	109.5
C1-N2-C10	122.1(3)	C11-C14-H14C	109.5
C3-N2-C10	125.8(3)	H14A-C14-H14C	109.5
C4-C3-N2	106.2(3)	H14B-C14-H14C	109.5
C4-C3-H3	126.9	C17-C15-C18	109.4(3)
N2-C3-H3	126.9	C17-C15-C16	108.5(3)
C3-C4-N5	108.3(3)	C18-C15-C16	107.7(3)
C3-C4-H4	125.9	C17-C15-P1	110.9(2)
N5-C4-H4	125.9	C18-C15-P1	113.1(2)
C1-N5-C4	110.0(3)	C16-C15-P1	107.1(2)
C1-N5-C6	127.9(2)	C15-C16-H16A	109.5
C4-N5-C6	122.1(3)	C15-C16-H16B	109.5
N5-C6-C8	107.9(3)	H16A-C16-H16B	109.5
N5-C6-C9	110.1(3)	C15-C16-H16C	109.5
C8-C6-C9	112.3(3)	H16A-C16-H16C	109.5
N5-C6-C7	108.5(3)	H16B-C16-H16C	109.5
C8-C6-C7	110.5(3)	C15-C17-H17A	109.5
C9-C6-C7	107.5(3)	C15-C17-H17B	109.5
C6-C7-H7A	109.5	H17A-C17-H17B	109.5
C6-C7-H7B	109.5	C15-C17-H17C	109.5
H7A-C7-H7B	109.5	H17A-C17-H17C	109.5
C6-C7-H7C	109.5	H17B-C17-H17C	109.5
H7A-C7-H7C	109.5	C15-C18-H18A	109.5
H7B-C7-H7C	109.5	C15-C18-H18B	109.5
C6-C8-H8A	109.5	H18A-C18-H18B	109.5
C6-C8-H8B	109.5	C15-C18-H18C	109.5
H8A-C8-H8B	109.5	H18A-C18-H18C	109.5
C6-C8-H8C	109.5	H18B-C18-H18C	109.5
H8A-C8-H8C	109.5	C21-C20-Ru1	126.3(2)
H8B-C8-H8C	109.5	C21-C20-H20	116.9
C6-C9-H9A	109.5	Ru1-C20-H20	116.9
C6-C9-H9B	109.5	C22-C21-C26	118.3(3)
H9A-C9-H9B	109.5	C22-C21-C20	123.3(3)
C6-C9-H9C	109.5	C26-C21-C20	118.4(3)
H9A-C9-H9C	109.5	C23-C22-C21	120.9(3)
H9B-C9-H9C	109.5	C23-C22-H22	119.6
N2-C10-P1	105.9(2)	C21-C22-H22	119.6
N2-C10-H10A	110.6	C24-C23-C22	119.8(3)
P1-C10-H10A	110.6	C24-C23-H23	120.1
N2-C10-H10B	110.6	C22-C23-H23	120.1
P1-C10-H10B	110.6	C23-C24-C25	120.4(3)
H10A-C10-H10B	108.7	C23-C24-H24	119.8
C12-C11-C14	107.6(3)	C25-C24-H24	119.8
C12-C11-C13	110.9(3)	C24-C25-C26	119.9(3)
C14-C11-C13	107.2(3)	C24-C25-H25	120.0
C12-C11-P1	110.9(3)	C26-C25-H25	120.0
C14-C11-P1	108.9(2)	C25-C26-C21	120.7(3)
C13-C11-P1	111.3(3)	C25-C26-H26	119.7
C11-C12-H12A	109.5	C21-C26-H26	119.7

Cl4-C31-Cl3	111.24(19)
Cl4-C31-H31A	109.4
Cl3-C31-H31A	109.4
Cl4-C31-H31B	109.4
Cl3-C31-H31B	109.4
H31A-C31-H31B	108.0

Crystal data for 7b:

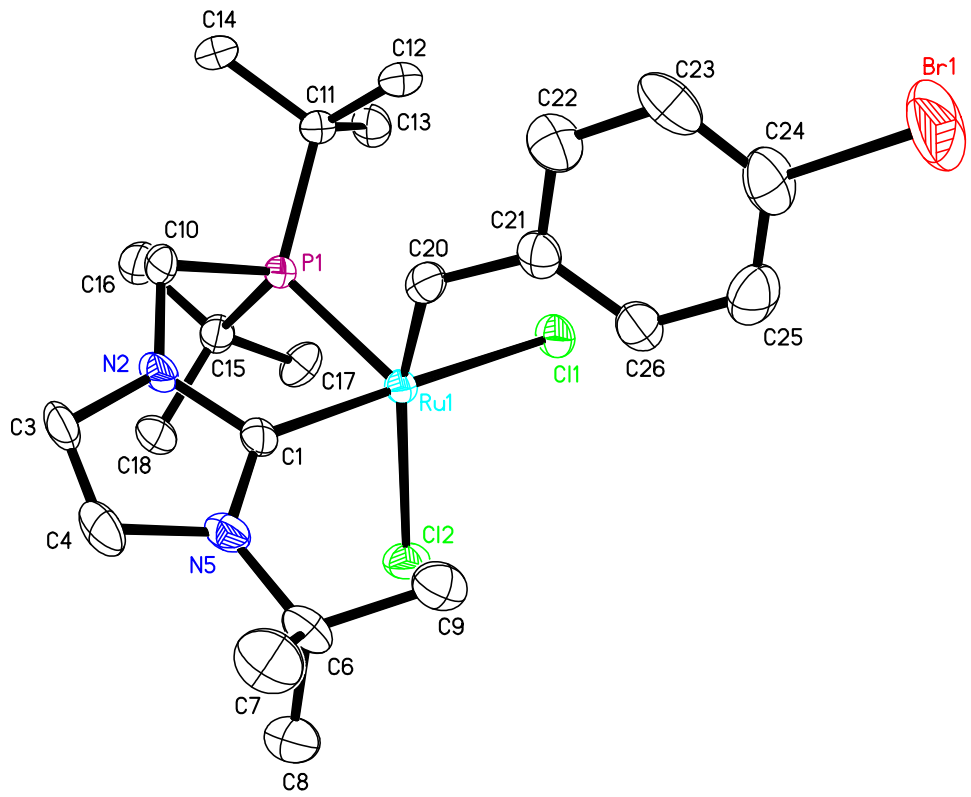


Table 1: Crystal data and structure refinement for **7b**.

Identification code	msi38
Empirical formula	$C_{23}H_{36}BrCl_2N_2PRu * (CH_2Cl_2)_{1.5}$
Formula weight	750.78
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Z	4
Unit cell dimensions	a = 9.6909(1) Å α = 90 deg. b = 26.8891(1) Å β =103.368(1) deg. c = 12.5386(2) Å γ = 90 deg.
Volume	3178.78(6) $Å^3$
Density (calculated)	1.57 g/cm^3
Absorption coefficient	2.24 mm^{-1}
Crystal shape	polyhedron
Crystal size	0.22 x 0.14 x 0.04 mm^3
Crystal colour	green
Theta range for data collection	1.8 to 24.7 deg.
Index ranges	$-11 \le h \le 11$, $-31 \le k \le 31$, $-14 \le l \le 14$
Reflections collected	24728
Independent reflections	5424 (R(int) = 0.0866)
Observed reflections	3792 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.92 and 0.64
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	5424 / 10 / 319

Goodness-of-fit on F^2	1.08
Final R indices ($I>2\sigma(I)$)	R1 = 0.063, wR2 = 0.126
Largest diff. peak and hole	1.37 and -1.27 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **7b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	-0.9629(1)	-0.1568(1)	-0.7805(1)	0.0187(2)
Cl1	-0.7089(2)	-0.1572(1)	-0.7176(2)	0.0297(4)
Cl2	-0.9695(2)	-0.1846(1)	-0.5916(2)	0.0311(5)
P1	-0.9854(2)	-0.2211(1)	-0.8963(2)	0.0195(4)
C1	-1.1794(7)	-0.1570(3)	-0.8301(5)	0.0221(16)
N2	-1.2443(6)	-0.1868(2)	-0.9170(5)	0.0244(14)
C3	-1.3904(7)	-0.1850(3)	-0.9323(6)	0.0310(19)
C4	-1.4175(7)	-0.1544(3)	-0.8555(6)	0.0331(19)
N5	-1.2880(6)	-0.1352(2)	-0.7948(5)	0.0253(14)
C6	-1.2798(8)	-0.0955(3)	-0.7114(7)	0.0297(18)
C7	-1.3963(9)	-0.0577(3)	-0.7573(8)	0.047(2)
C8	-1.3037(9)	-0.1174(3)	-0.6048(7)	0.041(2)
C9	-1.1355(8)	-0.0691(3)	-0.6912(7)	0.035(2)
C10	-1.1645(7)	-0.2121(3)	-0.9834(6)	0.0241(17)
C11	-0.8639(7)	-0.2275(3)	-0.9939(6)	0.0239(17)
C12	-0.8171(8)	-0.1765(3)	-1.0250(6)	0.0312(19)
C13	-0.7284(8)	-0.2564(3)	-0.9385(7)	0.0326(19)
C14	-0.9416(8)	-0.2537(3)	-1.1008(6)	0.0314(19)
C15	-1.0035(8)	-0.2824(3)	-0.8276(6)	0.0246(17)
C16	-1.0228(9)	-0.3273(3)	-0.9061(6)	0.036(2)
C17	-0.8734(8)	-0.2914(3)	-0.7329(6)	0.0322(19)
C18	-1.1360(8)	-0.2805(3)	-0.7786(6)	0.0318(19)
C20	-0.9739(7)	-0.1117(3)	-0.8975(6)	0.0254(17)
C21	-0.8922(8)	-0.0668(3)	-0.8955(6)	0.0273(18)
C22	-0.8790(9)	-0.0457(3)	-0.9953(7)	0.037(2)
C23	-0.7941(9)	-0.0050(3)	-0.9980(8)	0.046(2)
C24	-0.7251(9)	0.0167(3)	-0.9017(8)	0.042(2)
C25	-0.7383(9)	-0.0014(3)	-0.8010(8)	0.043(2)
C26	-0.8197(8)	-0.0436(3)	-0.7994(7)	0.0315(19)
Br1	-0.6114(1)	0.0738(1)	-0.9080(1)	0.0774(4)
C31	-0.9504(11)	-0.1180(7)	-1.3408(12)	0.133(7)
Cl3	-0.8051(4)	-0.0834(2)	-1.2773(4)	0.1121(13)
Cl4	-1.0971(4)	-0.1120(2)	-1.2860(3)	0.0940(11)
C32	-1.6491(17)	-0.0541(9)	-0.504(3)	0.123(11)
Cl5	-1.8066(10)	-0.0214(4)	-0.5255(8)	0.139(3)
Cl6	-1.5124(16)	-0.0114(5)	-0.4941(14)	0.154(4)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **7b**.

Atom	x	y	z	U_{eq}
H3	-1.4581	-0.2022	-0.9867	0.037
H4	-1.5087	-0.1469	-0.8439	0.040
H7A	-1.3908	-0.0483	-0.8318	0.070
H7B	-1.3835	-0.0281	-0.7105	0.070
H7C	-1.4892	-0.0726	-0.7593	0.070

H8A	-1.3968	-0.1336	-0.6188	0.061
H8B	-1.2999	-0.0908	-0.5508	0.061
H8C	-1.2296	-0.1420	-0.5763	0.061
H9A	-1.0607	-0.0919	-0.6544	0.053
H9B	-1.1366	-0.0398	-0.6450	0.053
H9C	-1.1169	-0.0587	-0.7615	0.053
H10A	-1.1604	-0.1919	-1.0486	0.029
H10B	-1.2086	-0.2445	-1.0083	0.029
H12A	-0.7512	-0.1805	-1.0730	0.047
H12B	-0.7698	-0.1586	-0.9586	0.047
H12C	-0.9003	-0.1576	-1.0635	0.047
H13A	-0.6620	-0.2563	-0.9867	0.049
H13B	-0.7534	-0.2907	-0.9248	0.049
H13C	-0.6840	-0.2404	-0.8688	0.049
H14A	-1.0171	-0.2321	-1.1412	0.047
H14B	-0.9829	-0.2850	-1.0827	0.047
H14C	-0.8739	-0.2608	-1.1461	0.047
H16A	-0.9372	-0.3316	-0.9342	0.053
H16B	-1.1045	-0.3216	-0.9674	0.053
H16C	-1.0389	-0.3574	-0.8665	0.053
H17A	-0.8570	-0.2621	-0.6852	0.048
H17B	-0.7899	-0.2974	-0.7627	0.048
H17C	-0.8904	-0.3204	-0.6905	0.048
H18A	-1.1390	-0.3104	-0.7344	0.048
H18B	-1.2216	-0.2791	-0.8382	0.048
H18C	-1.1314	-0.2509	-0.7323	0.048
H20	-1.0398	-0.1193	-0.9642	0.030
H22	-0.9300	-0.0599	-1.0623	0.044
H23	-0.7833	0.0079	-1.0661	0.055
H25	-0.6926	0.0148	-0.7348	0.052
H26	-0.8264	-0.0571	-0.7308	0.038
H31A	-0.9226	-0.1535	-1.3376	0.160
H31B	-0.9774	-0.1084	-1.4191	0.160
H32A	-1.6507	-0.0772	-0.5659	0.148
H32B	-1.6354	-0.0738	-0.4358	0.148

Table 4: Anisotropic displacement parameters ($Å^2$) for **7b**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{12}
Ru1	0.0139(3)	0.0250(3)	0.0170(3)	-0.0008(3)	0.0031(2)	-0.0015(3)	
Cl1	0.0143(9)	0.0453(12)	0.0273(10)	0.0005(9)	0.0002(7)	-0.0007(9)	
Cl2	0.0324(11)	0.0413(12)	0.0208(10)	0.0010(9)	0.0088(8)	0.0005(9)	
P1	0.0162(9)	0.0263(11)	0.0161(9)	-0.0017(8)	0.0037(7)	-0.0033(8)	
C1	0.023(4)	0.027(4)	0.016(4)	0.007(3)	0.004(3)	-0.008(3)	
N2	0.011(3)	0.037(4)	0.024(3)	0.002(3)	0.004(3)	0.002(3)	
C3	0.015(4)	0.046(5)	0.031(5)	0.005(4)	0.004(3)	-0.009(4)	
C4	0.012(4)	0.048(5)	0.037(5)	0.014(4)	0.002(3)	0.003(4)	
N5	0.019(3)	0.032(4)	0.027(3)	0.001(3)	0.010(3)	0.003(3)	
C6	0.022(4)	0.031(5)	0.040(5)	0.005(4)	0.014(4)	0.003(3)	
C7	0.040(5)	0.045(6)	0.056(6)	0.006(5)	0.013(5)	0.012(4)	
C8	0.041(5)	0.046(5)	0.039(5)	-0.003(4)	0.019(4)	-0.004(4)	
C9	0.038(5)	0.033(5)	0.038(5)	0.003(4)	0.015(4)	0.000(4)	
C10	0.017(4)	0.036(5)	0.017(4)	0.002(3)	-0.002(3)	-0.005(3)	
C11	0.023(4)	0.031(4)	0.018(4)	-0.001(3)	0.006(3)	-0.004(3)	
C12	0.032(4)	0.042(5)	0.023(4)	-0.008(4)	0.012(3)	-0.006(4)	

C13	0.025(4)	0.034(5)	0.041(5)	-0.012(4)	0.013(4)	-0.002(4)
C14	0.036(5)	0.041(5)	0.019(4)	-0.005(4)	0.010(3)	-0.007(4)
C15	0.025(4)	0.026(4)	0.022(4)	0.000(3)	0.003(3)	-0.004(3)
C16	0.041(5)	0.037(5)	0.029(5)	0.000(4)	0.007(4)	-0.009(4)
C17	0.036(5)	0.032(5)	0.024(4)	-0.001(4)	-0.003(4)	0.004(4)
C18	0.033(5)	0.037(5)	0.028(4)	0.005(4)	0.013(4)	-0.012(4)
C20	0.014(4)	0.039(5)	0.022(4)	-0.006(3)	0.001(3)	0.003(3)
C21	0.018(4)	0.029(4)	0.035(5)	-0.004(4)	0.008(3)	0.002(3)
C22	0.036(5)	0.036(5)	0.036(5)	0.015(4)	0.003(4)	0.001(4)
C23	0.045(5)	0.039(5)	0.059(6)	0.019(5)	0.023(5)	-0.002(4)
C24	0.044(5)	0.020(5)	0.064(7)	0.001(4)	0.017(5)	-0.002(4)
C25	0.044(5)	0.035(5)	0.051(6)	-0.014(5)	0.010(4)	0.000(4)
C26	0.030(4)	0.027(4)	0.040(5)	-0.001(4)	0.013(4)	-0.001(4)
Br1	0.0894(9)	0.0400(6)	0.1080(10)	0.0037(6)	0.0332(8)	-0.0300(6)
C31	0.093(9)	0.200(19)	0.101(12)	-0.090(12)	0.011(8)	0.002(10)
Cl3	0.115(3)	0.094(3)	0.139(4)	-0.024(3)	0.054(3)	-0.016(2)
Cl4	0.078(2)	0.112(3)	0.084(2)	-0.021(2)	0.0023(18)	0.009(2)

Table 5: Bond lengths (Å) and angles (deg) for **7b**.

Ru1-C20	1.887(8)	C20-Ru1-Cl1	97.3(2)
Ru1-C1	2.046(7)	C1-Ru1-Cl1	178.57(19)
Ru1-P1	2.2369(19)	P1-Ru1-Cl1	98.53(7)
Ru1-Cl1	2.4047(17)	C20-Ru1-Cl2	156.9(2)
Ru1-Cl2	2.4987(19)	C1-Ru1-Cl2	92.21(19)
P1-C10	1.841(7)	P1-Ru1-Cl2	111.34(7)
P1-C15	1.886(8)	Cl1-Ru1-Cl2	86.36(6)
P1-C11	1.892(7)	C10-P1-C15	102.3(3)
C1-N5	1.365(9)	C10-P1-C11	105.7(3)
C1-N2	1.381(9)	C15-P1-C11	110.7(3)
N2-C3	1.384(9)	C10-P1-Ru1	102.7(2)
N2-C10	1.432(9)	C15-P1-Ru1	112.6(2)
C3-C4	1.340(11)	C11-P1-Ru1	120.6(2)
C4-N5	1.406(9)	N5-C1-N2	105.1(6)
N5-C6	1.485(10)	N5-C1-Ru1	135.6(5)
C6-C8	1.527(11)	N2-C1-Ru1	119.3(5)
C6-C7	1.528(11)	C1-N2-C3	110.8(6)
C6-C9	1.537(10)	C1-N2-C10	121.7(6)
C11-C12	1.524(11)	C3-N2-C10	127.4(6)
C11-C13	1.545(10)	C4-C3-N2	106.6(7)
C11-C14	1.547(10)	C3-C4-N5	108.4(6)
C15-C17	1.538(10)	C1-N5-C4	109.0(6)
C15-C16	1.541(10)	C1-N5-C6	128.2(6)
C15-C18	1.547(10)	C4-N5-C6	122.7(6)
C20-C21	1.440(11)	N5-C6-C8	110.1(6)
C21-C26	1.394(11)	N5-C6-C7	107.3(7)
C21-C22	1.407(11)	C8-C6-C7	109.8(7)
C22-C23	1.373(12)	N5-C6-C9	110.3(6)
C23-C24	1.368(13)	C8-C6-C9	110.6(7)
C24-C25	1.386(12)	C7-C6-C9	108.7(7)
C24-Br1	1.902(8)	N2-C10-P1	106.3(5)
C25-C26	1.384(11)	C12-C11-C13	107.1(6)
C31-Cl3	1.723(11)	C12-C11-C14	107.6(6)
C31-Cl4	1.724(11)	C13-C11-C14	110.7(6)
C32-Cl5	1.728(16)	C12-C11-P1	110.5(5)
C32-Cl6	1.735(16)	C13-C11-P1	110.2(5)
C20-Ru1-C1	84.0(3)	C14-C11-P1	110.5(5)
C20-Ru1-P1	90.8(2)	C17-C15-C16	109.1(6)
C1-Ru1-P1	82.0(2)	C17-C15-C18	107.8(6)

C16-C15-C18	106.8(6)
C17-C15-P1	110.1(5)
C16-C15-P1	113.8(5)
C18-C15-P1	109.0(5)
C21-C20-Ru1	126.4(5)
C26-C21-C22	117.2(7)
C26-C21-C20	123.8(7)
C22-C21-C20	119.0(7)
C23-C22-C21	121.4(8)
C24-C23-C22	119.5(9)
C23-C24-C25	121.7(8)
C23-C24-Br1	118.5(7)
C25-C24-Br1	119.8(7)
C26-C25-C24	118.2(8)
C25-C26-C21	122.0(8)
Cl3-C31-Cl4	115.2(7)
Cl5-C32-Cl6	107.8(14)

Crystal data for 7c:

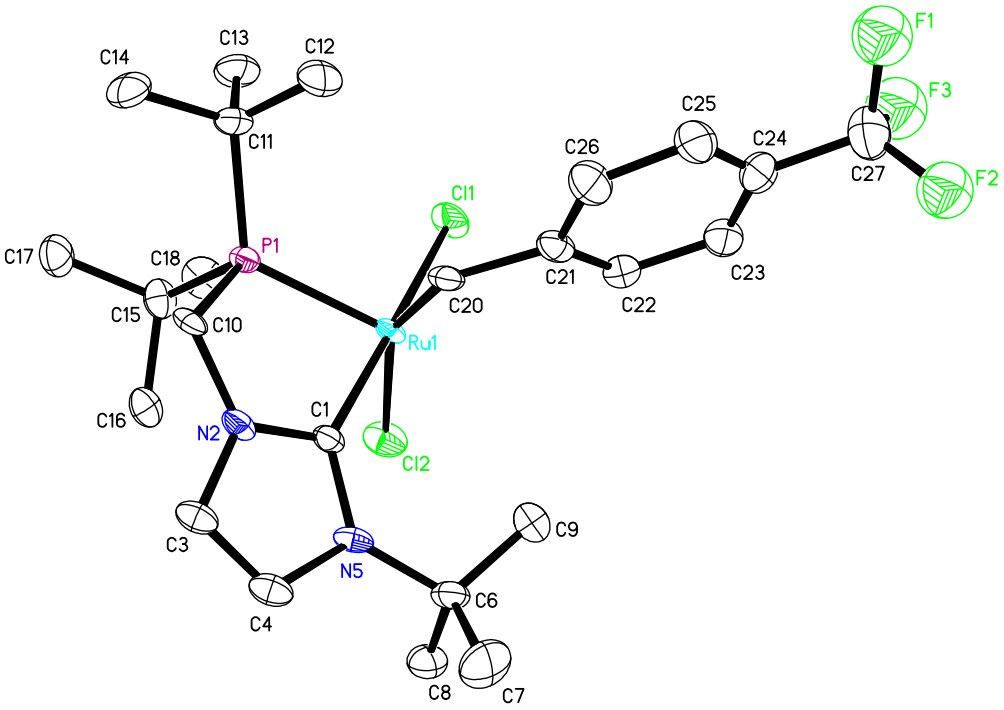


Table 1: Crystal data and structure refinement for **7c**.

Identification code	msi34
Empirical formula	$C_{24.50}H_{26.50}Cl_3F_3N_2OPRu$
Formula weight	660.37
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
Z	8
Unit cell dimensions	a = 9.5624(13) Å α = 90 deg. b = 27.160(4) Å β = 99.976(3) deg. c = 23.802(3) Å γ = 90 deg.
Volume	6088.1(15) $Å^3$
Density (calculated)	1.44 g/cm^3
Absorption coefficient	0.87 mm^{-1}
Crystal shape	needle
Crystal size	0.77 x 0.04 x 0.03 mm^3
Crystal colour	green
Theta range for data collection	1.7 to 22.5 deg.
Index ranges	$-10 \le h \le 10$, $-29 \le k \le 29$, $-25 \le l \le 25$
Reflections collected	37093
Independent reflections	7971 (R(int) = 0.1432)
Observed reflections	6469 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.55
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	7971 / 1087 / 636
Goodness-of-fit on F^2	1.35
Final R indices ($I>2\sigma(I)$)	R1 = 0.147, wR2 = 0.255

Largest diff. peak and hole	1.45 and -1.59 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **7c**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru11	0.7058(1)	0.2051(1)	0.4800(1)	0.0143(4)
Cl11	0.9263(5)	0.1848(2)	0.4515(2)	0.0283(11)
Cl21	0.5919(5)	0.1556(2)	0.3987(2)	0.0315(11)
P11	0.7038(5)	0.2847(2)	0.4606(2)	0.0165(9)
C11	0.5114(17)	0.2221(6)	0.4979(7)	0.017(2)
N21	0.4692(14)	0.2687(5)	0.5021(6)	0.019(2)
C31	0.3288(18)	0.2726(7)	0.5070(7)	0.023(3)
C41	0.2843(19)	0.2264(7)	0.5096(8)	0.025(3)
N51	0.3970(14)	0.1949(5)	0.5071(6)	0.020(2)
C61	0.3851(18)	0.1414(7)	0.5193(8)	0.024(3)
C71	0.309(2)	0.1349(8)	0.5689(9)	0.043(4)
C81	0.2970(19)	0.1177(7)	0.4661(8)	0.030(4)
C91	0.5280(19)	0.1180(7)	0.5322(8)	0.032(4)
C101	0.5670(16)	0.3088(6)	0.4981(7)	0.017(3)
C111	0.8628(18)	0.3240(7)	0.4847(8)	0.024(3)
C121	0.943(2)	0.3077(7)	0.5402(8)	0.034(4)
C131	0.966(2)	0.3212(7)	0.4414(9)	0.034(4)
C141	0.820(2)	0.3785(6)	0.4911(8)	0.031(4)
C151	0.6266(19)	0.2970(7)	0.3847(7)	0.025(3)
C161	0.4731(19)	0.2784(7)	0.3729(7)	0.025(3)
C171	0.618(2)	0.3515(7)	0.3671(8)	0.031(4)
C181	0.708(2)	0.2688(7)	0.3449(8)	0.034(4)
C201	0.7699(17)	0.2159(6)	0.5561(7)	0.020(3)
C211	0.8655(18)	0.1833(7)	0.5945(7)	0.022(3)
C221	0.8982(19)	0.1372(7)	0.5782(8)	0.028(3)
C231	0.9938(19)	0.1076(7)	0.6158(8)	0.030(4)
C241	1.057(2)	0.1275(7)	0.6676(8)	0.030(3)
C251	1.028(2)	0.1725(7)	0.6831(8)	0.033(4)
C261	0.928(2)	0.2003(8)	0.6469(8)	0.032(4)
C271	1.1615(18)	0.0961(6)	0.7046(7)	0.045(5)
F11	1.252(2)	0.1258(8)	0.7402(10)	0.058(9)
F21	1.108(2)	0.0693(9)	0.7416(9)	0.051(8)
F31	1.251(3)	0.0707(9)	0.6803(10)	0.070(9)
F1B1	1.158(3)	0.0484(8)	0.6877(12)	0.071(10)
F2B1	1.294(2)	0.1076(10)	0.7053(12)	0.067(10)
F3B1	1.130(3)	0.0919(12)	0.7562(9)	0.062(9)
Ru12	-0.0291(1)	0.0919(1)	0.1747(1)	0.0144(4)
Cl12	0.1907(5)	0.1003(2)	0.1390(2)	0.0308(11)
Cl22	-0.1512(5)	0.1149(2)	0.0783(2)	0.0298(11)
P12	-0.0031(5)	0.1559(2)	0.2329(2)	0.0165(9)
C12	-0.2151(17)	0.0864(6)	0.2030(7)	0.015(2)
N22	-0.2370(15)	0.1125(5)	0.2494(6)	0.020(3)
C32	-0.3705(19)	0.1049(7)	0.2607(8)	0.030(4)
C42	-0.431(2)	0.0728(7)	0.2242(8)	0.030(4)
N52	-0.3374(14)	0.0591(5)	0.1882(6)	0.022(3)
C62	-0.3714(19)	0.0210(7)	0.1438(8)	0.027(3)
C72	-0.459(2)	0.0437(7)	0.0922(8)	0.033(4)
C82	-0.446(2)	-0.0209(7)	0.1685(9)	0.041(4)
C92	-0.233(2)	-0.0013(7)	0.1307(8)	0.031(4)
C102	-0.1318(18)	0.1438(7)	0.2809(7)	0.021(3)

C112	0.1689(19)	0.1682(7)	0.2824(8)	0.026(3)
C122	0.237(2)	0.1184(7)	0.3030(8)	0.033(4)
C132	0.2730(19)	0.1950(7)	0.2507(8)	0.033(4)
C142	0.148(2)	0.1975(7)	0.3354(8)	0.032(4)
C152	-0.0711(19)	0.2133(6)	0.1955(7)	0.023(3)
C162	-0.062(2)	0.2590(7)	0.2360(8)	0.031(4)
C172	-0.2307(18)	0.2065(7)	0.1719(8)	0.028(3)
C182	0.005(2)	0.2249(7)	0.1459(8)	0.027(4)
C202	0.0355(16)	0.0507(6)	0.2354(8)	0.018(3)
C212	0.1134(19)	0.0047(6)	0.2339(8)	0.025(3)
C222	0.133(2)	-0.0178(7)	0.1825(9)	0.033(4)
C232	0.202(2)	-0.0624(7)	0.1851(9)	0.037(4)
C242	0.262(2)	-0.0826(8)	0.2364(10)	0.044(4)
C252	0.247(2)	-0.0605(8)	0.2857(10)	0.044(4)
C262	0.173(2)	-0.0168(8)	0.2848(9)	0.039(4)
C272	0.3386(18)	-0.1301(7)	0.2401(7)	0.055(5)
F12	0.408(3)	-0.1400(9)	0.2933(8)	0.073(9)
F22	0.443(2)	-0.1308(8)	0.2109(10)	0.055(8)
F32	0.2577(19)	-0.1685(6)	0.2253(11)	0.042(7)
F1B2	0.351(4)	-0.1419(13)	0.1863(9)	0.089(13)
F2B2	0.262(2)	-0.1666(8)	0.2552(13)	0.036(8)
F3B2	0.469(2)	-0.1309(14)	0.2677(16)	0.097(14)
C31	-0.170(4)	0.0547(15)	0.4201(18)	0.136(8)
Cl11	-0.2202(15)	0.0205(5)	0.4719(6)	0.163(5)
Cl12	-0.0353(14)	0.0392(4)	0.3952(5)	0.146(4)
O1	0.163(2)	0.0233(8)	0.0345(9)	0.101(7)
O2	-0.067(2)	0.0696(7)	-0.0362(8)	0.089(6)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **7c**.

Atom	x	y	z	U_{eq}
H31	0.2750	0.3018	0.5082	0.027
H41	0.1906	0.2166	0.5127	0.030
H7A1	0.2146	0.1500	0.5599	0.064
H7B1	0.3634	0.1508	0.6027	0.064
H7C1	0.2990	0.0997	0.5764	0.064
H8A1	0.3463	0.1218	0.4336	0.045
H8B1	0.2038	0.1336	0.4577	0.045
H8C1	0.2847	0.0825	0.4731	0.045
H9A1	0.5774	0.1227	0.4998	0.048
H9B1	0.5174	0.0827	0.5389	0.048
H9C1	0.5831	0.1332	0.5663	0.048
H10A1	0.6101	0.3205	0.5366	0.020
H10B1	0.5168	0.3368	0.4767	0.020
H12A1	0.9723	0.2733	0.5374	0.051
H12B1	0.8832	0.3106	0.5695	0.051
H12C1	1.0277	0.3284	0.5506	0.051
H13A1	0.9165	0.3316	0.4037	0.051
H13B1	0.9999	0.2873	0.4393	0.051
H13C1	1.0471	0.3431	0.4538	0.051
H14A1	0.7670	0.3905	0.4548	0.046
H14B1	0.9058	0.3985	0.5021	0.046
H14C1	0.7605	0.3811	0.5206	0.046
H16A1	0.4174	0.2958	0.3976	0.038
H16B1	0.4716	0.2430	0.3807	0.038
H16C1	0.4319	0.2844	0.3329	0.038

H17A1	0.7138	0.3655	0.3726	0.047
H17B1	0.5606	0.3694	0.3907	0.047
H17C1	0.5739	0.3542	0.3269	0.047
H18A1	0.8069	0.2800	0.3512	0.051
H18B1	0.6641	0.2749	0.3052	0.051
H18C1	0.7050	0.2335	0.3530	0.051
H201	0.7385	0.2450	0.5722	0.024
H221	0.8569	0.1250	0.5417	0.034
H231	1.0142	0.0749	0.6058	0.036
H251	1.0736	0.1857	0.7184	0.039
H261	0.9033	0.2319	0.6589	0.039
H32	-0.4111	0.1203	0.2899	0.036
H42	-0.5250	0.0606	0.2223	0.037
H7A2	-0.4032	0.0695	0.0774	0.049
H7B2	-0.5447	0.0581	0.1024	0.049
H7C2	-0.4847	0.0184	0.0629	0.049
H8A2	-0.3839	-0.0344	0.2020	0.061
H8B2	-0.4698	-0.0468	0.1397	0.061
H8C2	-0.5338	-0.0086	0.1798	0.061
H9A2	-0.1798	-0.0161	0.1654	0.046
H9B2	-0.1763	0.0247	0.1171	0.046
H9C2	-0.2558	-0.0266	0.1012	0.046
H10A2	-0.0848	0.1273	0.3162	0.025
H10B2	-0.1750	0.1749	0.2912	0.025
H12A2	0.1725	0.0997	0.3226	0.050
H12B2	0.3267	0.1243	0.3293	0.050
H12C2	0.2568	0.0995	0.2700	0.050
H13A2	0.2331	0.2270	0.2372	0.049
H13B2	0.2890	0.1752	0.2181	0.049
H13C2	0.3633	0.2001	0.2766	0.049
H14A2	0.0808	0.1801	0.3550	0.047
H14B2	0.1110	0.2302	0.3238	0.047
H14C2	0.2395	0.2008	0.3611	0.047
H16A2	0.0378	0.2659	0.2517	0.046
H16B2	-0.1137	0.2521	0.2672	0.046
H16C2	-0.1041	0.2877	0.2144	0.046
H17A2	-0.2810	0.1988	0.2033	0.042
H17B2	-0.2432	0.1796	0.1441	0.042
H17C2	-0.2690	0.2370	0.1532	0.042
H18A2	0.1070	0.2293	0.1604	0.040
H18B2	-0.0336	0.2552	0.1270	0.040
H18C2	-0.0081	0.1977	0.1186	0.040
H202	0.0157	0.0605	0.2715	0.021
H222	0.0993	-0.0026	0.1469	0.040
H232	0.2083	-0.0794	0.1508	0.044
H252	0.2868	-0.0751	0.3211	0.053
H262	0.1629	-0.0014	0.3198	0.047
H31A	-0.2505	0.0560	0.3880	0.163
H31B	-0.1536	0.0887	0.4350	0.163

Table 4: Anisotropic displacement parameters ($Å^2$) for **7c**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{12}
Ru11	0.0077(7)	0.0216(8)	0.0137(7)	0.0001(6)	0.0026(6)	0.0016(6)	
Cl11	0.016(2)	0.036(3)	0.035(3)	0.001(2)	0.010(2)	0.0074(19)	

Cl21	0.027(2)	0.035(3)	0.032(3)	-0.014(2)	0.002(2)	-0.002(2)
P11	0.012(2)	0.018(2)	0.019(2)	-0.0020(17)	0.0020(18)	-0.0003(17)
C11	0.011(4)	0.023(4)	0.017(6)	0.003(5)	0.002(4)	0.001(3)
N21	0.011(4)	0.025(4)	0.019(6)	0.002(5)	0.003(5)	0.004(3)
C31	0.013(5)	0.031(4)	0.026(8)	-0.003(6)	0.007(6)	0.002(4)
C41	0.015(5)	0.033(5)	0.029(8)	-0.002(6)	0.009(6)	0.001(4)
N51	0.011(4)	0.028(4)	0.024(6)	-0.003(4)	0.006(5)	-0.002(3)
C61	0.015(6)	0.031(4)	0.026(6)	0.004(6)	0.004(5)	-0.004(4)
C71	0.045(8)	0.050(9)	0.039(6)	0.011(6)	0.022(7)	-0.003(7)
C81	0.024(7)	0.027(7)	0.038(6)	-0.003(6)	0.000(5)	-0.005(6)
C91	0.025(5)	0.033(7)	0.037(8)	0.006(7)	0.000(5)	0.003(6)
C101	0.010(5)	0.021(4)	0.018(6)	-0.006(6)	-0.003(5)	0.001(4)
C111	0.015(5)	0.026(4)	0.032(6)	0.000(6)	0.003(4)	-0.005(4)
C121	0.030(7)	0.033(7)	0.034(6)	-0.006(6)	-0.009(5)	-0.005(6)
C131	0.021(6)	0.039(8)	0.046(7)	0.002(7)	0.012(6)	-0.007(6)
C141	0.033(8)	0.024(5)	0.032(8)	-0.007(5)	0.000(6)	-0.009(5)
C151	0.030(6)	0.026(5)	0.019(4)	0.000(4)	0.002(4)	0.005(5)
C161	0.027(5)	0.032(7)	0.015(7)	0.004(6)	-0.001(4)	0.005(5)
C171	0.032(8)	0.032(5)	0.028(7)	0.009(5)	0.004(7)	0.005(5)
C181	0.036(7)	0.042(7)	0.027(5)	-0.006(6)	0.011(6)	0.004(6)
C201	0.012(6)	0.024(6)	0.022(3)	0.000(4)	0.000(3)	-0.005(5)
C211	0.016(7)	0.031(6)	0.019(5)	0.002(5)	0.003(5)	-0.002(5)
C221	0.025(7)	0.024(6)	0.034(6)	0.002(5)	0.000(5)	-0.005(5)
C231	0.024(7)	0.030(6)	0.037(6)	0.004(5)	0.006(5)	0.000(5)
C241	0.029(7)	0.037(6)	0.026(6)	0.012(5)	0.009(5)	-0.004(5)
C251	0.033(7)	0.039(6)	0.023(6)	0.005(5)	-0.003(5)	-0.006(6)
C261	0.034(7)	0.036(6)	0.024(6)	0.000(5)	-0.003(5)	-0.001(6)
C271	0.046(8)	0.048(7)	0.039(7)	0.012(7)	0.002(6)	0.003(6)
Ru12	0.0097(7)	0.0158(7)	0.0188(8)	-0.0002(6)	0.0053(6)	-0.0006(6)
Cl12	0.023(2)	0.035(3)	0.039(3)	-0.006(2)	0.019(2)	-0.005(2)
Cl22	0.032(2)	0.034(3)	0.022(2)	0.0022(19)	0.0033(19)	-0.003(2)
P12	0.013(2)	0.019(2)	0.018(2)	-0.0032(17)	0.0044(17)	-0.0043(17)
C12	0.011(4)	0.011(6)	0.023(5)	0.001(4)	0.003(4)	0.001(4)
N22	0.019(5)	0.023(6)	0.019(6)	-0.002(4)	0.010(4)	-0.005(4)
C32	0.022(5)	0.035(7)	0.037(7)	-0.007(5)	0.014(5)	-0.005(5)
C42	0.022(5)	0.037(7)	0.035(7)	-0.003(5)	0.012(5)	-0.010(5)
N52	0.011(4)	0.026(5)	0.028(5)	-0.002(4)	0.002(4)	-0.005(4)
C62	0.022(6)	0.028(6)	0.029(6)	-0.003(4)	0.000(4)	-0.008(4)
C72	0.028(7)	0.034(8)	0.033(6)	-0.007(5)	-0.005(6)	-0.002(6)
C82	0.040(8)	0.032(6)	0.050(8)	0.000(6)	0.005(7)	-0.016(6)
C92	0.033(6)	0.018(7)	0.040(8)	-0.004(6)	0.004(6)	0.000(5)
C102	0.020(5)	0.031(7)	0.013(6)	-0.002(4)	0.004(4)	-0.003(5)
C112	0.021(5)	0.031(6)	0.025(6)	-0.005(4)	0.003(4)	-0.008(4)
C122	0.030(7)	0.041(6)	0.024(8)	-0.002(5)	-0.007(6)	0.001(6)
C132	0.022(6)	0.039(7)	0.038(8)	-0.009(6)	0.010(6)	-0.012(6)
C142	0.032(8)	0.041(7)	0.021(6)	-0.007(6)	0.002(5)	-0.008(6)
C152	0.027(5)	0.018(4)	0.025(6)	-0.002(4)	0.009(4)	-0.001(5)
C162	0.035(8)	0.025(5)	0.036(7)	-0.007(5)	0.016(6)	0.003(6)
C172	0.025(5)	0.028(7)	0.032(8)	0.003(6)	0.006(5)	0.007(5)
C182	0.031(7)	0.027(7)	0.024(6)	0.000(5)	0.011(6)	-0.002(6)
C202	0.005(6)	0.020(4)	0.025(5)	0.000(4)	-0.005(4)	-0.007(4)
C212	0.024(7)	0.021(6)	0.031(5)	0.010(4)	0.007(6)	-0.001(5)
C222	0.030(8)	0.029(6)	0.040(5)	-0.004(5)	0.008(6)	-0.006(5)
C232	0.029(8)	0.033(6)	0.048(5)	-0.004(5)	0.011(6)	-0.004(6)
C242	0.039(8)	0.037(7)	0.057(6)	0.007(5)	0.008(6)	-0.004(6)
C252	0.042(8)	0.040(7)	0.048(6)	0.017(5)	0.000(7)	0.009(6)
C262	0.036(8)	0.041(7)	0.039(5)	0.015(5)	-0.002(6)	0.008(6)
C272	0.057(9)	0.039(7)	0.066(9)	0.003(6)	0.002(7)	0.001(6)
C31	0.136(11)	0.139(13)	0.142(11)	0.013(8)	0.049(9)	0.001(8)
Cl11	0.188(8)	0.147(8)	0.171(8)	0.026(6)	0.083(6)	0.008(7)
Cl12	0.174(8)	0.128(7)	0.153(7)	0.022(6)	0.073(6)	0.031(6)
O1	0.105(10)	0.097(10)	0.100(10)	-0.009(8)	0.015(8)	-0.019(8)

O2	0.101(10)	0.085(9)	0.083(9)	0.006(8)	0.026(8)	-0.013(8)

Table 5: Bond lengths (Å) and angles (deg) for **7c**.

Ru11-C201	1.833(17)	C62-C92	1.53(3)
Ru11-C11	2.031(16)	C112-C142	1.53(2)
Ru11-P11	2.212(5)	C112-C132	1.53(2)
Ru11-Cl11	2.389(4)	C112-C122	1.55(3)
Ru11-Cl21	2.452(5)	C152-C182	1.52(2)
P11-C101	1.827(16)	C152-C172	1.54(2)
P11-C151	1.859(18)	C152-C162	1.56(2)
P11-C111	1.863(18)	C202-C212	1.46(2)
C11-N21	1.34(2)	C212-C262	1.38(3)
C11-N51	1.37(2)	C212-C222	1.41(3)
N21-C31	1.37(2)	C222-C232	1.37(3)
N21-C101	1.45(2)	C232-C242	1.37(3)
C31-C41	1.33(2)	C242-C252	1.35(3)
C41-N51	1.39(2)	C242-C272	1.48(3)
N51-C61	1.49(2)	C252-C262	1.38(3)
C61-C91	1.49(2)	C272-F3B2	1.305(15)
C61-C71	1.50(3)	C272-F32	1.312(14)
C61-C81	1.53(2)	C272-F22	1.312(15)
C111-C121	1.48(2)	C272-F2B2	1.317(15)
C111-C131	1.55(2)	C272-F1B2	1.346(15)
C111-C141	1.55(2)	C272-F12	1.352(15)
C151-C181	1.53(2)	C31-Cl12	1.56(4)
C151-C161	1.53(2)	C31-Cl11	1.68(4)
C151-C171	1.54(2)	C201-Ru11-C11	85.3(7)
C201-C211	1.47(2)	C201-Ru11-P11	92.3(6)
C211-C221	1.36(2)	C11-Ru11-P11	81.2(5)
C211-C261	1.37(2)	C201-Ru11-Cl11	99.1(5)
C221-C231	1.41(3)	C11-Ru11-Cl11	175.6(5)
C231-C241	1.38(3)	P11-Ru11-Cl11	98.16(17)
C241-C251	1.32(3)	C201-Ru11-Cl21	153.5(5)
C241-C271	1.48(3)	C11-Ru11-Cl21	89.6(5)
C251-C261	1.39(3)	P11-Ru11-Cl21	112.61(17)
C271-F2B1	1.301(15)	Cl11-Ru11-Cl21	86.69(17)
C271-F31	1.307(15)	C101-P11-C151	102.3(8)
C271-F21	1.310(15)	C101-P11-C111	105.0(8)
C271-F3B1	1.317(15)	C151-P11-C111	111.3(8)
C271-F1B1	1.357(15)	C101-P11-Ru11	103.3(6)
C271-F11	1.363(15)	C151-P11-Ru11	111.4(6)
Ru12-C202	1.848(17)	C111-P11-Ru11	121.2(6)
Ru12-C12	2.014(16)	N21-C11-N51	103.8(13)
Ru12-P12	2.211(5)	N21-C11-Ru11	122.0(12)
Ru12-Cl12	2.411(5)	N51-C11-Ru11	134.2(12)
Ru12-Cl22	2.468(5)	C11-N21-C31	113.0(14)
P12-C102	1.847(17)	C11-N21-C101	120.0(13)
P12-C152	1.856(18)	C31-N21-C101	126.9(14)
P12-C112	1.880(18)	C41-C31-N21	105.0(16)
C12-N22	1.36(2)	C31-C41-N51	108.8(16)
C12-N52	1.38(2)	C11-N51-C41	108.9(14)
N22-C32	1.36(2)	C11-N51-C61	130.3(14)
N22-C102	1.43(2)	C41-N51-C61	120.5(14)
C32-C42	1.29(2)	C91-C61-N51	110.9(14)
C42-N52	1.40(2)	C91-C61-C71	110.0(16)
N52-C62	1.47(2)	N51-C61-C71	109.3(15)
C62-C72	1.49(3)	C91-C61-C81	110.1(16)
C62-C82	1.52(3)	N51-C61-C81	107.3(14)

C71-C61-C81	109.1(16)	N22-C12-N52	104.2(14)
N21-C101-P11	106.7(11)	N22-C12-Ru12	120.3(11)
C121-C111-C131	106.7(15)	N52-C12-Ru12	135.4(12)
C121-C111-C141	107.6(15)	C12-N22-C32	111.3(14)
C131-C111-C141	108.7(15)	C12-N22-C102	122.9(14)
C121-C111-P11	112.1(13)	C32-N22-C102	125.8(15)
C131-C111-P11	110.4(13)	C42-C32-N22	107.3(17)
C141-C111-P11	111.2(12)	C32-C42-N52	109.2(16)
C181-C151-C161	107.2(15)	C12-N52-C42	107.8(14)
C181-C151-C171	108.8(15)	C12-N52-C62	129.3(14)
C161-C151-C171	105.2(15)	C42-N52-C62	122.8(14)
C181-C151-P11	110.7(13)	N52-C62-C72	108.7(15)
C161-C151-P11	109.0(12)	N52-C62-C82	108.1(15)
C171-C151-P11	115.5(13)	C72-C62-C82	113.3(16)
C211-C201-Ru11	125.7(13)	N52-C62-C92	109.4(14)
C221-C211-C261	118.9(18)	C72-C62-C92	111.9(16)
C221-C211-C201	121.6(17)	C82-C62-C92	105.4(16)
C261-C211-C201	119.5(17)	N22-C102-P12	105.5(11)
C211-C221-C231	119.8(18)	C142-C112-C132	110.3(15)
C241-C231-C221	118.5(18)	C142-C112-C122	107.6(15)
C251-C241-C231	121.8(19)	C132-C112-C122	107.2(15)
C251-C241-C271	121.3(18)	C142-C112-P12	112.6(13)
C231-C241-C271	116.8(17)	C132-C112-P12	110.3(13)
C241-C251-C261	119.0(19)	C122-C112-P12	108.6(12)
C211-C261-C251	121.9(19)	C182-C152-C172	108.6(15)
F2B1-C271-F31	54.8(14)	C182-C152-C162	109.3(14)
F2B1-C271-F21	128(2)	C172-C152-C162	105.4(14)
F31-C271-F21	111.2(18)	C182-C152-P12	111.7(12)
F2B1-C271-F3B1	112.8(19)	C172-C152-P12	108.5(12)
F31-C271-F3B1	130(2)	C162-C152-P12	113.2(13)
F21-C271-F3B1	31.7(14)	C212-C202-Ru12	127.0(14)
F2B1-C271-F1B1	102.0(17)	C262-C212-C222	118.8(18)
F31-C271-F1B1	49.4(14)	C262-C212-C202	118.5(18)
F21-C271-F1B1	70.9(16)	C222-C212-C202	122.7(17)
F3B1-C271-F1B1	101.1(17)	C232-C222-C212	118.6(19)
F2B1-C271-F11	48.8(14)	C242-C232-C222	121(2)
F31-C271-F11	101.3(16)	C252-C242-C232	120(2)
F21-C271-F11	100.9(16)	C252-C242-C272	118(2)
F3B1-C271-F11	72.3(16)	C232-C242-C272	122(2)
F1B1-C271-F11	137(2)	C242-C252-C262	120(2)
F2B1-C271-C241	115.2(18)	C212-C262-C252	121(2)
F31-C271-C241	117.7(18)	F3B2-C272-F32	126(2)
F21-C271-C241	114.7(17)	F3B2-C272-F22	61.1(17)
F3B1-C271-C241	111.5(19)	F32-C272-F22	108.2(17)
F1B1-C271-C241	113.1(19)	F3B2-C272-F2B2	112(2)
F11-C271-C241	108.7(18)	F32-C272-F2B2	31.3(12)
C202-Ru12-C12	83.6(7)	F22-C272-F2B2	130(2)
C202-Ru12-P12	90.0(5)	F3B2-C272-F1B2	103.8(19)
C12-Ru12-P12	81.8(5)	F32-C272-F1B2	72.5(17)
C202-Ru12-Cl12	98.0(5)	F22-C272-F1B2	44.8(15)
C12-Ru12-Cl12	178.3(5)	F2B2-C272-F1B2	103.0(17)
P12-Ru12-Cl12	97.81(17)	F3B2-C272-F12	41.5(16)
C202-Ru12-Cl22	157.1(5)	F32-C272-F12	105.4(16)
C12-Ru12-Cl22	91.6(5)	F22-C272-F12	101.2(16)
P12-Ru12-Cl22	111.53(17)	F2B2-C272-F12	78.5(16)
Cl12-Ru12-Cl22	87.09(17)	F1B2-C272-F12	137(2)
C102-P12-C152	103.3(8)	F3B2-C272-C242	118(2)
C102-P12-C112	104.4(8)	F32-C272-C242	114.6(17)
C152-P12-C112	110.3(8)	F22-C272-C242	113.4(17)
C102-P12-Ru12	103.4(6)	F2B2-C272-C242	112.5(18)
C152-P12-Ru12	111.6(6)	F1B2-C272-C242	106(2)
C112-P12-Ru12	121.6(6)	F12-C272-C242	112.9(19)

Cl12-C31-Cl11	119(3)

Crystal data for 7e:

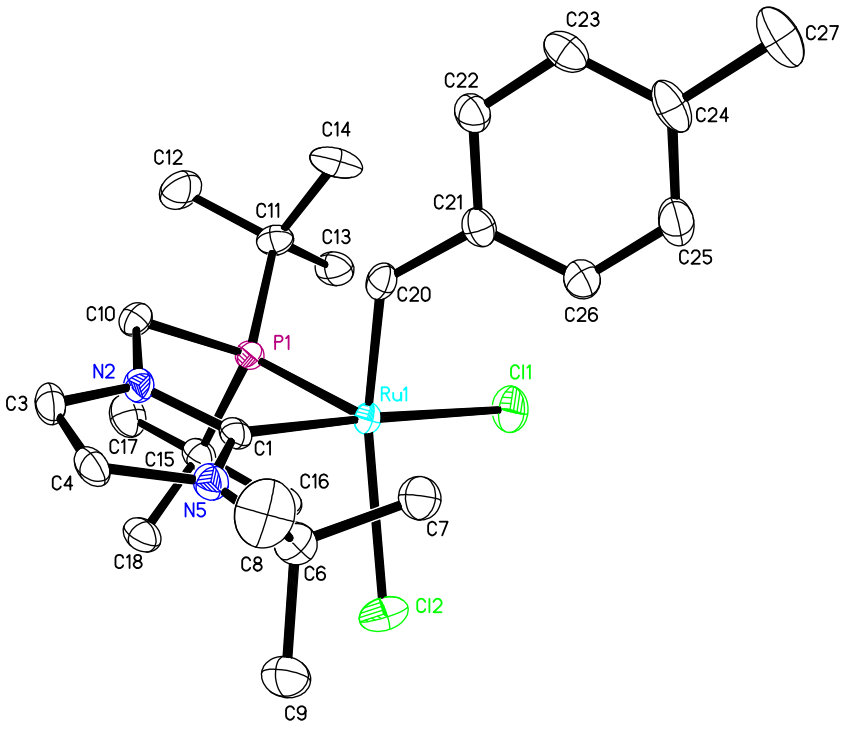


Table 1: Crystal data and structure refinement for **7e**.

Identification code	msi35	
Empirical formula	$C_{24}H_{39}Cl_2N_2PRu$	
Formula weight	558.51	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	4	
Unit cell dimensions	a = 10.0971(1) Å	α = 90 deg.
	b = 21.0977(2) Å	β = 96.574(1) deg.
	c = 11.9795(2) Å	γ = 90 deg.
Volume	2535.16(5) $Å^3$	
Density (calculated)	1.46 g/cm^3	
Absorption coefficient	0.91 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.18 x 0.18 x 0.10 mm^3	
Crystal colour	green	
Theta range for data collection	1.9 to 27.5 deg.	
Index ranges	$-13 \le h \le 12$, $-27 \le k \le 27$, $-15 \le l \le 15$	
Reflections collected	25082	
Independent reflections	5794 (R(int) = 0.0839)	
Observed reflections	4607 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5794 / 0 / 284	
Goodness-of-fit on F^2	1.05	
Final R indices ($I > 2\sigma(I)$)	R1 = 0.035, wR2 = 0.079	
Largest diff. peak and hole	0.60 and -0.57 $eÅ^{-3}$	

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **7e**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.5375(1)	0.3184(1)	0.4147(1)	0.0168(1)
Cl1	0.7778(1)	0.3161(1)	0.4220(1)	0.0354(2)
Cl2	0.5736(1)	0.3608(1)	0.6110(1)	0.0318(2)
P1	0.4984(1)	0.2147(1)	0.4098(1)	0.0159(1)
C1	0.3351(2)	0.3218(1)	0.4147(2)	0.0167(5)
N2	0.2592(2)	0.2683(1)	0.3944(2)	0.0172(4)
C3	0.1251(2)	0.2803(1)	0.3977(2)	0.0217(6)
C4	0.1147(2)	0.3425(1)	0.4182(2)	0.0209(6)
N5	0.2431(2)	0.3683(1)	0.4257(2)	0.0186(4)
C6	0.2683(3)	0.4379(1)	0.4386(2)	0.0234(6)
C7	0.3979(3)	0.4553(1)	0.3909(2)	0.0271(6)
C8	0.1543(3)	0.4738(2)	0.3702(3)	0.0409(8)
C9	0.2739(3)	0.4563(2)	0.5620(2)	0.0349(7)
C10	0.3176(2)	0.2087(1)	0.3634(2)	0.0183(5)
C11	0.5777(3)	0.1608(1)	0.3096(2)	0.0217(6)
C12	0.4941(3)	0.1008(1)	0.2816(3)	0.0346(7)
C13	0.7199(3)	0.1436(1)	0.3592(2)	0.0283(6)
C14	0.5892(3)	0.1949(2)	0.1988(2)	0.0336(7)
C15	0.5141(3)	0.1791(1)	0.5553(2)	0.0214(6)
C16	0.6529(3)	0.1935(1)	0.6156(2)	0.0271(6)
C17	0.4892(3)	0.1075(1)	0.5561(3)	0.0304(7)
C18	0.4075(3)	0.2101(1)	0.6205(2)	0.0254(6)
C20	0.4953(2)	0.3215(1)	0.2579(2)	0.0188(5)
H20	0.431(3)	0.2986(14)	0.222(2)	0.023
C21	0.5484(2)	0.3630(1)	0.1764(2)	0.0195(5)
C22	0.5081(3)	0.3528(1)	0.0614(2)	0.0217(6)
C23	0.5519(3)	0.3914(1)	-0.0208(2)	0.0242(6)
C24	0.6361(3)	0.4424(1)	0.0087(2)	0.0264(6)
C25	0.6775(3)	0.4524(1)	0.1220(2)	0.0290(6)
C26	0.6359(3)	0.4133(1)	0.2045(2)	0.0259(6)
C27	0.6801(3)	0.4855(2)	-0.0813(3)	0.0371(8)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **7e**.

Atom	x	y	z	U_{eq}
H3	0.0544	0.2504	0.3875	0.026
H4	0.0348	0.3650	0.4262	0.025
H7A	0.4734	0.4353	0.4363	0.041
H7B	0.4093	0.5015	0.3927	0.041
H7C	0.3938	0.4403	0.3131	0.041
H8A	0.1473	0.4600	0.2917	0.061
H8B	0.1725	0.5194	0.3744	0.061
H8C	0.0704	0.4649	0.4010	0.061
H9A	0.1911	0.4433	0.5909	0.052
H9B	0.2844	0.5024	0.5695	0.052
H9C	0.3497	0.4352	0.6050	0.052

H10A	0.3018	0.2022	0.2811	0.022
H10B	0.2781	0.1727	0.4011	0.022
H12A	0.4042	0.1130	0.2489	0.052
H12B	0.4884	0.0764	0.3504	0.052
H12C	0.5362	0.0750	0.2276	0.052
H13A	0.7639	0.1199	0.3035	0.042
H13B	0.7166	0.1174	0.4264	0.042
H13C	0.7701	0.1824	0.3796	0.042
H14A	0.6321	0.1669	0.1485	0.050
H14B	0.6428	0.2334	0.2131	0.050
H14C	0.5000	0.2063	0.1636	0.050
H16A	0.6607	0.1756	0.6915	0.041
H16B	0.6660	0.2395	0.6202	0.041
H16C	0.7207	0.1746	0.5735	0.041
H17A	0.5611	0.0856	0.5232	0.046
H17B	0.4037	0.0980	0.5120	0.046
H17C	0.4870	0.0931	0.6336	0.046
H18A	0.3185	0.1999	0.5833	0.038
H18B	0.4198	0.2562	0.6219	0.038
H18C	0.4165	0.1939	0.6976	0.038
H20	0.431(3)	0.2986(14)	0.222(2)	0.023
H22	0.4495	0.3187	0.0394	0.026
H23	0.5241	0.3830	-0.0978	0.029
H25	0.7356	0.4867	0.1435	0.035
H26	0.6673	0.4209	0.2811	0.031
H27A	0.6590	0.4656	-0.1551	0.056
H27B	0.7764	0.4927	-0.0669	0.056
H27C	0.6332	0.5262	-0.0800	0.056

Table 4: Anisotropic displacement parameters ($Å^2$) for **7e**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{12}
Ru1	0.0132(1)	0.0202(1)	0.0168(1)	-0.0013(1)	0.0015(1)	-0.0035(1)	
Cl1	0.0139(3)	0.0523(5)	0.0400(4)	-0.0031(4)	0.0030(3)	-0.0069(3)	
Cl2	0.0389(4)	0.0317(4)	0.0233(4)	-0.0075(3)	-0.0034(3)	0.0003(3)	
P1	0.0137(3)	0.0196(3)	0.0143(3)	-0.0002(3)	0.0007(2)	-0.0006(2)	
C1	0.0178(12)	0.0203(13)	0.0121(12)	0.0031(10)	0.0025(10)	-0.0006(10)	
N2	0.0132(10)	0.0219(11)	0.0162(11)	0.0021(9)	0.0000(8)	-0.0013(8)	
C3	0.0146(12)	0.0299(15)	0.0204(14)	0.0055(11)	0.0013(10)	-0.0043(11)	
C4	0.0136(12)	0.0314(15)	0.0184(13)	0.0025(11)	0.0049(10)	0.0017(11)	
N5	0.0165(10)	0.0213(11)	0.0181(11)	0.0004(9)	0.0021(8)	0.0000(9)	
C6	0.0269(14)	0.0180(13)	0.0259(15)	0.0006(11)	0.0057(12)	0.0025(11)	
C7	0.0345(16)	0.0214(14)	0.0261(15)	0.0011(12)	0.0068(12)	-0.0034(12)	
C8	0.0387(18)	0.0292(17)	0.053(2)	0.0091(15)	-0.0012(16)	0.0081(14)	
C9	0.0446(18)	0.0305(17)	0.0322(17)	-0.0084(13)	0.0161(14)	-0.0054(14)	
C10	0.0183(12)	0.0174(13)	0.0185(13)	0.0013(10)	-0.0015(10)	-0.0004(10)	
C11	0.0236(14)	0.0214(13)	0.0201(14)	-0.0042(11)	0.0018(11)	0.0031(11)	
C12	0.0370(17)	0.0290(16)	0.0379(18)	-0.0134(14)	0.0046(14)	-0.0029(13)	
C13	0.0245(15)	0.0341(17)	0.0267(15)	-0.0045(13)	0.0051(12)	0.0047(12)	
C14	0.050(2)	0.0348(18)	0.0175(15)	-0.0011(12)	0.0094(13)	0.0112(14)	
C15	0.0192(13)	0.0276(15)	0.0175(13)	0.0025(11)	0.0026(10)	0.0018(11)	
C16	0.0198(14)	0.0437(18)	0.0169(14)	0.0009(12)	-0.0015(11)	0.0022(12)	
C17	0.0283(15)	0.0313(17)	0.0318(17)	0.0097(13)	0.0042(13)	0.0012(12)	
C18	0.0230(14)	0.0360(16)	0.0175(14)	0.0022(12)	0.0033(11)	0.0018(12)	
C20	0.0136(12)	0.0190(13)	0.0237(14)	-0.0025(11)	0.0015(10)	-0.0015(10)	

C21	0.0163(12)	0.0198(13)	0.0232(14)	0.0011(11)	0.0061(10)	0.0026(10)
C22	0.0188(13)	0.0246(15)	0.0224(14)	0.0004(11)	0.0055(11)	-0.0004(11)
C23	0.0229(14)	0.0294(16)	0.0213(14)	0.0042(11)	0.0065(11)	0.0068(11)
C24	0.0243(14)	0.0239(14)	0.0341(17)	0.0090(12)	0.0166(12)	0.0073(11)
C25	0.0289(15)	0.0246(15)	0.0360(17)	0.0000(13)	0.0142(13)	-0.0047(12)
C26	0.0273(15)	0.0260(15)	0.0259(15)	-0.0035(12)	0.0089(12)	-0.0053(12)
C27	0.0392(18)	0.0353(18)	0.0399(19)	0.0172(14)	0.0174(15)	0.0059(14)

Table 5: Bond lengths (Å) and angles (deg) for **7e**.

Ru1-C20	1.880(3)	N5-C1-N2	103.6(2)
Ru1-C1	2.045(2)	N5-C1-Ru1	135.69(18)
Ru1-P1	2.2236(7)	N2-C1-Ru1	120.63(17)
Ru1-Cl1	2.4182(7)	C1-N2-C3	112.0(2)
Ru1-Cl2	2.5024(7)	C1-N2-C10	121.5(2)
P1-C10	1.850(2)	C3-N2-C10	126.3(2)
P1-C15	1.887(3)	C4-C3-N2	106.4(2)
P1-C11	1.897(3)	C3-C4-N5	107.4(2)
C1-N5	1.367(3)	C1-N5-C4	110.5(2)
C1-N2	1.371(3)	C1-N5-C6	127.2(2)
N2-C3	1.382(3)	C4-N5-C6	122.2(2)
N2-C10	1.456(3)	N5-C6-C9	109.7(2)
C3-C4	1.342(4)	N5-C6-C7	109.9(2)
C4-N5	1.399(3)	C9-C6-C7	111.3(2)
N5-C6	1.496(3)	N5-C6-C8	108.7(2)
C6-C9	1.523(4)	C9-C6-C8	109.5(2)
C6-C7	1.531(4)	C7-C6-C8	107.6(2)
C6-C8	1.534(4)	N2-C10-P1	106.22(16)
C11-C14	1.526(4)	C14-C11-C13	106.7(2)
C11-C13	1.533(4)	C14-C11-C12	107.0(2)
C11-C12	1.536(4)	C13-C11-C12	110.9(2)
C15-C16	1.531(4)	C14-C11-P1	110.32(19)
C15-C17	1.532(4)	C13-C11-P1	109.95(18)
C15-C18	1.545(4)	C12-C11-P1	111.72(19)
C20-C21	1.458(4)	C16-C15-C17	109.5(2)
C21-C26	1.397(4)	C16-C15-C18	109.3(2)
C21-C22	1.407(4)	C17-C15-C18	106.8(2)
C22-C23	1.388(4)	C16-C15-P1	109.43(18)
C23-C24	1.392(4)	C17-C15-P1	113.62(19)
C24-C25	1.389(4)	C18-C15-P1	107.98(18)
C24-C27	1.515(4)	C21-C20-Ru1	129.15(19)
C25-C26	1.388(4)	C26-C21-C22	117.1(2)
C20-Ru1-C1	83.46(10)	C26-C21-C20	124.4(2)
C20-Ru1-P1	89.36(8)	C22-C21-C20	118.5(2)
C1-Ru1-P1	81.96(7)	C23-C22-C21	121.7(3)
C20-Ru1-Cl1	98.54(8)	C22-C23-C24	120.6(3)
C1-Ru1-Cl1	177.79(7)	C25-C24-C23	118.1(2)
P1-Ru1-Cl1	98.97(3)	C25-C24-C27	121.6(3)
C20-Ru1-Cl2	156.70(8)	C23-C24-C27	120.3(3)
C1-Ru1-Cl2	91.46(7)	C26-C25-C24	121.6(3)
P1-Ru1-Cl2	112.51(3)	C25-C26-C21	120.9(3)
Cl1-Ru1-Cl2	86.33(3)		
C10-P1-C15	103.10(12)		
C10-P1-C11	104.04(12)		
C15-P1-C11	110.45(12)		
C10-P1-Ru1	103.96(8)		
C15-P1-Ru1	111.74(9)		
C11-P1-Ru1	121.34(9)		

Crystal data for 7f:

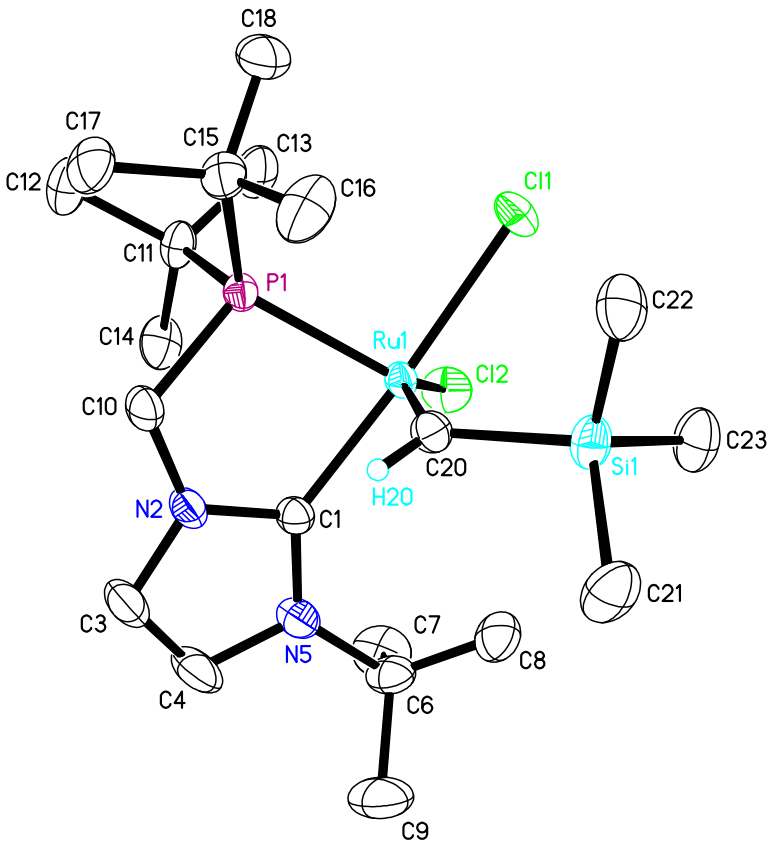


Table 1: Crystal data and structure refinement for **7f**.

Identification code	msi27	
Empirical formula	$C_{21}H_{43}Cl_4N_2PRuSi$	
Formula weight	625.50	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Z	4	
Unit cell dimensions	a = 10.9174(1) Å	α = 90 deg.
	b = 16.107 Å	β = 90 deg.
	c = 16.7379(1) Å	γ = 90 deg.
Volume	2943.38(3) $Å^3$	
Density (calculated)	1.41 g/cm^3	
Absorption coefficient	1.00 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.26 x 0.24 x 0.14 mm^3	
Crystal colour	colorless	
Theta range for data collection	1.8 to 27.5 deg.	
Index ranges	$-14 \le h \le 14$, $-20 \le k \le 20$, $-21 \le l \le 21$	
Reflections collected	29950	
Independent reflections	6745 (R(int) = 0.0475)	
Observed reflections	6272 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.87 and 0.78	

Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6745 / 7 / 315
Goodness-of-fit on F^2	1.10
Final R indices ($I>2\sigma(I)$)	R1 = 0.027, wR2 = 0.060
Absolute structure parameter	0.03(2)
Largest diff. peak and hole	0.53 and -0.54 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **7f**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.7470(1)	1.0094(1)	0.4198(1)	0.0184(1)
Cl1	0.8499(1)	1.1092(1)	0.5044(1)	0.0313(2)
Cl2	0.7953(1)	0.9074(1)	0.5254(1)	0.0345(2)
P1	0.8762(1)	1.0216(1)	0.3168(1)	0.0198(1)
Si1	0.5383(1)	1.1539(1)	0.4397(1)	0.0286(2)
C1	0.6689(2)	0.9212(2)	0.3446(2)	0.0226(5)
N2	0.7040(2)	0.9201(1)	0.2659(1)	0.0268(5)
C3	0.6471(3)	0.8575(2)	0.2237(2)	0.0408(8)
C4	0.5736(3)	0.8192(2)	0.2759(2)	0.0431(8)
N5	0.5845(2)	0.8586(2)	0.3494(1)	0.0287(5)
C6	0.5055(3)	0.8328(2)	0.4192(2)	0.0330(6)
C7	0.5702(3)	0.7621(2)	0.4635(2)	0.0485(8)
C8	0.4822(3)	0.9064(2)	0.4727(2)	0.0384(7)
C9	0.3817(3)	0.8022(2)	0.3866(2)	0.0540(10)
C10	0.7893(2)	0.9792(2)	0.2319(1)	0.0277(6)
C11	1.0081(2)	0.9471(2)	0.3300(2)	0.0271(6)
C12	1.1012(3)	0.9494(2)	0.2605(2)	0.0387(7)
C13	1.0742(3)	0.9653(2)	0.4092(2)	0.0365(7)
C14	0.9563(3)	0.8584(2)	0.3340(2)	0.0348(7)
C15	0.9317(3)	1.1250(2)	0.2776(2)	0.0288(6)
C16	0.8259(3)	1.1869(2)	0.2856(2)	0.0450(8)
C17	0.9682(3)	1.1192(2)	0.1884(2)	0.0362(7)
C18	1.0407(3)	1.1566(2)	0.3269(2)	0.0427(8)
C20	0.6320(2)	1.0802(2)	0.3758(2)	0.0239(5)
H20	0.605(3)	1.0752(17)	0.3261(17)	0.023(7)
C21	0.3776(3)	1.1531(2)	0.4009(2)	0.0443(8)
C22	0.6051(3)	1.2599(2)	0.4280(2)	0.0408(7)
C23	0.5341(3)	1.1249(2)	0.5476(2)	0.0426(8)
C31	0.4066(16)	1.0023(14)	0.1276(11)	0.082(8)
Cl3	0.4212(8)	1.0579(8)	0.2059(6)	0.134(3)
Cl4	0.2797(5)	0.9783(3)	0.0850(3)	0.0598(13)
C31B	0.4281(13)	0.9969(8)	0.1180(7)	0.034(2)
Cl3B	0.4270(5)	1.0281(8)	0.2182(4)	0.124(3)
Cl4B	0.2710(5)	1.0116(10)	0.0829(3)	0.111(3)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **7f**.

Atom	x	y	z	U_{eq}
H3	0.6579	0.8444	0.1688	0.049
H4	0.5225	0.7729	0.2646	0.052

H7A	0.5923	0.7183	0.4255	0.073
H7B	0.5152	0.7392	0.5042	0.073
H7C	0.6445	0.7834	0.4893	0.073
H8A	0.5600	0.9257	0.4953	0.058
H8B	0.4269	0.8901	0.5160	0.058
H8C	0.4447	0.9512	0.4415	0.058
H9A	0.3483	0.8435	0.3495	0.081
H9B	0.3245	0.7942	0.4310	0.081
H9C	0.3935	0.7494	0.3585	0.081
H10A	0.7449	1.0240	0.2036	0.033
H10B	0.8450	0.9514	0.1937	0.033
H12A	1.1461	1.0020	0.2618	0.058
H12B	1.0576	0.9443	0.2096	0.058
H12C	1.1590	0.9032	0.2662	0.058
H13A	1.0154	0.9623	0.4534	0.055
H13B	1.1102	1.0209	0.4073	0.055
H13C	1.1391	0.9241	0.4176	0.055
H14A	1.0227	0.8194	0.3460	0.052
H14B	0.9192	0.8440	0.2825	0.052
H14C	0.8941	0.8554	0.3761	0.052
H16A	0.8024	1.1916	0.3420	0.068
H16B	0.7557	1.1673	0.2544	0.068
H16C	0.8520	1.2413	0.2657	0.068
H17A	0.8965	1.1035	0.1566	0.054
H17B	1.0325	1.0773	0.1819	0.054
H17C	0.9988	1.1732	0.1703	0.054
H18A	1.0566	1.2149	0.3136	0.064
H18B	1.1134	1.1233	0.3146	0.064
H18C	1.0217	1.1519	0.3839	0.064
H20	0.605(3)	1.0752(17)	0.3261(17)	0.023(7)
H21A	0.3283	1.1935	0.4306	0.066
H21B	0.3424	1.0975	0.4077	0.066
H21C	0.3777	1.1677	0.3441	0.066
H22A	0.5524	1.3005	0.4548	0.061
H22B	0.6108	1.2736	0.3711	0.061
H22C	0.6870	1.2612	0.4519	0.061
H23A	0.6173	1.1265	0.5696	0.064
H23B	0.5007	1.0687	0.5532	0.064
H23C	0.4821	1.1642	0.5767	0.064
H31A	0.4476	0.9490	0.1397	0.099
H31B	0.4569	1.0296	0.0860	0.099
H31C	0.4528	0.9380	0.1132	0.041
H31D	0.4858	1.0313	0.0865	0.041

Table 4: Anisotropic displacement parameters ($Å^2$) for **7f**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0204(1)	0.0204(1)	0.0143(1)	-0.0008(1)	-0.0008(1)	0.0001(1)
Cl1	0.0361(4)	0.0309(3)	0.0267(3)	-0.0087(3)	-0.0079(3)	-0.0023(3)
Cl2	0.0380(4)	0.0368(4)	0.0288(3)	0.0117(3)	-0.0068(3)	-0.0019(3)
P1	0.0225(3)	0.0191(3)	0.0177(3)	-0.0004(2)	0.0012(2)	-0.0001(2)
Si1	0.0293(4)	0.0309(4)	0.0258(4)	0.0000(3)	0.0021(3)	0.0091(3)
C1	0.0241(13)	0.0240(13)	0.0198(12)	0.0008(10)	-0.0013(10)	-0.0025(10)
N2	0.0331(11)	0.0290(12)	0.0185(10)	-0.0044(9)	-0.0008(9)	-0.0074(9)
C3	0.053(2)	0.0426(17)	0.0265(15)	-0.0112(13)	-0.0015(14)	-0.0174(15)
C4	0.059(2)	0.0372(17)	0.0333(16)	-0.0079(13)	-0.0052(15)	-0.0226(15)

N5	0.0348(13)	0.0283(12)	0.0230(12)	0.0010(10)	-0.0027(10)	-0.0088(10)
C6	0.0296(14)	0.0386(15)	0.0309(15)	0.0076(14)	-0.0003(13)	-0.0115(11)
C7	0.058(2)	0.0385(18)	0.049(2)	0.0146(15)	-0.0038(17)	-0.0074(15)
C8	0.0377(16)	0.0469(18)	0.0305(15)	0.0041(14)	0.0069(13)	-0.0028(14)
C9	0.0409(19)	0.066(2)	0.055(2)	0.0073(18)	-0.0036(16)	-0.0256(18)
C10	0.0351(13)	0.0313(14)	0.0166(11)	-0.0011(10)	0.0001(10)	-0.0054(11)
C11	0.0268(13)	0.0310(14)	0.0235(13)	0.0001(11)	0.0035(11)	0.0083(11)
C12	0.0358(16)	0.0482(18)	0.0320(16)	-0.0007(14)	0.0073(13)	0.0134(13)
C13	0.0283(14)	0.0508(17)	0.0303(15)	0.0000(13)	-0.0007(12)	0.0116(12)
C14	0.0444(18)	0.0224(14)	0.0376(17)	0.0006(12)	0.0074(14)	0.0107(12)
C15	0.0369(15)	0.0222(13)	0.0272(14)	0.0040(11)	0.0055(12)	-0.0037(11)
C16	0.054(2)	0.0266(15)	0.055(2)	0.0132(14)	0.0214(16)	0.0066(14)
C17	0.0463(18)	0.0341(16)	0.0281(15)	0.0064(12)	0.0097(13)	-0.0039(13)
C18	0.051(2)	0.0389(17)	0.0382(17)	-0.0034(14)	0.0036(15)	-0.0202(15)
C20	0.0245(13)	0.0274(13)	0.0198(13)	0.0006(10)	-0.0021(11)	-0.0006(11)
C21	0.0302(16)	0.055(2)	0.048(2)	0.0036(15)	0.0008(14)	0.0113(14)
C22	0.0487(18)	0.0320(15)	0.0417(18)	-0.0028(14)	0.0068(15)	0.0094(13)
C23	0.0470(19)	0.054(2)	0.0272(15)	0.0021(14)	0.0057(14)	0.0096(15)
C31	0.040(7)	0.137(15)	0.070(9)	-0.050(8)	0.012(5)	0.019(7)
Cl3	0.120(5)	0.192(6)	0.091(5)	-0.091(5)	0.005(3)	-0.054(4)
Cl4	0.045(2)	0.097(3)	0.0375(18)	-0.0202(19)	-0.0003(12)	-0.0124(15)
C31B	0.020(4)	0.053(5)	0.029(4)	-0.013(4)	-0.001(4)	0.010(3)
Cl3B	0.0432(19)	0.288(9)	0.0416(16)	-0.044(3)	-0.0109(11)	0.003(3)
Cl4B	0.0327(15)	0.254(8)	0.0468(19)	0.042(3)	0.0012(12)	0.018(3)

Table 5: Bond lengths (Å) and angles (deg) for **7f**.

Ru1-C20	1.849(3)	C20-Ru1-C1	84.39(11)
Ru1-C1	2.080(2)	C20-Ru1-P1	93.88(8)
Ru1-P1	2.2354(6)	C1-Ru1-P1	81.52(7)
Ru1-Cl1	2.4203(6)	C20-Ru1-Cl1	97.95(8)
Ru1-Cl2	2.4704(7)	C1-Ru1-Cl1	176.53(7)
P1-C10	1.839(3)	P1-Ru1-Cl1	95.74(2)
P1-C11	1.888(3)	C20-Ru1-Cl2	147.12(8)
P1-C15	1.889(3)	C1-Ru1-Cl2	93.80(7)
Si1-C22	1.866(3)	P1-Ru1-Cl2	118.39(3)
Si1-C23	1.867(3)	Cl1-Ru1-Cl2	85.61(2)
Si1-C21	1.871(3)	C10-P1-C11	104.31(12)
Si1-C20	1.897(3)	C10-P1-C15	102.95(12)
C1-N5	1.369(3)	C11-P1-C15	110.86(13)
C1-N2	1.372(3)	C10-P1-Ru1	103.74(8)
N2-C3	1.379(3)	C11-P1-Ru1	109.60(8)
N2-C10	1.448(3)	C15-P1-Ru1	123.21(9)
C3-C4	1.337(4)	C22-Si1-C23	109.91(16)
C4-N5	1.390(4)	C22-Si1-C21	109.69(15)
N5-C6	1.509(4)	C23-Si1-C21	108.12(15)
C6-C8	1.507(4)	C22-Si1-C20	107.60(13)
C6-C7	1.533(4)	C23-Si1-C20	113.68(13)
C6-C9	1.539(4)	C21-Si1-C20	107.78(14)
C11-C14	1.537(4)	N5-C1-N2	103.6(2)
C11-C13	1.539(4)	N5-C1-Ru1	138.03(19)
C11-C12	1.544(4)	N2-C1-Ru1	118.38(18)
C15-C16	1.532(4)	C1-N2-C3	112.1(2)
C15-C18	1.535(4)	C1-N2-C10	123.2(2)
C15-C17	1.548(4)	C3-N2-C10	124.7(2)
C31-Cl3	1.595(14)	C4-C3-N2	105.9(3)
C31-Cl4	1.605(14)	C3-C4-N5	108.4(3)
C31B-Cl3B	1.752(13)	C1-N5-C4	110.0(2)
C31B-Cl4B	1.828(14)	C1-N5-C6	129.2(2)

C4-N5-C6	120.7(2)
C8-C6-N5	109.9(2)
C8-C6-C7	112.0(3)
N5-C6-C7	108.4(3)
C8-C6-C9	108.3(3)
N5-C6-C9	108.4(2)
C7-C6-C9	109.7(3)
N2-C10-P1	105.80(16)
C14-C11-C13	108.1(2)
C14-C11-C12	107.3(2)
C13-C11-C12	109.6(2)
C14-C11-P1	108.38(19)
C13-C11-P1	109.73(18)
C12-C11-P1	113.53(19)
C16-C15-C18	108.7(3)
C16-C15-C17	108.6(2)
C18-C15-C17	109.7(2)
C16-C15-P1	107.54(19)
C18-C15-P1	110.8(2)
C17-C15-P1	111.42(19)
Ru1-C20-Si1	121.89(14)
Cl3-C31-Cl4	125.9(13)
Cl3B-C31B-Cl4B	105.3(9)

Crystal data for 8:

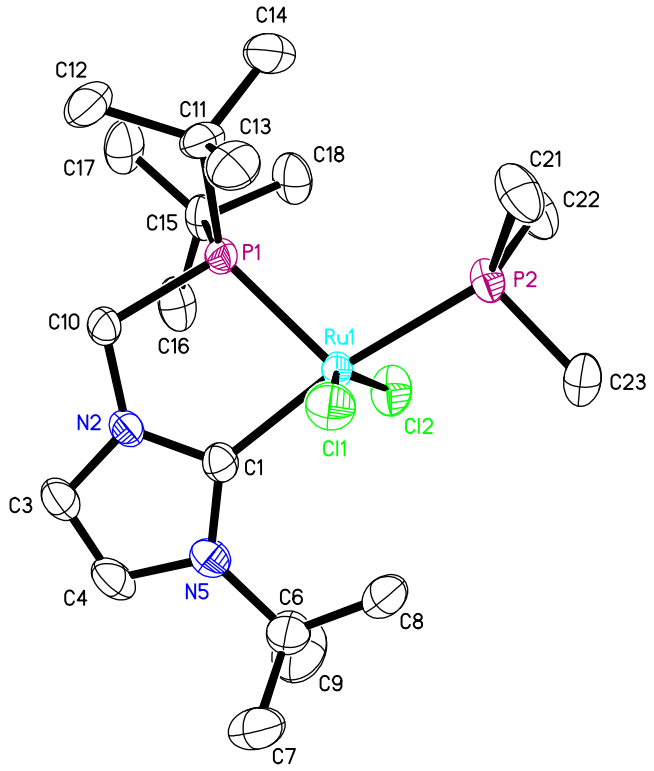


Table 1: Crystal data and structure refinement for **8**.

Identification code	msi26	
Empirical formula	$C_{19}H_{40}Cl_2N_2P_2Ru$	
Formula weight	530.44	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$Pca2_1$	
Z	4	
Unit cell dimensions	a = 13.1234(2) Å	α = 90 deg.
	b = 15.9143(2) Å	β = 90 deg.
	c = 12.1529(1) Å	γ = 90 deg.
Volume	2538.13(5) $Å^3$	
Density (calculated)	1.39 g/cm^3	
Absorption coefficient	0.96 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.42 x 0.24 x 0.10 mm^3	
Crystal colour	green	
Theta range for data collection	2.6 to 27.5 deg.	
Index ranges	$-17\leq h\leq 17$, $-20\leq k\leq 20$, $-15\leq l\leq 15$	
Reflections collected	25223	
Independent reflections	5794 (R(int) = 0.0398)	
Observed reflections	5129 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.91 and 0.69	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	5794 / 1 / 247	
Goodness-of-fit on F^2	1.05	

Final R indices (I>2σ(I))	R1 = 0.026, wR2 = 0.049
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	0.34 and -0.41 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **8**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.0264(1)	0.2704(1)	0.5039(1)	0.0227(1)
P1	0.0915(1)	0.1825(1)	0.3814(1)	0.0241(1)
P2	-0.1351(1)	0.2154(1)	0.5495(1)	0.0290(2)
Cl2	-0.0651(1)	0.3715(1)	0.3922(1)	0.0417(2)
Cl1	0.0909(1)	0.2123(1)	0.6722(1)	0.0364(2)
C1	0.1635(2)	0.3296(2)	0.4817(2)	0.0276(6)
N2	0.2404(2)	0.2912(1)	0.4268(2)	0.0278(5)
C3	0.3245(2)	0.3429(2)	0.4139(2)	0.0347(7)
C4	0.3003(2)	0.4149(2)	0.4642(2)	0.0395(7)
N5	0.2026(2)	0.4066(1)	0.5073(3)	0.0347(5)
C6	0.1538(3)	0.4729(2)	0.5767(3)	0.0454(8)
C7	0.2305(3)	0.4984(2)	0.6675(3)	0.0636(11)
C8	0.0591(3)	0.4387(2)	0.6336(3)	0.0517(9)
C9	0.1269(3)	0.5462(2)	0.5012(5)	0.0761(12)
C10	0.2306(2)	0.2042(2)	0.3910(2)	0.0282(6)
C11	0.0912(2)	0.0638(2)	0.4010(2)	0.0343(7)
C12	0.1842(2)	0.0212(2)	0.3462(3)	0.0495(9)
C13	0.0983(2)	0.0440(2)	0.5246(3)	0.0406(8)
C14	-0.0081(2)	0.0259(2)	0.3553(3)	0.0458(8)
C15	0.0644(2)	0.2061(2)	0.2307(2)	0.0334(7)
C16	0.1081(2)	0.2943(2)	0.2062(2)	0.0433(8)
C17	0.1142(2)	0.1460(2)	0.1480(2)	0.0499(9)
C18	-0.0511(2)	0.2072(2)	0.2108(3)	0.0442(8)
C21	-0.1543(2)	0.1138(2)	0.6157(3)	0.0466(8)
C22	-0.2397(2)	0.2166(2)	0.4509(3)	0.0462(8)
C23	-0.1805(3)	0.2857(2)	0.6576(3)	0.0537(10)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **8**.

Atom	x	y	z	U_{eq}
H3	0.3864	0.3300	0.3770	0.042
H4	0.3425	0.4633	0.4695	0.047
H7A	0.2482	0.4489	0.7116	0.095
H7B	0.1996	0.5411	0.7150	0.095
H7C	0.2922	0.5213	0.6334	0.095
H8A	0.0773	0.3889	0.6768	0.078
H8B	0.0082	0.4234	0.5782	0.078
H8C	0.0309	0.4818	0.6825	0.078
H9A	0.0988	0.5924	0.5451	0.114
H9B	0.0764	0.5279	0.4470	0.114
H9C	0.1885	0.5655	0.4631	0.114
H10A	0.2631	0.1660	0.4448	0.034
H10B	0.2636	0.1962	0.3186	0.034
H12A	0.2470	0.0425	0.3797	0.074
H12B	0.1843	0.0338	0.2673	0.074

H12C	0.1801	-0.0397	0.3570	0.074
H13A	0.0977	-0.0170	0.5354	0.061
H13B	0.0400	0.0691	0.5629	0.061
H13C	0.1617	0.0674	0.5543	0.061
H14A	-0.0120	-0.0337	0.3752	0.069
H14B	-0.0090	0.0315	0.2750	0.069
H14C	-0.0666	0.0558	0.3866	0.069
H16A	0.0862	0.3124	0.1328	0.065
H16B	0.1827	0.2922	0.2089	0.065
H16C	0.0832	0.3343	0.2613	0.065
H17A	0.0865	0.0893	0.1582	0.075
H17B	0.1880	0.1450	0.1599	0.075
H17C	0.0998	0.1651	0.0729	0.075
H18A	-0.0651	0.2283	0.1366	0.066
H18B	-0.0839	0.2438	0.2652	0.066
H18C	-0.0781	0.1500	0.2180	0.066
H21A	-0.2239	0.1107	0.6449	0.070
H21B	-0.1055	0.1073	0.6761	0.070
H21C	-0.1440	0.0688	0.5618	0.070
H22A	-0.2277	0.1738	0.3943	0.069
H22B	-0.2438	0.2721	0.4162	0.069
H22C	-0.3038	0.2044	0.4890	0.069
H23A	-0.2489	0.2685	0.6806	0.081
H23B	-0.1827	0.3434	0.6296	0.081
H23C	-0.1341	0.2829	0.7208	0.081

Table 4: Anisotropic displacement parameters ($Å^2$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0202(1)	0.0222(1)	0.0258(1)	0.0001(1)	0.0036(1)	0.0007(1)
P1	0.0195(3)	0.0286(3)	0.0241(3)	-0.0041(3)	-0.0013(3)	0.0018(3)
P2	0.0223(4)	0.0314(4)	0.0332(4)	0.0060(3)	0.0042(3)	-0.0007(3)
Cl2	0.0403(4)	0.0343(4)	0.0503(4)	0.0142(3)	0.0064(4)	0.0100(3)
Cl1	0.0363(4)	0.0443(4)	0.0287(3)	-0.0011(3)	-0.0075(3)	0.0003(3)
C1	0.0265(13)	0.0302(13)	0.0262(17)	0.0016(11)	0.0033(11)	-0.0012(10)
N2	0.0213(12)	0.0345(12)	0.0278(11)	-0.0036(10)	0.0004(9)	-0.0054(9)
C3	0.0257(15)	0.0469(17)	0.0315(16)	-0.0006(13)	0.0021(12)	-0.0090(13)
C4	0.0330(17)	0.0455(18)	0.0401(17)	0.0016(14)	0.0022(13)	-0.0173(14)
N5	0.0334(11)	0.0293(10)	0.0415(12)	-0.0012(15)	0.0063(14)	-0.0089(9)
C6	0.045(2)	0.0303(16)	0.061(2)	-0.0062(15)	0.0138(17)	-0.0065(14)
C7	0.069(3)	0.055(2)	0.066(3)	-0.028(2)	0.014(2)	-0.017(2)
C8	0.055(2)	0.0425(18)	0.058(2)	-0.0190(17)	0.0188(17)	-0.0059(16)
C9	0.088(3)	0.0384(17)	0.102(3)	0.011(3)	0.031(3)	0.0086(17)
C10	0.0202(13)	0.0372(14)	0.0273(14)	-0.0074(12)	-0.0025(11)	0.0018(11)
C11	0.0370(17)	0.0255(14)	0.0406(17)	-0.0089(13)	-0.0022(14)	0.0023(12)
C12	0.044(2)	0.0400(19)	0.064(2)	-0.0210(17)	-0.0043(16)	0.0123(15)
C13	0.0468(17)	0.0272(14)	0.048(2)	0.0073(14)	-0.0023(15)	0.0050(12)
C14	0.044(2)	0.0366(17)	0.057(2)	-0.0100(15)	-0.0052(15)	-0.0057(14)
C15	0.0234(14)	0.0528(18)	0.0240(14)	-0.0015(13)	-0.0028(11)	0.0023(13)
C16	0.0332(17)	0.067(2)	0.0292(15)	0.0119(15)	0.0024(13)	0.0027(15)
C17	0.0380(19)	0.084(3)	0.0274(16)	-0.0151(16)	0.0005(13)	0.0052(17)
C18	0.0281(17)	0.071(2)	0.0338(16)	-0.0013(16)	-0.0090(13)	0.0032(15)
C21	0.0358(18)	0.0472(19)	0.057(2)	0.0193(16)	0.0042(15)	-0.0071(15)
C22	0.0285(17)	0.057(2)	0.0529(19)	0.0107(16)	-0.0038(14)	-0.0052(14)
C23	0.042(2)	0.054(2)	0.064(2)	-0.0132(18)	0.0248(18)	-0.0029(16)

Table 5: Bond lengths (Å) and angles (deg) for **8**.

Ru1-C1	2.049(2)	C1-N5-C4	110.2(2)
Ru1-P1	2.2153(7)	C1-N5-C6	126.9(2)
Ru1-P2	2.3586(7)	C4-N5-C6	122.8(2)
Ru1-Cl1	2.3990(7)	N5-C6-C8	110.7(2)
Ru1-Cl2	2.4239(7)	N5-C6-C9	107.4(3)
P1-C10	1.861(3)	C8-C6-C9	111.0(3)
P1-C15	1.902(3)	N5-C6-C7	108.0(3)
P1-C11	1.904(3)	C8-C6-C7	107.5(3)
P2-C22	1.822(3)	C9-C6-C7	112.2(3)
P2-C21	1.824(3)	N2-C10-P1	106.38(17)
P2-C23	1.825(3)	C13-C11-C14	108.9(3)
C1-N2	1.356(3)	C13-C11-C12	106.4(2)
C1-N5	1.365(3)	C14-C11-C12	110.0(2)
N2-C3	1.386(3)	C13-C11-P1	108.95(19)
N2-C10	1.456(3)	C14-C11-P1	110.2(2)
C3-C4	1.336(4)	C12-C11-P1	112.3(2)
C4-N5	1.391(3)	C18-C15-C17	108.9(2)
N5-C6	1.495(4)	C18-C15-C16	109.1(2)
C6-C8	1.523(4)	C17-C15-C16	106.4(3)
C6-C9	1.526(5)	C18-C15-P1	109.8(2)
C6-C7	1.547(5)	C17-C15-P1	115.3(2)
C11-C13	1.538(4)	C16-C15-P1	107.22(19)
C11-C14	1.540(4)		
C11-C12	1.546(4)		
C15-C18	1.535(4)		
C15-C17	1.535(4)		
C15-C16	1.545(4)		
C1-Ru1-P1	82.12(7)		
C1-Ru1-P2	172.13(7)		
P1-Ru1-P2	105.67(3)		
C1-Ru1-Cl1	88.83(7)		
P1-Ru1-Cl1	101.16(3)		
P2-Ru1-Cl1	88.50(3)		
C1-Ru1-Cl2	93.21(7)		
P1-Ru1-Cl2	103.52(3)		
P2-Ru1-Cl2	86.15(3)		
Cl1-Ru1-Cl2	155.28(3)		
C10-P1-C15	101.97(13)		
C10-P1-C11	100.29(12)		
C15-P1-C11	108.43(13)		
C10-P1-Ru1	102.63(9)		
C15-P1-Ru1	116.73(10)		
C11-P1-Ru1	122.81(9)		
C22-P2-C21	101.25(15)		
C22-P2-C23	102.80(17)		
C21-P2-C23	100.37(16)		
C22-P2-Ru1	121.23(11)		
C21-P2-Ru1	123.86(11)		
C23-P2-Ru1	103.58(11)		
N2-C1-N5	103.7(2)		
N2-C1-Ru1	120.73(18)		
N5-C1-Ru1	135.52(19)		
C1-N2-C3	112.4(2)		
C1-N2-C10	120.7(2)		
C3-N2-C10	127.0(2)		
C4-C3-N2	105.6(3)		
C3-C4-N5	108.0(2)		

Crystal data for 9b:

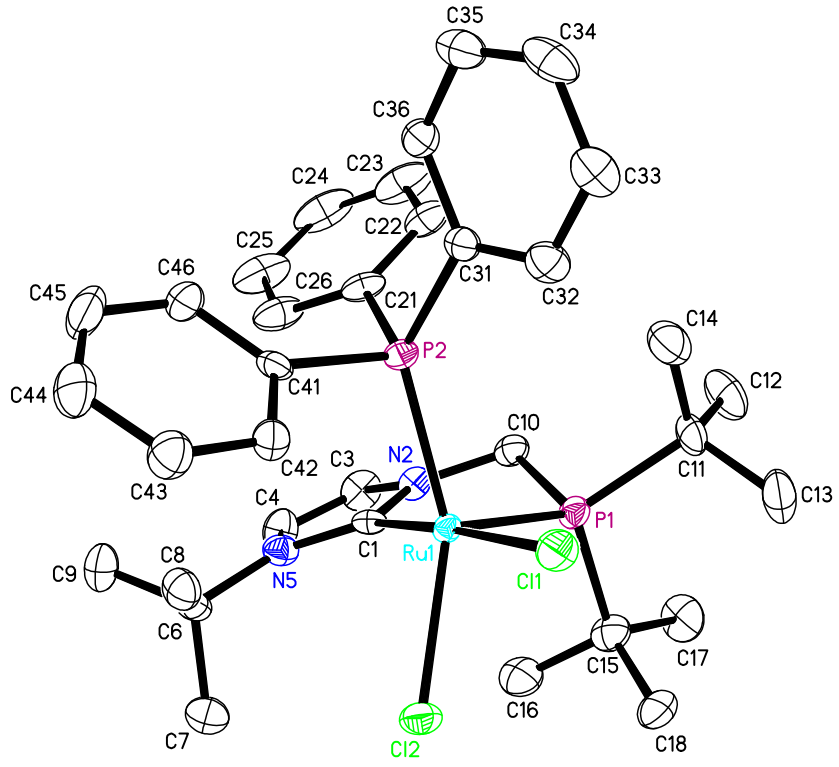


Table 1: Crystal data and structure refinement for **9b**.

Identification code	msi29	
Empirical formula	$C_{36}H_{50}Cl_6N_2P_2Ru$	
Formula weight	886.49	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/c$	
Z	4	
Unit cell dimensions	a = 13.3716(8) Å	α = 90 deg.
	b = 14.0724(9) Å	β = 99.899(2) deg.
	c = 21.8737(14) Å	γ = 90 deg.
Volume	4054.7(4) $Å^3$	
Density (calculated)	1.45 g/cm^3	
Absorption coefficient	0.89 mm^{-1}	
Crystal shape	plate	
Crystal size	0.23 x 0.15 x 0.01 mm^3	
Crystal colour	violet	
Theta range for data collection	1.5 to 28.4 deg.	
Index ranges	$-17 \le h \le 17$, $-18 \le k \le 18$, $-29 \le l \le 29$	
Reflections collected	41839	
Independent reflections	10107 (R(int) = 0.0892)	
Observed reflections	8446 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.99 and 0.82	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	10107 / 0 / 433	
Goodness-of-fit on F^2	1.36	

Final R indices (I>2σ(I))	R1 = 0.102, wR2 = 0.150
Largest diff. peak and hole	0.96 and -1.59 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **9b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.2724(1)	0.9841(1)	0.2571(1)	0.0144(1)
Cl1	0.1999(1)	1.0778(1)	0.3326(1)	0.0275(3)
Cl2	0.3700(1)	1.1279(1)	0.2477(1)	0.0263(3)
P1	0.3745(1)	0.8921(1)	0.3242(1)	0.0194(3)
P2	0.1301(1)	0.8894(1)	0.2293(1)	0.0171(3)
C1	0.3421(4)	0.9110(4)	0.1959(3)	0.0173(11)
N2	0.3884(3)	0.8260(3)	0.2140(2)	0.0205(10)
C3	0.4377(4)	0.7872(4)	0.1699(3)	0.0272(13)
C4	0.4218(5)	0.8466(4)	0.1216(3)	0.0299(14)
N5	0.3626(3)	0.9214(3)	0.1365(2)	0.0219(10)
C6	0.3390(4)	1.0024(4)	0.0913(3)	0.0230(12)
C7	0.4318(5)	1.0676(5)	0.0990(3)	0.0349(15)
C8	0.2446(4)	1.0558(4)	0.1018(3)	0.0282(13)
C9	0.3197(6)	0.9616(5)	0.0254(3)	0.0394(17)
C10	0.3923(4)	0.7890(4)	0.2757(3)	0.0225(12)
C11	0.3366(5)	0.8370(4)	0.3956(3)	0.0268(13)
C12	0.3898(6)	0.7410(5)	0.4130(3)	0.0428(18)
C13	0.3582(6)	0.9050(5)	0.4509(3)	0.0420(17)
C14	0.2237(5)	0.8192(5)	0.3831(3)	0.0396(17)
C15	0.5087(4)	0.9404(4)	0.3461(3)	0.0284(14)
C16	0.5535(5)	0.9550(5)	0.2867(3)	0.0348(15)
C17	0.5816(5)	0.8728(5)	0.3877(3)	0.0399(17)
C18	0.5068(5)	1.0363(4)	0.3804(3)	0.0352(16)
C21	0.1494(4)	0.7747(4)	0.1926(3)	0.0229(12)
C22	0.1473(5)	0.6905(4)	0.2253(3)	0.0292(14)
C23	0.1732(5)	0.6050(5)	0.2003(4)	0.0441(19)
C24	0.2008(5)	0.6026(5)	0.1432(4)	0.045(2)
C25	0.2022(5)	0.6855(5)	0.1098(4)	0.0423(19)
C26	0.1769(5)	0.7717(5)	0.1343(3)	0.0332(15)
C31	0.0237(4)	0.8617(4)	0.2704(3)	0.0197(11)
C32	0.0106(5)	0.9105(4)	0.3238(3)	0.0270(13)
C33	-0.0720(5)	0.8920(4)	0.3518(3)	0.0306(14)
C34	-0.1458(5)	0.8272(5)	0.3263(3)	0.0343(16)
C35	-0.1349(5)	0.7820(4)	0.2722(3)	0.0312(14)
C36	-0.0520(4)	0.7979(4)	0.2448(3)	0.0242(12)
C41	0.0543(4)	0.9602(4)	0.1669(3)	0.0189(11)
C42	0.0457(4)	1.0571(4)	0.1775(3)	0.0247(13)
C43	-0.0107(5)	1.1149(5)	0.1332(3)	0.0311(14)
C44	-0.0604(5)	1.0765(5)	0.0787(3)	0.0401(17)
C45	-0.0563(5)	0.9797(5)	0.0689(3)	0.0403(16)
C46	-0.0004(5)	0.9217(4)	0.1130(3)	0.0275(13)
C51	-0.0788(8)	0.8707(7)	0.5464(4)	0.075(3)
Cl3	-0.0717(3)	0.7734(2)	0.5000(1)	0.1058(12)
Cl4	-0.1348(3)	0.9707(2)	0.5081(1)	0.0941(10)
C52	0.7044(8)	0.8029(7)	0.1272(4)	0.074(3)
Cl5	0.6427(2)	0.7715(2)	0.0530(1)	0.0938(10)
Cl6	0.6986(2)	0.9235(2)	0.1420(1)	0.0846(8)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **9b**.

Atom	x	y	z	U_{eq}
H3	0.4755	0.7297	0.1730	0.033
H4	0.4466	0.8391	0.0837	0.036
H7A	0.4413	1.0974	0.1401	0.052
H7B	0.4215	1.1169	0.0669	0.052
H7C	0.4922	1.0302	0.0950	0.052
H8A	0.1873	1.0116	0.0984	0.042
H8B	0.2289	1.1058	0.0704	0.042
H8C	0.2567	1.0844	0.1432	0.042
H9A	0.3835	0.9373	0.0151	0.059
H9B	0.2929	1.0116	-0.0041	0.059
H9C	0.2702	0.9097	0.0230	0.059
H10A	0.4587	0.7584	0.2906	0.027
H10B	0.3378	0.7417	0.2765	0.027
H12A	0.3716	0.7177	0.4519	0.064
H12B	0.4635	0.7495	0.4183	0.064
H12C	0.3681	0.6948	0.3799	0.064
H13A	0.3289	0.9675	0.4387	0.063
H13B	0.4317	0.9113	0.4642	0.063
H13C	0.3277	0.8799	0.4853	0.063
H14A	0.2035	0.7881	0.4192	0.059
H14B	0.2065	0.7781	0.3466	0.059
H14C	0.1877	0.8798	0.3753	0.059
H16A	0.6196	0.9865	0.2970	0.052
H16B	0.5075	0.9946	0.2576	0.052
H16C	0.5621	0.8932	0.2676	0.052
H17A	0.5818	0.8107	0.3675	0.060
H17B	0.5591	0.8654	0.4278	0.060
H17C	0.6504	0.8994	0.3944	0.060
H18A	0.5724	1.0683	0.3824	0.053
H18B	0.4940	1.0248	0.4226	0.053
H18C	0.4529	1.0765	0.3580	0.053
H22	0.1281	0.6913	0.2651	0.035
H23	0.1715	0.5478	0.2232	0.053
H24	0.2191	0.5441	0.1266	0.055
H25	0.2205	0.6837	0.0697	0.051
H26	0.1785	0.8286	0.1111	0.040
H32	0.0589	0.9569	0.3409	0.032
H33	-0.0785	0.9240	0.3892	0.037
H34	-0.2026	0.8145	0.3458	0.041
H35	-0.1858	0.7390	0.2535	0.037
H36	-0.0457	0.7650	0.2077	0.029
H42	0.0788	1.0838	0.2155	0.030
H43	-0.0150	1.1812	0.1406	0.037
H44	-0.0976	1.1163	0.0479	0.048
H45	-0.0921	0.9529	0.0316	0.048
H46	0.0005	0.8550	0.1064	0.033
H51A	-0.0092	0.8876	0.5670	0.091
H51B	-0.1177	0.8529	0.5793	0.091
H52A	0.6733	0.7676	0.1583	0.089
H52B	0.7765	0.7834	0.1320	0.089

Table 4: Anisotropic displacement parameters ($Å^2$) for **9b**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{12}
Ru1	0.0159(2)	0.0120(2)	0.0147(2)	-0.0010(2)	0.0005(1)	0.0002(2)	
Cl1	0.0370(8)	0.0220(7)	0.0254(7)	-0.0070(6)	0.0105(6)	-0.0025(6)	
Cl2	0.0283(7)	0.0205(7)	0.0303(8)	-0.0037(6)	0.0057(6)	-0.0063(6)	
P1	0.0189(7)	0.0186(7)	0.0189(7)	0.0007(5)	-0.0015(6)	0.0007(6)	
P2	0.0182(7)	0.0133(6)	0.0197(7)	-0.0033(5)	0.0026(6)	-0.0005(5)	
C1	0.016(3)	0.012(2)	0.024(3)	-0.001(2)	0.004(2)	-0.003(2)	
N2	0.018(2)	0.021(2)	0.022(2)	-0.0032(19)	0.0017(19)	0.0025(19)	
C3	0.021(3)	0.028(3)	0.033(3)	-0.007(3)	0.008(3)	0.010(2)	
C4	0.032(3)	0.034(3)	0.024(3)	-0.006(3)	0.006(3)	0.007(3)	
N5	0.022(2)	0.021(2)	0.024(3)	-0.0017(19)	0.008(2)	-0.0026(19)	
C6	0.028(3)	0.017(3)	0.025(3)	0.001(2)	0.006(2)	-0.003(2)	
C7	0.032(4)	0.037(4)	0.037(4)	0.003(3)	0.009(3)	-0.008(3)	
C8	0.025(3)	0.029(3)	0.030(3)	0.007(3)	0.003(3)	0.004(3)	
C9	0.046(4)	0.049(4)	0.021(3)	0.000(3)	0.001(3)	-0.003(3)	
C10	0.020(3)	0.019(3)	0.026(3)	0.001(2)	-0.002(2)	0.000(2)	
C11	0.030(3)	0.030(3)	0.020(3)	0.010(2)	0.002(2)	0.004(3)	
C12	0.049(4)	0.040(4)	0.040(4)	0.022(3)	0.009(3)	0.009(3)	
C13	0.052(4)	0.054(5)	0.020(3)	0.006(3)	0.006(3)	-0.001(4)	
C14	0.032(4)	0.052(4)	0.035(4)	0.011(3)	0.008(3)	-0.006(3)	
C15	0.022(3)	0.028(3)	0.033(3)	0.001(3)	-0.003(3)	0.001(3)	
C16	0.021(3)	0.040(4)	0.042(4)	0.004(3)	0.000(3)	-0.002(3)	
C17	0.020(3)	0.054(4)	0.042(4)	0.015(3)	-0.008(3)	0.007(3)	
C18	0.035(4)	0.036(4)	0.030(3)	0.001(3)	-0.008(3)	-0.010(3)	
C21	0.017(3)	0.016(3)	0.035(3)	-0.009(2)	0.004(2)	-0.002(2)	
C22	0.027(3)	0.021(3)	0.036(4)	-0.007(3)	-0.003(3)	-0.002(2)	
C23	0.036(4)	0.017(3)	0.072(5)	-0.010(3)	-0.012(4)	0.004(3)	
C24	0.028(4)	0.033(4)	0.072(6)	-0.031(4)	0.000(4)	0.004(3)	
C25	0.024(3)	0.050(5)	0.057(5)	-0.030(4)	0.017(3)	-0.006(3)	
C26	0.027(3)	0.031(3)	0.043(4)	-0.018(3)	0.011(3)	-0.008(3)	
C31	0.017(3)	0.019(3)	0.023(3)	0.005(2)	0.002(2)	0.001(2)	
C32	0.032(3)	0.020(3)	0.031(3)	0.001(2)	0.007(3)	0.000(2)	
C33	0.037(4)	0.023(3)	0.034(4)	0.002(3)	0.014(3)	0.005(3)	
C34	0.025(3)	0.034(4)	0.048(4)	0.015(3)	0.018(3)	0.007(3)	
C35	0.025(3)	0.029(3)	0.040(4)	0.007(3)	0.008(3)	-0.002(3)	
C36	0.021(3)	0.027(3)	0.024(3)	0.003(2)	0.002(2)	0.000(2)	
C41	0.019(3)	0.015(3)	0.023(3)	0.006(2)	0.005(2)	-0.003(2)	
C42	0.024(3)	0.028(3)	0.021(3)	0.002(2)	0.002(2)	-0.001(2)	
C43	0.030(3)	0.031(3)	0.031(3)	0.001(3)	0.002(3)	0.002(3)	
C44	0.040(4)	0.040(4)	0.035(4)	0.010(3)	-0.009(3)	0.003(3)	
C45	0.044(4)	0.042(4)	0.028(3)	-0.002(3)	-0.014(3)	-0.003(3)	
C46	0.032(3)	0.029(3)	0.021(3)	-0.005(2)	0.003(3)	-0.007(3)	
C51	0.087(7)	0.099(8)	0.045(5)	0.009(5)	0.022(5)	0.036(6)	
Cl3	0.194(4)	0.0578(16)	0.0589(16)	0.0083(12)	0.0027(19)	0.0190(19)	
Cl4	0.135(3)	0.095(2)	0.0632(16)	0.0180(14)	0.0501(17)	0.0584(19)	
C52	0.081(7)	0.073(7)	0.066(6)	0.022(5)	0.004(5)	0.035(6)	
Cl5	0.114(2)	0.115(2)	0.0521(15)	0.0102(15)	0.0122(15)	0.0428(19)	
Cl6	0.0865(19)	0.0708(17)	0.095(2)	0.0240(15)	0.0104(16)	0.0090(14)	

Table 5: Bond lengths (Å) and angles (deg) for **9b**.

Ru1-C1	2.036(5)	Ru1-P2	2.3164(14)
Ru1-P1	2.2380(15)	Ru1-Cl2	2.4364(14)

Ru1-Cl1	2.4416(15)	C21-P2-C31	101.8(3)
P1-C10	1.837(6)	C41-P2-C31	95.9(2)
P1-C11	1.889(6)	C21-P2-Ru1	116.67(18)
P1-C15	1.902(6)	C41-P2-Ru1	101.83(17)
P2-C21	1.841(5)	C31-P2-Ru1	131.21(19)
P2-C41	1.846(5)	N2-C1-N5	102.2(4)
P2-C31	1.851(6)	N2-C1-Ru1	119.0(4)
C1-N2	1.373(7)	N5-C1-Ru1	138.7(4)
C1-N5	1.381(7)	C3-N2-C1	113.0(5)
N2-C3	1.372(7)	C3-N2-C10	124.9(5)
N2-C10	1.439(7)	C1-N2-C10	121.8(5)
C3-C4	1.336(8)	C4-C3-N2	106.1(5)
C4-N5	1.389(7)	C3-C4-N5	108.0(5)
N5-C6	1.506(7)	C1-N5-C4	110.7(5)
C6-C8	1.520(8)	C1-N5-C6	130.2(5)
C6-C7	1.529(8)	C4-N5-C6	118.8(5)
C6-C9	1.532(8)	N5-C6-C8	111.1(5)
C11-C14	1.509(9)	N5-C6-C7	107.8(5)
C11-C13	1.531(9)	C8-C6-C7	111.5(5)
C11-C12	1.544(8)	N5-C6-C9	108.5(5)
C15-C16	1.535(9)	C8-C6-C9	108.5(5)
C15-C17	1.543(8)	C7-C6-C9	109.4(5)
C15-C18	1.547(9)	N2-C10-P1	105.6(4)
C21-C26	1.386(8)	C14-C11-C13	107.1(6)
C21-C22	1.387(8)	C14-C11-C12	107.7(6)
C22-C23	1.389(9)	C13-C11-C12	109.7(5)
C23-C24	1.362(11)	C14-C11-P1	108.7(4)
C24-C25	1.378(11)	C13-C11-P1	110.9(4)
C25-C26	1.392(9)	C12-C11-P1	112.7(4)
C31-C32	1.390(8)	C16-C15-C17	106.5(5)
C31-C36	1.397(8)	C16-C15-C18	109.6(5)
C32-C33	1.378(8)	C17-C15-C18	108.2(5)
C33-C34	1.389(9)	C16-C15-P1	108.9(4)
C34-C35	1.373(9)	C17-C15-P1	113.7(4)
C35-C36	1.366(8)	C18-C15-P1	109.9(4)
C41-C46	1.385(8)	C26-C21-C22	118.7(5)
C41-C42	1.391(8)	C26-C21-P2	120.5(5)
C42-C43	1.385(8)	C22-C21-P2	120.5(5)
C43-C44	1.372(9)	C21-C22-C23	120.6(7)
C44-C45	1.381(10)	C24-C23-C22	120.5(7)
C45-C46	1.382(9)	C23-C24-C25	119.7(6)
C51-Cl3	1.717(10)	C24-C25-C26	120.4(7)
C51-Cl4	1.742(9)	C21-C26-C25	120.1(7)
C52-Cl6	1.733(10)	C32-C31-C36	117.8(5)
C52-Cl5	1.746(10)	C32-C31-P2	121.5(4)
C1-Ru1-P1	80.95(15)	C36-C31-P2	120.3(4)
C1-Ru1-P2	89.14(15)	C33-C32-C31	120.5(6)
P1-Ru1-P2	102.71(5)	C32-C33-C34	120.9(6)
C1-Ru1-Cl2	93.00(15)	C35-C34-C33	118.5(6)
P1-Ru1-Cl2	105.10(5)	C36-C35-C34	121.1(6)
P2-Ru1-Cl2	152.09(5)	C35-C36-C31	121.1(6)
C1-Ru1-Cl1	175.99(15)	C46-C41-C42	118.5(5)
P1-Ru1-Cl1	97.85(5)	C46-C41-P2	124.1(4)
P2-Ru1-Cl1	94.87(5)	C42-C41-P2	117.1(4)
Cl2-Ru1-Cl1	83.60(5)	C43-C42-C41	120.7(6)
C10-P1-C11	103.5(3)	C44-C43-C42	120.0(6)
C10-P1-C15	102.5(3)	C43-C44-C45	119.8(6)
C11-P1-C15	108.3(3)	C44-C45-C46	120.3(6)
C10-P1-Ru1	101.67(18)	C45-C46-C41	120.4(6)
C11-P1-Ru1	124.1(2)	Cl3-C51-Cl4	115.0(5)
C15-P1-Ru1	113.65(19)	Cl6-C52-Cl5	113.1(5)
C21-P2-C41	104.5(3)		

Crystal data for 11:

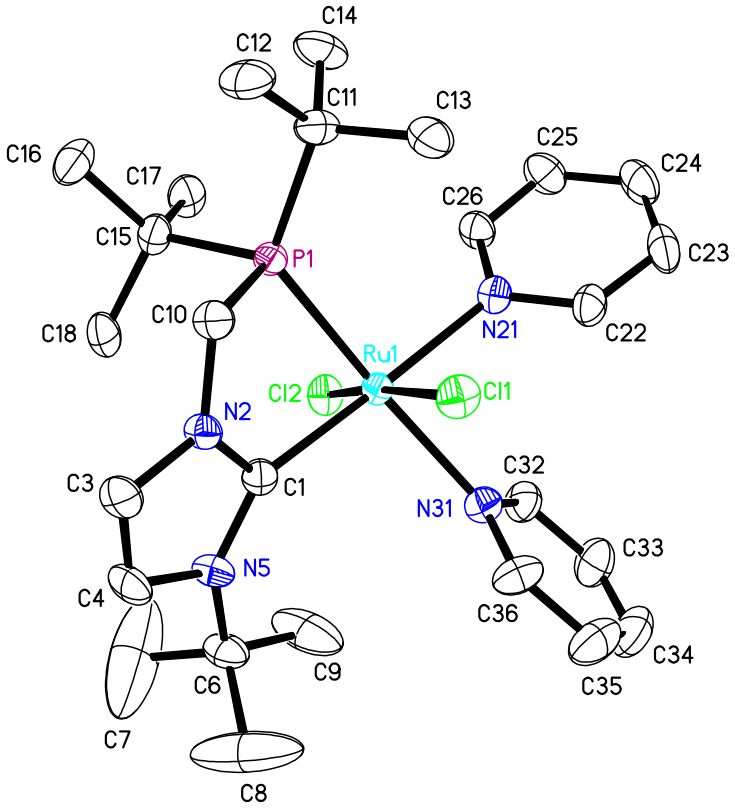


Table 1: Crystal data and structure refinement for **11**.

Identification code	msi25	
Empirical formula	$C_{31}H_{46}Cl_2N_5PRu$	
Formula weight	691.67	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	4	
Unit cell dimensions	a = 18.1448(6) Å	α = 90 deg.
	b = 9.1268(3) Å	β = 93.872(1) deg.
	c = 19.6120(6) Å	γ = 90 deg.
Volume	3240.41(18) $Å^3$	
Density (calculated)	1.42 g/cm^3	
Absorption coefficient	0.73 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.22 x 0.12 x 0.08 mm^3	
Crystal colour	orange	
Theta range for data collection	1.5 to 27.5 deg.	
Index ranges	$-23 \le h \le 23$, $-11 \le k \le 11$, $-25 \le l \le 25$	
Reflections collected	32713	
Independent reflections	7426 (R(int) = 0.1334)	
Observed reflections	5517 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.94 and 0.86	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	7426 / 0 / 371	

Goodness-of-fit on F^2	1.13
Final R indices ($I>2\sigma(I)$)	R1 = 0.052, wR2 = 0.105
Largest diff. peak and hole	0.69 and -0.85 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **11**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.5009(1)	0.6482(1)	0.7264(1)	0.0184(1)
P1	0.5870(1)	0.6788(1)	0.8178(1)	0.0204(2)
Cl1	0.5918(1)	0.5130(1)	0.6643(1)	0.0286(2)
Cl2	0.4007(1)	0.7842(1)	0.7733(1)	0.0274(2)
C1	0.4848(2)	0.4515(4)	0.7775(2)	0.0227(9)
N2	0.5474(2)	0.3991(4)	0.8139(2)	0.0217(7)
C3	0.5356(3)	0.2662(5)	0.8451(2)	0.0294(10)
C4	0.4654(3)	0.2318(5)	0.8283(2)	0.0320(10)
N5	0.4339(2)	0.3428(4)	0.7874(2)	0.0248(7)
C6	0.3523(2)	0.3301(5)	0.7686(2)	0.0325(10)
C7	0.3133(4)	0.3221(16)	0.8325(4)	0.169(7)
C8	0.3396(4)	0.1895(7)	0.7287(5)	0.115(4)
C9	0.3213(3)	0.4511(7)	0.7252(4)	0.068(2)
C10	0.6142(2)	0.4845(4)	0.8271(2)	0.0252(9)
C11	0.6816(2)	0.7684(5)	0.8100(2)	0.0292(10)
C12	0.7439(2)	0.6891(6)	0.8510(3)	0.0396(12)
C13	0.7006(3)	0.7672(6)	0.7351(2)	0.0370(11)
C14	0.6814(3)	0.9292(5)	0.8327(3)	0.0409(12)
C15	0.5552(2)	0.7246(5)	0.9066(2)	0.0272(9)
C16	0.6147(3)	0.7064(6)	0.9657(2)	0.0405(12)
C17	0.5243(3)	0.8812(5)	0.9080(2)	0.0328(10)
C18	0.4917(3)	0.6183(5)	0.9204(2)	0.0321(10)
N21	0.5270(2)	0.8485(4)	0.6737(2)	0.0248(7)
C22	0.5443(2)	0.8465(5)	0.6080(2)	0.0289(9)
C23	0.5598(3)	0.9729(6)	0.5725(2)	0.0364(11)
C24	0.5574(3)	1.1072(5)	0.6046(3)	0.0381(12)
C25	0.5394(3)	1.1101(5)	0.6721(3)	0.0357(11)
C26	0.5235(2)	0.9803(5)	0.7037(2)	0.0278(9)
N31	0.4291(2)	0.6115(4)	0.6340(2)	0.0256(8)
C32	0.3823(2)	0.7181(5)	0.6107(2)	0.0313(10)
C33	0.3414(3)	0.7089(6)	0.5487(2)	0.0421(12)
C34	0.3485(3)	0.5877(7)	0.5082(3)	0.0492(14)
C35	0.3954(3)	0.4768(7)	0.5314(3)	0.0475(14)
C36	0.4342(3)	0.4933(5)	0.5947(2)	0.0361(11)
N51	0.1873(4)	0.3645(9)	0.4739(4)	0.101(2)
C52	0.2304(4)	0.2736(8)	0.4463(3)	0.0602(17)
C53	0.2636(3)	0.1563(8)	0.4746(4)	0.0662(19)
C54	0.2523(5)	0.1338(10)	0.5458(5)	0.100(3)
C55	0.2062(4)	0.2376(10)	0.5746(3)	0.073(2)
C56	0.1768(4)	0.3430(10)	0.5373(5)	0.085(2)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **11**.

Atom	x	y	z	U_{eq}
H3	0.5704	0.2109	0.8728	0.035

H4	0.4410	0.1457	0.8419	0.038
H7A	0.3286	0.2335	0.8578	0.253
H7B	0.2598	0.3191	0.8212	0.253
H7C	0.3255	0.4086	0.8606	0.253
H8A	0.3633	0.1080	0.7543	0.173
H8B	0.3609	0.1985	0.6843	0.173
H8C	0.2864	0.1710	0.7218	0.173
H9A	0.2672	0.4443	0.7216	0.101
H9B	0.3398	0.4437	0.6795	0.101
H9C	0.3363	0.5453	0.7457	0.101
H10A	0.6510	0.4590	0.7939	0.030
H10B	0.6362	0.4653	0.8738	0.030
H12A	0.7904	0.7421	0.8469	0.059
H12B	0.7486	0.5894	0.8333	0.059
H12C	0.7328	0.6847	0.8992	0.059
H13A	0.6657	0.8297	0.7082	0.055
H13B	0.6974	0.6668	0.7175	0.055
H13C	0.7509	0.8043	0.7318	0.055
H14A	0.6752	0.9342	0.8819	0.061
H14B	0.6405	0.9809	0.8079	0.061
H14C	0.7283	0.9752	0.8229	0.061
H16A	0.5925	0.7228	1.0093	0.061
H16B	0.6543	0.7778	0.9606	0.061
H16C	0.6350	0.6071	0.9649	0.061
H17A	0.4878	0.8949	0.8694	0.049
H17B	0.5647	0.9515	0.9046	0.049
H17C	0.5008	0.8970	0.9509	0.049
H18A	0.5109	0.5180	0.9239	0.048
H18B	0.4534	0.6242	0.8829	0.048
H18C	0.4706	0.6452	0.9634	0.048
H22	0.5460	0.7549	0.5851	0.035
H23	0.5720	0.9672	0.5262	0.044
H24	0.5677	1.1950	0.5810	0.046
H25	0.5380	1.2002	0.6963	0.043
H26	0.5093	0.9842	0.7494	0.033
H32	0.3772	0.8029	0.6381	0.038
H33	0.3086	0.7858	0.5343	0.051
H34	0.3216	0.5804	0.4650	0.059
H35	0.4010	0.3911	0.5048	0.057
H36	0.4660	0.4161	0.6107	0.043
H52	0.2397	0.2924	0.4001	0.072
H53	0.2927	0.0918	0.4495	0.079
H54	0.2744	0.0550	0.5715	0.119
H55	0.1964	0.2305	0.6214	0.087
H56	0.1451	0.4092	0.5585	0.102

Table 4: Anisotropic displacement parameters ($Å^2$) for msi25. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0205(2)	0.0153(2)	0.0192(2)	-0.0006(1)	0.0011(1)	0.0018(1)
P1	0.0227(5)	0.0176(5)	0.0209(5)	0.0000(4)	0.0006(4)	-0.0005(4)
Cl1	0.0280(5)	0.0274(5)	0.0309(5)	-0.0059(4)	0.0052(4)	0.0048(4)
Cl2	0.0292(5)	0.0269(5)	0.0267(5)	0.0001(4)	0.0058(4)	0.0070(4)
C1	0.026(2)	0.020(2)	0.022(2)	-0.0014(17)	0.0026(17)	0.0016(16)
N2	0.0212(17)	0.0161(16)	0.0274(18)	0.0032(14)	-0.0023(14)	0.0020(13)

C3	0.035(2)	0.017(2)	0.036(2)	0.0041(18)	-0.001(2)	0.0035(18)
C4	0.038(3)	0.017(2)	0.041(3)	0.0073(19)	0.003(2)	-0.0024(19)
N5	0.0215(17)	0.0184(17)	0.0346(19)	-0.0004(15)	0.0014(15)	-0.0020(14)
C6	0.022(2)	0.031(3)	0.044(3)	0.003(2)	-0.0006(19)	-0.0061(19)
C7	0.031(4)	0.42(2)	0.057(4)	0.059(8)	0.014(3)	0.011(7)
C8	0.071(5)	0.042(4)	0.220(11)	-0.027(5)	-0.085(6)	0.007(4)
C9	0.028(3)	0.046(4)	0.125(6)	0.030(4)	-0.021(3)	-0.008(3)
C10	0.024(2)	0.020(2)	0.030(2)	0.0020(17)	-0.0025(18)	0.0032(17)
C11	0.025(2)	0.029(2)	0.033(2)	-0.0073(19)	0.0028(19)	-0.0046(18)
C12	0.024(2)	0.044(3)	0.049(3)	-0.001(2)	-0.008(2)	-0.005(2)
C13	0.031(2)	0.043(3)	0.037(3)	-0.002(2)	0.008(2)	-0.010(2)
C14	0.042(3)	0.028(3)	0.054(3)	-0.009(2)	0.010(2)	-0.012(2)
C15	0.036(2)	0.024(2)	0.021(2)	-0.0001(17)	0.0009(18)	0.0027(19)
C16	0.046(3)	0.047(3)	0.027(2)	0.000(2)	-0.009(2)	-0.002(2)
C17	0.046(3)	0.026(2)	0.027(2)	-0.0051(18)	0.007(2)	0.001(2)
C18	0.038(3)	0.035(3)	0.024(2)	0.0042(19)	0.010(2)	0.000(2)
N21	0.0262(18)	0.0258(18)	0.0225(17)	0.0002(15)	0.0023(14)	0.0016(16)
C22	0.030(2)	0.035(2)	0.022(2)	-0.0017(19)	0.0060(17)	0.001(2)
C23	0.033(2)	0.049(3)	0.027(2)	0.015(2)	0.007(2)	0.001(2)
C24	0.041(3)	0.032(3)	0.041(3)	0.018(2)	0.003(2)	-0.001(2)
C25	0.041(3)	0.023(2)	0.043(3)	0.005(2)	0.006(2)	-0.001(2)
C26	0.035(2)	0.020(2)	0.028(2)	0.0017(18)	0.0032(19)	0.0005(18)
N31	0.0257(18)	0.0238(19)	0.0270(18)	-0.0012(15)	0.0002(15)	0.0015(15)
C32	0.030(2)	0.035(3)	0.028(2)	0.004(2)	-0.0029(19)	0.003(2)
C33	0.045(3)	0.049(3)	0.031(3)	0.008(2)	-0.009(2)	0.006(3)
C34	0.042(3)	0.076(4)	0.029(3)	-0.003(3)	-0.006(2)	-0.005(3)
C35	0.047(3)	0.056(4)	0.040(3)	-0.020(3)	0.000(2)	-0.001(3)
C36	0.034(3)	0.034(3)	0.039(3)	-0.014(2)	-0.003(2)	0.001(2)
N51	0.095(5)	0.115(6)	0.097(5)	0.014(5)	0.027(4)	0.023(5)
C52	0.082(5)	0.066(4)	0.033(3)	0.001(3)	0.006(3)	0.002(4)
C53	0.049(4)	0.067(4)	0.084(5)	-0.029(4)	0.012(3)	-0.005(3)
C54	0.098(6)	0.097(7)	0.099(6)	0.044(5)	-0.026(5)	0.016(5)
C55	0.069(5)	0.112(7)	0.039(3)	0.003(4)	0.014(3)	-0.008(5)
C56	0.065(5)	0.107(7)	0.083(6)	-0.016(5)	0.017(4)	0.000(5)

Table 5: Bond lengths (Å) and angles (deg) for **11**.

Ru1-C1	2.086(4)	C15-C17	1.536(6)
Ru1-N21	2.169(4)	C15-C16	1.538(6)
Ru1-N31	2.186(4)	C15-C18	1.544(6)
Ru1-P1	2.3139(11)	N21-C26	1.342(5)
Ru1-Cl2	2.4319(10)	N21-C22	1.347(5)
Ru1-Cl1	2.4488(10)	C22-C23	1.386(6)
P1-C10	1.847(4)	C23-C24	1.379(7)
P1-C11	1.916(4)	C24-C25	1.386(7)
P1-C15	1.917(4)	C25-C26	1.375(6)
C1-N5	1.378(5)	N31-C36	1.333(6)
C1-N2	1.385(5)	N31-C32	1.350(6)
N2-C3	1.382(5)	C32-C33	1.385(6)
N2-C10	1.449(5)	C33-C34	1.373(8)
C3-C4	1.332(6)	C34-C35	1.380(8)
C4-N5	1.391(6)	C35-C36	1.394(7)
N5-C6	1.504(5)	N51-C52	1.284(9)
C6-C7	1.482(8)	N51-C56	1.285(10)
C6-C9	1.483(7)	C52-C53	1.330(9)
C6-C8	1.512(8)	C53-C54	1.441(10)
C11-C12	1.526(6)	C54-C55	1.407(11)
C11-C13	1.532(6)	C55-C56	1.301(11)
C11-C14	1.533(6)	C1-Ru1-N21	175.37(14)

C1-Ru1-N31	99.90(15)
N21-Ru1-N31	82.56(13)
C1-Ru1-P1	80.85(12)
N21-Ru1-P1	96.29(10)
N31-Ru1-P1	173.99(9)
C1-Ru1-Cl2	97.21(11)
N21-Ru1-Cl2	86.75(9)
N31-Ru1-Cl2	88.47(9)
P1-Ru1-Cl2	97.36(4)
C1-Ru1-Cl1	85.73(11)
N21-Ru1-Cl1	90.65(9)
N31-Ru1-Cl1	83.91(9)
P1-Ru1-Cl1	90.21(4)
Cl2-Ru1-Cl1	172.21(4)
C10-P1-C11	100.52(19)
C10-P1-C15	102.41(19)
C11-P1-C15	107.77(19)
C10-P1-Ru1	97.03(14)
C11-P1-Ru1	123.46(15)
C15-P1-Ru1	120.08(15)
N5-C1-N2	102.4(3)
N5-C1-Ru1	143.5(3)
N2-C1-Ru1	114.0(3)
C3-N2-C1	112.6(3)
C3-N2-C10	123.1(4)
C1-N2-C10	123.6(3)
C4-C3-N2	105.8(4)
C3-C4-N5	108.7(4)
C1-N5-C4	110.6(4)
C1-N5-C6	132.7(4)
C4-N5-C6	116.4(3)
C7-C6-C9	109.7(6)
C7-C6-N5	108.4(4)
C9-C6-N5	114.4(4)
C7-C6-C8	109.3(8)
C9-C6-C8	107.2(5)
N5-C6-C8	107.8(4)
N2-C10-P1	106.5(3)
C12-C11-C13	107.1(4)
C12-C11-C14	108.5(4)
C13-C11-C14	106.9(4)
C12-C11-P1	113.0(3)
C13-C11-P1	109.5(3)
C14-C11-P1	111.4(3)
C17-C15-C16	109.0(4)
C17-C15-C18	107.7(4)
C16-C15-C18	107.1(4)
C17-C15-P1	110.6(3)
C16-C15-P1	115.0(3)
C18-C15-P1	107.2(3)
C26-N21-C22	116.9(4)
C26-N21-Ru1	121.9(3)
C22-N21-Ru1	121.1(3)
N21-C22-C23	122.4(4)
C24-C23-C22	119.8(4)
C23-C24-C25	118.0(4)
C26-C25-C24	118.9(4)
N21-C26-C25	123.9(4)
C36-N31-C32	117.1(4)
C36-N31-Ru1	122.9(3)
C32-N31-Ru1	119.7(3)
N31-C32-C33	122.7(5)
C34-C33-C32	119.4(5)
C33-C34-C35	118.7(5)
C34-C35-C36	118.6(5)
N31-C36-C35	123.4(5)
C52-N51-C56	116.3(8)
N51-C52-C53	128.0(6)
C52-C53-C54	115.4(6)
C55-C54-C53	114.8(7)
C56-C55-C54	120.4(7)
N51-C56-C55	125.0(8)

Crystal data for 13:

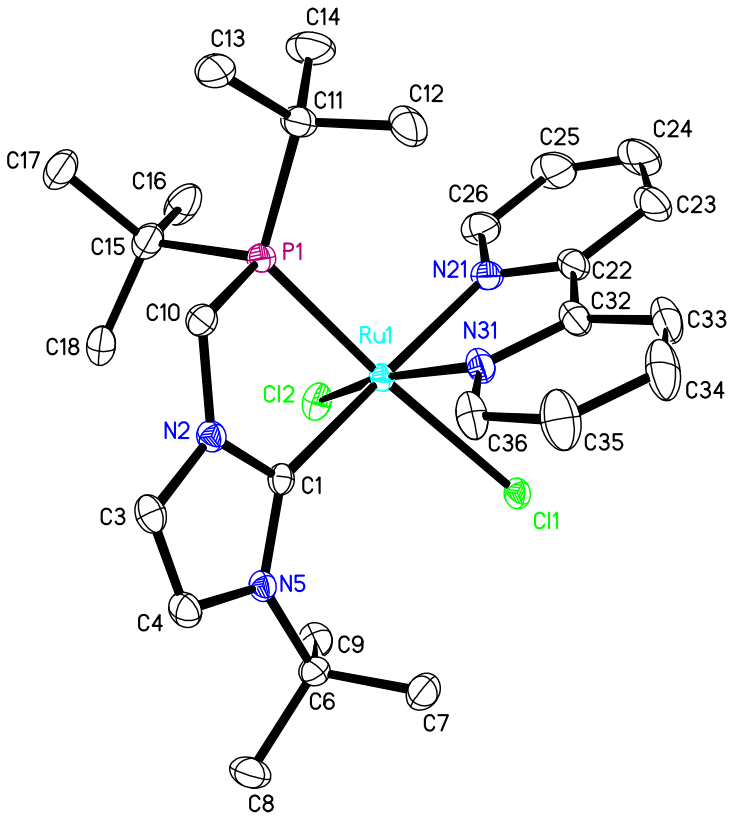


Table 1: Crystal data and structure refinement for **13**.

Identification code	abo9	
Empirical formula	$C_{27}H_{41}Cl_4N_4PRu$	
Formula weight	695.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Z	4	
Unit cell dimensions	a = 12.6218(14) Å	α = 90 deg.
	b = 16.0062(17) Å	β = 99.837(2) deg.
	c = 16.0036(17) Å	γ = 90 deg.
Volume	3185.6(6) $Å^3$	
Density (calculated)	1.45 g/cm^3	
Absorption coefficient	0.90 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.28 x 0.23 x 0.17 mm^3	
Crystal colour	black	
Theta range for data collection	1.8 to 28.3 deg.	
Index ranges	$-16 \le h \le 16$, $-21 \le k \le 21$, $-21 \le l \le 21$	
Reflections collected	33225	
Independent reflections	7905 (R(int) = 0.0261)	
Observed reflections	7151 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.86 and 0.79	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	7905 / 88 / 400	

Goodness-of-fit on F^2	1.08
Final R indices ($I>2\sigma(I)$)	R1 = 0.033, wR2 = 0.076
Largest diff. peak and hole	1.71 and -0.71 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **13**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ru1	0.3568(1)	0.1613(1)	0.2913(1)	0.0135(1)
Cl1	0.2888(1)	0.0308(1)	0.3528(1)	0.0163(1)
Cl2	0.2871(1)	0.0974(1)	0.1553(1)	0.0206(1)
P1	0.4305(1)	0.2771(1)	0.2389(1)	0.0175(1)
C1	0.2301(2)	0.2451(1)	0.2945(1)	0.0138(4)
N2	0.2554(1)	0.3290(1)	0.2949(1)	0.0148(3)
C3	0.1725(2)	0.3800(1)	0.3084(1)	0.0178(4)
C4	0.0909(2)	0.3289(1)	0.3170(1)	0.0189(4)
N5	0.1246(1)	0.2470(1)	0.3074(1)	0.0147(3)
C6	0.0517(2)	0.1747(1)	0.3161(1)	0.0182(4)
C7	0.0834(2)	0.1387(2)	0.4053(2)	0.0251(5)
C8	-0.0654(2)	0.2057(2)	0.3056(2)	0.0278(5)
C9	0.0576(2)	0.1122(1)	0.2453(2)	0.0214(4)
C10	0.3605(2)	0.3612(1)	0.2860(1)	0.0175(4)
C11	0.5762(2)	0.3090(2)	0.2772(2)	0.0286(5)
C12	0.6125(2)	0.2800(2)	0.3689(2)	0.0369(7)
C13	0.5932(2)	0.4046(2)	0.2776(2)	0.0316(6)
C14	0.6501(2)	0.2683(2)	0.2219(2)	0.0424(8)
C15	0.3966(2)	0.3002(1)	0.1210(2)	0.0232(5)
C16	0.4398(2)	0.2312(2)	0.0689(2)	0.0317(6)
C17	0.4365(2)	0.3852(2)	0.0934(2)	0.0288(5)
C18	0.2730(2)	0.3025(1)	0.0992(1)	0.0225(4)
N21	0.4951(2)	0.0869(1)	0.3074(1)	0.0205(4)
C22	0.5419(2)	0.0771(1)	0.3898(2)	0.0234(5)
C23	0.6321(2)	0.0263(2)	0.4130(2)	0.0332(6)
C24	0.6745(2)	-0.0148(2)	0.3501(2)	0.0407(7)
C25	0.6267(2)	-0.0047(2)	0.2662(2)	0.0384(7)
C26	0.5369(2)	0.0465(2)	0.2471(2)	0.0285(5)
N31	0.4167(1)	0.1822(1)	0.4160(1)	0.0184(4)
C32	0.4949(2)	0.1271(1)	0.4508(2)	0.0215(5)
C33	0.5296(2)	0.1226(2)	0.5381(2)	0.0283(5)
C34	0.4882(2)	0.1766(2)	0.5909(2)	0.0347(6)
C35	0.4109(2)	0.2335(2)	0.5560(2)	0.0334(6)
C36	0.3766(2)	0.2339(1)	0.4691(2)	0.0236(5)
C51	-0.3234(11)	0.0175(10)	0.0160(10)	0.067(4)
Cl3	-0.4573(3)	-0.0035(3)	0.0201(2)	0.0883(15)
Cl4	-0.2654(5)	0.0893(3)	0.0925(3)	0.0562(12)
C51B	-0.316(3)	0.0063(15)	0.021(2)	0.056(8)
Cl3B	-0.3965(6)	-0.0629(4)	0.0629(3)	0.058(2)
Cl4B	-0.2952(11)	0.1023(8)	0.0685(7)	0.052(3)
C51C	-0.1156(9)	0.0096(14)	0.0086(8)	0.201(9)
Cl3C	0.0116(5)	0.0253(3)	0.0261(2)	0.142(2)
Cl4C	-0.2205(5)	0.0501(3)	0.0455(4)	0.161(3)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **13**.

Atom	x	y	z	U_{eq}
H3	0.1729	0.4393	0.3111	0.021
H4	0.0222	0.3456	0.3277	0.023
H7A	0.1581	0.1195	0.4133	0.038
H7B	0.0362	0.0916	0.4125	0.038
H7C	0.0761	0.1820	0.4472	0.038
H8A	-0.0732	0.2432	0.3525	0.042
H8B	-0.1137	0.1578	0.3057	0.042
H8C	-0.0837	0.2359	0.2517	0.042
H9A	0.0346	0.1393	0.1903	0.032
H9B	0.0103	0.0648	0.2509	0.032
H9C	0.1317	0.0924	0.2492	0.032
H10A	0.4015	0.3772	0.3420	0.021
H10B	0.3528	0.4110	0.2488	0.021
H12A	0.6147	0.2188	0.3707	0.055
H12B	0.5616	0.3003	0.4042	0.055
H12C	0.6842	0.3023	0.3905	0.055
H13A	0.5502	0.4307	0.3159	0.047
H13B	0.5709	0.4265	0.2201	0.047
H13C	0.6695	0.4171	0.2970	0.047
H14A	0.7254	0.2783	0.2473	0.064
H14B	0.6357	0.2925	0.1649	0.064
H14C	0.6365	0.2080	0.2184	0.064
H16A	0.4190	0.1764	0.0881	0.048
H16B	0.5184	0.2348	0.0767	0.048
H16C	0.4096	0.2384	0.0087	0.048
H17A	0.4061	0.3955	0.0338	0.043
H17B	0.5151	0.3846	0.1004	0.043
H17C	0.4136	0.4296	0.1286	0.043
H18A	0.2510	0.3090	0.0378	0.034
H18B	0.2459	0.3497	0.1283	0.034
H18C	0.2436	0.2503	0.1175	0.034
H23	0.6639	0.0201	0.4709	0.040
H24	0.7358	-0.0496	0.3644	0.049
H25	0.6549	-0.0324	0.2222	0.046
H26	0.5039	0.0531	0.1895	0.034
H33	0.5819	0.0823	0.5610	0.034
H34	0.5123	0.1747	0.6504	0.042
H35	0.3817	0.2719	0.5912	0.040
H36	0.3221	0.2724	0.4459	0.028
H51A	-0.3180	0.0395	-0.0409	0.080
H51B	-0.2821	-0.0353	0.0240	0.080
H51C	-0.3479	0.0153	-0.0393	0.068
H51D	-0.2452	-0.0204	0.0222	0.068
H51E	-0.1219	-0.0511	0.0189	0.242
H51F	-0.1354	0.0165	-0.0536	0.242

Table 4: Anisotropic displacement parameters ($Å^2$) for **13**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	0.0129(1)	0.0104(1)	0.0170(1)	0.0014(1)	0.0020(1)	0.0016(1)
Cl1	0.0166(2)	0.0125(2)	0.0190(2)	0.0024(2)	0.0008(2)	0.0003(2)
Cl2	0.0304(3)	0.0148(2)	0.0172(2)	-0.0009(2)	0.0058(2)	0.0020(2)
P1	0.0141(2)	0.0133(2)	0.0258(3)	0.0041(2)	0.0052(2)	0.0018(2)

C1	0.0158(9)	0.0137(9)	0.0113(8)	0.0005(7)	0.0002(7)	0.0001(7)
N2	0.0146(8)	0.0126(8)	0.0168(8)	0.0000(6)	0.0016(6)	0.0007(6)
C3	0.0199(10)	0.0133(9)	0.0193(10)	-0.0017(7)	0.0010(8)	0.0037(8)
C4	0.0194(10)	0.0166(10)	0.0211(10)	-0.0004(8)	0.0048(8)	0.0049(8)
N5	0.0152(8)	0.0125(8)	0.0160(8)	0.0011(6)	0.0019(6)	0.0015(6)
C6	0.0163(10)	0.0159(10)	0.0230(10)	0.0025(8)	0.0052(8)	-0.0002(8)
C7	0.0298(12)	0.0229(11)	0.0253(11)	0.0063(9)	0.0126(10)	0.0055(9)
C8	0.0157(10)	0.0245(12)	0.0439(15)	0.0029(10)	0.0076(10)	0.0005(9)
C9	0.0207(10)	0.0170(10)	0.0250(11)	-0.0011(8)	0.0000(9)	-0.0022(8)
C10	0.0165(10)	0.0122(9)	0.0235(10)	0.0016(8)	0.0023(8)	-0.0015(7)
C11	0.0151(10)	0.0195(11)	0.0504(16)	0.0103(11)	0.0038(10)	0.0001(8)
C12	0.0211(12)	0.0248(12)	0.0582(18)	0.0146(12)	-0.0120(12)	-0.0072(10)
C13	0.0191(11)	0.0212(12)	0.0538(17)	0.0100(11)	0.0037(11)	-0.0038(9)
C14	0.0201(12)	0.0277(13)	0.083(2)	0.0087(14)	0.0180(14)	0.0049(10)
C15	0.0282(12)	0.0182(10)	0.0260(11)	0.0048(9)	0.0129(9)	0.0042(9)
C16	0.0432(15)	0.0237(12)	0.0343(13)	0.0047(10)	0.0240(12)	0.0057(11)
C17	0.0346(13)	0.0213(11)	0.0345(13)	0.0092(10)	0.0172(11)	0.0033(10)
C18	0.0296(12)	0.0192(10)	0.0189(10)	0.0035(8)	0.0044(9)	0.0041(9)
N21	0.0160(9)	0.0135(8)	0.0329(10)	0.0038(7)	0.0066(8)	0.0018(7)
C22	0.0153(10)	0.0151(10)	0.0382(13)	0.0078(9)	0.0005(9)	-0.0004(8)
C23	0.0174(11)	0.0241(12)	0.0558(17)	0.0136(12)	-0.0003(11)	0.0036(9)
C24	0.0212(12)	0.0286(14)	0.073(2)	0.0131(14)	0.0104(13)	0.0129(10)
C25	0.0289(13)	0.0273(13)	0.064(2)	0.0052(13)	0.0214(13)	0.0109(11)
C26	0.0246(12)	0.0198(11)	0.0441(15)	0.0024(10)	0.0146(11)	0.0041(9)
N31	0.0160(8)	0.0139(8)	0.0228(9)	0.0029(7)	-0.0031(7)	-0.0004(7)
C32	0.0160(10)	0.0133(9)	0.0322(12)	0.0042(9)	-0.0045(9)	-0.0019(8)
C33	0.0252(12)	0.0199(11)	0.0336(13)	0.0072(9)	-0.0124(10)	-0.0031(9)
C34	0.0427(15)	0.0309(13)	0.0230(12)	0.0026(10)	-0.0158(11)	-0.0008(11)
C35	0.0445(16)	0.0275(13)	0.0238(12)	-0.0034(10)	-0.0066(11)	0.0055(11)
C36	0.0286(12)	0.0175(10)	0.0214(11)	0.0006(8)	-0.0051(9)	0.0037(9)
C51	0.099(8)	0.056(8)	0.042(7)	-0.008(5)	0.005(6)	-0.017(8)
Cl3	0.091(2)	0.105(3)	0.076(2)	-0.054(2)	0.0331(18)	-0.019(2)
Cl4	0.085(3)	0.0402(18)	0.048(2)	-0.0127(15)	0.026(2)	-0.0227(19)
C51B	0.13(2)	0.021(9)	0.037(14)	-0.012(8)	0.055(14)	0.016(9)
Cl3B	0.087(5)	0.052(4)	0.036(3)	-0.011(2)	0.015(3)	-0.028(3)
Cl4B	0.071(6)	0.045(4)	0.044(6)	-0.016(4)	0.021(4)	-0.005(4)
C51C	0.152(9)	0.35(3)	0.084(9)	0.161(13)	-0.030(7)	-0.056(11)
Cl3C	0.239(5)	0.110(3)	0.0594(19)	0.0056(17)	-0.026(2)	-0.099(3)
Cl4C	0.184(5)	0.102(3)	0.162(5)	0.068(4)	-0.073(4)	-0.043(3)

Table 5: Bond lengths (Å) and angles (deg) for **13**.

Ru1-N31	2.0372(19)	C6-C7	1.527(3)
Ru1-N21	2.0924(18)	C6-C8	1.540(3)
Ru1-C1	2.094(2)	C11-C12	1.533(4)
Ru1-P1	2.2962(6)	C11-C14	1.536(4)
Ru1-Cl2	2.4292(6)	C11-C13	1.544(3)
Ru1-Cl1	2.5217(5)	C15-C18	1.539(3)
P1-C10	1.841(2)	C15-C16	1.539(3)
P1-C15	1.899(2)	C15-C17	1.541(3)
P1-C11	1.907(2)	N21-C26	1.343(3)
C1-N2	1.380(3)	N21-C22	1.358(3)
C1-N5	1.383(3)	C22-C23	1.397(3)
N2-C3	1.374(3)	C22-C32	1.464(3)
N2-C10	1.452(3)	C23-C24	1.385(4)
C3-C4	1.340(3)	C24-C25	1.385(5)
C4-N5	1.396(3)	C25-C26	1.390(3)
N5-C6	1.499(3)	N31-C36	1.345(3)
C6-C9	1.523(3)	N31-C32	1.369(3)

C32-C33	1.393(3)
C33-C34	1.373(4)
C34-C35	1.381(4)
C35-C36	1.385(3)
C51-Cl3	1.736(11)
C51-Cl4	1.746(10)
Cl3-Cl3#1	1.162(7)
C51B-Cl3B	1.714(14)
C51B-Cl4B	1.715(13)
C51C-Cl3C	1.602(12)
C51C-Cl4C	1.671(13)
N31-Ru1-N21	79.10(8)
N31-Ru1-C1	91.59(7)
N21-Ru1-C1	170.34(8)
N31-Ru1-P1	96.85(5)
N21-Ru1-P1	97.03(5)
C1-Ru1-P1	81.40(6)
N31-Ru1-Cl2	164.54(5)
N21-Ru1-Cl2	92.15(6)
C1-Ru1-Cl2	97.50(6)
P1-Ru1-Cl2	96.85(2)
N31-Ru1-Cl1	81.27(5)
N21-Ru1-Cl1	79.25(5)
C1-Ru1-Cl1	102.06(6)
P1-Ru1-Cl1	176.072(19)
Cl2-Ru1-Cl1	84.604(18)
C10-P1-C15	102.83(10)
C10-P1-C11	100.18(11)
C15-P1-C11	108.00(11)
C10-P1-Ru1	100.81(7)
C15-P1-Ru1	118.94(8)
C11-P1-Ru1	121.85(8)
N2-C1-N5	101.89(16)
N2-C1-Ru1	116.54(14)
N5-C1-Ru1	140.94(15)
C3-N2-C1	113.43(17)
C3-N2-C10	122.55(17)
C1-N2-C10	123.96(17)
C4-C3-N2	105.83(18)
C3-C4-N5	107.96(19)
C1-N5-C4	110.87(17)
C1-N5-C6	128.26(17)
C4-N5-C6	120.77(17)
N5-C6-C9	109.17(17)
N5-C6-C7	108.14(18)
C9-C6-C7	114.15(18)
N5-C6-C8	109.49(17)
C9-C6-C8	107.32(19)
C7-C6-C8	108.50(19)
N2-C10-P1	106.96(14)
C12-C11-C14	108.1(2)
C12-C11-C13	106.1(2)
C14-C11-C13	109.0(2)
C12-C11-P1	109.90(17)
C14-C11-P1	110.4(2)
C13-C11-P1	113.13(16)
C18-C15-C16	109.5(2)
C18-C15-C17	106.38(19)
C16-C15-C17	108.38(19)
C18-C15-P1	106.13(15)
C16-C15-P1	110.97(16)
C17-C15-P1	115.27(18)
C26-N21-C22	118.9(2)
C26-N21-Ru1	127.41(17)
C22-N21-Ru1	113.58(15)
N21-C22-C23	121.7(2)
N21-C22-C32	115.20(19)
C23-C22-C32	123.0(2)
C24-C23-C22	118.7(3)
C25-C24-C23	119.5(2)
C24-C25-C26	119.0(3)
N21-C26-C25	122.1(3)
C36-N31-C32	117.5(2)
C36-N31-Ru1	127.08(15)
C32-N31-Ru1	114.42(15)
N31-C32-C33	121.5(2)
N31-C32-C22	115.3(2)
C33-C32-C22	123.1(2)
C34-C33-C32	119.8(2)
C33-C34-C35	118.9(2)
C34-C35-C36	119.1(3)
N31-C36-C35	123.0(2)
Cl3-C51-Cl4	113.3(7)
Cl3#1-Cl3-C51	141.0(8)
Cl3B-C51B-Cl4B	117.5(11)
Cl3C-C51C-Cl4C	135.2(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x-1,-y,-z

Crystal data for 16a:

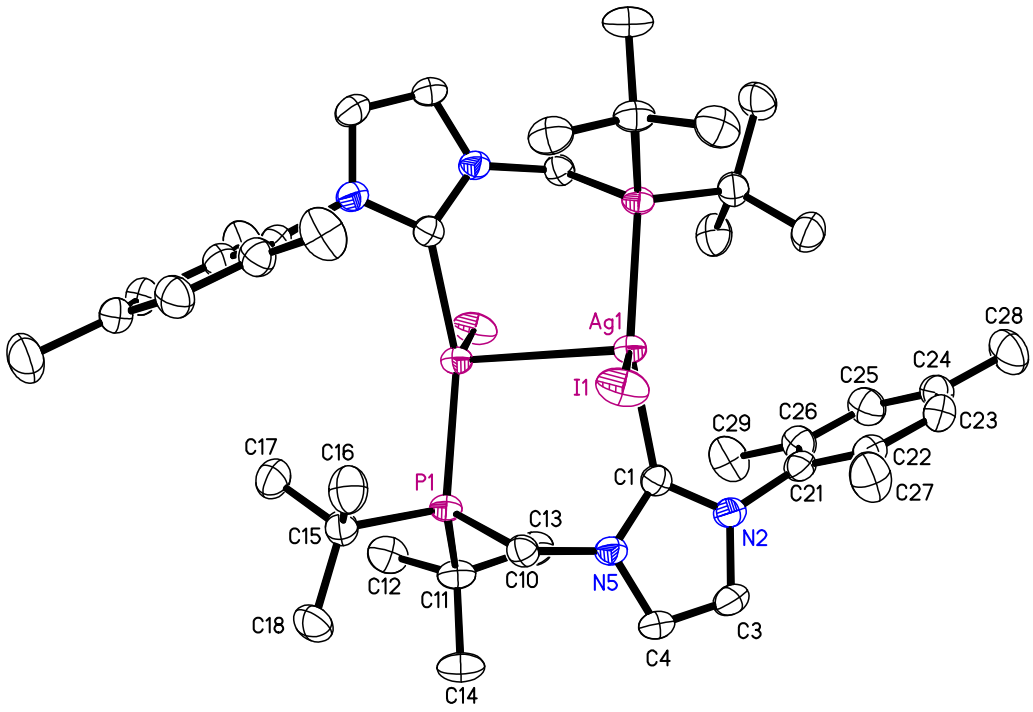


Table 1: Crystal data and structure refinement for **16a**.

Identification code	ek29
Empirical formula	$C_{46}H_{76}Ag_2I_2N_4OP_2$
Formula weight	1232.59
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	$P\bar{1}$
Z	1
Unit cell dimensions	a = 9.7387(9) Å α = 65.277(2) deg. b = 11.1342(10) Å β = 77.942(2) deg. c = 13.2867(16) Å γ = 85.113(2) deg.
Volume	1279.8(2) $Å^3$
Density (calculated)	1.60 g/cm^3
Absorption coefficient	2.07 mm^{-1}
Crystal shape	polyhedron
Crystal size	0.17 x 0.14 x 0.14 mm^3
Crystal colour	colourless
Theta range for data collection	1.7 to 28.3 deg.
Index ranges	$-12 \le h \le 12$, $-14 \le k \le 14$, $-17 \le l \le 17$
Reflections collected	13678
Independent reflections	6314 (R(int) = 0.0521)
Observed reflections	5470 ($I > 2\sigma(I)$)
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.76 and 0.72
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	6314 / 34 / 283
Goodness-of-fit on F^2	1.03
Final R indices ($I > 2\sigma(I)$)	R1 = 0.027, wR2 = 0.072

Largest diff. peak and hole	1.20 and -1.00 eÅ^{-3}

Table 2: Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **16a**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ag1	0.9788(1)	0.9691(1)	0.4007(1)	0.0262(1)
I1	0.7486(1)	0.7757(1)	0.4696(1)	0.0395(1)
P1	0.7872(1)	1.1244(1)	0.6109(1)	0.0231(1)
C1	0.8388(2)	1.1358(2)	0.3465(2)	0.0245(4)
N2	0.8317(2)	1.2214(2)	0.2390(2)	0.0287(4)
C3	0.7077(3)	1.2927(3)	0.2342(2)	0.0378(6)
C4	0.6354(2)	1.2523(2)	0.3402(2)	0.0334(5)
N5	0.7174(2)	1.1576(2)	0.4074(2)	0.0252(4)
C10	0.6747(2)	1.0897(2)	0.5296(2)	0.0256(4)
C11	0.7787(2)	1.3082(2)	0.5685(2)	0.0305(5)
C12	0.8437(3)	1.3388(3)	0.6508(2)	0.0401(6)
C13	0.8729(3)	1.3727(2)	0.4510(2)	0.0369(6)
C14	0.6321(3)	1.3697(2)	0.5614(3)	0.0409(6)
C15	0.6865(2)	1.0304(2)	0.7582(2)	0.0299(5)
C16	0.6602(3)	0.8912(3)	0.7692(2)	0.0418(6)
C17	0.7787(3)	1.0171(3)	0.8424(2)	0.0406(6)
C18	0.5459(3)	1.0915(3)	0.7895(2)	0.0403(6)
C21	0.9329(2)	1.2367(2)	0.1384(2)	0.0293(5)
C22	0.9093(3)	1.1711(3)	0.0749(2)	0.0333(5)
C23	1.0009(3)	1.1948(3)	-0.0271(2)	0.0360(5)
C24	1.1129(3)	1.2810(3)	-0.0648(2)	0.0366(6)
C25	1.1340(3)	1.3423(3)	0.0025(2)	0.0401(6)
C26	1.0447(3)	1.3233(2)	0.1044(2)	0.0343(5)
C27	0.7889(3)	1.0753(3)	0.1159(2)	0.0475(7)
C28	1.2120(4)	1.3051(3)	-0.1758(2)	0.0543(8)
C29	1.0690(3)	1.3941(3)	0.1739(3)	0.0497(7)
O30	0.4423(8)	1.5254(6)	-0.0203(5)	0.0920(19)
C31	0.5518(9)	1.4811(13)	-0.0741(8)	0.109(5)
C32	0.5691(10)	1.4685(11)	-0.1651(9)	0.092(3)
C33	0.423(2)	1.5826(13)	0.0454(10)	0.126(5)
C34	0.403(2)	1.6395(16)	0.0920(14)	0.167(7)

Table 3: Hydrogen coordinates and isotropic displacement parameters (Å^2) for **16a**.

Atom	x	y	z	U_{eq}
H3	0.6795	1.3578	0.1684	0.045
H4	0.5458	1.2826	0.3644	0.040
H10A	0.6751	0.9932	0.5505	0.031
H10B	0.5771	1.1154	0.5518	0.031
H12A	0.9370	1.2985	0.6549	0.048
H12B	0.7836	1.3027	0.7259	0.048
H12C	0.8521	1.4348	0.6242	0.048
H13A	0.8340	1.3551	0.3962	0.044
H13B	0.9677	1.3356	0.4539	0.044
H13C	0.8771	1.4683	0.4282	0.044

H14A	0.5922	1.3500	0.5080	0.049
H14B	0.6391	1.4657	0.5354	0.049
H14C	0.5713	1.3326	0.6361	0.049
H16A	0.7498	0.8515	0.7497	0.050
H16B	0.5984	0.8967	0.7180	0.050
H16C	0.6157	0.8365	0.8471	0.050
H17A	0.8691	0.9780	0.8235	0.049
H17B	0.7317	0.9601	0.9189	0.049
H17C	0.7945	1.1047	0.8388	0.049
H18A	0.5621	1.1806	0.7826	0.048
H18B	0.5020	1.0364	0.8674	0.048
H18C	0.4839	1.0967	0.7385	0.048
H23	0.9862	1.1508	-0.0717	0.043
H25	1.2125	1.3995	-0.0219	0.048
H27A	0.7948	1.0079	0.1915	0.071
H27B	0.7937	1.0326	0.0640	0.071
H27C	0.6999	1.1230	0.1191	0.071
H28A	1.2917	1.2443	-0.1620	0.081
H28B	1.2463	1.3965	-0.2107	0.081
H28C	1.1622	1.2902	-0.2264	0.081
H29A	1.1043	1.3314	0.2406	0.075
H29B	0.9804	1.4322	0.1978	0.075
H29C	1.1381	1.4649	0.1286	0.075
H31A	0.6315	1.5369	-0.0836	0.130
H31B	0.5703	1.3920	-0.0179	0.130
H32A	0.6621	1.4310	-0.1793	0.137
H32B	0.5619	1.5552	-0.2268	0.137
H32C	0.4968	1.4093	-0.1605	0.137
H33A	0.3692	1.5067	0.1074	0.151
H33B	0.5201	1.5638	0.0596	0.151
H34A	0.4657	1.6129	0.1464	0.251
H34B	0.3050	1.6263	0.1326	0.251
H34C	0.4181	1.7331	0.0411	0.251

Table 4: Anisotropic displacement parameters ($Å^2$) for **16a**. The anisotropic displacement factor exponent takes the form: $-2\,pi^2\,(h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag1	0.0220(1)	0.0285(1)	0.0286(1)	-0.0124(1)	-0.0063(1)	0.0045(1)
I1	0.0251(1)	0.0350(1)	0.0615(1)	-0.0248(1)	-0.0026(1)	-0.0042(1)
P1	0.0189(2)	0.0232(3)	0.0277(3)	-0.0109(2)	-0.0046(2)	0.0007(2)
C1	0.0234(10)	0.0252(10)	0.0259(10)	-0.0111(9)	-0.0052(8)	-0.0009(8)
N2	0.0250(9)	0.0305(10)	0.0262(9)	-0.0081(8)	-0.0052(7)	0.0043(8)
C3	0.0326(13)	0.0430(14)	0.0315(12)	-0.0088(11)	-0.0115(10)	0.0110(11)
C4	0.0256(11)	0.0396(13)	0.0339(12)	-0.0141(11)	-0.0099(9)	0.0107(10)
N5	0.0196(8)	0.0281(9)	0.0272(9)	-0.0108(8)	-0.0052(7)	0.0017(7)
C10	0.0215(10)	0.0294(11)	0.0268(10)	-0.0128(9)	-0.0029(8)	-0.0021(8)
C11	0.0245(11)	0.0261(11)	0.0427(13)	-0.0151(10)	-0.0089(10)	0.0016(9)
C12	0.0399(14)	0.0361(13)	0.0519(16)	-0.0251(12)	-0.0081(12)	-0.0035(11)
C13	0.0348(13)	0.0261(12)	0.0435(14)	-0.0078(11)	-0.0068(11)	-0.0025(10)
C14	0.0314(13)	0.0288(12)	0.0631(17)	-0.0192(12)	-0.0123(12)	0.0074(10)
C15	0.0281(11)	0.0345(12)	0.0276(11)	-0.0133(10)	-0.0047(9)	-0.0016(9)
C16	0.0512(16)	0.0340(13)	0.0333(13)	-0.0077(11)	-0.0029(11)	-0.0096(11)
C17	0.0405(14)	0.0493(16)	0.0329(13)	-0.0156(12)	-0.0123(11)	0.0016(12)
C18	0.0262(12)	0.0542(16)	0.0405(14)	-0.0224(13)	0.0007(10)	-0.0009(11)
C21	0.0269(11)	0.0310(11)	0.0245(11)	-0.0066(9)	-0.0052(9)	0.0041(9)

C22	0.0289(12)	0.0389(13)	0.0315(12)	-0.0129(10)	-0.0087(9)	0.0031(10)
C23	0.0385(13)	0.0408(14)	0.0288(12)	-0.0138(11)	-0.0092(10)	0.0033(11)
C24	0.0385(13)	0.0365(13)	0.0277(12)	-0.0090(10)	-0.0032(10)	0.0072(11)
C25	0.0388(14)	0.0368(13)	0.0363(13)	-0.0105(11)	0.0026(11)	-0.0051(11)
C26	0.0358(13)	0.0315(12)	0.0326(12)	-0.0114(10)	-0.0031(10)	-0.0019(10)
C27	0.0411(15)	0.0606(18)	0.0469(16)	-0.0284(14)	-0.0019(12)	-0.0150(13)
C28	0.062(2)	0.0552(18)	0.0346(15)	-0.0152(13)	0.0083(13)	-0.0014(15)
C29	0.0476(16)	0.0540(18)	0.0514(17)	-0.0281(15)	0.0022(13)	-0.0148(14)
O30	0.143(6)	0.079(4)	0.079(4)	-0.045(3)	-0.063(4)	0.042(4)
C31	0.030(4)	0.178(13)	0.062(5)	0.002(6)	-0.010(4)	0.017(5)
C32	0.069(5)	0.116(8)	0.136(8)	-0.092(8)	-0.043(6)	0.042(6)
C33	0.181(14)	0.101(10)	0.085(8)	-0.025(6)	-0.011(8)	-0.053(9)
C34	0.218(18)	0.164(15)	0.150(14)	-0.114(11)	0.029(12)	-0.048(13)

Table 5: Bond lengths (Å) and angles (deg) for **16a**.

Ag1-C1	2.164(2)	C21-C22	1.388(4)
Ag1-P1#1	2.4255(6)	C21-C26	1.388(3)
Ag1-I1	2.9697(3)	C22-C23	1.392(3)
Ag1-Ag1#1	3.1028(4)	C22-C27	1.506(4)
P1-C10	1.853(2)	C23-C24	1.382(4)
P1-C11	1.881(2)	C23-H23	0.9500
P1-C15	1.883(2)	C24-C25	1.385(4)
P1-Ag1#1	2.4255(6)	C24-C28	1.515(4)
C1-N5	1.352(3)	C25-C26	1.390(3)
C1-N2	1.359(3)	C25-H25	0.9500
N2-C3	1.385(3)	C26-C29	1.505(4)
N2-C21	1.440(3)	C27-H27A	0.9800
C3-C4	1.338(3)	C27-H27B	0.9800
C3-H3	0.9500	C27-H27C	0.9800
C4-N5	1.383(3)	C28-H28A	0.9800
C4-H4	0.9500	C28-H28B	0.9800
N5-C10	1.457(3)	C28-H28C	0.9800
C10-H10A	0.9900	C29-H29A	0.9800
C10-H10B	0.9900	C29-H29B	0.9800
C11-C12	1.533(3)	C29-H29C	0.9800
C11-C14	1.534(3)	O30-C33	1.256(12)
C11-C13	1.539(3)	O30-C31	1.334(10)
C12-H12A	0.9800	C31-C32	1.250(11)
C12-H12B	0.9800	C31-H31A	0.9900
C12-H12C	0.9800	C31-H31B	0.9900
C13-H13A	0.9800	C32-H32A	0.9800
C13-H13B	0.9800	C32-H32B	0.9800
C13-H13C	0.9800	C32-H32C	0.9800
C14-H14A	0.9800	C33-C34	1.040(12)
C14-H14B	0.9800	C33-H33A	0.9900
C14-H14C	0.9800	C33-H33B	0.9900
C15-C17	1.530(3)	C34-H34A	0.9800
C15-C16	1.533(4)	C34-H34B	0.9800
C15-C18	1.533(3)	C34-H34C	0.9800
C16-H16A	0.9800	C1-Ag1-P1#1	150.15(6)
C16-H16B	0.9800	C1-Ag1-I1	92.38(6)
C16-H16C	0.9800	P1#1-Ag1-I1	114.410(16)
C17-H17A	0.9800	C1-Ag1-Ag1#1	91.50(6)
C17-H17B	0.9800	P1#1-Ag1-Ag1#1	90.271(15)
C17-H17C	0.9800	I1-Ag1-Ag1#1	112.114(10)
C18-H18A	0.9800	C10-P1-C11	106.08(10)
C18-H18B	0.9800	C10-P1-C15	99.48(10)
C18-H18C	0.9800	C11-P1-C15	111.95(11)

C10-P1-Ag1#1	114.84(7)	H17A-C17-H17B	109.5
C11-P1-Ag1#1	115.73(7)	C15-C17-H17C	109.5
C15-P1-Ag1#1	107.65(8)	H17A-C17-H17C	109.5
N5-C1-N2	103.27(18)	H17B-C17-H17C	109.5
N5-C1-Ag1	127.16(15)	C15-C18-H18A	109.5
N2-C1-Ag1	127.57(15)	C15-C18-H18B	109.5
C1-N2-C3	111.50(19)	H18A-C18-H18B	109.5
C1-N2-C21	126.82(18)	C15-C18-H18C	109.5
C3-N2-C21	121.62(19)	H18A-C18-H18C	109.5
C4-C3-N2	106.8(2)	H18B-C18-H18C	109.5
C4-C3-H3	126.6	C22-C21-C26	122.4(2)
N2-C3-H3	126.6	C22-C21-N2	118.4(2)
C3-C4-N5	106.2(2)	C26-C21-N2	119.1(2)
C3-C4-H4	126.9	C21-C22-C23	118.2(2)
N5-C4-H4	126.9	C21-C22-C27	120.9(2)
C1-N5-C4	112.17(18)	C23-C22-C27	120.9(2)
C1-N5-C10	124.88(18)	C24-C23-C22	121.4(2)
C4-N5-C10	122.95(18)	C24-C23-H23	119.3
N5-C10-P1	114.49(14)	C22-C23-H23	119.3
N5-C10-H10A	108.6	C23-C24-C25	118.4(2)
P1-C10-H10A	108.6	C23-C24-C28	120.7(3)
N5-C10-H10B	108.6	C25-C24-C28	120.9(3)
P1-C10-H10B	108.6	C24-C25-C26	122.5(3)
H10A-C10-H10B	107.6	C24-C25-H25	118.7
C12-C11-C14	110.3(2)	C26-C25-H25	118.7
C12-C11-C13	107.4(2)	C21-C26-C25	117.1(2)
C14-C11-C13	108.1(2)	C21-C26-C29	121.9(2)
C12-C11-P1	108.16(16)	C25-C26-C29	121.0(2)
C14-C11-P1	115.60(16)	C22-C27-H27A	109.5
C13-C11-P1	106.91(16)	C22-C27-H27B	109.5
C11-C12-H12A	109.5	H27A-C27-H27B	109.5
C11-C12-H12B	109.5	C22-C27-H27C	109.5
H12A-C12-H12B	109.5	H27A-C27-H27C	109.5
C11-C12-H12C	109.5	H27B-C27-H27C	109.5
H12A-C12-H12C	109.5	C24-C28-H28A	109.5
H12B-C12-H12C	109.5	C24-C28-H28B	109.5
C11-C13-H13A	109.5	H28A-C28-H28B	109.5
C11-C13-H13B	109.5	C24-C28-H28C	109.5
H13A-C13-H13B	109.5	H28A-C28-H28C	109.5
C11-C13-H13C	109.5	H28B-C28-H28C	109.5
H13A-C13-H13C	109.5	C26-C29-H29A	109.5
H13B-C13-H13C	109.5	C26-C29-H29B	109.5
C11-C14-H14A	109.5	H29A-C29-H29B	109.5
C11-C14-H14B	109.5	C26-C29-H29C	109.5
H14A-C14-H14B	109.5	H29A-C29-H29C	109.5
C11-C14-H14C	109.5	H29B-C29-H29C	109.5
H14A-C14-H14C	109.5	C33-O30-C31	136.8(13)
H14B-C14-H14C	109.5	C32-C31-O30	130.8(8)
C17-C15-C16	107.8(2)	C32-C31-H31A	104.6
C17-C15-C18	108.5(2)	O30-C31-H31A	104.6
C16-C15-C18	109.1(2)	C32-C31-H31B	104.6
C17-C15-P1	108.68(17)	O30-C31-H31B	104.6
C16-C15-P1	107.03(16)	H31A-C31-H31B	105.7
C18-C15-P1	115.44(17)	C31-C32-H32A	109.5
C15-C16-H16A	109.5	C31-C32-H32B	109.5
C15-C16-H16B	109.5	H32A-C32-H32B	109.5
H16A-C16-H16B	109.5	C31-C32-H32C	109.5
C15-C16-H16C	109.5	H32A-C32-H32C	109.5
H16A-C16-H16C	109.5	H32B-C32-H32C	109.5
H16B-C16-H16C	109.5	C34-C33-O30	173(2)
C15-C17-H17A	109.5	C34-C33-H33A	92.2
C15-C17-H17B	109.5	O30-C33-H33A	92.2

C34-C33-H33B	92.2
O30-C33-H33B	92.2
H33A-C33-H33B	103.0
C33-C34-H34A	109.5
C33-C34-H34B	109.5
H34A-C34-H34B	109.5
C33-C34-H34C	109.5
H34A-C34-H34C	109.5
H34B-C34-H34C	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1

Crystal data for 16b:

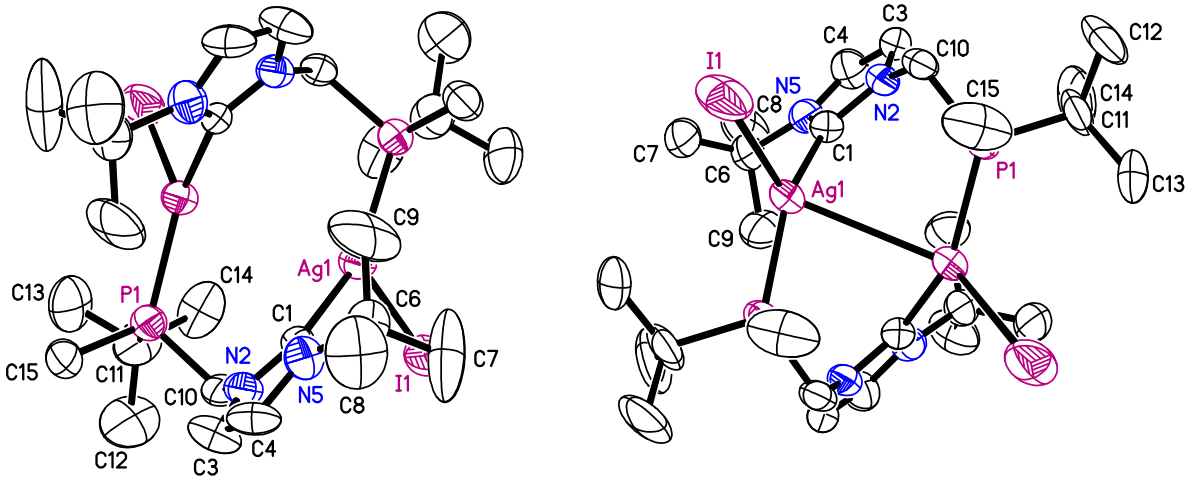


Table 1: Crystal data and structure refinement for **16b**.

Identification code	mbi10	
Empirical formula	$C_{38}H_{74}Ag_2I_2N_4O_3P_2$	
Formula weight	1166.49	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	C222	
Z	8	
Unit cell dimensions	a = 18.139(4) Å	α = 90 deg.
	b = 21.706(4) Å	β = 90 deg.
	c = 24.619(5) Å	γ = 90 deg.
Volume	9693(4) $Å^3$	
Density (calculated)	1.60 g/cm^3	
Absorption coefficient	2.18 mm^{-1}	
Crystal shape	polyhedron	
Crystal size	0.18 x 0.09 x 0.04 mm^3	
Crystal colour	colourless	
Theta range for data collection	0.8 to 25.8 deg.	
Index ranges	$-22 \le h \le 22$, $-26 \le k \le 26$, $-29 \le l \le 30$	
Reflections collected	42272	
Independent reflections	9282 (R(int) = 0.0577)	
Observed reflections	6847 ($I > 2\sigma(I)$)	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.92 and 0.69	
Refinement method	Full-matrix least-squares on F^2	
Data/restraints/parameters	9282 / 337 / 458	
Goodness-of-fit on F^2	1.08	
Final R indices ($I > 2\sigma(I)$)	R1 = 0.058, wR2 = 0.132	
Absolute structure parameter	0.11(5)	
Largest diff. peak and hole	0.74 and -0.76 $eÅ^{-3}$	

Table 2: Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **16b**. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
Ag11	0.0321(1)	0.0742(1)	0.2644(1)	0.0465(2)
I11	0.1302(1)	0.1222(1)	0.1837(1)	0.0770(3)
P11	0.0936(2)	-0.1038(1)	0.2472(1)	0.0482(7)
C11	0.1084(6)	0.0328(4)	0.3222(5)	0.041(2)
N21	0.1548(5)	-0.0130(4)	0.3117(4)	0.045(2)
C31	0.1951(7)	-0.0285(7)	0.3544(5)	0.068(4)
C41	0.1761(6)	0.0096(7)	0.3956(5)	0.061(3)
N51	0.1206(6)	0.0458(4)	0.3762(4)	0.050(2)
C61	0.0874(6)	0.0997(5)	0.4052(4)	0.057(3)
C71	0.1181(11)	0.1583(5)	0.3794(6)	0.130(7)
C81	0.1100(10)	0.0980(7)	0.4645(4)	0.100(6)
C91	0.0056(7)	0.0965(7)	0.4025(7)	0.119(6)
C101	0.1604(6)	-0.0409(5)	0.2589(4)	0.047(2)
C111	0.1183(6)	-0.1286(5)	0.1758(5)	0.075(3)
C121	0.2012(6)	-0.1378(7)	0.1656(6)	0.111(5)
C131	0.0774(7)	-0.1893(5)	0.1679(6)	0.091(4)
C141	0.0848(8)	-0.0802(5)	0.1382(5)	0.086(4)
C151	0.1269(6)	-0.1641(5)	0.2923(5)	0.069(3)
Ag12	-0.0336(1)	0.4320(1)	0.2385(1)	0.0476(2)
I12	-0.1277(1)	0.3771(1)	0.3204(1)	0.0983(4)
P12	-0.0867(2)	0.5902(1)	0.2702(1)	0.0512(7)
C12	-0.1071(6)	0.4693(5)	0.1788(4)	0.042(2)
N22	-0.1544(5)	0.5163(4)	0.1916(4)	0.047(2)
C32	-0.1958(6)	0.5318(5)	0.1450(5)	0.047(2)
C42	-0.1726(7)	0.4952(6)	0.1053(5)	0.057(3)
N52	-0.1208(5)	0.4549(4)	0.1267(4)	0.046(2)
C62	-0.0836(6)	0.4045(5)	0.0967(4)	0.055(3)
C72	-0.0980(7)	0.3459(5)	0.1274(5)	0.074(3)
C82	-0.1126(8)	0.4040(7)	0.0396(4)	0.086(4)
C92	-0.0008(6)	0.4167(6)	0.0955(5)	0.069(3)
C102	-0.1662(6)	0.5427(5)	0.2448(4)	0.048(3)
C112	-0.1166(6)	0.6701(5)	0.2617(5)	0.094(4)
C122	-0.1854(7)	0.6866(7)	0.2942(8)	0.158(7)
C132	-0.0525(7)	0.7124(5)	0.2800(7)	0.102(5)
C142	-0.1342(9)	0.6800(6)	0.2020(6)	0.136(6)
C152	-0.0987(8)	0.5766(8)	0.3429(5)	0.097(5)
C21	0.121(3)	0.231(2)	0.035(2)	0.40(3)
C22	-0.011(3)	0.1956(19)	0.028(2)	0.36(3)
C23	0.0000	0.2709(18)	0.0000	0.163(12)
C31	-0.0444(17)	0.3173(18)	0.4706(15)	0.221(13)
C32	-0.109(3)	0.293(2)	0.5159(19)	0.44(4)
C33	0.0343(14)	0.2568(14)	0.5321(16)	0.243(19)
C41	-0.209(2)	0.2050(14)	0.4405(10)	0.246(18)
C42	-0.2500	0.2500	0.4033(10)	0.129(10)
C43	-0.2500	0.2500	0.4910(14)	0.23(2)
C51	0.246(3)	0.282(2)	0.0681(16)	0.30(3)
C52	0.254(3)	0.2213(19)	0.0018(14)	0.26(2)
C61	-0.4074(9)	0.5279(11)	0.0140(14)	0.163(13)
C62	-0.3240(9)	0.5579(9)	0.0172(9)	0.118(6)
C63	-0.2775(10)	0.5000	0.0000	0.062(5)
C71	0.3877(12)	-0.0338(14)	0.4842(12)	0.179(13)
C72	0.3205(12)	-0.0404(11)	0.4872(11)	0.143(9)
C73	0.2801(13)	0.0000	0.5000	0.065(5)

Table 3: Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **16b**.

Atom	x	y	z	U_{eq}
H31	0.2308	-0.0605	0.3559	0.082
H41	0.1972	0.0108	0.4309	0.073
H7A1	0.1721	0.1575	0.3810	0.194
H7B1	0.0998	0.1943	0.3993	0.194
H7C1	0.1022	0.1607	0.3415	0.194
H8A1	0.1638	0.1010	0.4672	0.150
H8B1	0.0934	0.0593	0.4809	0.150
H8C1	0.0874	0.1328	0.4837	0.150
H9A1	-0.0101	0.0954	0.3645	0.178
H9B1	-0.0155	0.1329	0.4203	0.178
H9C1	-0.0114	0.0592	0.4211	0.178
H10A1	0.2109	-0.0575	0.2543	0.056
H10B1	0.1529	-0.0088	0.2309	0.056
H12A1	0.2272	-0.0988	0.1715	0.167
H12B1	0.2089	-0.1515	0.1281	0.167
H12C1	0.2203	-0.1690	0.1907	0.167
H13A1	0.0245	-0.1829	0.1740	0.136
H13B1	0.0960	-0.2198	0.1939	0.136
H13C1	0.0853	-0.2043	0.1308	0.136
H14A1	0.0320	-0.0763	0.1458	0.129
H14B1	0.0919	-0.0927	0.1004	0.129
H14C1	0.1091	-0.0404	0.1444	0.129
H15A1	0.0952	-0.2004	0.2890	0.104
H15B1	0.1259	-0.1492	0.3299	0.104
H15C1	0.1775	-0.1751	0.2823	0.104
H32	-0.2331	0.5624	0.1425	0.056
H42	-0.1886	0.4964	0.0686	0.069
H7A2	-0.0752	0.3484	0.1634	0.111
H7B2	-0.0768	0.3110	0.1074	0.111
H7C2	-0.1512	0.3399	0.1313	0.111
H8A2	-0.1024	0.4439	0.0224	0.129
H8B2	-0.1659	0.3968	0.0401	0.129
H8C2	-0.0883	0.3712	0.0189	0.129
H9A2	0.0182	0.4179	0.1327	0.104
H9B2	0.0086	0.4563	0.0777	0.104
H9C2	0.0239	0.3838	0.0752	0.104
H10A2	-0.1756	0.5089	0.2710	0.058
H10B2	-0.2108	0.5689	0.2436	0.058
H12A2	-0.1753	0.6815	0.3331	0.237
H12B2	-0.2260	0.6595	0.2836	0.237
H12C2	-0.1990	0.7296	0.2870	0.237
H13A2	-0.0424	0.7055	0.3187	0.153
H13B2	-0.0662	0.7556	0.2742	0.153
H13C2	-0.0083	0.7028	0.2587	0.153
H14A2	-0.0905	0.6706	0.1801	0.203
H14B2	-0.1488	0.7229	0.1961	0.203
H14C2	-0.1747	0.6527	0.1913	0.203
H15A2	-0.0838	0.5344	0.3517	0.145
H15B2	-0.1507	0.5825	0.3526	0.145
H15C2	-0.0682	0.6057	0.3634	0.145

Table 4: Anisotropic displacement parameters ($Å^2$) for **16b**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ (h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12})$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

Ag11	0.0391(5)	0.0477(4)	0.0526(5)	-0.0047(4)	-0.0004(4)	0.0027(4)
I11	0.0588(6)	0.0641(5)	0.1082(8)	0.0152(5)	0.0316(6)	0.0079(4)
P11	0.0439(15)	0.0438(14)	0.0569(18)	-0.0052(12)	0.0029(12)	0.0016(11)
C11	0.031(6)	0.033(5)	0.058(5)	-0.010(4)	-0.002(4)	-0.002(4)
N21	0.035(5)	0.049(5)	0.051(5)	-0.005(4)	-0.002(4)	0.003(4)
C31	0.045(8)	0.090(9)	0.069(7)	0.002(7)	-0.009(6)	0.023(6)
C41	0.033(6)	0.090(9)	0.060(7)	-0.001(6)	-0.013(6)	0.001(5)
N51	0.057(6)	0.048(5)	0.046(5)	-0.001(4)	0.000(4)	0.003(4)
C61	0.071(7)	0.055(6)	0.044(6)	-0.005(5)	0.008(6)	-0.001(5)
C71	0.26(2)	0.040(6)	0.090(10)	-0.006(6)	0.070(13)	-0.004(9)
C81	0.149(16)	0.103(12)	0.048(6)	-0.022(6)	-0.010(8)	0.000(11)
C91	0.077(7)	0.137(13)	0.143(14)	-0.091(12)	-0.001(8)	0.041(8)
C101	0.033(5)	0.049(5)	0.058(6)	-0.009(5)	0.018(5)	0.001(4)
C111	0.074(7)	0.080(8)	0.072(6)	-0.027(5)	0.017(6)	-0.009(6)
C121	0.094(8)	0.113(12)	0.126(12)	-0.063(10)	0.050(8)	0.006(7)
C131	0.120(10)	0.058(6)	0.094(10)	-0.027(6)	-0.008(9)	-0.005(7)
C141	0.124(11)	0.088(8)	0.045(6)	-0.001(6)	-0.001(7)	-0.028(7)
C151	0.051(6)	0.049(6)	0.108(8)	0.018(6)	0.019(7)	0.008(5)
Ag12	0.0389(5)	0.0431(4)	0.0606(6)	-0.0002(4)	0.0024(4)	0.0086(3)
I12	0.0720(7)	0.1021(8)	0.1207(9)	0.0505(7)	0.0489(7)	0.0286(6)
P12	0.0382(14)	0.0452(14)	0.0701(19)	-0.0175(14)	-0.0034(14)	0.0098(11)
C12	0.037(6)	0.041(5)	0.049(5)	0.000(4)	0.003(4)	0.000(4)
N22	0.035(5)	0.042(5)	0.064(5)	-0.010(4)	0.000(4)	0.005(4)
C32	0.041(6)	0.038(5)	0.062(6)	0.000(5)	0.004(5)	-0.001(4)
C42	0.062(8)	0.056(7)	0.054(6)	-0.003(5)	-0.008(6)	0.006(5)
N52	0.045(5)	0.047(5)	0.048(5)	-0.009(4)	0.006(4)	-0.003(4)
C62	0.053(6)	0.045(6)	0.065(6)	-0.012(5)	0.009(6)	0.003(5)
C72	0.062(7)	0.050(6)	0.110(9)	-0.014(6)	0.025(7)	-0.002(5)
C82	0.087(10)	0.100(11)	0.072(7)	-0.035(6)	0.002(7)	0.028(9)
C92	0.058(6)	0.078(8)	0.071(8)	-0.010(7)	0.020(6)	-0.005(6)
C102	0.032(6)	0.048(5)	0.064(6)	-0.011(5)	-0.002(5)	0.009(4)
C112	0.068(7)	0.046(5)	0.170(10)	-0.046(7)	-0.042(7)	0.031(5)
C122	0.072(8)	0.094(11)	0.31(2)	-0.096(14)	-0.015(11)	0.046(7)
C132	0.095(8)	0.039(5)	0.172(14)	-0.037(8)	-0.010(9)	0.002(6)
C142	0.145(15)	0.046(7)	0.216(12)	0.008(9)	-0.092(11)	0.034(9)
C152	0.070(8)	0.162(13)	0.058(6)	-0.033(7)	-0.007(6)	0.022(9)
C21	0.48(7)	0.34(5)	0.39(5)	0.26(4)	0.09(5)	-0.04(5)
C22	0.23(4)	0.31(3)	0.53(8)	0.19(4)	0.15(5)	0.07(4)
C23	0.057(14)	0.20(2)	0.24(3)	0.000	0.04(2)	0.000
C31	0.16(2)	0.25(3)	0.25(3)	0.00(3)	-0.05(2)	0.03(3)
C32	0.56(7)	0.43(6)	0.34(5)	0.29(4)	0.19(5)	0.24(5)
C33	0.108(18)	0.22(3)	0.40(4)	0.21(3)	0.00(2)	-0.019(18)
C41	0.42(5)	0.17(3)	0.15(2)	-0.014(17)	-0.10(2)	0.11(3)
C42	0.21(3)	0.101(18)	0.081(13)	0.000	0.000	0.009(17)
C43	0.26(5)	0.37(6)	0.078(14)	0.000	0.000	-0.01(4)
C51	0.21(3)	0.35(7)	0.35(4)	-0.14(4)	-0.04(5)	-0.03(5)
C52	0.28(4)	0.30(5)	0.21(2)	-0.11(3)	0.07(4)	0.09(4)
C61	0.060(8)	0.21(3)	0.21(3)	0.08(3)	0.038(14)	0.020(10)
C62	0.072(9)	0.148(15)	0.134(17)	-0.010(13)	-0.008(11)	0.022(9)
C63	0.028(7)	0.122(14)	0.034(9)	-0.013(10)	0.000	0.000
C71	0.101(11)	0.27(4)	0.16(2)	0.01(2)	0.018(16)	0.080(16)
C72	0.093(11)	0.19(2)	0.149(19)	-0.055(16)	-0.054(14)	0.036(12)
C73	0.065(11)	0.097(15)	0.033(10)	0.000(10)	0.000	0.000

Table 5: Bond lengths (Å) and angles (deg) for **16b**.

Ag11-C11	2.179(11)	Ag11-I11	2.8617(13)
Ag11-P11#1	2.407(3)	P11-C151	1.819(11)

P11-C101	1.848(11)	C72-H7B2	0.9800
P11-C111	1.891(11)	C72-H7C2	0.9800
P11-Ag11#1	2.407(3)	C82-H8A2	0.9800
C11-N21	1.328(13)	C82-H8B2	0.9800
C11-N51	1.376(14)	C82-H8C2	0.9800
N21-C31	1.325(14)	C92-H9A2	0.9800
N21-C101	1.439(13)	C92-H9B2	0.9800
C31-C41	1.353(18)	C92-H9C2	0.9800
C31-H31	0.9500	C102-H10A2	0.9900
C41-N51	1.364(15)	C102-H10B2	0.9900
C41-H41	0.9500	C112-C142	1.519(12)
N51-C61	1.497(14)	C112-C122	1.525(12)
C61-C91	1.485(11)	C112-C132	1.548(11)
C61-C81	1.517(11)	C122-H12A2	0.9800
C61-C71	1.526(11)	C122-H12B2	0.9800
C71-H7A1	0.9800	C122-H12C2	0.9800
C71-H7B1	0.9800	C132-H13A2	0.9800
C71-H7C1	0.9800	C132-H13B2	0.9800
C81-H8A1	0.9800	C132-H13C2	0.9800
C81-H8B1	0.9800	C142-H14A2	0.9800
C81-H8C1	0.9800	C142-H14B2	0.9800
C91-H9A1	0.9800	C142-H14C2	0.9800
C91-H9B1	0.9800	C152-H15A2	0.9800
C91-H9C1	0.9800	C152-H15B2	0.9800
C101-H10A1	0.9900	C152-H15C2	0.9800
C101-H10B1	0.9900	C22-C22#3	1.44(10)
C111-C141	1.525(11)	C22-C23	1.78(5)
C111-C131	1.525(11)	C23-C22#3	1.78(5)
C111-C121	1.537(11)	C31-C33#4	1.33(4)
C121-H12A1	0.9800	C31-C32	1.70(5)
C121-H12B1	0.9800	C32-C33#4	1.96(5)
C121-H12C1	0.9800	C33-C31#4	1.33(4)
C131-H13A1	0.9800	C33-C32#4	1.96(5)
C131-H13B1	0.9800	C33-C33#4	2.01(7)
C131-H13C1	0.9800	C41-C42	1.53(3)
C141-H14A1	0.9800	C41-C43	1.75(4)
C141-H14B1	0.9800	C42-C41#5	1.53(3)
C141-H14C1	0.9800	C43-C41#5	1.75(4)
C151-H15A1	0.9800	C51-C51#6	1.38(10)
C151-H15B1	0.9800	C51-C52#6	1.63(4)
C151-H15C1	0.9800	C52-C52#6	1.26(8)
Ag12-C12	2.144(11)	C52-C51#6	1.63(4)
Ag12-P12#2	2.367(3)	C61-C61#7	1.39(5)
Ag12-I12	2.8980(13)	C61-C62	1.65(2)
Ag12-Ag12#2	3.1951(17)	C62-C63	1.57(2)
P12-C152	1.828(13)	C63-C62#7	1.57(2)
P12-C112	1.830(11)	C71-C72	1.23(3)
P12-C102	1.879(11)	C71-C71#8	1.66(6)
P12-Ag12#2	2.367(3)	C72-C73	1.19(2)
C12-N52	1.342(14)	C72-C72#8	1.86(5)
C12-N22	1.369(13)	C73-C72#8	1.19(2)
N22-C32	1.412(14)	C11-Ag11-P11#1	145.8(3)
N22-C102	1.446(13)	C11-Ag11-I11	102.0(3)
C32-C42	1.329(16)	P11#1-Ag11-I11	111.70(8)
C32-H32	0.9500	C151-P11-C101	102.6(5)
C42-N52	1.387(15)	C151-P11-C111	106.5(5)
C42-H42	0.9500	C101-P11-C111	101.5(5)
N52-C62	1.483(14)	C151-P11-Ag11#1	113.5(4)
C62-C72	1.502(11)	C101-P11-Ag11#1	113.4(3)
C62-C82	1.502(11)	C111-P11-Ag11#1	117.6(3)
C62-C92	1.525(11)	N21-C11-N51	103.9(9)
C72-H7A2	0.9800	N21-C11-Ag11	125.7(8)

N51-C11-Ag11	130.4(8)
C31-N21-C11	112.7(10)
C31-N21-C101	124.8(10)
C11-N21-C101	122.4(10)
N21-C31-C41	107.3(11)
N21-C31-H31	126.3
C41-C31-H31	126.3
C31-C41-N51	106.2(11)
C31-C41-H41	126.9
N51-C41-H41	126.9
C41-N51-C11	109.8(10)
C41-N51-C61	125.5(10)
C11-N51-C61	123.8(9)
C91-C61-N51	110.1(9)
C91-C61-C81	108.1(11)
N51-C61-C81	109.4(10)
C91-C61-C71	112.7(12)
N51-C61-C71	107.8(9)
C81-C61-C71	108.7(10)
C61-C71-H7A1	109.5
C61-C71-H7B1	109.5
H7A1-C71-H7B1	109.5
C61-C71-H7C1	109.5
H7A1-C71-H7C1	109.5
H7B1-C71-H7C1	109.5
C61-C81-H8A1	109.5
C61-C81-H8B1	109.5
H8A1-C81-H8B1	109.5
C61-C81-H8C1	109.5
H8A1-C81-H8C1	109.5
H8B1-C81-H8C1	109.5
C61-C91-H9A1	109.5
C61-C91-H9B1	109.5
H9A1-C91-H9B1	109.5
C61-C91-H9C1	109.5
H9A1-C91-H9C1	109.5
H9B1-C91-H9C1	109.5
N21-C101-P11	113.9(7)
N21-C101-H10A1	108.8
P11-C101-H10A1	108.8
N21-C101-H10B1	108.8
P11-C101-H10B1	108.8
H10A1-C101-H10B1	107.7
C141-C111-C131	108.9(9)
C141-C111-C121	112.3(11)
C131-C111-C121	110.0(10)
C141-C111-P11	105.9(7)
C131-C111-P11	104.4(8)
C121-C111-P11	114.9(8)
C111-C121-H12A1	109.5
C111-C121-H12B1	109.5
H12A1-C121-H12B1	109.5
C111-C121-H12C1	109.5
H12A1-C121-H12C1	109.5
H12B1-C121-H12C1	109.5
C111-C131-H13A1	109.5
C111-C131-H13B1	109.5
H13A1-C131-H13B1	109.5
C111-C131-H13C1	109.5
H13A1-C131-H13C1	109.5
H13B1-C131-H13C1	109.5
C111-C141-H14A1	109.5
C111-C141-H14B1	109.5
H14A1-C141-H14B1	109.5
C111-C141-H14C1	109.5
H14A1-C141-H14C1	109.5
H14B1-C141-H14C1	109.5
P11-C151-H15A1	109.5
P11-C151-H15B1	109.5
H15A1-C151-H15B1	109.5
P11-C151-H15C1	109.5
H15A1-C151-H15C1	109.5
H15B1-C151-H15C1	109.5
C12-Ag12-P12#2	151.2(3)
C12-Ag12-I12	105.5(3)
P12#2-Ag12-I12	103.30(8)
C12-Ag12-Ag12#2	83.5(3)
P12#2-Ag12-Ag12#2	80.56(8)
I12-Ag12-Ag12#2	127.19(4)
C152-P12-C112	103.2(7)
C152-P12-C102	98.3(6)
C112-P12-C102	104.8(5)
C152-P12-Ag12#2	113.6(5)
C112-P12-Ag12#2	115.4(4)
C102-P12-Ag12#2	119.1(3)
N52-C12-N22	106.1(10)
N52-C12-Ag12	132.9(8)
N22-C12-Ag12	120.9(8)
C12-N22-C32	108.9(10)
C12-N22-C102	126.6(10)
C32-N22-C102	124.3(8)
C42-C32-N22	106.6(10)
C42-C32-H32	126.7
N22-C32-H32	126.7
C32-C42-N52	108.2(11)
C32-C42-H42	125.9
N52-C42-H42	125.9
C12-N52-C42	109.9(10)
C12-N52-C62	124.3(10)
C42-N52-C62	125.7(9)
N52-C62-C72	107.2(8)
N52-C62-C82	108.2(9)
C72-C62-C82	113.9(10)
N52-C62-C92	109.3(9)
C72-C62-C92	109.2(9)
C82-C62-C92	109.1(10)
C62-C72-H7A2	109.5
C62-C72-H7B2	109.5
H7A2-C72-H7B2	109.5
C62-C72-H7C2	109.5
H7A2-C72-H7C2	109.5
H7B2-C72-H7C2	109.5
C62-C82-H8A2	109.5
C62-C82-H8B2	109.5
H8A2-C82-H8B2	109.5
C62-C82-H8C2	109.5
H8A2-C82-H8C2	109.5
H8B2-C82-H8C2	109.5
C62-C92-H9A2	109.5
C62-C92-H9B2	109.5
H9A2-C92-H9B2	109.5
C62-C92-H9C2	109.5
H9A2-C92-H9C2	109.5
H9B2-C92-H9C2	109.5

N22-C102-P12	113.9(8)
N22-C102-H10A2	108.8
P12-C102-H10A2	108.8
N22-C102-H10B2	108.8
P12-C102-H10B2	108.8
H10A2-C102-H10B2	107.7
C142-C112-C122	107.7(11)
C142-C112-C132	110.9(11)
C122-C112-C132	108.8(10)
C142-C112-P12	107.8(7)
C122-C112-P12	113.9(10)
C132-C112-P12	107.8(7)
C112-C122-H12A2	109.5
C112-C122-H12B2	109.5
H12A2-C122-H12B2	109.5
C112-C122-H12C2	109.5
H12A2-C122-H12C2	109.5
H12B2-C122-H12C2	109.5
C112-C132-H13A2	109.5
C112-C132-H13B2	109.5
H13A2-C132-H13B2	109.5
C112-C132-H13C2	109.5
H13A2-C132-H13C2	109.5
H13B2-C132-H13C2	109.5
C112-C142-H14A2	109.5
C112-C142-H14B2	109.5
H14A2-C142-H14B2	109.5
C112-C142-H14C2	109.5
H14A2-C142-H14C2	109.5
H14B2-C142-H14C2	109.5
P12-C152-H15A2	109.5
P12-C152-H15B2	109.5
H15A2-C152-H15B2	109.5
P12-C152-H15C2	109.5
H15A2-C152-H15C2	109.5
H15B2-C152-H15C2	109.5
C22#3-C22-C23	66.3(17)
C22#3-C23-C22	47(3)
C33#4-C31-C32	80(3)
C31-C32-C33#4	41.7(18)
C31#4-C33-C32#4	59(2)
C31#4-C33-C33#4	93(2)
C32#4-C33-C33#4	87(3)
C42-C41-C43	81.9(19)
C41#5-C42-C41	107(3)
C41#5-C43-C41	89(2)
C51#6-C51-C52#6	88(2)
C52#6-C52-C51#6	92(2)
C61#7-C61-C62	111.5(14)
C63-C62-C61	99.4(16)
C62#7-C63-C62	115.2(18)
C72-C71-C71#8	94.3(18)
C73-C72-C71	123(3)
C73-C72-C72#8	38.2(15)
C71-C72-C72#8	84.9(19)
C72-C73-C72#8	104(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,z
#2 -x,-y+1,z
#3 -x,y,-z
#4 -x,y,-z+1
#5 -x-1/2,-y+1/2,z
#6 -x+1/2,-y+1/2,z
#7 x,-y+1,-z
#8 x,-y,-z+1

Crystal data for dicarbonyl A :