Mono- and dimeric complexes of an asymmetric heterotopic P,C_{NHC},pyr ligand

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Supporting Information

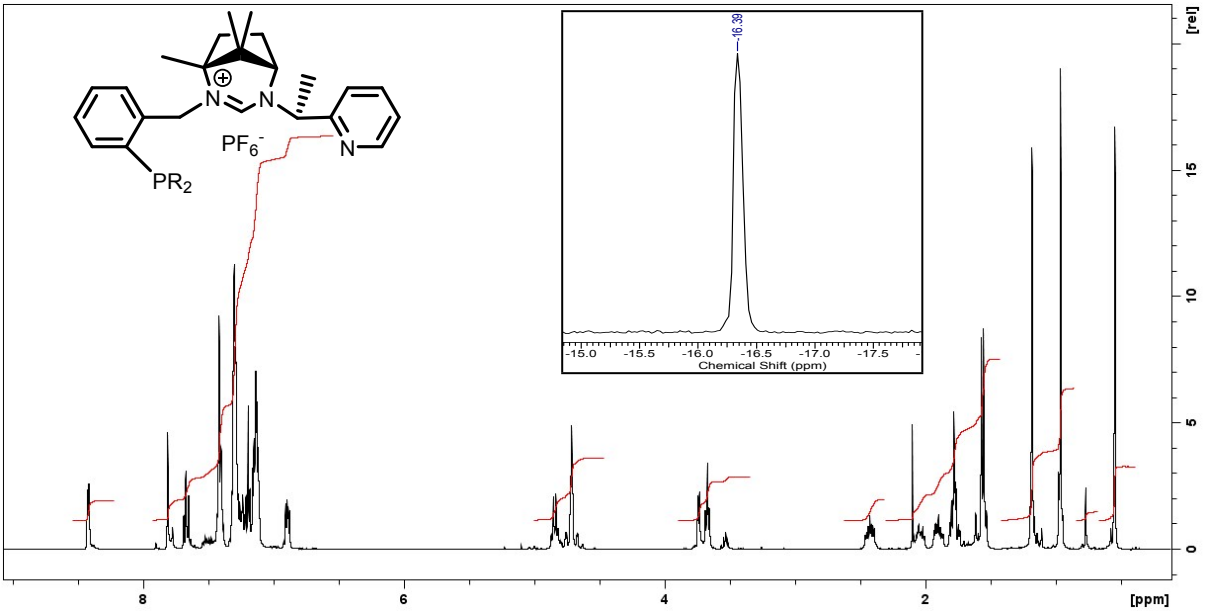

Figure S1. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of *S*-[N^{Me}CHP]PF_6 recorded in $CDCl_3$.

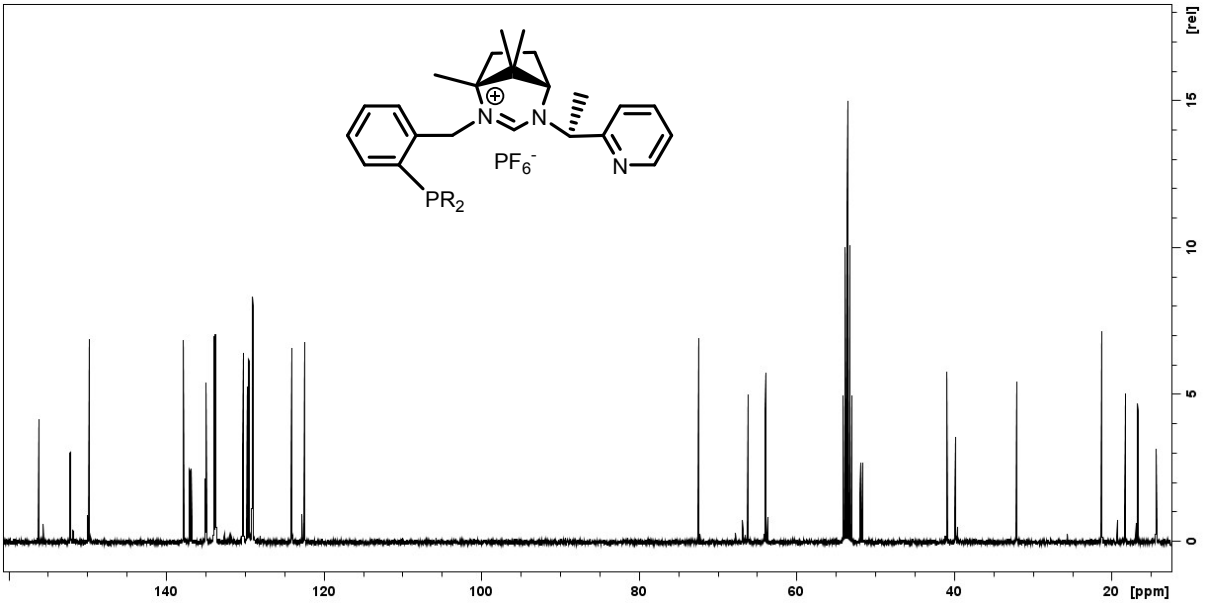

Figure S2. $^{13}C\{^{1}H\}$ (100 MHz) spectrum of *S*-[N^{Me}CHP]PF_6 recorded in CD_2Cl_2.

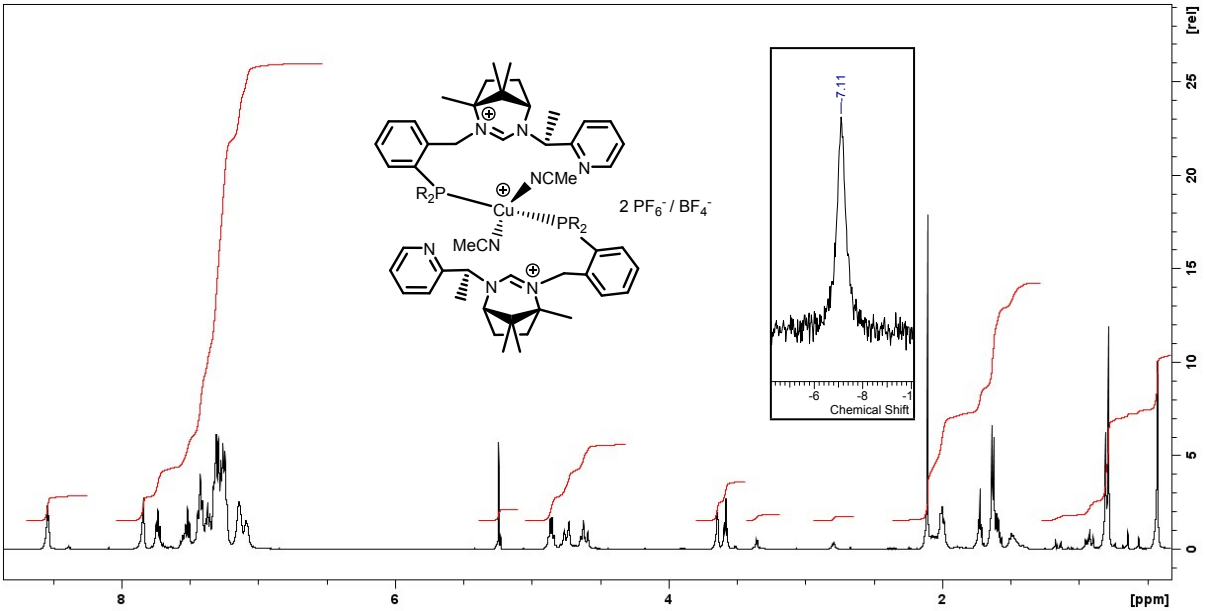

Figure S3. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of $[Cu(\kappa\text{-}P\text{-}N^{Me}CHP)_2(MeCN)_2]BF_4.(PF_6)_2$, **1**, recorded in CD_2Cl_2.

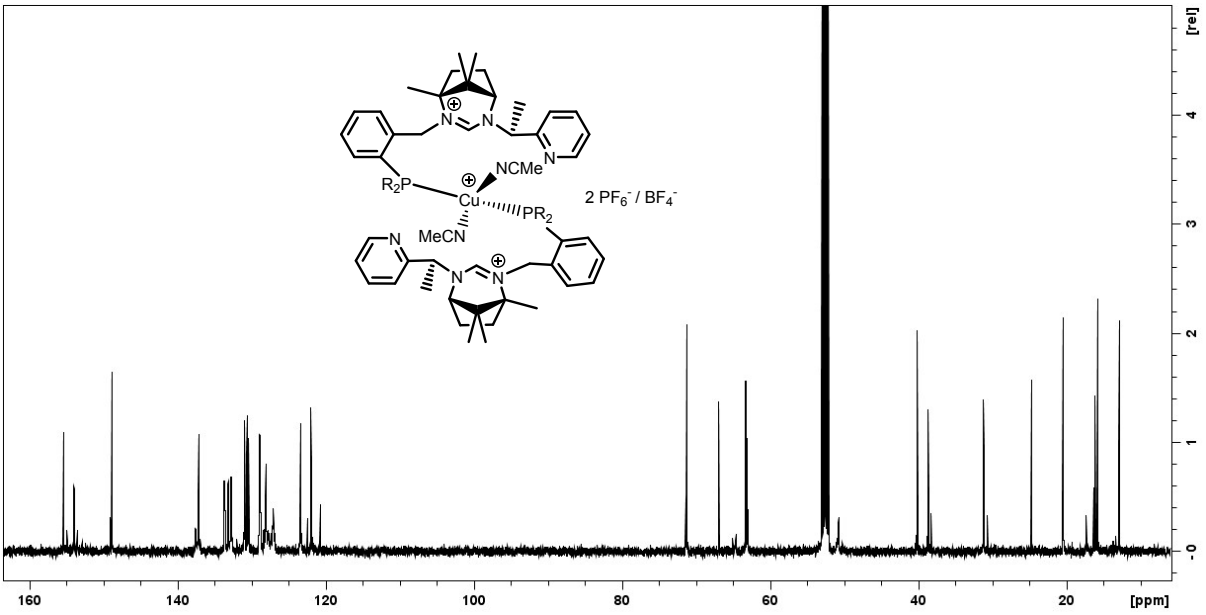

Figure S4. $^{13}C\{^{1}H\}$ (125.8 MHz) spectrum of $[Cu(\kappa\text{-}P\text{-}N^{Me}CHP)_2(MeCN)_2]BF_4.(PF_6)_2$, **1**, recorded in CD_2Cl_2.

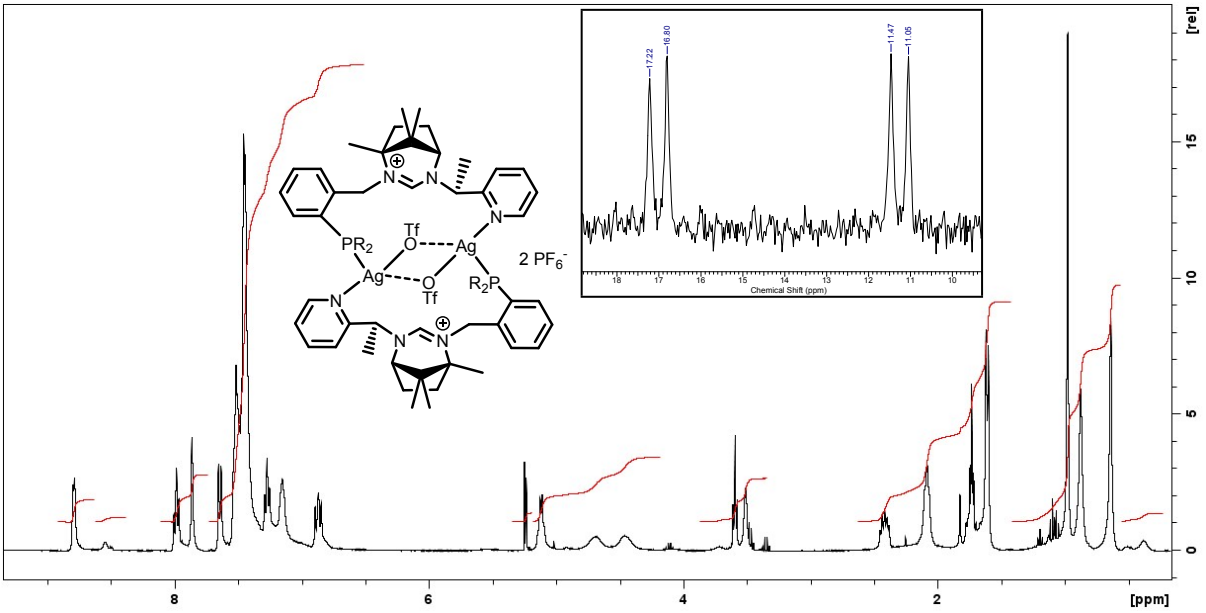

Figure S5. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of *H,T*-[Ag_2(μ-*N,P*-$N^{Me}CHP)_2$(μ-OTf)$_2$](PF_6)$_2$, **2.OTf**, recorded in CD_2Cl_2. Peaks at approximately 3.55 and 1.70 ppm are from residual THF.

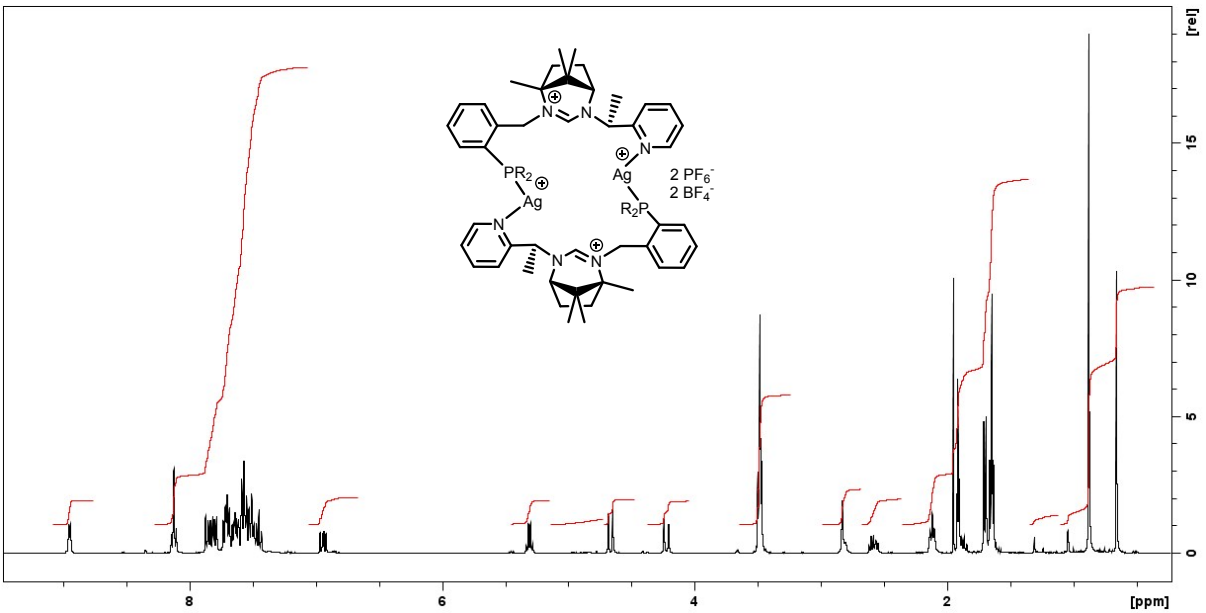

Figure S6. ^{1}H (400.1 MHz) spectrum of *H,T*-[Ag_2(μ-*N,P*-$N^{Me}CHP)_2$](BF_4)$_2$(PF_6)$_2$, **2.BF$_4$**, recorded in CD_3CN. Peaks at approximately 3.50 and 1.65 ppm are from residual THF.

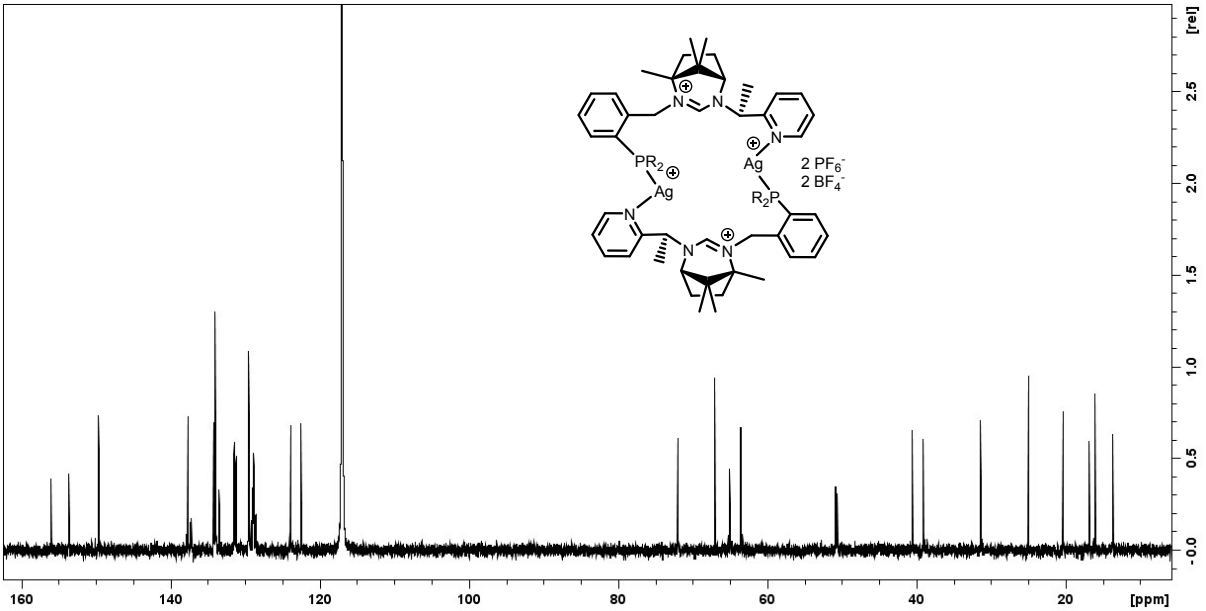

Figure S7. $^{13}C\{^{1}H\}$ (125.8 MHz) spectrum of *H,T*-$[Ag_2(\mu\text{-}N,P\text{-}N^{Me}CHP)_2](BF_4)_2(PF_6)_2$, **2.BF$_4$**, recorded in CD_3CN. Peaks at approximately 67 and 25 ppm are from residual THF.

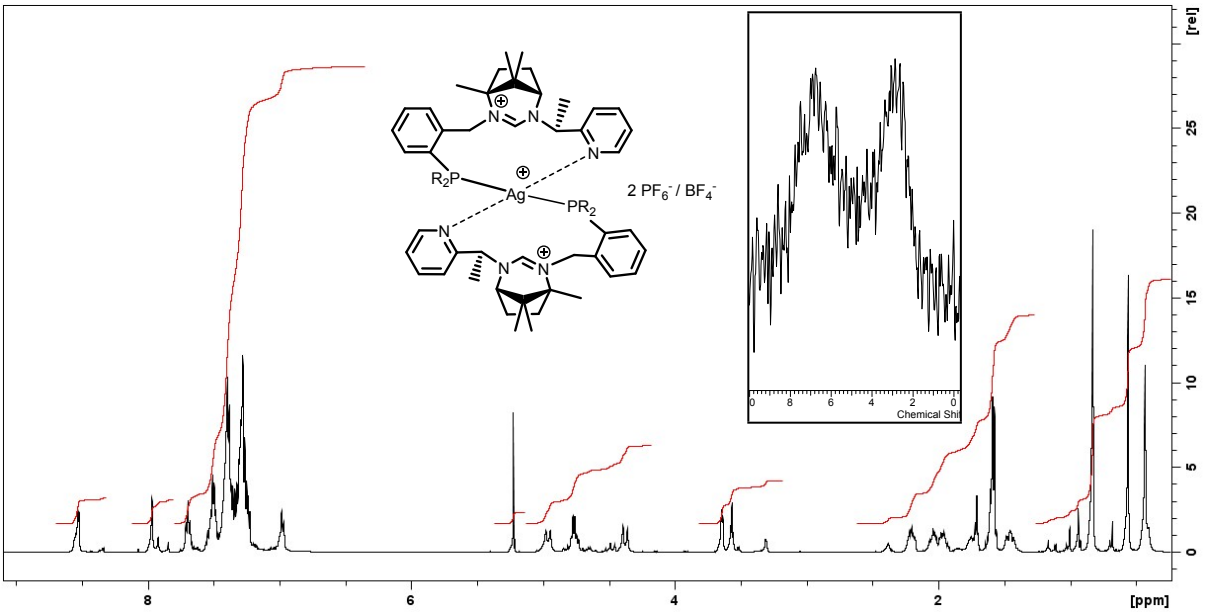

Figure S8. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of $[Ag(\kappa\text{-}P\text{-}N^{Me}CHP)_2](BF_4)(PF_6)_2$, **3**, recorded in CD_2Cl_2. Peaks at approximately 3.55 and 1.70 ppm are from residual THF.

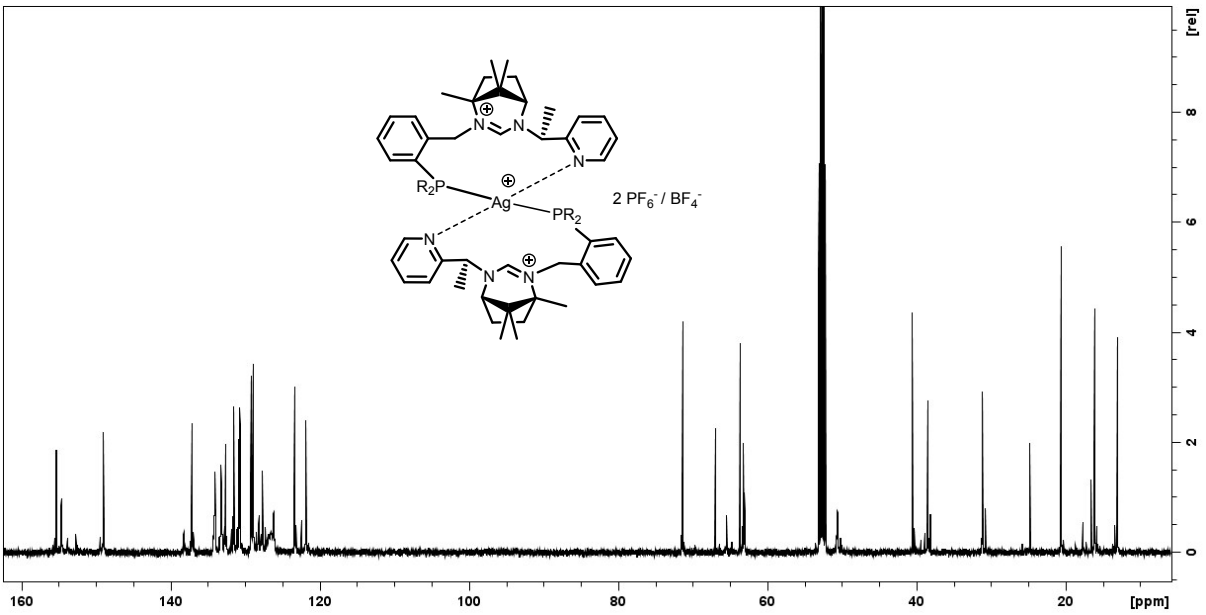

Figure S9. $^{13}C\{^{1}H\}$ (125.8 MHz) spectrum of $[Ag(\kappa\text{-}P\text{-}N^{Me}CHP)_2](BF_4)(PF_6)_2$, **3**, recorded in CD_2Cl_2. Peaks at approximately 67 and 25 ppm are from residual THF.

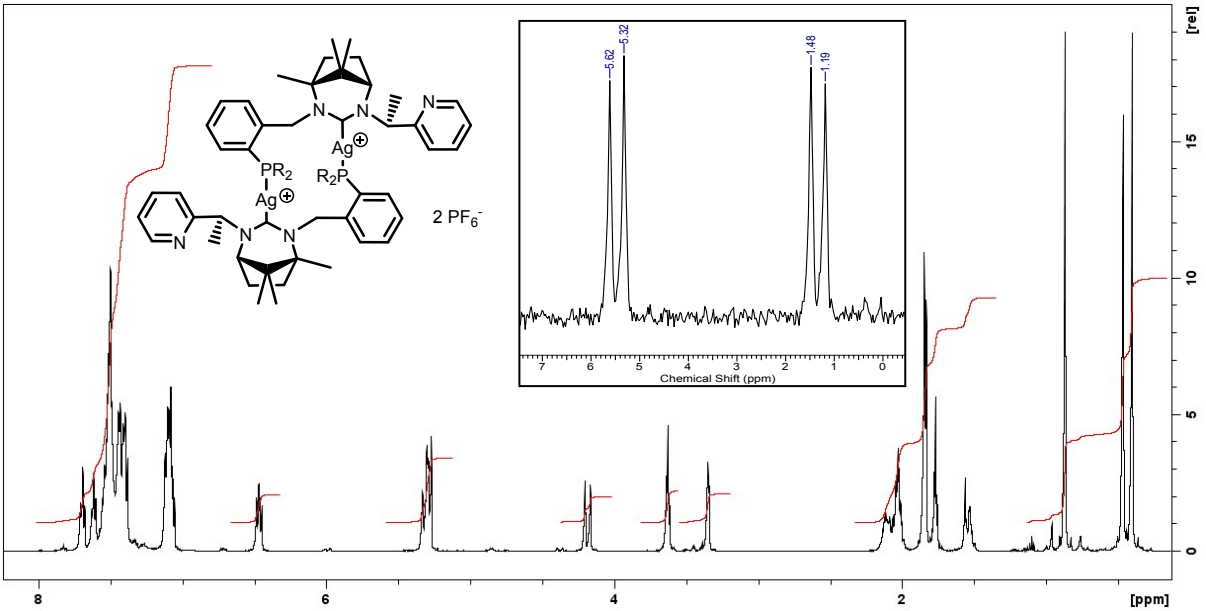

Figure S10. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of *H,T*-[Ag_2(μ-*C,P*-$N^{Me}CP)_2$]$(PF_6)_2$, **4**, recorded in CD_2Cl_2. Peaks at approximately 3.60 and 1.75 ppm are from residual THF.

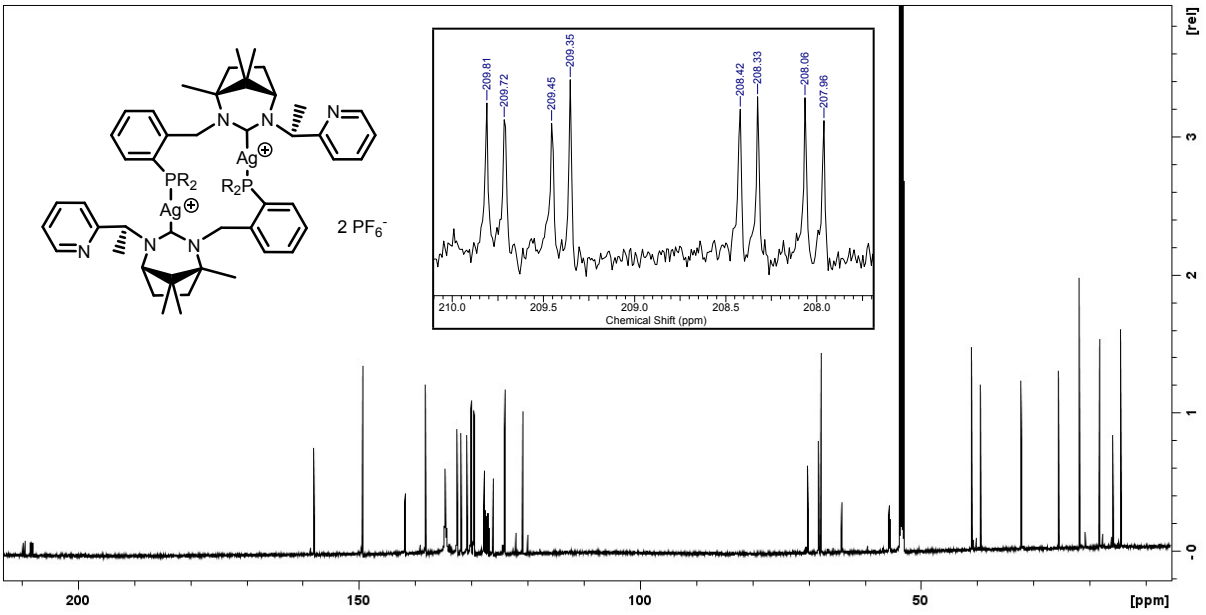

Figure S11. $^{13}C\{^{1}H\}$ (150.9 MHz) spectrum of *H,T*-[Ag_2(μ-*C,P*-$N^{Me}CP)_2$]$(PF_6)_2$, **4**, recorded in CD_2Cl_2. Peaks at approximately 67 and 25 ppm are from residual THF.

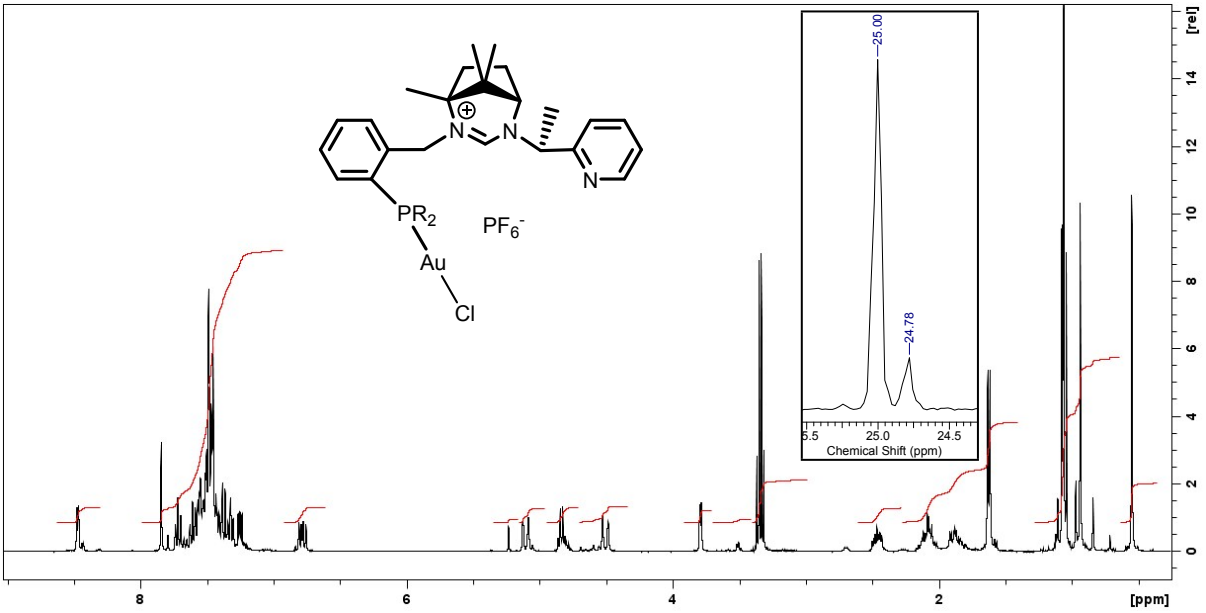

Figure S12. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of [Au(κ-*P*-N^{Me}CHP)Cl]PF_6, **5**, recorded in CD_2Cl_2. The triplet at 1.06 ppm and quartet at 3.35 ppm are assigned to lattice Et_2O.

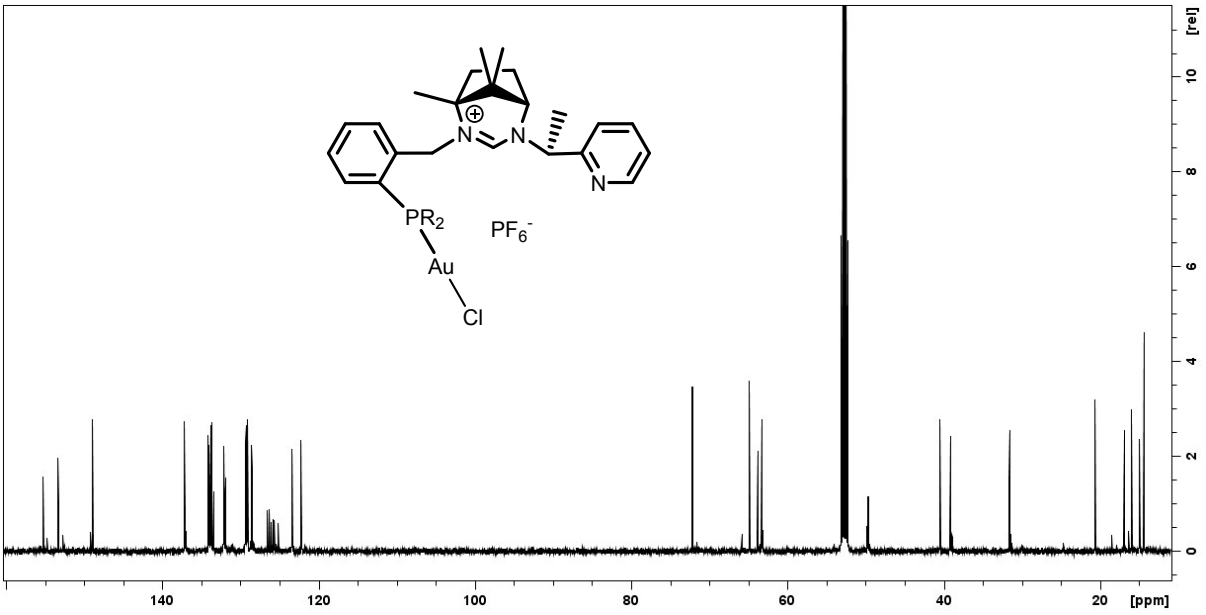

Figure S13. $^{13}C\{^{1}H\}$ (125.8 MHz) NMR spectrum of [Au(κ-*P*-N^{Me}CHP)Cl]PF_6, **5**, recorded in CD_2Cl_2. The peaks at 64.9 ppm and 14.4 ppm are assigned to lattice Et_2O.

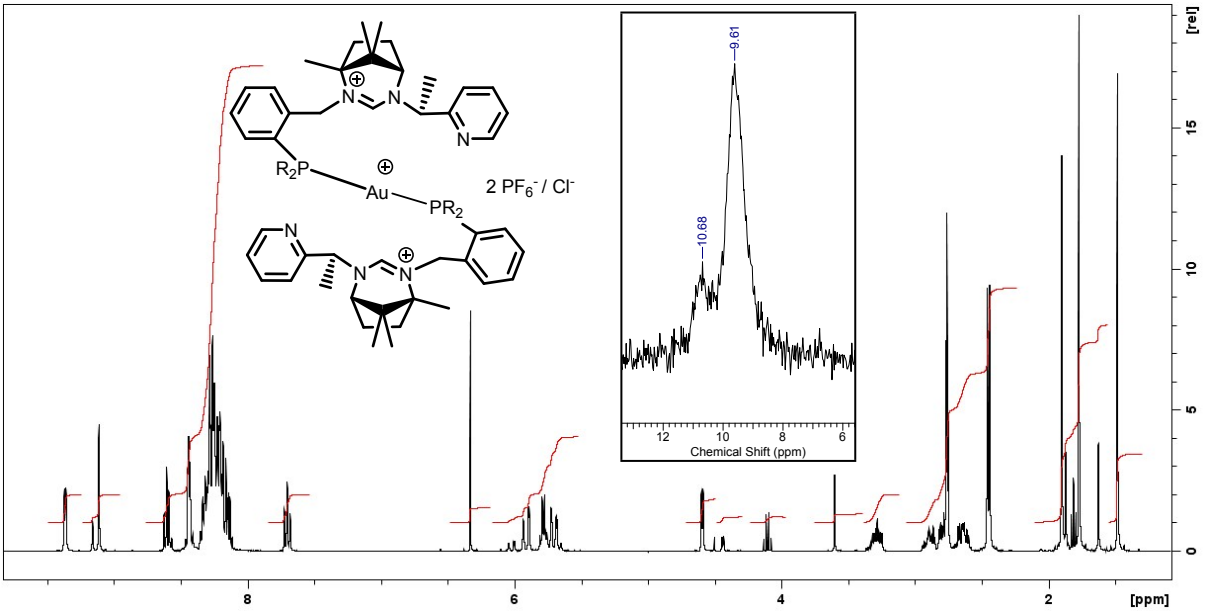

Figure S14. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of $[Au(\kappa\text{-}P\text{-}N^{Me}CHP)_2]Cl(PF_6)_2$, **6**, recorded in $(CD_3)_2CO$.

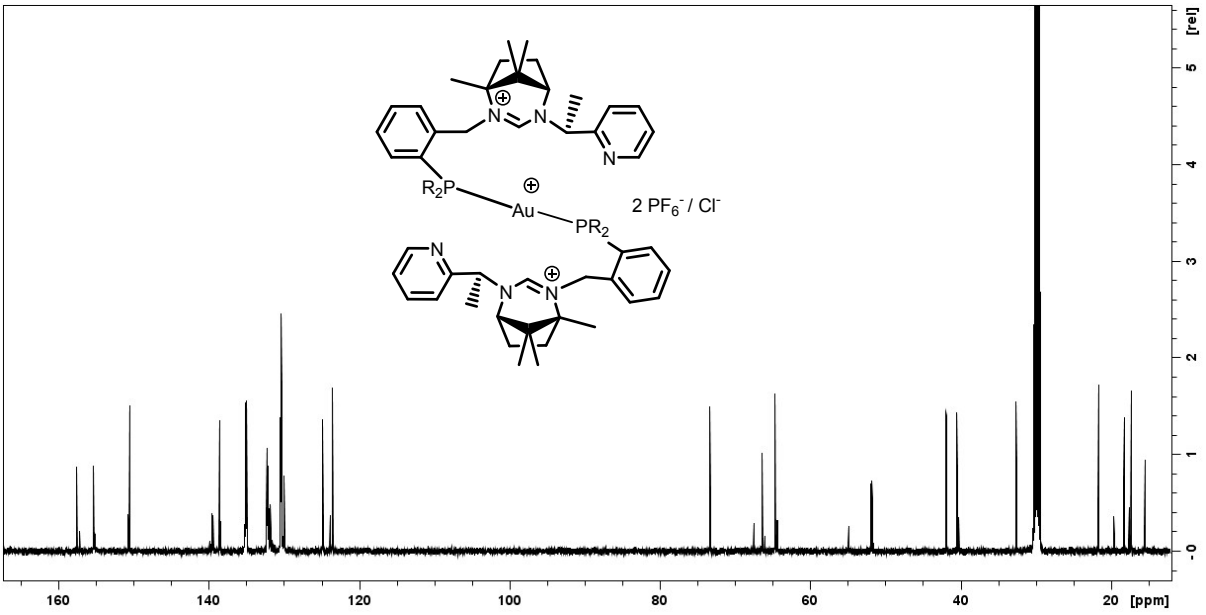

Figure S15. $^{13}C\{^{1}H\}$ (125.8 MHz) NMR spectrum of $[Au(\kappa\text{-}P\text{-}N^{Me}CHP)_2]Cl(PF_6)_2$, **6**, recorded in $(CD_3)_2CO$.

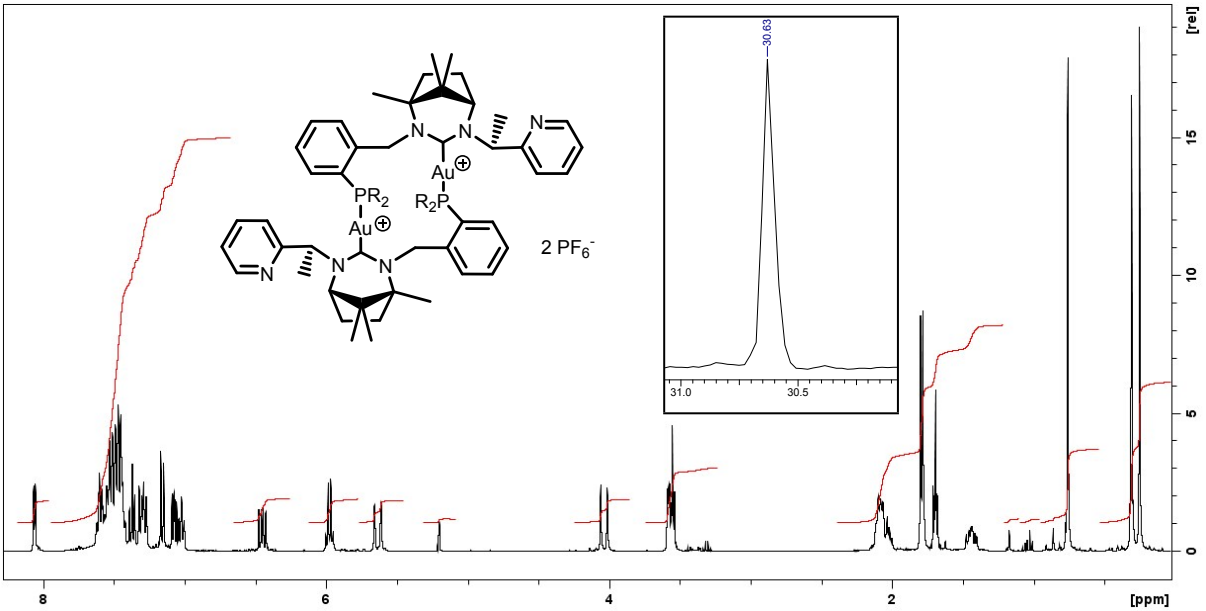

Figure S16. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of *H,T*-[Au_2(μ-*C,P*-$N^{Me}CP)_2$]($PF_6)_2$, **7**, recorded in CD_2Cl_2. Peaks at approximately 3.55 and 1.70 ppm are from residual THF.

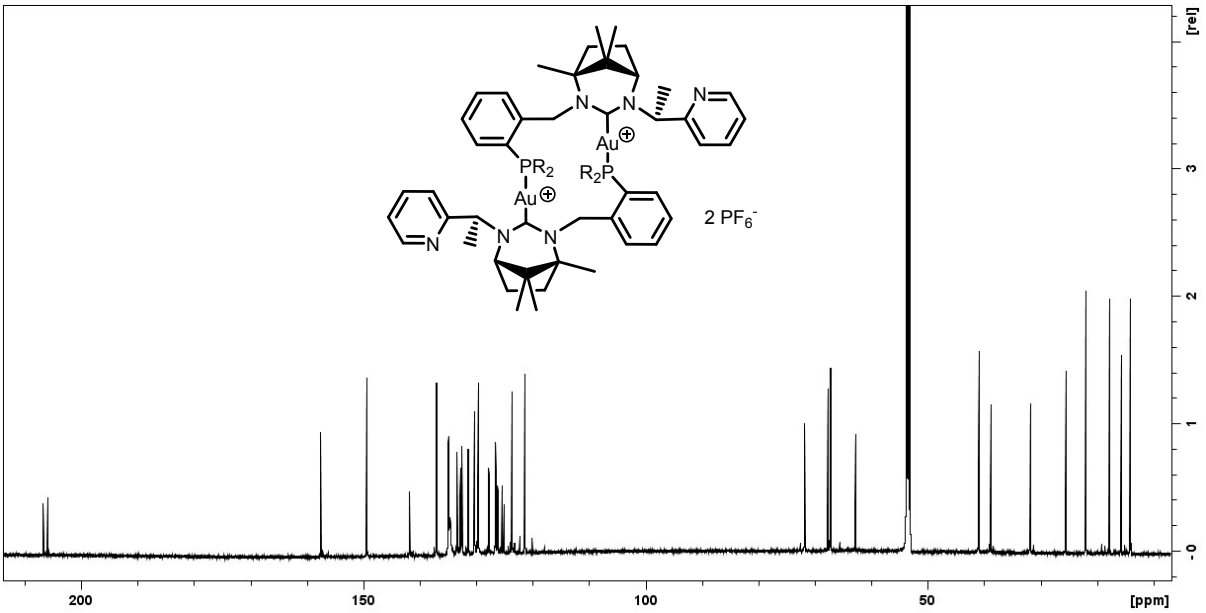

Figure S17. $^{13}C\{^{1}H\}$ (150.9 MHz) NMR spectrum of *H,T*-[Au_2(μ-*C,P*-$N^{Me}CP)_2$]($PF_6)_2$, **7**, recorded in CD_2Cl_2. Peaks at approximately 67 and 25 ppm are from residual THF.

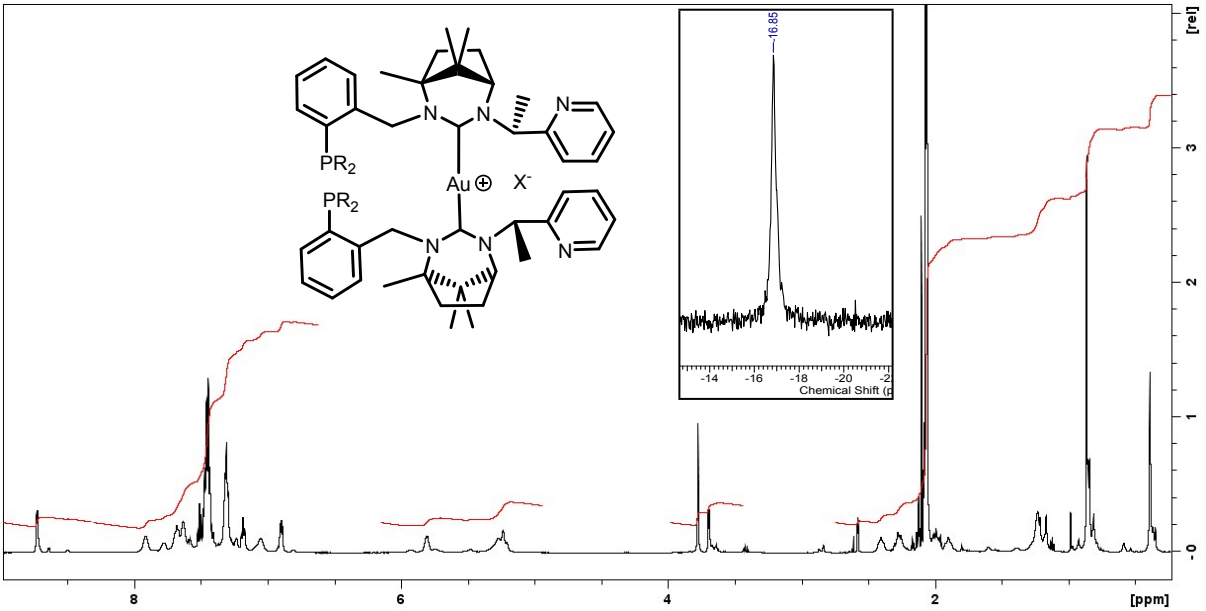

Figure S18. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of [Au(κ-*C*-$N^{Me}CP)_2$](PF_6), **8**, recorded in d_6-acetone.

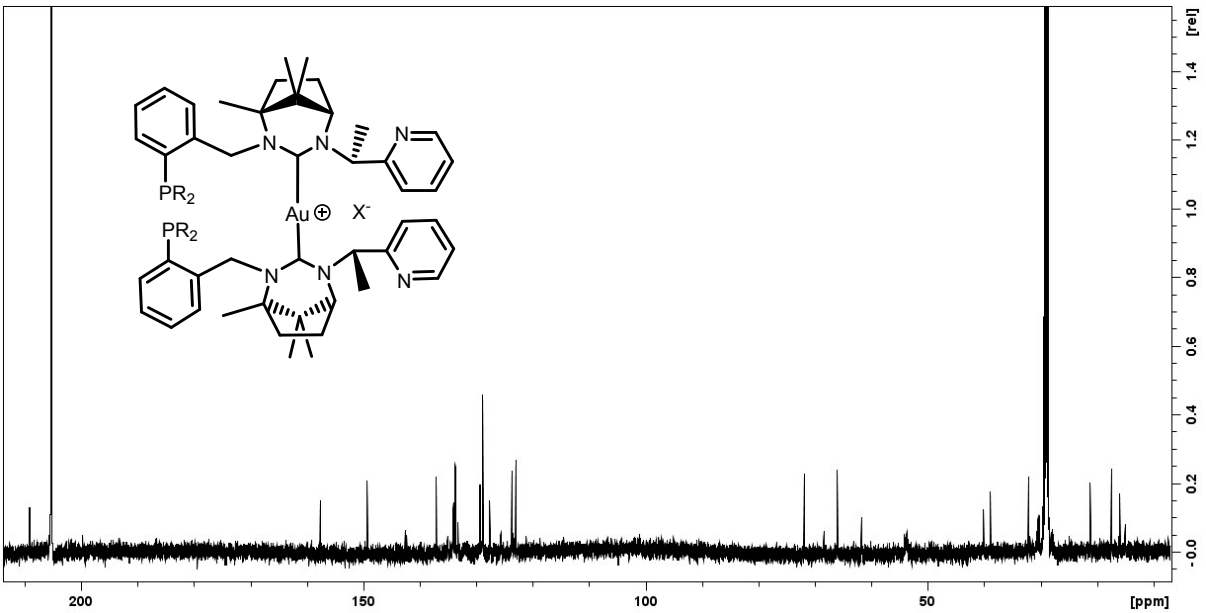

Figure S19. $^{13}C\{^{1}H\}$ (150.9 MHz) NMR spectrum of [Au(κ-*C*-$N^{Me}CP)_2$](PF_6), **8**, recorded in d_6-acetone.

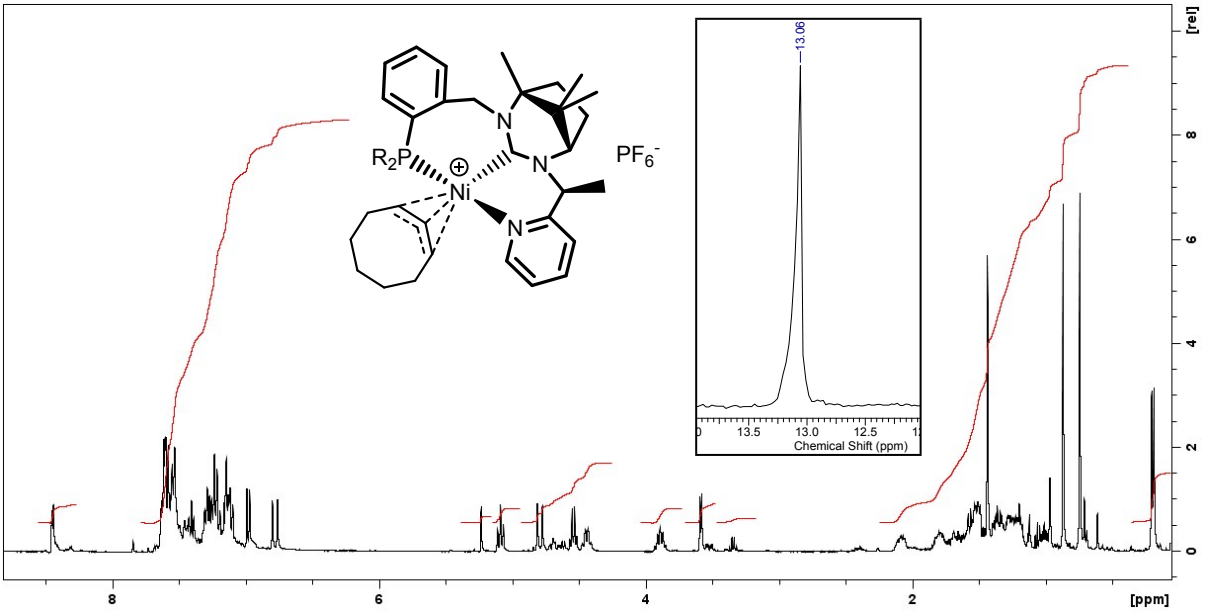

Figure S20. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of [Ni(κ^3-*N,C,P*-N^{Me}CP)(η^3-C_8H_{13})]PF_6, **9**, recorded in CD_2Cl_2.

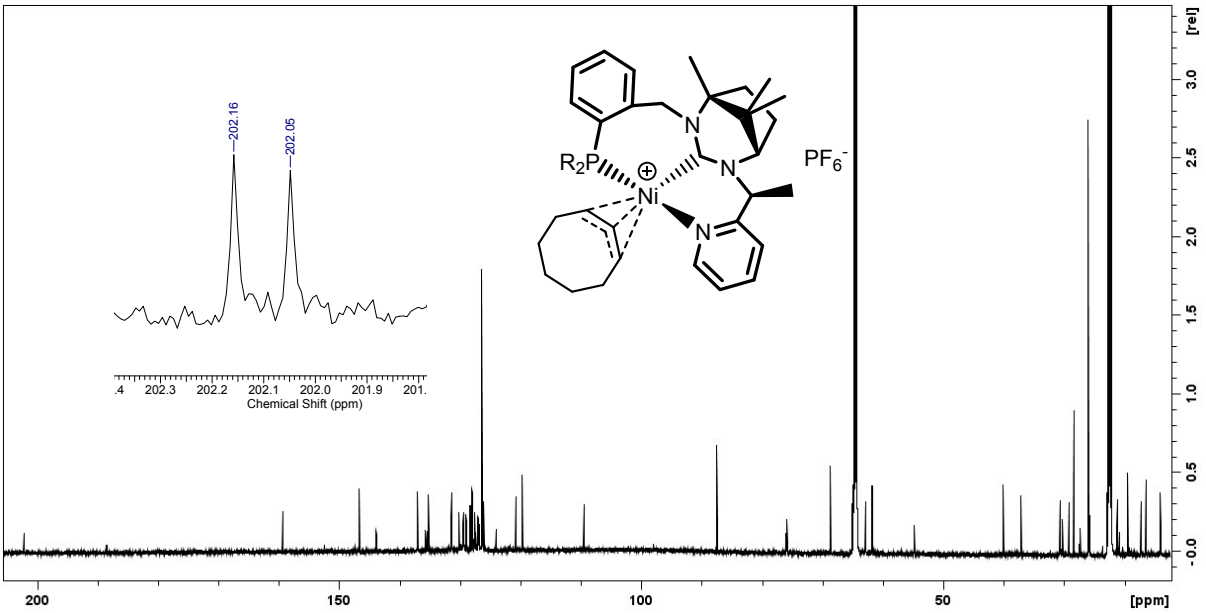

Figure S21. $^{13}C\{^{1}H\}$ (150.9 MHz) NMR spectrum of [Ni(κ^3-*N,C,P*-N^{Me}CP)(η^3-C_8H_{13})]PF_6, **9**, recorded in CD_2Cl_2. The peaks at ~126 and 26 ppm are assigned to residual 1,5-cyclooctadiene.

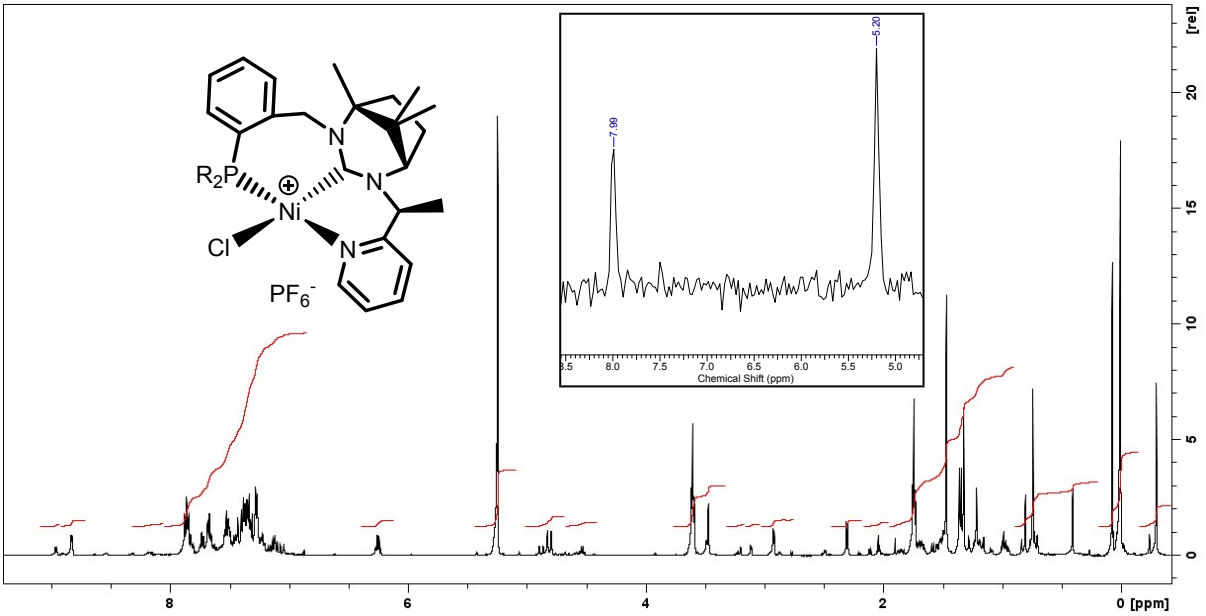

Figure S22. ^{1}H (500.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of an approximately 3:1 mixture of the two isomers of [Ni(κ^{3}-*N,C,P*-N^{Me}CP)Cl]PF_6, **10**, recorded in CD_2Cl_2. Peaks at approximately 3.25 and 1.50 ppm are from residual THF.

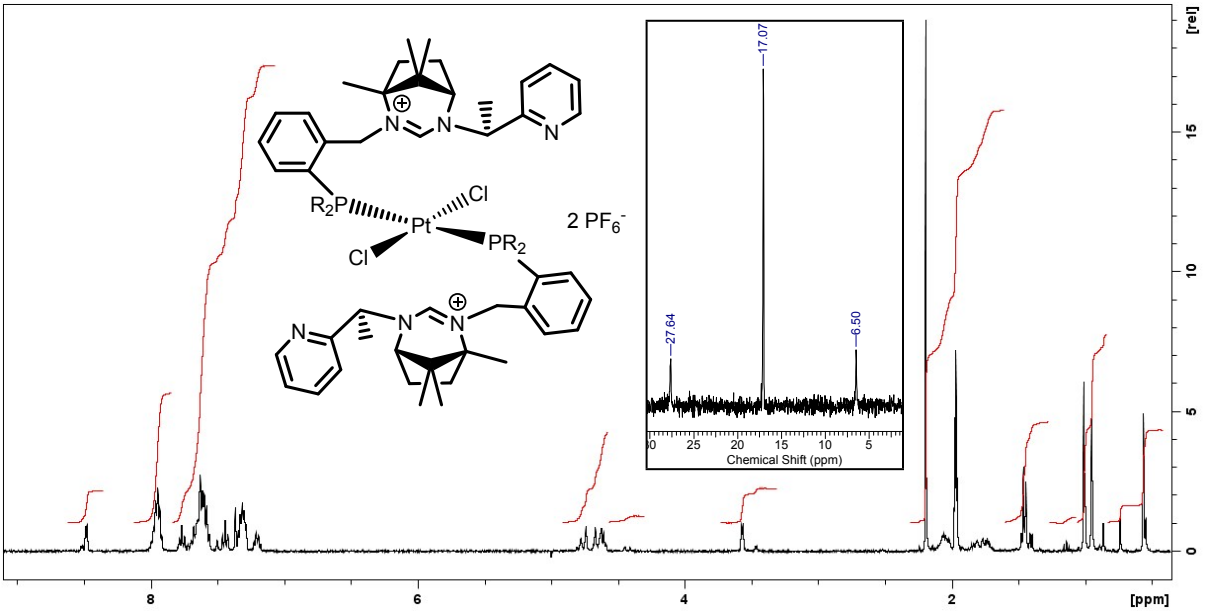

Figure S23. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of *trans*-[Pt(κ-*P*-$N^{Me}CHP)_2Cl_2$]$(PF_6)_2$, **11**, recorded in CD_3CN.

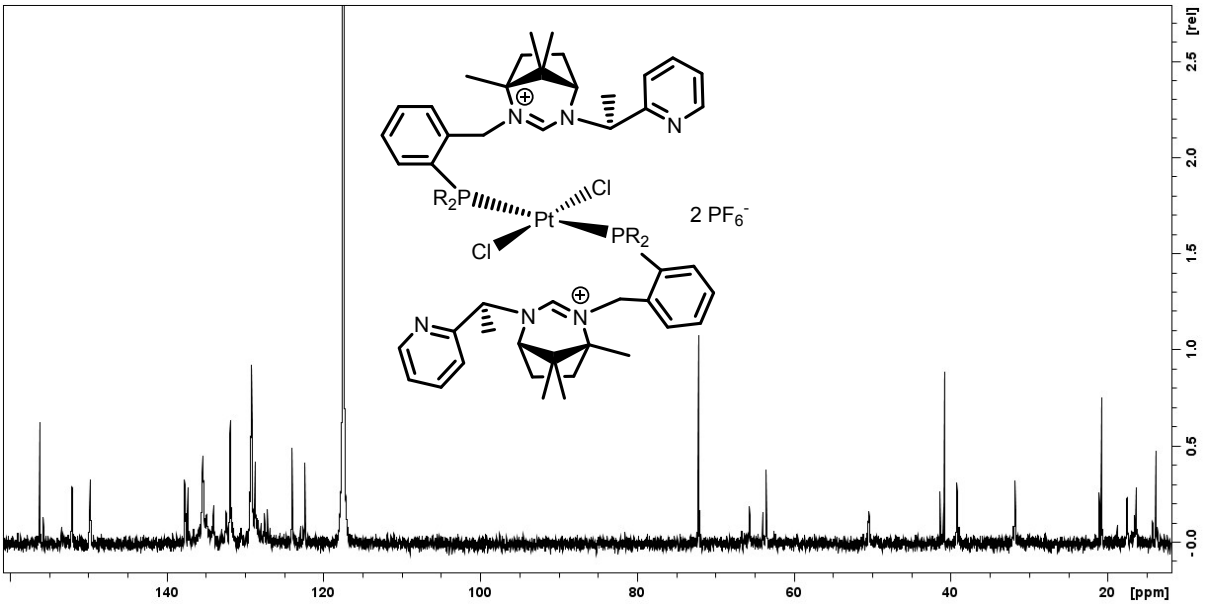

Figure S24. $^{13}C\{^{1}H\}$ (75.5 MHz) NMR spectrum of *trans*-[Pt(κ-*P*-$N^{Me}CHP)_2Cl_2$]$(PF_6)_2$, **11**, recorded in CD_3CN.

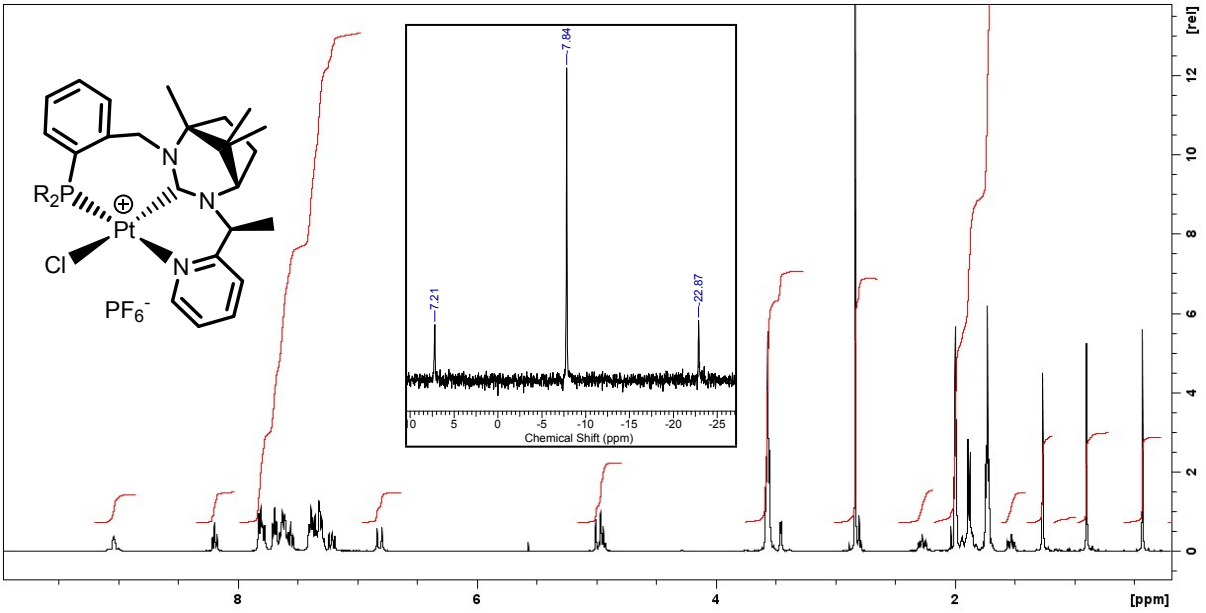

Figure S25. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of [Pt(κ^{3}-*N,C,P*-N^{Me}CP)Cl]PF_6, **12**, recorded in CD_3CN. Peaks at approximately 3.55 and 1.70 ppm are from residual THF.

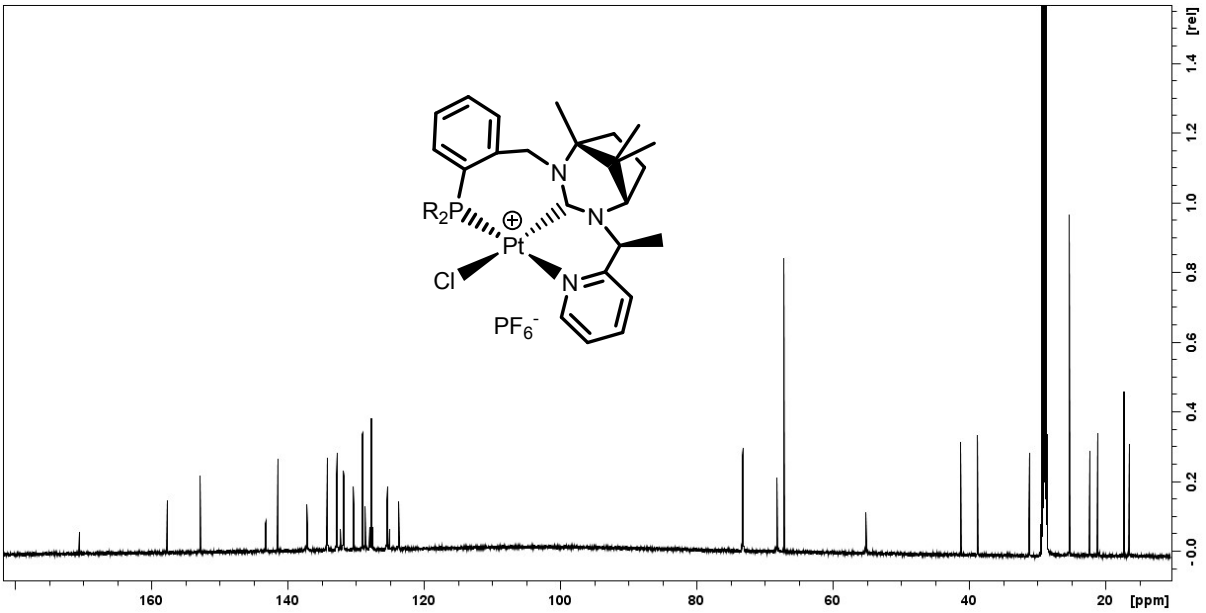

Figure S26. $^{13}C\{^{1}H\}$ (150.9 MHz) NMR spectrum of [Pt(κ^{3}-*N,C,P*-N^{Me}CP)Cl]PF_6, **12**, recorded in CD_3CN. Peaks at approximately 67 and 25 ppm are from residual THF.

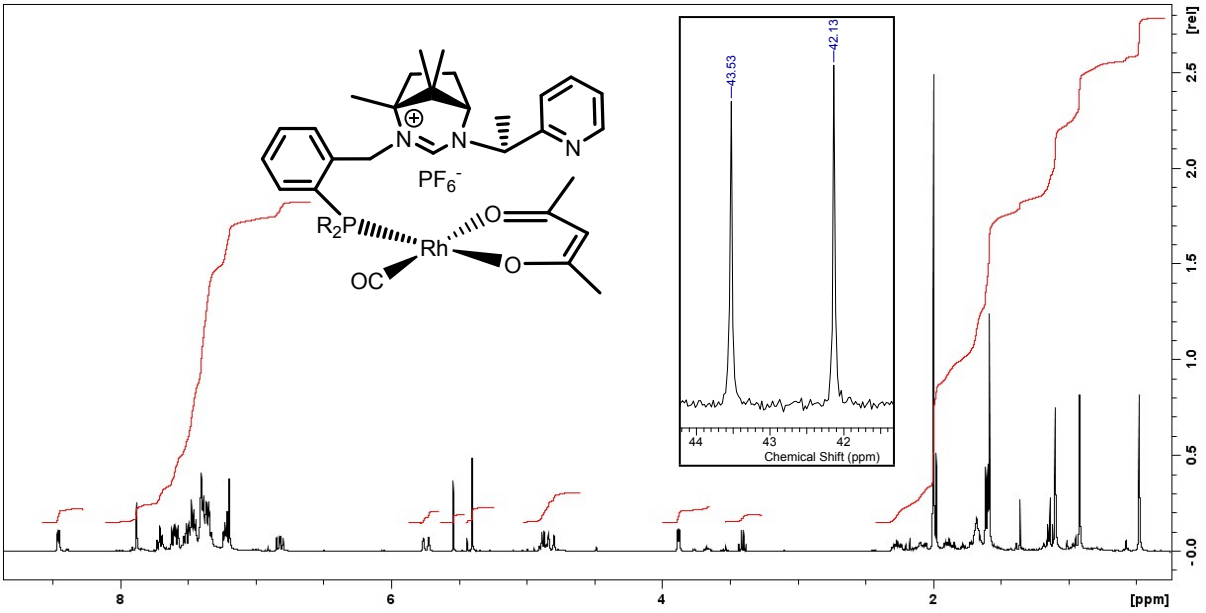

Figure S27. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of [Rh(κ-*P*-N^{Me}CHP)(acac)(CO)]PF_6, **13**, recorded in $CDCl_3$.

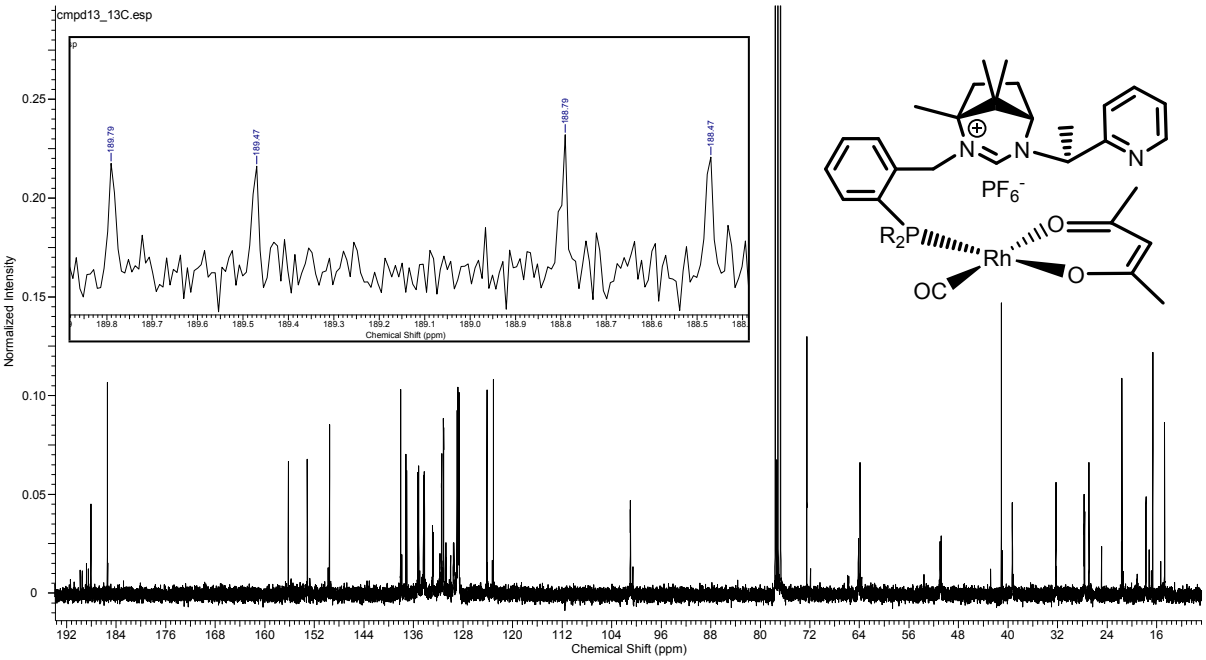

Figure S28. $^{13}C\{^{1}H\}$ (75.5 MHz) NMR spectrum of [Rh(κ-*P*-N^{Me}CHP)(acac)(CO)]PF_6, **13**, recorded in $CDCl_3$.

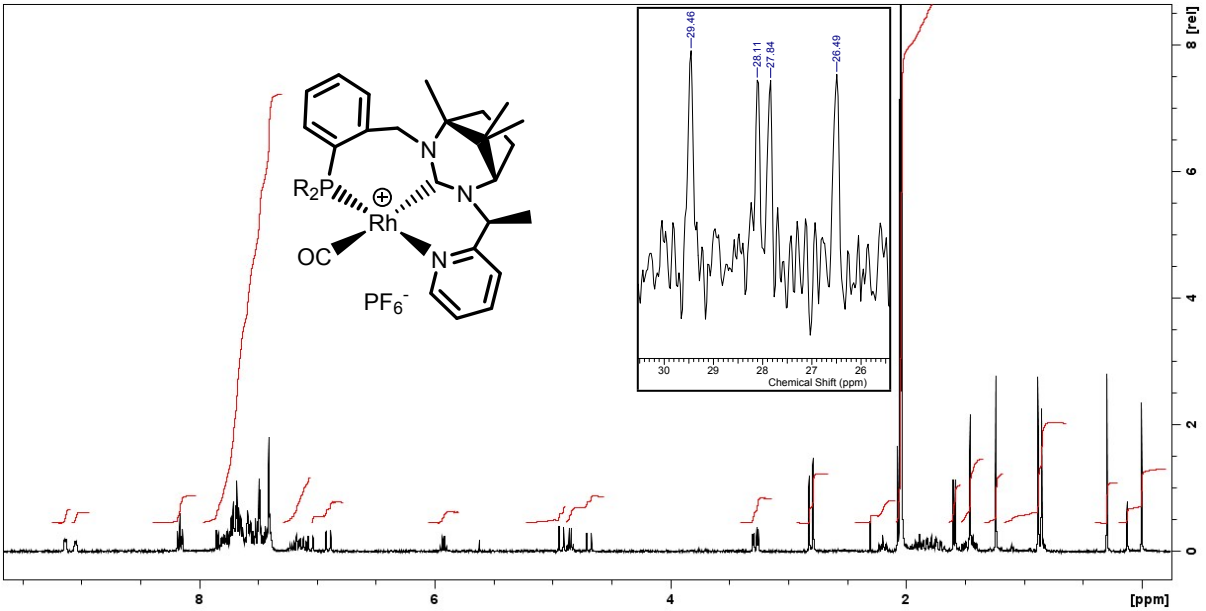

Figure S29. ^{1}H (400.1 MHz) and $^{31}P\{^{1}H\}$ (inset, 121.7 MHz) spectra of an approximately 1:1 mixture of the two diastereomers of [Rh(κ^{3}-*N,C,P*-N^{Me}CP)(CO)]PF_6, **14**, recorded in d_6-acetone.

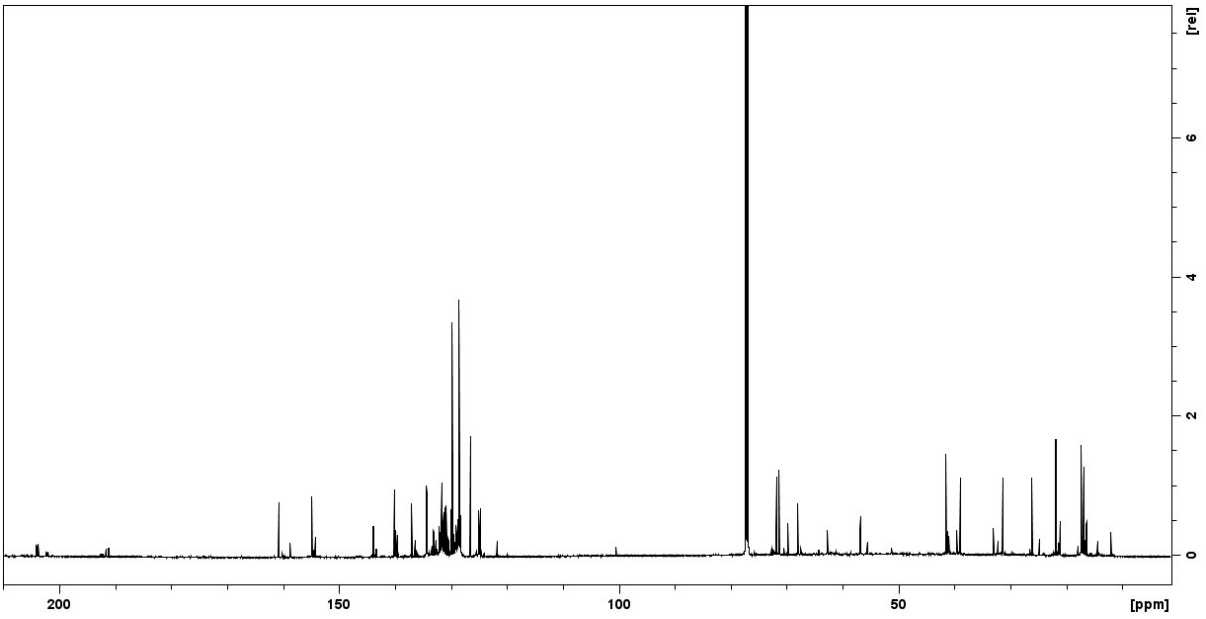

Figure S30. $^{13}C\{^{1}H\}$ (150.9 MHz) NMR spectrum of an approximately 3:1 mixture of the two diastereomers of [Rh(κ^{3}-*N,C,P*-N^{Me}CP)(CO)]PF_6, **14**, recorded in $CDCl_3$. See main text for details.

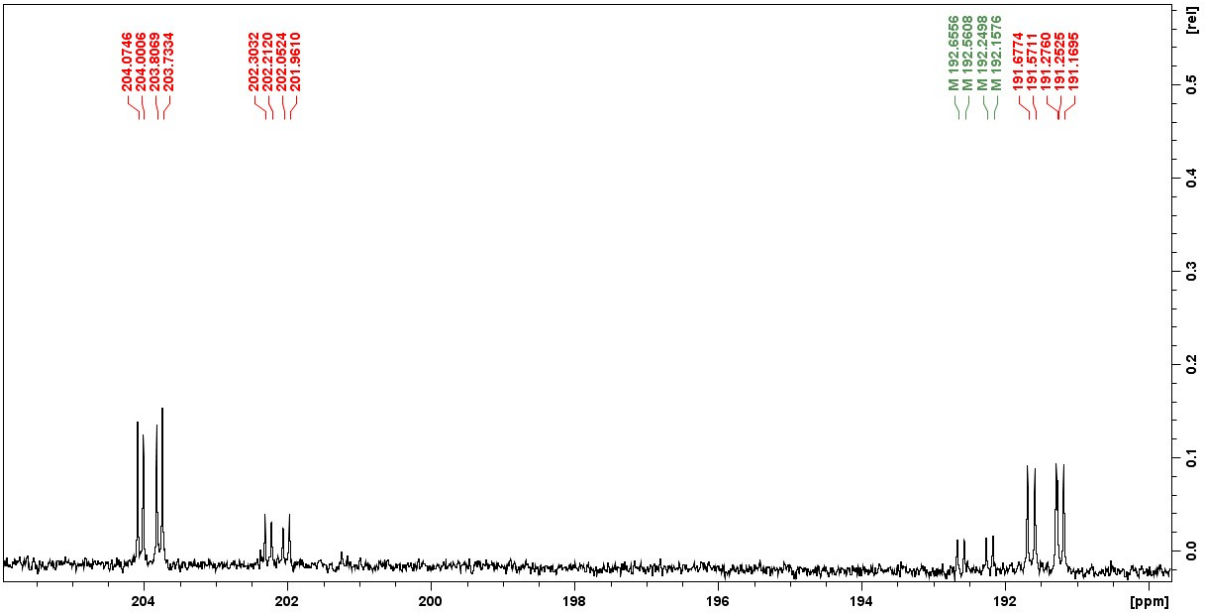

Figure S31. Expansion of the carbonyl and NHC region of the $^{13}C\{^{1}H\}$ (150.9 MHz) NMR spectrum of an approximately 3:1 mixture of the two diastereomers of [Rh(κ^3-*N,C,P*-N^{Me}CP)(CO)]PF_6, **14**, recorded in $CDCl_3$.

Table 1. Crystal data and structure refinement for cmpd2.

Identification code	cmpd2	
Empirical formula	C78 H90 Ag2 Cl10 F18 N6 O7 P4 S2	
Formula weight	2323.79	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 19.7186(6) Å	α= 90°.
	b = 10.8796(2) Å	β= 93.680(2)°.
	c = 23.3108(6) Å	γ = 90°.
Volume	4990.6(2) $Å^3$	
Z	2	
Density (calculated)	1.546 Mg/m^3	
Absorption coefficient	7.352 mm^{-1}	
F(000)	2348	
Crystal size	0.280 x 0.224 x 0.120 mm^3	
Theta range for data collection	3.800 to 73.554°.	
Index ranges	-24<=h<=20, -11<=k<=13, -28<=l<=19	
Reflections collected	21155	
Independent reflections	14570 [R(int) = 0.0431]	
Completeness to theta = 67.684°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.49787	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14570 / 14 / 1153	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0870, wR2 = 0.2411	
R indices (all data)	R1 = 0.0941, wR2 = 0.2493	
Absolute structure parameter	0.074(8)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.638 and -0.984 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cmpd2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2278(6)	6105(13)	3329(6)	37(3)
C(2)	1741(8)	5300(15)	3344(8)	55(4)
C(3)	1219(9)	5620(14)	3654(9)	58(4)
C(4)	1220(7)	6725(14)	3949(7)	47(3)
C(5)	1782(6)	7466(12)	3921(5)	31(2)
C(6)	1830(7)	8668(12)	4247(6)	43(3)
C(7)	1858(8)	8456(16)	4907(6)	54(3)
C(8)	1141(7)	9610(12)	3502(5)	35(3)
C(9)	888(7)	10360(12)	4428(5)	38(3)
C(10)	1203(8)	11638(14)	4371(7)	48(3)
C(11)	788(8)	12225(13)	3838(7)	48(3)
C(12)	291(7)	11195(13)	3644(6)	40(3)
C(13)	161(8)	10482(12)	4200(6)	42(3)
C(14)	-219(8)	9251(13)	4103(7)	49(3)
C(15)	-243(9)	11244(18)	4608(7)	61(4)
C(16)	-383(9)	11683(19)	3322(8)	63(4)
C(17)	693(7)	10604(15)	2653(6)	42(3)
C(18)	239(6)	9825(13)	2267(6)	38(3)
C(19)	220(7)	9976(12)	1663(6)	38(3)
C(20)	-203(7)	9213(15)	1308(7)	49(3)
C(21)	-593(8)	8297(19)	1533(9)	65(5)
C(22)	-582(8)	8139(14)	2119(8)	51(4)
C(23)	-166(7)	8863(12)	2480(7)	42(3)
C(24)	301(8)	12580(13)	1614(6)	41(3)
C(25)	675(9)	13592(13)	1815(7)	53(4)
C(26)	359(11)	14580(15)	2040(8)	65(5)
C(27)	-335(12)	14595(16)	2067(7)	66(5)
C(28)	-713(9)	13605(18)	1840(8)	62(4)
C(29)	-395(8)	12607(17)	1651(8)	56(4)
C(30)	538(7)	11103(16)	601(6)	46(3)
C(31)	910(11)	10230(19)	292(8)	70(5)
C(32)	748(12)	10110(20)	-276(10)	80(6)
C(33)	241(14)	10870(30)	-576(9)	93(8)

C(34)	-111(14)	11700(30)	-284(8)	88(7)
C(35)	60(11)	11813(19)	287(7)	69(5)
C(36)	2811(7)	13512(15)	1673(7)	47(3)
C(37)	3322(8)	14399(15)	1725(7)	52(4)
C(38)	3873(8)	14230(15)	1406(8)	55(4)
C(39)	3907(8)	13227(14)	1056(7)	50(3)
C(40)	3375(7)	12361(11)	1032(6)	37(3)
C(41)	3438(7)	11256(14)	628(5)	40(3)
C(42)	2800(8)	10645(15)	405(6)	50(3)
C(43)	3960(6)	10205(12)	1488(6)	35(3)
C(44)	4403(8)	9691(12)	569(6)	46(3)
C(45)	5094(9)	10221(15)	652(6)	54(4)
C(46)	5434(8)	9663(19)	1213(8)	63(4)
C(47)	4891(8)	8755(13)	1420(6)	45(3)
C(48)	4490(8)	8386(14)	849(6)	49(3)
C(49)	3836(10)	7707(14)	916(8)	64(5)
C(50)	4937(11)	7580(15)	470(7)	65(5)
C(51)	5175(12)	7710(20)	1760(9)	85(7)
C(52)	4331(7)	9297(12)	2376(5)	35(3)
C(53)	4802(6)	10052(11)	2759(6)	35(3)
C(54)	4880(7)	9744(13)	3357(6)	37(3)
C(55)	5324(7)	10443(14)	3732(6)	42(3)
C(56)	5696(8)	11385(17)	3502(7)	56(4)
C(57)	5616(9)	11685(15)	2925(8)	54(4)
C(58)	5166(7)	11042(13)	2560(6)	46(3)
C(59)	4820(7)	7148(15)	3370(6)	38(3)
C(60)	4444(8)	6128(16)	3191(6)	47(3)
C(61)	4763(10)	5081(16)	2958(7)	58(4)
C(62)	5441(10)	5130(18)	2891(8)	60(5)
C(63)	5810(10)	6139(16)	3062(8)	65(5)
C(64)	5506(8)	7145(14)	3315(6)	45(3)
C(65)	4609(5)	8520(14)	4404(5)	34(3)
C(66)	4234(8)	9294(14)	4749(6)	46(3)
C(67)	4397(10)	9314(16)	5352(6)	55(4)
C(68)	4921(10)	8662(18)	5590(7)	65(5)
C(69)	5263(10)	7873(17)	5269(7)	59(4)
C(70)	5123(9)	7780(19)	4663(7)	57(4)
C(71)	3179(7)	12567(14)	3388(7)	44(3)

C(72)	1963(8)	7036(16)	1593(6)	45(3)
C(73)	7631(15)	6150(30)	2128(17)	137(14)
C(74)	7631(17)	3010(30)	3230(12)	108(9)
C(75)	7503(12)	7060(20)	4168(11)	85(6)
C(76)	3213(17)	4880(20)	5058(12)	116(10)
C(77)	2097(19)	3950(40)	9530(20)	180(20)
C(78)	8126(12)	770(30)	2077(10)	95(7)
N(1)	2300(5)	7176(10)	3605(5)	34(2)
N(2)	1247(5)	9492(10)	4065(5)	35(2)
N(3)	678(5)	10376(10)	3271(5)	34(2)
N(4)	2844(5)	12491(10)	1325(5)	35(2)
N(5)	3929(6)	10362(10)	920(4)	35(2)
N(6)	4394(6)	9500(11)	1756(4)	38(2)
O(1)	2593(6)	10451(10)	3384(5)	49(2)
O(2)	3059(9)	11179(13)	2505(5)	81(4)
O(3)	2047(6)	12110(12)	2834(6)	65(3)
O(4)	1825(5)	8586(11)	2425(4)	50(3)
O(5)	2935(5)	7686(10)	2311(4)	43(2)
O(6)	2488(6)	9194(9)	1638(5)	50(2)
O(7)	7879(13)	1310(30)	1502(12)	190(12)
F(1)	2901(9)	12891(12)	3866(5)	97(4)
F(2)	3803(6)	12121(14)	3538(7)	104(5)
F(3)	3275(6)	13585(10)	3116(5)	76(3)
F(4)	2356(6)	6677(11)	1207(4)	72(3)
F(5)	1827(6)	6060(9)	1908(5)	69(3)
F(6)	1360(5)	7445(14)	1341(5)	81(4)
F(7)	5333(6)	4238(13)	782(5)	80(3)
F(8)	6473(8)	4610(20)	863(7)	121(6)
F(9)	6560(7)	3585(15)	1717(7)	107(5)
F(10)	5453(8)	3177(17)	1632(7)	115(6)
F(11)	5810(11)	5113(14)	1556(6)	122(6)
F(12)	6084(9)	2650(16)	944(13)	187(13)
F(13)	8579(6)	4926(14)	4017(5)	82(3)
F(14)	8588(6)	6310(20)	3303(7)	133(8)
F(15)	9704(5)	6259(14)	3341(6)	85(4)
F(16)	9696(7)	4843(12)	4066(6)	89(4)
F(17)	9111(10)	4482(17)	3227(6)	119(6)
F(18)	9156(8)	6605(11)	4155(5)	94(4)

P(1)	737(2)	11198(3)	1362(1)	37(1)
P(2)	4385(1)	8471(3)	3640(1)	30(1)
P(3)	5958(3)	3897(5)	1239(2)	63(1)
P(4)	9138(2)	5587(5)	3676(2)	56(1)
S(1)	2673(2)	11460(3)	2988(1)	39(1)
S(2)	2348(2)	8254(3)	2048(1)	35(1)
Ag(1)	3193(1)	8386(1)	3449(1)	38(1)
Ag(2)	1944(1)	11226(1)	1526(1)	43(1)
Cl(1)	7183(8)	7747(17)	1906(7)	217(6)
Cl(2)	8015(4)	5918(8)	1410(6)	161(5)
Cl(3)	7017(3)	3872(6)	3537(5)	121(3)
Cl(4)	7745(4)	1607(7)	3675(4)	110(2)
Cl(5)	7215(3)	8259(8)	3679(3)	104(2)
Cl(6)	6958(3)	6732(6)	4662(3)	93(2)
Cl(7)	2301(3)	4884(5)	4908(2)	78(1)
Cl(8)	3575(4)	6215(7)	4824(3)	105(2)
Cl(9)	2931(5)	4199(14)	9803(5)	172(5)
Cl(10)	1595(6)	3609(11)	10051(6)	168(5)

Table 3. Bond lengths [Å] and angles [°] for cmpd2.

C(1)-N(1)	1.330(18)
C(1)-C(2)	1.38(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.34(2)
C(2)-H(2)	0.9500
C(3)-C(4)	1.38(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.377(18)
C(4)-H(4)	0.9500
C(5)-N(1)	1.335(15)
C(5)-C(6)	1.512(18)
C(6)-N(2)	1.497(17)
C(6)-C(7)	1.553(19)
C(6)-H(6)	1.0000
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-N(2)	1.321(17)
C(8)-N(3)	1.325(17)
C(9)-N(2)	1.479(15)
C(9)-C(13)	1.50(2)
C(9)-C(10)	1.532(19)
C(9)-H(9)	1.0000
C(10)-C(11)	1.58(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.54(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(3)	1.490(16)
C(12)-C(13)	1.545(18)
C(12)-C(16)	1.58(2)
C(13)-C(15)	1.523(19)
C(13)-C(14)	1.544(19)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800

C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-N(3)	1.463(17)
C(17)-C(18)	1.492(19)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.42(2)
C(18)-C(23)	1.424(19)
C(19)-C(20)	1.41(2)
C(19)-P(1)	1.841(15)
C(20)-C(21)	1.38(2)
C(20)-H(20)	0.9500
C(21)-C(22)	1.37(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.38(2)
C(22)-H(22)	0.9500
C(23)-H(23)	0.9500
C(24)-C(29)	1.38(2)
C(24)-C(25)	1.39(2)
C(24)-P(1)	1.846(15)
C(25)-C(26)	1.36(2)
C(25)-H(25)	0.9500
C(26)-C(27)	1.37(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.40(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.34(3)
C(28)-H(28)	0.9500
C(29)-H(29)	0.9500
C(30)-C(35)	1.39(2)
C(30)-C(31)	1.42(3)
C(30)-P(1)	1.794(14)
C(31)-C(32)	1.35(3)

C(31)-H(31)	0.9500
C(32)-C(33)	1.45(4)
C(32)-H(32)	0.9500
C(33)-C(34)	1.35(4)
C(33)-H(33)	0.9500
C(34)-C(35)	1.36(2)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-N(4)	1.379(19)
C(36)-C(37)	1.39(2)
C(36)-H(36)	0.9500
C(37)-C(38)	1.37(2)
C(37)-H(37)	0.9500
C(38)-C(39)	1.37(2)
C(38)-H(38)	0.9500
C(39)-C(40)	1.41(2)
C(39)-H(39)	0.9500
C(40)-N(4)	1.293(16)
C(40)-C(41)	1.537(19)
C(41)-C(42)	1.49(2)
C(41)-N(5)	1.504(16)
C(41)-H(41)	1.0000
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-N(6)	1.282(18)
C(43)-N(5)	1.333(17)
C(44)-N(5)	1.473(17)
C(44)-C(45)	1.48(2)
C(44)-C(48)	1.567(19)
C(44)-H(44)	1.0000
C(45)-C(46)	1.55(3)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.56(2)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(51)	1.47(2)

C(47)-N(6)	1.527(17)
C(47)-C(48)	1.56(2)
C(48)-C(49)	1.50(2)
C(48)-C(50)	1.559(19)
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-N(6)	1.476(15)
C(52)-C(53)	1.492(17)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(58)	1.390(17)
C(53)-C(54)	1.43(2)
C(54)-C(55)	1.417(19)
C(54)-P(2)	1.841(14)
C(55)-C(56)	1.39(2)
C(55)-H(55)	0.9500
C(56)-C(57)	1.38(3)
C(56)-H(56)	0.9500
C(57)-C(58)	1.38(2)
C(57)-H(57)	0.9500
C(58)-H(58)	0.9500
C(59)-C(64)	1.37(2)
C(59)-C(60)	1.38(2)
C(59)-P(2)	1.810(16)
C(60)-C(61)	1.42(2)
C(60)-H(60)	0.9500
C(61)-C(62)	1.36(3)
C(61)-H(61)	0.9500
C(62)-C(63)	1.36(3)
C(62)-H(62)	0.9500
C(63)-C(64)	1.40(2)

C(63)-H(63)	0.9500
C(64)-H(64)	0.9500
C(65)-C(70)	1.40(2)
C(65)-C(66)	1.407(19)
C(65)-P(2)	1.806(11)
C(66)-C(67)	1.42(2)
C(66)-H(66)	0.9500
C(67)-C(68)	1.34(3)
C(67)-H(67)	0.9500
C(68)-C(69)	1.35(3)
C(68)-H(68)	0.9500
C(69)-C(70)	1.42(2)
C(69)-H(69)	0.9500
C(70)-H(70)	0.9500
C(71)-F(3)	1.30(2)
C(71)-F(1)	1.320(18)
C(71)-F(2)	1.349(19)
C(71)-S(1)	1.788(15)
C(72)-F(4)	1.285(18)
C(72)-F(5)	1.328(18)
C(72)-F(6)	1.364(18)
C(72)-S(2)	1.833(17)
C(73)-Cl(2)	1.90(3)
C(73)-Cl(1)	2.01(4)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(74)-Cl(3)	1.72(3)
C(74)-Cl(4)	1.85(3)
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-Cl(6)	1.66(2)
C(75)-Cl(5)	1.80(3)
C(75)-H(75A)	0.9900
C(75)-H(75B)	0.9900
C(76)-Cl(8)	1.72(3)
C(76)-Cl(7)	1.81(3)
C(76)-H(76A)	0.9900
C(76)-H(76B)	0.9900

C(77)-Cl(10)	1.66(5)
C(77)-Cl(9)	1.75(3)
C(77)-H(77A)	0.9900
C(77)-H(77B)	0.9900
C(78)-O(7)	1.519(12)
C(78)-H(78A)	0.9800
C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
N(1)-Ag(1)	2.247(10)
N(4)-Ag(2)	2.319(10)
O(1)-S(1)	1.449(11)
O(1)-Ag(1)	2.538(11)
O(2)-S(1)	1.433(11)
O(3)-S(1)	1.447(12)
O(4)-S(2)	1.443(10)
O(5)-S(2)	1.416(11)
O(6)-S(2)	1.439(10)
O(6)-Ag(2)	2.464(11)
F(7)-P(3)	1.621(14)
F(8)-P(3)	1.583(15)
F(9)-P(3)	1.610(15)
F(10)-P(3)	1.600(14)
F(11)-P(3)	1.552(15)
F(12)-P(3)	1.549(14)
F(13)-P(4)	1.575(11)
F(14)-P(4)	1.559(14)
F(15)-P(4)	1.581(11)
F(16)-P(4)	1.601(13)
F(17)-P(4)	1.593(16)
F(18)-P(4)	1.571(13)
P(1)-Ag(2)	2.386(3)
P(2)-Ag(1)	2.367(3)

N(1)-C(1)-C(2)	123.1(12)
N(1)-C(1)-H(1)	118.4
C(2)-C(1)-H(1)	118.4
C(3)-C(2)-C(1)	117.8(15)
C(3)-C(2)-H(2)	121.1

C(1)-C(2)-H(2)	121.1
C(2)-C(3)-C(4)	121.1(15)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	117.4(14)
C(5)-C(4)-H(4)	121.3
C(3)-C(4)-H(4)	121.3
N(1)-C(5)-C(4)	122.3(12)
N(1)-C(5)-C(6)	117.2(11)
C(4)-C(5)-C(6)	120.5(12)
N(2)-C(6)-C(5)	110.7(11)
N(2)-C(6)-C(7)	110.4(11)
C(5)-C(6)-C(7)	111.5(11)
N(2)-C(6)-H(6)	108.0
C(5)-C(6)-H(6)	108.0
C(7)-C(6)-H(6)	108.0
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(2)-C(8)-N(3)	121.8(12)
N(2)-C(9)-C(13)	109.6(11)
N(2)-C(9)-C(10)	108.6(10)
C(13)-C(9)-C(10)	105.8(11)
N(2)-C(9)-H(9)	110.9
C(13)-C(9)-H(9)	110.9
C(10)-C(9)-H(9)	110.9
C(9)-C(10)-C(11)	104.1(12)
C(9)-C(10)-H(10A)	110.9
C(11)-C(10)-H(10A)	110.9
C(9)-C(10)-H(10B)	110.9
C(11)-C(10)-H(10B)	110.9
H(10A)-C(10)-H(10B)	109.0
C(12)-C(11)-C(10)	103.0(11)
C(12)-C(11)-H(11A)	111.2
C(10)-C(11)-H(11A)	111.2

C(12)-C(11)-H(11B)	111.2
C(10)-C(11)-H(11B)	111.2
H(11A)-C(11)-H(11B)	109.1
N(3)-C(12)-C(11)	105.5(10)
N(3)-C(12)-C(13)	108.0(11)
C(11)-C(12)-C(13)	104.9(11)
N(3)-C(12)-C(16)	111.7(12)
C(11)-C(12)-C(16)	113.4(13)
C(13)-C(12)-C(16)	112.8(12)
C(9)-C(13)-C(15)	110.6(12)
C(9)-C(13)-C(14)	114.7(11)
C(15)-C(13)-C(14)	107.2(13)
C(9)-C(13)-C(12)	97.7(11)
C(15)-C(13)-C(12)	111.8(11)
C(14)-C(13)-C(12)	114.7(12)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(12)-C(16)-H(16A)	109.5
C(12)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(12)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(3)-C(17)-C(18)	116.6(12)
N(3)-C(17)-H(17A)	108.2
C(18)-C(17)-H(17A)	108.2
N(3)-C(17)-H(17B)	108.2
C(18)-C(17)-H(17B)	108.2

H(17A)-C(17)-H(17B)	107.3
C(19)-C(18)-C(23)	116.8(13)
C(19)-C(18)-C(17)	120.7(12)
C(23)-C(18)-C(17)	122.4(13)
C(20)-C(19)-C(18)	119.5(14)
C(20)-C(19)-P(1)	121.6(11)
C(18)-C(19)-P(1)	118.9(10)
C(21)-C(20)-C(19)	121.8(16)
C(21)-C(20)-H(20)	119.1
C(19)-C(20)-H(20)	119.1
C(22)-C(21)-C(20)	119.5(15)
C(22)-C(21)-H(21)	120.2
C(20)-C(21)-H(21)	120.2
C(21)-C(22)-C(23)	120.3(15)
C(21)-C(22)-H(22)	119.9
C(23)-C(22)-H(22)	119.9
C(22)-C(23)-C(18)	122.1(15)
C(22)-C(23)-H(23)	119.0
C(18)-C(23)-H(23)	119.0
C(29)-C(24)-C(25)	118.0(15)
C(29)-C(24)-P(1)	121.5(13)
C(25)-C(24)-P(1)	120.4(13)
C(26)-C(25)-C(24)	120.6(17)
C(26)-C(25)-H(25)	119.7
C(24)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	120.5(18)
C(25)-C(26)-H(26)	119.8
C(27)-C(26)-H(26)	119.8
C(26)-C(27)-C(28)	118.9(17)
C(26)-C(27)-H(27)	120.5
C(28)-C(27)-H(27)	120.5
C(29)-C(28)-C(27)	119.9(17)
C(29)-C(28)-H(28)	120.1
C(27)-C(28)-H(28)	120.1
C(28)-C(29)-C(24)	121.7(17)
C(28)-C(29)-H(29)	119.1
C(24)-C(29)-H(29)	119.1
C(35)-C(30)-C(31)	117.2(16)

C(35)-C(30)-P(1)	125.9(14)
C(31)-C(30)-P(1)	116.9(14)
C(32)-C(31)-C(30)	118(2)
C(32)-C(31)-H(31)	121.1
C(30)-C(31)-H(31)	121.1
C(31)-C(32)-C(33)	122(2)
C(31)-C(32)-H(32)	119.0
C(33)-C(32)-H(32)	119.0
C(34)-C(33)-C(32)	120.3(19)
C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	117(2)
C(33)-C(34)-H(34)	121.6
C(35)-C(34)-H(34)	121.6
C(34)-C(35)-C(30)	126(2)
C(34)-C(35)-H(35)	117.1
C(30)-C(35)-H(35)	117.1
N(4)-C(36)-C(37)	123.2(13)
N(4)-C(36)-H(36)	118.4
C(37)-C(36)-H(36)	118.4
C(38)-C(37)-C(36)	117.0(15)
C(38)-C(37)-H(37)	121.5
C(36)-C(37)-H(37)	121.5
C(39)-C(38)-C(37)	120.1(14)
C(39)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9
C(38)-C(39)-C(40)	119.6(13)
C(38)-C(39)-H(39)	120.2
C(40)-C(39)-H(39)	120.2
N(4)-C(40)-C(39)	122.1(13)
N(4)-C(40)-C(41)	120.7(12)
C(39)-C(40)-C(41)	117.2(12)
C(42)-C(41)-N(5)	112.0(12)
C(42)-C(41)-C(40)	117.6(11)
N(5)-C(41)-C(40)	107.7(10)
C(42)-C(41)-H(41)	106.3
N(5)-C(41)-H(41)	106.3
C(40)-C(41)-H(41)	106.3

C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(6)-C(43)-N(5)	123.2(12)
N(5)-C(44)-C(45)	110.2(12)
N(5)-C(44)-C(48)	105.9(10)
C(45)-C(44)-C(48)	102.8(13)
N(5)-C(44)-H(44)	112.4
C(45)-C(44)-H(44)	112.4
C(48)-C(44)-H(44)	112.4
C(44)-C(45)-C(46)	107.5(12)
C(44)-C(45)-H(45A)	110.2
C(46)-C(45)-H(45A)	110.2
C(44)-C(45)-H(45B)	110.2
C(46)-C(45)-H(45B)	110.2
H(45A)-C(45)-H(45B)	108.5
C(45)-C(46)-C(47)	104.0(13)
C(45)-C(46)-H(46A)	111.0
C(47)-C(46)-H(46A)	111.0
C(45)-C(46)-H(46B)	111.0
C(47)-C(46)-H(46B)	111.0
H(46A)-C(46)-H(46B)	109.0
C(51)-C(47)-N(6)	111.6(12)
C(51)-C(47)-C(46)	114.3(16)
N(6)-C(47)-C(46)	107.4(12)
C(51)-C(47)-C(48)	114.5(15)
N(6)-C(47)-C(48)	105.5(11)
C(46)-C(47)-C(48)	102.7(12)
C(49)-C(48)-C(47)	115.5(12)
C(49)-C(48)-C(50)	107.6(14)
C(47)-C(48)-C(50)	110.8(13)
C(49)-C(48)-C(44)	114.5(13)
C(47)-C(48)-C(44)	99.2(12)
C(50)-C(48)-C(44)	108.9(11)
C(48)-C(49)-H(49A)	109.5

C(48)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(48)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(48)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(47)-C(51)-H(51A)	109.5
C(47)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(47)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
N(6)-C(52)-C(53)	114.5(11)
N(6)-C(52)-H(52A)	108.6
C(53)-C(52)-H(52A)	108.6
N(6)-C(52)-H(52B)	108.6
C(53)-C(52)-H(52B)	108.6
H(52A)-C(52)-H(52B)	107.6
C(58)-C(53)-C(54)	118.7(13)
C(58)-C(53)-C(52)	122.8(13)
C(54)-C(53)-C(52)	118.5(11)
C(55)-C(54)-C(53)	119.9(13)
C(55)-C(54)-P(2)	120.1(11)
C(53)-C(54)-P(2)	119.9(10)
C(56)-C(55)-C(54)	118.7(14)
C(56)-C(55)-H(55)	120.7
C(54)-C(55)-H(55)	120.7
C(57)-C(56)-C(55)	121.2(15)
C(57)-C(56)-H(56)	119.4
C(55)-C(56)-H(56)	119.4
C(58)-C(57)-C(56)	120.6(15)
C(58)-C(57)-H(57)	119.7
C(56)-C(57)-H(57)	119.7

C(57)-C(58)-C(53)	120.8(14)
C(57)-C(58)-H(58)	119.6
C(53)-C(58)-H(58)	119.6
C(64)-C(59)-C(60)	118.9(15)
C(64)-C(59)-P(2)	121.9(12)
C(60)-C(59)-P(2)	119.2(11)
C(59)-C(60)-C(61)	121.1(15)
C(59)-C(60)-H(60)	119.5
C(61)-C(60)-H(60)	119.5
C(62)-C(61)-C(60)	118.3(17)
C(62)-C(61)-H(61)	120.9
C(60)-C(61)-H(61)	120.9
C(61)-C(62)-C(63)	120.6(17)
C(61)-C(62)-H(62)	119.7
C(63)-C(62)-H(62)	119.7
C(62)-C(63)-C(64)	121.3(17)
C(62)-C(63)-H(63)	119.3
C(64)-C(63)-H(63)	119.3
C(59)-C(64)-C(63)	119.7(16)
C(59)-C(64)-H(64)	120.2
C(63)-C(64)-H(64)	120.2
C(70)-C(65)-C(66)	119.4(12)
C(70)-C(65)-P(2)	122.1(11)
C(66)-C(65)-P(2)	118.5(10)
C(65)-C(66)-C(67)	118.7(15)
C(65)-C(66)-H(66)	120.6
C(67)-C(66)-H(66)	120.6
C(68)-C(67)-C(66)	121.2(15)
C(68)-C(67)-H(67)	119.4
C(66)-C(67)-H(67)	119.4
C(67)-C(68)-C(69)	120.4(15)
C(67)-C(68)-H(68)	119.8
C(69)-C(68)-H(68)	119.8
C(68)-C(69)-C(70)	121.6(17)
C(68)-C(69)-H(69)	119.2
C(70)-C(69)-H(69)	119.2
C(65)-C(70)-C(69)	118.4(15)
C(65)-C(70)-H(70)	120.8

C(69)-C(70)-H(70)	120.8
F(3)-C(71)-F(1)	105.5(13)
F(3)-C(71)-F(2)	105.9(14)
F(1)-C(71)-F(2)	107.4(15)
F(3)-C(71)-S(1)	114.5(11)
F(1)-C(71)-S(1)	111.8(11)
F(2)-C(71)-S(1)	111.3(11)
F(4)-C(72)-F(5)	107.2(14)
F(4)-C(72)-F(6)	110.3(13)
F(5)-C(72)-F(6)	107.3(14)
F(4)-C(72)-S(2)	112.2(11)
F(5)-C(72)-S(2)	110.3(10)
F(6)-C(72)-S(2)	109.3(12)
Cl(2)-C(73)-Cl(1)	94.6(17)
Cl(2)-C(73)-H(73A)	112.8
Cl(1)-C(73)-H(73A)	112.8
Cl(2)-C(73)-H(73B)	112.8
Cl(1)-C(73)-H(73B)	112.8
H(73A)-C(73)-H(73B)	110.3
Cl(3)-C(74)-Cl(4)	106.1(15)
Cl(3)-C(74)-H(74A)	110.5
Cl(4)-C(74)-H(74A)	110.5
Cl(3)-C(74)-H(74B)	110.5
Cl(4)-C(74)-H(74B)	110.5
H(74A)-C(74)-H(74B)	108.7
Cl(6)-C(75)-Cl(5)	113.7(14)
Cl(6)-C(75)-H(75A)	108.8
Cl(5)-C(75)-H(75A)	108.8
Cl(6)-C(75)-H(75B)	108.8
Cl(5)-C(75)-H(75B)	108.8
H(75A)-C(75)-H(75B)	107.7
Cl(8)-C(76)-Cl(7)	111.5(15)
Cl(8)-C(76)-H(76A)	109.3
Cl(7)-C(76)-H(76A)	109.3
Cl(8)-C(76)-H(76B)	109.3
Cl(7)-C(76)-H(76B)	109.3
H(76A)-C(76)-H(76B)	108.0
Cl(10)-C(77)-Cl(9)	111(2)

Cl(10)-C(77)-H(77A)	109.5
Cl(9)-C(77)-H(77A)	109.5
Cl(10)-C(77)-H(77B)	109.5
Cl(9)-C(77)-H(77B)	109.5
H(77A)-C(77)-H(77B)	108.1
O(7)-C(78)-H(78A)	109.5
O(7)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
O(7)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(1)-N(1)-C(5)	118.2(11)
C(1)-N(1)-Ag(1)	115.9(8)
C(5)-N(1)-Ag(1)	125.8(9)
C(8)-N(2)-C(9)	117.0(11)
C(8)-N(2)-C(6)	114.2(11)
C(9)-N(2)-C(6)	127.4(11)
C(8)-N(3)-C(17)	116.8(11)
C(8)-N(3)-C(12)	120.2(11)
C(17)-N(3)-C(12)	121.1(11)
C(40)-N(4)-C(36)	118.0(11)
C(40)-N(4)-Ag(2)	134.2(9)
C(36)-N(4)-Ag(2)	107.1(8)
C(43)-N(5)-C(44)	119.9(11)
C(43)-N(5)-C(41)	121.2(10)
C(44)-N(5)-C(41)	118.8(10)
C(43)-N(6)-C(52)	118.2(11)
C(43)-N(6)-C(47)	119.9(11)
C(52)-N(6)-C(47)	121.3(11)
S(1)-O(1)-Ag(1)	129.8(6)
S(2)-O(6)-Ag(2)	127.4(6)
C(30)-P(1)-C(19)	104.1(7)
C(30)-P(1)-C(24)	106.6(7)
C(19)-P(1)-C(24)	100.7(6)
C(30)-P(1)-Ag(2)	108.2(5)
C(19)-P(1)-Ag(2)	121.2(4)
C(24)-P(1)-Ag(2)	114.7(5)
C(65)-P(2)-C(59)	106.0(6)

C(65)-P(2)-C(54)	103.4(6)
C(59)-P(2)-C(54)	101.5(6)
C(65)-P(2)-Ag(1)	111.3(3)
C(59)-P(2)-Ag(1)	113.0(5)
C(54)-P(2)-Ag(1)	120.3(5)
F(12)-P(3)-F(11)	177.2(13)
F(12)-P(3)-F(8)	93.1(13)
F(11)-P(3)-F(8)	89.7(11)
F(12)-P(3)-F(10)	87.1(13)
F(11)-P(3)-F(10)	90.1(10)
F(8)-P(3)-F(10)	178.6(10)
F(12)-P(3)-F(9)	89.4(12)
F(11)-P(3)-F(9)	90.2(10)
F(8)-P(3)-F(9)	90.9(9)
F(10)-P(3)-F(9)	87.7(9)
F(12)-P(3)-F(7)	92.6(11)
F(11)-P(3)-F(7)	87.7(9)
F(8)-P(3)-F(7)	90.7(8)
F(10)-P(3)-F(7)	90.7(7)
F(9)-P(3)-F(7)	177.4(8)
F(14)-P(4)-F(18)	91.5(11)
F(14)-P(4)-F(13)	91.5(7)
F(18)-P(4)-F(13)	87.0(8)
F(14)-P(4)-F(15)	88.9(7)
F(18)-P(4)-F(15)	92.3(8)
F(13)-P(4)-F(15)	179.2(9)
F(14)-P(4)-F(17)	91.2(12)
F(18)-P(4)-F(17)	175.7(8)
F(13)-P(4)-F(17)	89.5(8)
F(15)-P(4)-F(17)	91.2(8)
F(14)-P(4)-F(16)	179.2(8)
F(18)-P(4)-F(16)	88.2(8)
F(13)-P(4)-F(16)	87.7(7)
F(15)-P(4)-F(16)	91.9(7)
F(17)-P(4)-F(16)	89.1(9)
O(2)-S(1)-O(3)	113.3(9)
O(2)-S(1)-O(1)	115.1(8)
O(3)-S(1)-O(1)	113.8(7)

O(2)-S(1)-C(71)	104.3(8)
O(3)-S(1)-C(71)	103.8(7)
O(1)-S(1)-C(71)	105.0(7)
O(5)-S(2)-O(6)	114.3(6)
O(5)-S(2)-O(4)	116.2(6)
O(6)-S(2)-O(4)	113.7(7)
O(5)-S(2)-C(72)	103.4(7)
O(6)-S(2)-C(72)	102.6(7)
O(4)-S(2)-C(72)	104.4(7)
N(1)-Ag(1)-P(2)	140.5(3)
N(1)-Ag(1)-O(1)	99.3(4)
P(2)-Ag(1)-O(1)	115.5(3)
N(4)-Ag(2)-P(1)	138.1(3)
N(4)-Ag(2)-O(6)	102.7(4)
P(1)-Ag(2)-O(6)	115.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cmpd2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	47(6)	27(6)	40(6)	1(6)	13(5)	0(5)
C(2)	59(9)	33(8)	74(11)	-12(8)	1(7)	-10(7)
C(3)	62(9)	17(6)	98(13)	14(8)	14(8)	-1(6)
C(4)	45(7)	29(7)	68(9)	7(7)	16(6)	-4(6)
C(5)	30(5)	25(6)	40(6)	0(5)	19(4)	3(4)
C(6)	58(8)	26(7)	46(7)	2(5)	6(6)	5(5)
C(7)	77(9)	43(8)	41(7)	-6(7)	4(6)	14(8)
C(8)	45(6)	25(6)	35(6)	3(5)	7(5)	-5(5)
C(9)	58(7)	22(6)	37(6)	-5(5)	22(5)	0(5)
C(10)	60(8)	29(7)	56(8)	-6(6)	17(7)	-7(6)
C(11)	70(9)	23(6)	53(8)	1(6)	17(7)	-1(6)
C(12)	55(7)	20(6)	45(7)	-1(6)	14(5)	2(6)
C(13)	70(8)	17(6)	42(7)	0(5)	18(6)	4(6)
C(14)	62(8)	27(7)	61(9)	8(6)	18(7)	-4(6)
C(15)	71(9)	51(9)	64(9)	12(8)	29(7)	21(9)
C(16)	63(10)	53(10)	74(11)	4(9)	5(8)	17(8)
C(17)	41(6)	38(7)	45(7)	8(6)	3(5)	-5(6)
C(18)	41(6)	25(6)	50(8)	6(6)	5(5)	-1(5)
C(19)	52(7)	21(6)	39(7)	-2(5)	-7(5)	2(5)
C(20)	51(8)	35(8)	60(9)	1(7)	-7(6)	-8(6)
C(21)	63(9)	47(10)	84(12)	-17(10)	-4(8)	-22(9)
C(22)	55(8)	31(8)	69(10)	-3(7)	12(7)	-13(6)
C(23)	49(7)	19(6)	60(8)	3(6)	8(6)	-1(5)
C(24)	69(9)	20(6)	35(6)	7(5)	4(6)	4(6)
C(25)	85(10)	20(7)	54(8)	4(6)	-4(7)	-5(7)
C(26)	96(14)	23(7)	73(12)	0(8)	-8(10)	15(8)
C(27)	127(17)	27(8)	44(9)	1(7)	15(9)	10(9)
C(28)	70(10)	45(10)	72(11)	3(8)	1(8)	0(8)
C(29)	50(8)	42(9)	74(11)	13(8)	-2(7)	1(7)
C(30)	46(7)	46(9)	47(7)	-7(7)	2(5)	-12(7)
C(31)	99(14)	54(11)	58(10)	-14(9)	11(9)	-29(10)
C(32)	105(16)	47(11)	89(15)	-17(10)	17(12)	-21(11)
C(33)	130(20)	92(19)	51(11)	-18(12)	-21(12)	-25(16)

C(34)	135(19)	89(17)	37(9)	10(11)	-25(10)	-6(15)
C(35)	109(15)	55(11)	40(8)	8(8)	-18(9)	2(10)
C(36)	52(7)	31(7)	60(8)	4(7)	13(6)	5(6)
C(37)	75(10)	27(7)	55(9)	3(6)	17(7)	4(7)
C(38)	54(8)	29(7)	84(11)	1(7)	17(8)	-11(6)
C(39)	57(8)	25(7)	72(9)	4(7)	22(7)	-1(6)
C(40)	48(7)	16(6)	48(7)	8(5)	17(5)	2(5)
C(41)	55(7)	34(7)	31(6)	9(5)	9(5)	8(6)
C(42)	68(9)	38(7)	44(7)	1(6)	0(6)	-5(7)
C(43)	42(6)	29(7)	36(6)	0(5)	10(5)	-4(5)
C(44)	85(10)	21(6)	34(6)	4(5)	19(6)	8(6)
C(45)	82(11)	37(8)	46(8)	7(6)	34(7)	10(7)
C(46)	55(9)	67(11)	69(10)	-5(9)	27(8)	-7(8)
C(47)	65(8)	35(8)	36(6)	4(6)	13(6)	15(6)
C(48)	79(9)	29(7)	41(7)	-4(6)	23(6)	12(7)
C(49)	104(14)	21(7)	68(11)	-3(7)	21(9)	2(8)
C(50)	119(15)	27(7)	50(8)	-8(6)	28(9)	18(8)
C(51)	114(16)	77(15)	66(11)	36(11)	25(11)	51(13)
C(52)	63(7)	17(5)	26(5)	0(4)	-1(5)	-9(5)
C(53)	39(6)	16(5)	51(7)	-6(5)	14(5)	-9(5)
C(54)	45(7)	29(7)	37(7)	-6(6)	4(5)	-3(5)
C(55)	52(7)	35(7)	39(7)	-12(6)	-1(5)	-6(6)
C(56)	59(8)	44(9)	66(10)	-12(8)	9(7)	-15(7)
C(57)	62(9)	26(7)	77(11)	-13(7)	26(8)	-13(6)
C(58)	61(8)	27(7)	52(8)	10(6)	20(6)	-7(6)
C(59)	40(7)	46(8)	30(6)	12(6)	11(5)	0(6)
C(60)	66(8)	42(8)	33(6)	-4(7)	-2(5)	-5(7)
C(61)	99(13)	29(8)	46(8)	-10(7)	17(8)	10(8)
C(62)	81(12)	48(10)	53(9)	11(8)	17(8)	22(9)
C(63)	88(11)	29(8)	81(11)	20(8)	37(9)	26(8)
C(64)	57(8)	31(7)	48(8)	2(6)	12(6)	1(6)
C(65)	30(5)	44(7)	28(5)	7(6)	7(4)	2(5)
C(66)	77(9)	29(7)	32(6)	-4(5)	8(6)	0(6)
C(67)	96(12)	44(9)	28(6)	-5(6)	15(7)	2(8)
C(68)	106(13)	55(11)	32(7)	-1(7)	-3(7)	0(10)
C(69)	87(12)	47(9)	42(8)	7(7)	-14(8)	-5(8)
C(70)	66(9)	65(11)	38(7)	-5(8)	-2(6)	22(8)
C(71)	52(8)	28(7)	52(8)	-6(6)	8(6)	-1(6)

C(72)	57(8)	40(9)	39(7)	8(6)	0(6)	0(6)
C(73)	130(20)	70(17)	220(40)	-10(20)	100(20)	-32(17)
C(74)	160(30)	67(15)	101(18)	-11(14)	36(17)	20(16)
C(75)	88(14)	68(14)	97(16)	-15(12)	5(12)	-18(11)
C(76)	200(30)	51(13)	98(19)	25(13)	36(19)	8(17)
C(77)	180(40)	100(30)	230(50)	60(30)	-90(30)	-30(30)
C(78)	95(13)	90(15)	105(14)	-5(12)	52(12)	5(12)
N(1)	38(5)	27(5)	36(5)	9(4)	11(4)	-8(4)
N(2)	45(6)	26(5)	34(5)	1(4)	10(4)	2(4)
N(3)	44(5)	20(5)	39(5)	1(4)	6(4)	2(4)
N(4)	42(5)	21(5)	40(6)	3(4)	7(4)	-6(4)
N(5)	58(6)	18(5)	32(5)	1(4)	9(4)	3(4)
N(6)	59(6)	28(6)	29(5)	3(4)	11(4)	-1(5)
O(1)	67(6)	34(6)	49(6)	4(5)	19(5)	0(5)
O(2)	153(12)	42(7)	55(7)	-18(6)	56(8)	-10(8)
O(3)	52(6)	50(7)	89(9)	12(6)	-14(6)	-2(5)
O(4)	65(6)	48(7)	37(5)	-1(5)	5(4)	7(5)
O(5)	47(5)	43(6)	40(5)	4(4)	9(4)	-9(4)
O(6)	73(7)	23(5)	55(6)	14(5)	12(5)	-2(5)
O(7)	148(16)	180(20)	240(20)	-33(19)	-64(16)	-27(17)
F(1)	189(14)	50(7)	52(6)	-30(5)	21(7)	-3(8)
F(2)	79(7)	77(9)	149(13)	-16(9)	-58(8)	10(6)
F(3)	91(7)	39(6)	95(8)	-7(6)	1(6)	-23(5)
F(4)	109(8)	57(6)	52(5)	-22(5)	18(5)	3(6)
F(5)	94(7)	30(5)	82(7)	3(5)	1(5)	-24(5)
F(6)	67(6)	97(10)	75(7)	-16(7)	-28(5)	-1(6)
F(7)	90(7)	80(8)	71(7)	8(6)	24(6)	-2(7)
F(8)	101(10)	164(19)	103(10)	30(11)	31(8)	-34(11)
F(9)	106(9)	73(9)	137(12)	5(9)	-34(8)	-9(8)
F(10)	112(10)	103(12)	131(12)	64(11)	22(9)	-12(9)
F(11)	230(20)	64(9)	71(8)	-2(7)	41(10)	36(11)
F(12)	111(12)	83(12)	370(40)	-138(18)	30(16)	4(9)
F(13)	91(7)	87(9)	71(7)	17(6)	27(6)	-23(7)
F(14)	68(7)	210(20)	117(11)	103(14)	1(7)	-7(10)
F(15)	72(6)	87(9)	100(8)	26(8)	29(6)	-11(7)
F(16)	106(9)	61(7)	101(9)	22(7)	16(7)	23(7)
F(17)	188(16)	90(11)	86(9)	-15(8)	60(10)	-24(11)
F(18)	161(12)	46(6)	75(7)	-11(6)	20(8)	-3(7)

P(1)	48(2)	27(2)	34(2)	3(1)	0(1)	0(1)
P(2)	41(1)	24(1)	25(1)	2(1)	7(1)	0(1)
P(3)	83(3)	44(2)	65(3)	-5(2)	20(2)	-3(2)
P(4)	63(2)	47(2)	61(2)	4(2)	21(2)	-4(2)
S(1)	54(2)	26(2)	37(2)	-1(1)	4(1)	-5(1)
S(2)	50(2)	24(2)	32(1)	-2(1)	2(1)	-3(1)
Ag(1)	40(1)	34(1)	40(1)	2(1)	9(1)	-3(1)
Ag(2)	48(1)	34(1)	47(1)	3(1)	9(1)	-2(1)
Cl(1)	243(15)	180(15)	232(15)	5(13)	53(12)	34(12)
Cl(2)	90(4)	78(5)	317(16)	6(7)	19(6)	-7(4)
Cl(3)	73(3)	61(3)	225(9)	-34(5)	-12(4)	-6(3)
Cl(4)	104(4)	80(4)	147(6)	18(4)	25(4)	8(3)
Cl(5)	93(4)	108(5)	111(4)	-16(4)	0(3)	-8(4)
Cl(6)	87(3)	69(3)	125(5)	-11(3)	25(3)	-5(3)
Cl(7)	94(3)	56(3)	82(3)	9(2)	-7(3)	3(2)
Cl(8)	122(4)	80(4)	113(5)	45(4)	-3(4)	-20(4)
Cl(9)	140(7)	202(13)	172(9)	76(10)	2(6)	34(8)
Cl(10)	165(8)	121(8)	215(11)	75(8)	-10(8)	-17(7)

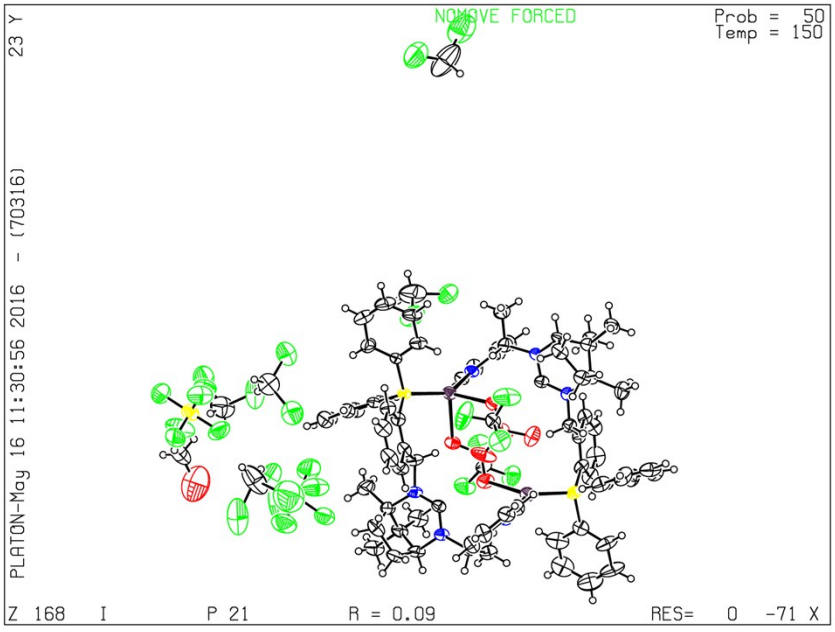

Table 5. Crystal data and structure refinement for cmpd7.

Identification code	cmpd7	
Empirical formula	C70 H76 Au2 F12 N6 P4	
Formula weight	1747.18	
Temperature	150(2) K	
Wavelength	1.54184 Å	
Crystal system	Tetragonal	
Space group	$P4_32_12$	
Unit cell dimensions	a = 14.4471(2) Å	α= 90°.
	b = 14.4471(2) Å	β= 90°.
	c = 69.8751(12) Å	γ = 90°.
Volume	14584.2(5) $Å^3$	
Z	8	
Density (calculated)	1.591 Mg/m^3	
Absorption coefficient	8.923 mm^{-1}	
F(000)	6912	
Crystal size	0.166 x 0.125 x 0.081 mm^3	
Theta range for data collection	3.310 to 73.213°.	
Index ranges	-17<=h<=17, -16<=k<=13, -86<=l<=85	
Reflections collected	54253	
Independent reflections	14470 [R(int) = 0.0393]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.76697	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14470 / 791 / 979	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0749, wR2 = 0.1874	
R indices (all data)	R1 = 0.0838, wR2 = 0.1941	
Absolute structure parameter	-0.008(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.285 and -1.904 $e.Å^{-3}$	

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cmpd7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	990(13)	5339(17)	9628(3)	78(6)
C(2)	174(15)	5066(19)	9540(3)	86(6)
C(3)	-140(20)	4190(20)	9529(4)	112(8)
C(4)	510(20)	3522(19)	9597(4)	100(7)
C(5)	1310(20)	3720(20)	9681(4)	111(8)
C(6)	1623(18)	4666(16)	9698(3)	91(6)
C(7)	1681(12)	6804(12)	9881(3)	60(4)
C(8)	2499(14)	6442(14)	9953(3)	79(5)
C(9)	2785(16)	6619(17)	10136(3)	85(6)
C(10)	2246(16)	7198(16)	10248(3)	82(6)
C(11)	1437(17)	7564(16)	10174(3)	85(6)
C(12)	1158(11)	7389(12)	9992(2)	61(4)
C(13)	2336(12)	6658(15)	9488(3)	70(5)
C(14)	2852(11)	7531(16)	9478(3)	71(5)
C(15)	3618(12)	7570(20)	9365(3)	92(7)
C(16)	3933(17)	6840(20)	9260(4)	112(9)
C(17)	3434(15)	6020(20)	9264(4)	114(10)
C(18)	2649(13)	5909(17)	9381(3)	85(6)
C(19)	-1019(11)	8125(14)	9396(2)	61(4)
C(20)	-2606(12)	8628(16)	9372(2)	74(5)
C(21)	-2426(14)	9640(18)	9317(3)	94(7)
C(22)	-1936(15)	9560(20)	9119(3)	104(9)
C(23)	-1766(14)	8520(20)	9086(3)	96(9)
C(24)	-2634(13)	8070(20)	9182(3)	93(8)
C(25)	-1611(14)	8240(30)	8884(3)	117(11)
C(26)	-3540(13)	8380(30)	9077(3)	133(13)
C(27)	-2624(15)	7010(20)	9211(3)	96(8)
C(28)	-1978(12)	8009(14)	9687(2)	61(4)
C(29)	-2538(10)	7190(13)	9706(2)	63(4)
C(30)	-2195(18)	6274(17)	9707(3)	88(7)
C(31)	-2720(20)	5510(18)	9715(5)	120(10)
C(32)	-3700(30)	5610(20)	9704(8)	190(20)
C(33)	-4010(20)	6530(20)	9729(7)	160(16)

N(5)	-3489(11)	7309(16)	9714(4)	108(6)
C(34)	-2319(18)	8866(16)	9795(3)	85(7)
C(35)	-28(12)	8408(17)	9120(2)	75(6)
C(36)	442(11)	7560(20)	9047(3)	83(7)
C(37)	1290(14)	7640(30)	8948(3)	115(11)
C(38)	1750(20)	6860(30)	8891(5)	147(14)
C(39)	1352(18)	5960(30)	8918(6)	156(16)
C(40)	491(17)	5860(30)	9017(4)	123(11)
C(41)	88(17)	6720(20)	9071(3)	102(8)
C(42)	1014(14)	9428(12)	8772(3)	110(11)
C(43)	440(16)	9030(20)	8626(3)	106(9)
C(44)	-190(20)	9530(30)	8530(4)	121(12)
C(45)	-260(20)	10420(40)	8577(5)	141(16)
C(46)	260(20)	10820(30)	8710(4)	124(11)
C(47)	879(8)	10364(8)	8812(2)	110(10)
C(48)	2829(8)	8614(8)	8751(2)	94(4)
C(49)	2705(8)	8525(8)	8555(2)	99(5)
C(50)	3469(8)	8445(8)	8435(2)	99(5)
C(51)	4357(8)	8454(8)	8512(2)	96(5)
C(52)	4481(8)	8544(8)	8708(2)	93(4)
C(53)	3717(8)	8624(8)	8828(2)	91(4)
C(48A)	2829(8)	8614(8)	8751(2)	94(4)
C(49A)	2793(8)	7862(8)	8598(2)	96(5)
C(50A)	3560(8)	7781(8)	8479(2)	97(5)
C(51A)	4394(8)	8190(8)	8531(2)	96(5)
C(52A)	4462(8)	8680(8)	8702(2)	94(5)
C(53A)	3695(8)	8761(8)	8821(2)	92(4)
C(54)	2949(12)	9825(17)	9447(3)	74(5)
C(55)	3831(15)	10858(18)	9653(3)	83(6)
C(56)	3118(18)	10907(19)	9822(3)	96(7)
C(57)	3075(17)	9868(19)	9897(3)	94(7)
C(58)	3677(12)	9359(16)	9755(3)	72(5)
C(59)	4421(13)	10037(16)	9690(3)	72(5)
C(60)	4028(17)	8472(17)	9844(3)	88(6)
C(61)	5051(15)	10290(18)	9865(3)	90(7)
C(62)	5043(13)	9721(17)	9529(3)	79(6)
C(63)	3247(9)	11395(9)	9325(2)	106(9)
C(64)	4112(9)	11502(9)	9233(2)	97(7)

C(65)	4781(9)	12133(9)	9291(2)	122(10)
C(66)	5636(9)	12155(9)	9200(2)	137(11)
C(67)	5822(9)	11545(9)	9051(2)	125(10)
C(68)	5153(9)	10914(9)	8993(2)	146(12)
N(6)	4298(9)	10892(9)	9084(2)	119(7)
C(69)	2850(30)	12340(30)	9408(5)	157(15)
C(70)	2480(12)	8358(13)	9584(3)	67(4)
N(1)	-1808(9)	8262(11)	9484(2)	56(3)
N(2)	-952(8)	8272(14)	9208(2)	77(5)
N(3)	3288(12)	10657(13)	9470(2)	80(5)
N(4)	3079(9)	9187(11)	9579(2)	63(4)
P(1)	1315(3)	6563(4)	9637(1)	61(1)
P(2)	1832(4)	8780(6)	8910(1)	98(2)
Au(1)	110(1)	7455(1)	9528(1)	60(1)
Au(2)	2328(1)	9405(1)	9191(1)	86(1)
P(3)	-2131(6)	14193(8)	9137(2)	115(3)
F(1)	-2825(11)	13520(13)	9043(2)	112(6)
F(2)	-2313(17)	14929(14)	8972(3)	172(9)
F(3)	-1483(12)	14929(13)	9231(3)	139(7)
F(4)	-2011(17)	13539(15)	9306(3)	176(9)
F(5)	-1335(12)	13807(16)	9022(3)	172(8)
F(6)	-2966(13)	14665(17)	9246(3)	186(10)
P(3A)	-1730(20)	12270(20)	9093(4)	153(8)
F(1A)	-1300(30)	12760(40)	8918(5)	169(12)
F(2A)	-830(30)	11670(30)	9117(7)	173(15)
F(3A)	-2190(30)	11720(30)	9256(5)	161(15)
F(4A)	-2630(20)	12870(30)	9070(7)	127(11)
F(5A)	-1330(30)	13000(30)	9230(6)	147(10)
F(6A)	-2100(30)	11590(40)	8941(6)	152(15)
P(4)	4151(14)	3939(14)	9840(3)	182(7)
F(7)	3380(20)	3790(20)	9687(4)	207(13)
F(8)	4120(20)	4999(15)	9796(4)	184(9)
F(9)	4890(20)	3820(20)	9675(4)	174(12)
F(10)	4210(20)	2884(14)	9875(4)	182(9)
F(11)	3420(20)	4060(20)	9996(4)	189(10)
F(12)	4944(19)	4100(20)	9986(4)	172(9)
P(5)	221(10)	10241(10)	9864(2)	106(4)
F(13)	976(15)	9903(18)	9720(3)	128(10)

F(14)	-78(18)	9239(13)	9905(4)	122(7)
F(15)	956(15)	10200(20)	10028(3)	126(7)
F(16)	501(18)	11256(13)	9823(4)	129(7)
F(17)	-475(16)	10280(20)	9690(4)	141(10)
F(18)	-512(15)	10600(17)	10013(4)	101(6)

Table 7. Bond lengths [Å] and angles [°] for cmpd7.

C(1)-C(2)	1.39(3)
C(1)-C(6)	1.42(3)
C(1)-P(1)	1.83(2)
C(2)-C(3)	1.35(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.42(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.33(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.44(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(12)	1.37(2)
C(7)-C(8)	1.39(2)
C(7)-P(1)	1.821(19)
C(8)-C(9)	1.37(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.39(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.38(3)
C(10)-H(10)	0.9500
C(11)-C(12)	1.36(3)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(18)	1.39(3)
C(13)-C(14)	1.47(3)
C(13)-P(1)	1.809(18)
C(14)-C(15)	1.36(2)
C(14)-C(70)	1.51(3)
C(15)-C(16)	1.37(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.38(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.41(3)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500

C(19)-N(1)	1.31(2)
C(19)-N(2)	1.33(2)
C(19)-Au(1)	2.108(17)
C(20)-N(1)	1.49(2)
C(20)-C(21)	1.53(3)
C(20)-C(24)	1.56(3)
C(20)-H(20)	1.0000
C(21)-C(22)	1.55(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.54(4)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(25)	1.48(3)
C(23)-N(2)	1.50(2)
C(23)-C(24)	1.57(3)
C(24)-C(27)	1.54(4)
C(24)-C(26)	1.57(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(29)	1.44(3)
C(28)-N(1)	1.481(19)
C(28)-C(34)	1.53(3)
C(28)-H(28)	1.0000
C(29)-N(5)	1.386(13)
C(29)-C(30)	1.41(3)
C(30)-C(31)	1.34(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.42(4)
C(31)-H(31)	0.9500
C(32)-C(33)	1.42(4)

C(32)-H(32)	0.9500
C(33)-N(5)	1.35(3)
C(33)-H(33)	0.9500
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-N(2)	1.484(19)
C(35)-C(36)	1.49(3)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-C(41)	1.32(4)
C(36)-C(37)	1.41(3)
C(37)-C(38)	1.36(5)
C(37)-P(2)	1.84(4)
C(38)-C(39)	1.44(5)
C(38)-H(38)	0.9500
C(39)-C(40)	1.43(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.42(4)
C(40)-H(40)	0.9500
C(41)-H(41)	0.9500
C(42)-C(47)	1.393(13)
C(42)-C(43)	1.43(3)
C(42)-P(2)	1.79(2)
C(43)-C(44)	1.34(4)
C(43)-H(43)	0.9500
C(44)-C(45)	1.34(5)
C(44)-H(44)	0.9500
C(45)-C(46)	1.32(4)
C(45)-H(45)	0.9500
C(46)-C(47)	1.32(4)
C(46)-H(46)	0.9500
C(47)-H(47)	0.9500
C(48)-C(53)	1.3899
C(48)-C(49)	1.3900
C(49)-C(50)	1.3898
C(49)-H(49)	0.9500
C(50)-C(51)	1.3900

C(50)-H(50)	0.9500
C(51)-C(52)	1.3899
C(51)-H(51)	0.9500
C(52)-C(53)	1.3899
C(52)-H(52)	0.9500
C(53)-H(53)	0.9500
C(49A)-C(50A)	1.3900
C(49A)-H(49A)	0.9500
C(50A)-C(51A)	1.3900
C(50A)-H(50A)	0.9500
C(51A)-C(52A)	1.3899
C(51A)-H(51A)	0.9500
C(52A)-C(53A)	1.3898
C(52A)-H(52A)	0.9500
C(53A)-H(53A)	0.9500
C(54)-N(3)	1.31(3)
C(54)-N(4)	1.32(2)
C(54)-Au(2)	2.091(17)
C(55)-C(59)	1.48(3)
C(55)-N(3)	1.53(2)
C(55)-C(56)	1.57(3)
C(55)-H(55)	1.0000
C(56)-C(57)	1.59(4)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.51(3)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-C(60)	1.51(3)
C(58)-C(59)	1.52(3)
C(58)-N(4)	1.53(2)
C(59)-C(62)	1.51(3)
C(59)-C(61)	1.56(3)
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800

C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-C(64)	1.4111
C(63)-N(3)	1.48(2)
C(63)-C(69)	1.60(4)
C(63)-H(63)	1.0000
C(64)-C(65)	1.3900
C(64)-N(6)	1.3901
C(65)-C(66)	1.3900
C(65)-H(65)	0.9500
C(66)-C(67)	1.3900
C(66)-H(66)	0.9500
C(67)-C(68)	1.3900
C(67)-H(67)	0.9500
C(68)-N(6)	1.3900
C(68)-H(68)	0.9500
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-N(4)	1.48(2)
C(70)-H(70A)	0.9900
C(70)-H(70B)	0.9900
P(1)-Au(1)	2.296(5)
P(2)-Au(2)	2.281(6)
P(3)-F(5)	1.510(15)
P(3)-F(4)	1.527(14)
P(3)-F(1)	1.542(14)
P(3)-F(3)	1.563(14)
P(3)-F(6)	1.582(15)
P(3)-F(2)	1.589(15)
P(3A)-F(5A)	1.536(19)
P(3A)-F(3A)	1.537(18)
P(3A)-F(6A)	1.54(2)
P(3A)-F(1A)	1.546(19)
P(3A)-F(2A)	1.569(18)
P(3A)-F(4A)	1.569(18)

P(4)-F(11)#1	1.37(4)
P(4)-F(11)	1.528(16)
P(4)-F(10)	1.546(16)
P(4)-F(12)	1.550(17)
P(4)-F(7)	1.559(17)
P(4)-F(8)	1.564(17)
P(4)-F(9)	1.585(17)
P(4)-F(12)#1	1.89(4)
P(4)-P(4)#1	2.27(4)
F(8)-F(12)#1	1.53(5)
F(10)-F(11)#1	1.20(4)
F(11)-F(10)#1	1.20(4)
F(11)-F(11)#1	1.32(6)
F(11)-P(4)#1	1.37(4)
F(11)-F(12)#1	1.62(3)
F(12)-F(8)#1	1.53(5)
F(12)-F(11)#1	1.62(3)
F(12)-F(12)#1	1.73(6)
F(12)-P(4)#1	1.89(4)
P(5)-F(15)#2	1.28(3)
P(5)-F(18)#2	1.49(3)
P(5)-F(14)	1.537(16)
P(5)-F(16)	1.548(16)
P(5)-F(15)	1.560(16)
P(5)-F(13)	1.563(16)
P(5)-F(18)	1.57(2)
P(5)-F(17)	1.580(17)
P(5)-P(5)#2	1.90(3)
P(5)-F(14)#2	2.20(3)
F(14)-F(18)#2	1.19(3)
F(14)-P(5)#2	2.20(3)
F(15)-F(18)#2	1.19(3)
F(15)-F(16)#2	1.21(3)
F(15)-P(5)#2	1.28(3)
F(15)-F(15)#2	1.59(5)
F(16)-F(15)#2	1.21(3)
F(18)-F(14)#2	1.19(3)
F(18)-F(15)#2	1.19(3)

F(18)-P(5)#2	1.49(3)

C(2)-C(1)-C(6)	120(2)
C(2)-C(1)-P(1)	120(2)
C(6)-C(1)-P(1)	119.0(16)
C(3)-C(2)-C(1)	125(3)
C(3)-C(2)-H(2)	117.5
C(1)-C(2)-H(2)	117.5
C(2)-C(3)-C(4)	114(3)
C(2)-C(3)-H(3)	123.2
C(4)-C(3)-H(3)	123.2
C(5)-C(4)-C(3)	125(3)
C(5)-C(4)-H(4)	117.5
C(3)-C(4)-H(4)	117.5
C(4)-C(5)-C(6)	121(3)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(1)-C(6)-C(5)	115(3)
C(1)-C(6)-H(6)	122.6
C(5)-C(6)-H(6)	122.6
C(12)-C(7)-C(8)	119.9(18)
C(12)-C(7)-P(1)	119.2(13)
C(8)-C(7)-P(1)	120.9(15)
C(9)-C(8)-C(7)	122(2)
C(9)-C(8)-H(8)	119.2
C(7)-C(8)-H(8)	119.2
C(8)-C(9)-C(10)	118(2)
C(8)-C(9)-H(9)	120.9
C(10)-C(9)-H(9)	120.9
C(11)-C(10)-C(9)	120(2)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(12)-C(11)-C(10)	122(2)
C(12)-C(11)-H(11)	119.1
C(10)-C(11)-H(11)	119.1
C(11)-C(12)-C(7)	118.7(18)
C(11)-C(12)-H(12)	120.6
C(7)-C(12)-H(12)	120.6

C(18)-C(13)-C(14)	118.5(17)
C(18)-C(13)-P(1)	120.9(17)
C(14)-C(13)-P(1)	120.6(14)
C(15)-C(14)-C(13)	118(2)
C(15)-C(14)-C(70)	123(2)
C(13)-C(14)-C(70)	118.4(15)
C(14)-C(15)-C(16)	124(2)
C(14)-C(15)-H(15)	118.2
C(16)-C(15)-H(15)	118.2
C(15)-C(16)-C(17)	118(2)
C(15)-C(16)-H(16)	120.9
C(17)-C(16)-H(16)	120.9
C(16)-C(17)-C(18)	122(2)
C(16)-C(17)-H(17)	118.8
C(18)-C(17)-H(17)	118.8
C(13)-C(18)-C(17)	119(2)
C(13)-C(18)-H(18)	120.6
C(17)-C(18)-H(18)	120.6
N(1)-C(19)-N(2)	120.1(15)
N(1)-C(19)-Au(1)	122.5(12)
N(2)-C(19)-Au(1)	116.5(12)
N(1)-C(20)-C(21)	109.8(16)
N(1)-C(20)-C(24)	106.6(17)
C(21)-C(20)-C(24)	106.4(17)
N(1)-C(20)-H(20)	111.3
C(21)-C(20)-H(20)	111.3
C(24)-C(20)-H(20)	111.3
C(20)-C(21)-C(22)	103(2)
C(20)-C(21)-H(21A)	111.1
C(22)-C(21)-H(21A)	111.1
C(20)-C(21)-H(21B)	111.1
C(22)-C(21)-H(21B)	111.1
H(21A)-C(21)-H(21B)	109.1
C(23)-C(22)-C(21)	106(2)
C(23)-C(22)-H(22A)	110.4
C(21)-C(22)-H(22A)	110.4
C(23)-C(22)-H(22B)	110.4
C(21)-C(22)-H(22B)	110.4

H(22A)-C(22)-H(22B)	108.6
C(25)-C(23)-N(2)	111.0(19)
C(25)-C(23)-C(22)	116(2)
N(2)-C(23)-C(22)	105.8(19)
C(25)-C(23)-C(24)	115(2)
N(2)-C(23)-C(24)	106.5(17)
C(22)-C(23)-C(24)	102(2)
C(27)-C(24)-C(20)	113.6(19)
C(27)-C(24)-C(26)	111(2)
C(20)-C(24)-C(26)	106(2)
C(27)-C(24)-C(23)	118(2)
C(20)-C(24)-C(23)	97.4(19)
C(26)-C(24)-C(23)	110(2)
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(24)-C(26)-H(26A)	109.5
C(24)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(24)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-H(27A)	109.5
C(24)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(24)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(29)-C(28)-N(1)	112.6(15)
C(29)-C(28)-C(34)	115.9(16)
N(1)-C(28)-C(34)	109.1(15)
C(29)-C(28)-H(28)	106.1
N(1)-C(28)-H(28)	106.1
C(34)-C(28)-H(28)	106.1
N(5)-C(29)-C(30)	118(2)

N(5)-C(29)-C(28)	117.3(17)
C(30)-C(29)-C(28)	125.0(17)
C(31)-C(30)-C(29)	125(2)
C(31)-C(30)-H(30)	117.5
C(29)-C(30)-H(30)	117.5
C(30)-C(31)-C(32)	119(3)
C(30)-C(31)-H(31)	120.7
C(32)-C(31)-H(31)	120.7
C(31)-C(32)-C(33)	114(3)
C(31)-C(32)-H(32)	123.2
C(33)-C(32)-H(32)	123.2
N(5)-C(33)-C(32)	127(3)
N(5)-C(33)-H(33)	116.7
C(32)-C(33)-H(33)	116.7
C(33)-N(5)-C(29)	117(2)
C(28)-C(34)-H(34A)	109.5
C(28)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(28)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
N(2)-C(35)-C(36)	116.2(19)
N(2)-C(35)-H(35A)	108.2
C(36)-C(35)-H(35A)	108.2
N(2)-C(35)-H(35B)	108.2
C(36)-C(35)-H(35B)	108.2
H(35A)-C(35)-H(35B)	107.4
C(41)-C(36)-C(37)	118(3)
C(41)-C(36)-C(35)	122.3(18)
C(37)-C(36)-C(35)	119(2)
C(38)-C(37)-C(36)	120(3)
C(38)-C(37)-P(2)	119(2)
C(36)-C(37)-P(2)	121(2)
C(37)-C(38)-C(39)	121(3)
C(37)-C(38)-H(38)	119.5
C(39)-C(38)-H(38)	119.5
C(40)-C(39)-C(38)	120(3)
C(40)-C(39)-H(39)	120.0

C(38)-C(39)-H(39)	120.0
C(41)-C(40)-C(39)	113(3)
C(41)-C(40)-H(40)	123.3
C(39)-C(40)-H(40)	123.3
C(36)-C(41)-C(40)	127(2)
C(36)-C(41)-H(41)	116.4
C(40)-C(41)-H(41)	116.4
C(47)-C(42)-C(43)	117(2)
C(47)-C(42)-P(2)	119.4(14)
C(43)-C(42)-P(2)	123.8(18)
C(44)-C(43)-C(42)	122(3)
C(44)-C(43)-H(43)	118.9
C(42)-C(43)-H(43)	118.9
C(45)-C(44)-C(43)	117(3)
C(45)-C(44)-H(44)	121.6
C(43)-C(44)-H(44)	121.6
C(46)-C(45)-C(44)	123(4)
C(46)-C(45)-H(45)	118.5
C(44)-C(45)-H(45)	118.5
C(47)-C(46)-C(45)	123(4)
C(47)-C(46)-H(46)	118.4
C(45)-C(46)-H(46)	118.4
C(46)-C(47)-C(42)	118.1(19)
C(46)-C(47)-H(47)	121.0
C(42)-C(47)-H(47)	121.0
C(53)-C(48)-C(49)	120.0
C(50)-C(49)-C(48)	120.0
C(50)-C(49)-H(49)	120.0
C(48)-C(49)-H(49)	120.0
C(49)-C(50)-C(51)	120.0
C(49)-C(50)-H(50)	120.0
C(51)-C(50)-H(50)	120.0
C(52)-C(51)-C(50)	120.0
C(52)-C(51)-H(51)	120.0
C(50)-C(51)-H(51)	120.0
C(53)-C(52)-C(51)	120.0
C(53)-C(52)-H(52)	120.0
C(51)-C(52)-H(52)	120.0

C(52)-C(53)-C(48)	120.0
C(52)-C(53)-H(53)	120.0
C(48)-C(53)-H(53)	120.0
C(50A)-C(49A)-H(49A)	121.6
C(49A)-C(50A)-C(51A)	120.0
C(49A)-C(50A)-H(50A)	120.0
C(51A)-C(50A)-H(50A)	120.0
C(52A)-C(51A)-C(50A)	120.0
C(52A)-C(51A)-H(51A)	120.0
C(50A)-C(51A)-H(51A)	120.0
C(53A)-C(52A)-C(51A)	120.0
C(53A)-C(52A)-H(52A)	120.0
C(51A)-C(52A)-H(52A)	120.0
C(52A)-C(53A)-H(53A)	119.7
N(3)-C(54)-N(4)	120.2(16)
N(3)-C(54)-Au(2)	122.2(14)
N(4)-C(54)-Au(2)	117.2(15)
C(59)-C(55)-N(3)	106.9(18)
C(59)-C(55)-C(56)	106.4(19)
N(3)-C(55)-C(56)	107.4(17)
C(59)-C(55)-H(55)	111.9
N(3)-C(55)-H(55)	111.9
C(56)-C(55)-H(55)	111.9
C(55)-C(56)-C(57)	103.4(19)
C(55)-C(56)-H(56A)	111.1
C(57)-C(56)-H(56A)	111.1
C(55)-C(56)-H(56B)	111.1
C(57)-C(56)-H(56B)	111.1
H(56A)-C(56)-H(56B)	109.1
C(58)-C(57)-C(56)	102.8(19)
C(58)-C(57)-H(57A)	111.2
C(56)-C(57)-H(57A)	111.2
C(58)-C(57)-H(57B)	111.2
C(56)-C(57)-H(57B)	111.2
H(57A)-C(57)-H(57B)	109.1
C(57)-C(58)-C(60)	109.9(18)
C(57)-C(58)-C(59)	107(2)
C(60)-C(58)-C(59)	115.6(17)

C(57)-C(58)-N(4)	106.3(16)
C(60)-C(58)-N(4)	112.5(18)
C(59)-C(58)-N(4)	105.3(15)
C(55)-C(59)-C(62)	117.0(18)
C(55)-C(59)-C(58)	99.3(16)
C(62)-C(59)-C(58)	116.5(19)
C(55)-C(59)-C(61)	106.6(19)
C(62)-C(59)-C(61)	107.7(16)
C(58)-C(59)-C(61)	109.1(17)
C(58)-C(60)-H(60A)	109.5
C(58)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(58)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(59)-C(61)-H(61A)	109.5
C(59)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(59)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(59)-C(62)-H(62A)	109.5
C(59)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(59)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(64)-C(63)-N(3)	110.9(9)
C(64)-C(63)-C(69)	113.2(17)
N(3)-C(63)-C(69)	112.3(16)
C(64)-C(63)-H(63)	106.7
N(3)-C(63)-H(63)	106.7
C(69)-C(63)-H(63)	106.7
C(65)-C(64)-N(6)	120.0
C(65)-C(64)-C(63)	123.7
N(6)-C(64)-C(63)	116.2
C(64)-C(65)-C(66)	120.0
C(64)-C(65)-H(65)	120.0

C(66)-C(65)-H(65)	120.0
C(65)-C(66)-C(67)	120.0
C(65)-C(66)-H(66)	120.0
C(67)-C(66)-H(66)	120.0
C(68)-C(67)-C(66)	120.0
C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0
C(67)-C(68)-N(6)	120.0
C(67)-C(68)-H(68)	120.0
N(6)-C(68)-H(68)	120.0
C(68)-N(6)-C(64)	120.0
C(63)-C(69)-H(69A)	109.5
C(63)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(63)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
N(4)-C(70)-C(14)	115.0(15)
N(4)-C(70)-H(70A)	108.5
C(14)-C(70)-H(70A)	108.5
N(4)-C(70)-H(70B)	108.5
C(14)-C(70)-H(70B)	108.5
H(70A)-C(70)-H(70B)	107.5
C(19)-N(1)-C(28)	123.8(14)
C(19)-N(1)-C(20)	118.6(13)
C(28)-N(1)-C(20)	117.4(12)
C(19)-N(2)-C(35)	119.7(13)
C(19)-N(2)-C(23)	123.0(13)
C(35)-N(2)-C(23)	115.9(13)
C(54)-N(3)-C(63)	124.3(15)
C(54)-N(3)-C(55)	118.1(17)
C(63)-N(3)-C(55)	117.4(17)
C(54)-N(4)-C(70)	119.9(15)
C(54)-N(4)-C(58)	122.1(17)
C(70)-N(4)-C(58)	116.5(16)
C(13)-P(1)-C(7)	106.7(9)
C(13)-P(1)-C(1)	105.3(9)
C(7)-P(1)-C(1)	106.9(9)

C(13)-P(1)-Au(1)	112.6(7)
C(7)-P(1)-Au(1)	115.1(5)
C(1)-P(1)-Au(1)	109.7(7)
C(42)-P(2)-C(37)	105.4(11)
C(42)-P(2)-Au(2)	117.7(7)
C(37)-P(2)-Au(2)	111.2(8)
C(19)-Au(1)-P(1)	171.6(5)
C(54)-Au(2)-P(2)	171.0(6)
F(5)-P(3)-F(4)	95.7(11)
F(5)-P(3)-F(1)	92.1(10)
F(4)-P(3)-F(1)	90.7(10)
F(5)-P(3)-F(3)	91.1(10)
F(4)-P(3)-F(3)	91.4(10)
F(1)-P(3)-F(3)	175.9(12)
F(5)-P(3)-F(6)	175.5(13)
F(4)-P(3)-F(6)	88.7(10)
F(1)-P(3)-F(6)	88.9(9)
F(3)-P(3)-F(6)	87.6(10)
F(5)-P(3)-F(2)	89.3(10)
F(4)-P(3)-F(2)	174.9(13)
F(1)-P(3)-F(2)	90.4(10)
F(3)-P(3)-F(2)	87.1(14)
F(6)-P(3)-F(2)	86.4(10)
F(5A)-P(3A)-F(3A)	93.2(14)
F(5A)-P(3A)-F(6A)	175(2)
F(3A)-P(3A)-F(6A)	91.9(15)
F(5A)-P(3A)-F(1A)	91.6(15)
F(3A)-P(3A)-F(1A)	175(2)
F(6A)-P(3A)-F(1A)	83(2)
F(5A)-P(3A)-F(2A)	90.0(14)
F(3A)-P(3A)-F(2A)	89.9(12)
F(6A)-P(3A)-F(2A)	90.6(14)
F(1A)-P(3A)-F(2A)	90.1(10)
F(5A)-P(3A)-F(4A)	89.8(14)
F(3A)-P(3A)-F(4A)	90.4(12)
F(6A)-P(3A)-F(4A)	90(2)
F(1A)-P(3A)-F(4A)	89.7(12)
F(2A)-P(3A)-F(4A)	180(2)

F(11)#1-P(4)-F(11)	54(2)
F(11)#1-P(4)-F(10)	48.3(17)
F(11)-P(4)-F(10)	92.3(12)
F(11)#1-P(4)-F(12)	66.7(17)
F(11)-P(4)-F(12)	91.5(12)
F(10)-P(4)-F(12)	90.5(11)
F(11)#1-P(4)-F(7)	116(2)
F(11)-P(4)-F(7)	90.7(12)
F(10)-P(4)-F(7)	90.6(12)
F(12)-P(4)-F(7)	177.5(15)
F(11)#1-P(4)-F(8)	134.4(19)
F(11)-P(4)-F(8)	90.6(11)
F(10)-P(4)-F(8)	177.1(15)
F(12)-P(4)-F(8)	90.0(11)
F(7)-P(4)-F(8)	88.8(11)
F(11)#1-P(4)-F(9)	128(2)
F(11)-P(4)-F(9)	178.6(15)
F(10)-P(4)-F(9)	88.5(11)
F(12)-P(4)-F(9)	89.6(11)
F(7)-P(4)-F(9)	88.2(11)
F(8)-P(4)-F(9)	88.6(11)
F(11)#1-P(4)-F(12)#1	83.3(17)
F(11)-P(4)-F(12)#1	55.1(15)
F(10)-P(4)-F(12)#1	131.1(16)
F(12)-P(4)-F(12)#1	59.3(19)
F(7)-P(4)-F(12)#1	121.3(19)
F(8)-P(4)-F(12)#1	51.4(15)
F(9)-P(4)-F(12)#1	125.0(16)
F(11)#1-P(4)-P(4)#1	40.9(11)
F(11)-P(4)-P(4)#1	36.1(13)
F(10)-P(4)-P(4)#1	89.2(14)
F(12)-P(4)-P(4)#1	55.5(13)
F(7)-P(4)-P(4)#1	126.7(15)
F(8)-P(4)-P(4)#1	93.5(14)
F(9)-P(4)-P(4)#1	145.1(14)
F(12)#1-P(4)-P(4)#1	42.5(8)
F(12)#1-F(8)-P(4)	75.5(16)
F(11)#1-F(10)-P(4)	58(2)

F(10)#1-F(11)-F(11)#1	123(4)
F(10)#1-F(11)-P(4)#1	73(2)
F(11)#1-F(11)-P(4)#1	69(3)
F(10)#1-F(11)-P(4)	175(3)
F(11)#1-F(11)-P(4)	57.1(18)
P(4)#1-F(11)-P(4)	103(2)
F(10)#1-F(11)-F(12)#1	102(3)
F(11)#1-F(11)-F(12)#1	97.0(18)
P(4)#1-F(11)-F(12)#1	61.9(14)
P(4)-F(11)-F(12)#1	74.0(19)
F(8)#1-F(12)-P(4)	134(2)
F(8)#1-F(12)-F(11)#1	89(2)
P(4)-F(12)-F(11)#1	51.4(18)
F(8)#1-F(12)-F(12)#1	85(2)
P(4)-F(12)-F(12)#1	70.2(15)
F(11)#1-F(12)-F(12)#1	82.4(17)
F(8)#1-F(12)-P(4)#1	53.1(14)
P(4)-F(12)-P(4)#1	82.0(15)
F(11)#1-F(12)-P(4)#1	50.9(11)
F(12)#1-F(12)-P(4)#1	50.4(13)
F(15)#2-P(5)-F(18)#2	105.0(18)
F(15)#2-P(5)-F(14)	130.2(15)
F(18)#2-P(5)-F(14)	46.3(13)
F(15)#2-P(5)-F(16)	49.5(13)
F(18)#2-P(5)-F(16)	134.7(15)
F(14)-P(5)-F(16)	178.8(15)
F(15)#2-P(5)-F(15)	67(2)
F(18)#2-P(5)-F(15)	45.8(12)
F(14)-P(5)-F(15)	91.3(11)
F(16)-P(5)-F(15)	89.5(11)
F(15)#2-P(5)-F(13)	130.3(18)
F(18)#2-P(5)-F(13)	83.4(16)
F(14)-P(5)-F(13)	91.2(12)
F(16)-P(5)-F(13)	89.7(11)
F(15)-P(5)-F(13)	89.2(11)
F(15)#2-P(5)-F(18)	47.9(15)
F(18)#2-P(5)-F(18)	96.2(15)
F(14)-P(5)-F(18)	89.9(11)

F(16)-P(5)-F(18)	89.3(11)
F(15)-P(5)-F(18)	89.1(13)
F(13)-P(5)-F(18)	178.0(15)
F(15)#2-P(5)-F(17)	115(2)
F(18)#2-P(5)-F(17)	134.4(15)
F(14)-P(5)-F(17)	89.6(11)
F(16)-P(5)-F(17)	89.6(11)
F(15)-P(5)-F(17)	176.6(16)
F(13)-P(5)-F(17)	87.5(12)
F(18)-P(5)-F(17)	94.2(16)
F(15)#2-P(5)-P(5)#2	54.8(11)
F(18)#2-P(5)-P(5)#2	53.8(11)
F(14)-P(5)-P(5)#2	78.8(11)
F(16)-P(5)-P(5)#2	101.3(12)
F(15)-P(5)-P(5)#2	42.0(10)
F(13)-P(5)-P(5)#2	129.0(14)
F(18)-P(5)-P(5)#2	49.7(12)
F(17)-P(5)-P(5)#2	141.4(15)
F(15)#2-P(5)-F(14)#2	73.9(14)
F(18)#2-P(5)-F(14)#2	70.3(12)
F(14)-P(5)-F(14)#2	59.0(16)
F(16)-P(5)-F(14)#2	120.3(14)
F(15)-P(5)-F(14)#2	84.0(13)
F(13)-P(5)-F(14)#2	149.1(15)
F(18)-P(5)-F(14)#2	31.6(12)
F(17)-P(5)-F(14)#2	99.3(15)
P(5)#2-P(5)-F(14)#2	43.3(7)
F(18)#2-F(14)-P(5)	64.6(15)
F(18)#2-F(14)-P(5)#2	43.9(16)
P(5)-F(14)-P(5)#2	57.9(11)
F(18)#2-F(15)-F(16)#2	132(3)
F(18)#2-F(15)-P(5)#2	79(2)
F(16)#2-F(15)-P(5)#2	76.9(19)
F(18)#2-F(15)-P(5)	63.8(16)
F(16)#2-F(15)-P(5)	150(3)
P(5)#2-F(15)-P(5)	83.2(15)
F(18)#2-F(15)-F(15)#2	103.8(17)
F(16)#2-F(15)-F(15)#2	102(3)

P(5)#2-F(15)-F(15)#2	64.9(17)
P(5)-F(15)-F(15)#2	47.9(12)
F(15)#2-F(16)-P(5)	53.6(13)
F(14)#2-F(18)-F(15)#2	137(3)
F(14)#2-F(18)-P(5)#2	69.1(17)
F(15)#2-F(18)-P(5)#2	70.3(17)
F(14)#2-F(18)-P(5)	105(2)
F(15)#2-F(18)-P(5)	53.0(17)
P(5)#2-F(18)-P(5)	76.5(12)

Symmetry transformations used to generate equivalent atoms:

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

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cmpd7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	53(10)	100(16)	79(12)	-19(11)	10(9)	-4(10)
C(2)	77(13)	111(17)	70(11)	-26(12)	10(10)	-15(13)
C(3)	115(13)	113(13)	107(12)	-20(11)	-2(11)	-17(11)
C(4)	111(12)	93(11)	96(11)	-18(10)	15(10)	-13(10)
C(5)	118(13)	106(13)	108(12)	3(11)	18(11)	13(11)
C(6)	94(11)	83(11)	97(11)	-5(9)	18(9)	-9(9)
C(7)	52(9)	54(9)	76(10)	3(8)	-4(8)	14(7)
C(8)	64(12)	78(12)	95(13)	-5(10)	-15(11)	18(10)
C(9)	78(10)	94(11)	85(10)	7(9)	-24(9)	7(9)
C(10)	86(14)	87(14)	74(11)	19(11)	-25(11)	-12(11)
C(11)	109(16)	76(14)	69(11)	-3(10)	-2(11)	9(13)
C(12)	54(9)	55(9)	72(10)	-2(8)	-2(7)	7(8)
C(13)	38(8)	100(14)	73(11)	-20(10)	5(8)	8(9)
C(14)	44(8)	93(14)	74(10)	-10(11)	0(7)	-4(9)
C(15)	42(9)	130(20)	102(15)	-38(15)	21(9)	-26(12)
C(16)	68(14)	160(30)	106(18)	-10(18)	22(13)	-17(16)
C(17)	58(12)	150(20)	140(20)	-64(19)	46(14)	-12(14)
C(18)	43(9)	101(15)	111(15)	-28(12)	18(10)	-1(10)
C(19)	38(8)	95(13)	50(8)	2(8)	-3(6)	-10(8)
C(20)	39(8)	127(17)	57(9)	21(10)	4(7)	-6(10)
C(21)	60(11)	150(20)	73(11)	32(12)	12(9)	30(13)
C(22)	57(12)	180(30)	79(13)	37(16)	-7(10)	20(15)
C(23)	50(11)	190(30)	43(9)	9(13)	3(8)	-14(14)
C(24)	34(8)	190(30)	53(9)	0(13)	3(8)	1(13)
C(25)	45(10)	260(40)	49(10)	2(15)	4(8)	14(16)
C(26)	31(9)	290(40)	80(14)	40(20)	-2(9)	16(16)
C(27)	48(10)	160(30)	78(13)	-21(14)	-7(10)	-16(14)
C(28)	44(8)	89(12)	50(8)	7(8)	5(7)	8(8)
C(29)	51(9)	75(11)	65(9)	3(8)	21(8)	7(8)
C(30)	85(16)	94(16)	85(14)	-9(12)	9(12)	22(13)
C(31)	110(20)	68(14)	180(30)	14(16)	-20(20)	-8(14)
C(32)	120(30)	90(20)	370(70)	110(30)	60(40)	30(20)
C(33)	73(17)	77(18)	330(50)	0(20)	30(20)	-5(13)

N(5)	89(10)	94(11)	141(12)	13(10)	25(9)	5(9)
C(34)	97(16)	100(15)	59(10)	24(10)	20(10)	33(13)
C(35)	35(8)	139(19)	51(8)	-2(10)	8(7)	-4(10)
C(36)	38(8)	150(20)	60(9)	-7(12)	5(7)	-14(12)
C(37)	45(10)	200(30)	97(15)	-74(19)	8(10)	-14(15)
C(38)	75(18)	200(40)	170(30)	-70(30)	23(19)	-20(20)
C(39)	52(13)	200(40)	220(40)	-110(30)	-16(18)	12(18)
C(40)	61(13)	180(30)	130(20)	-70(20)	7(14)	-14(17)
C(41)	60(13)	170(30)	75(13)	-27(15)	14(11)	-9(16)
C(42)	51(11)	220(30)	56(11)	1(16)	10(9)	-50(17)
C(43)	60(12)	190(30)	67(12)	-15(16)	14(10)	-27(16)
C(44)	80(17)	220(40)	66(14)	30(20)	1(12)	-40(20)
C(45)	77(18)	240(50)	100(20)	50(30)	-20(16)	-50(30)
C(46)	130(30)	150(30)	87(17)	2(18)	3(17)	-60(20)
C(47)	102(19)	170(30)	63(13)	-2(16)	3(13)	-30(20)
C(48)	87(5)	106(6)	90(5)	-11(5)	11(5)	-7(5)
C(49)	90(7)	110(7)	96(7)	-11(6)	9(6)	-9(6)
C(50)	90(7)	110(7)	97(7)	-9(6)	9(6)	-7(6)
C(51)	86(7)	106(7)	95(7)	-8(6)	13(6)	-9(6)
C(52)	82(7)	105(7)	92(7)	-2(6)	10(6)	-4(6)
C(53)	83(7)	105(7)	86(7)	-2(6)	11(6)	-2(6)
C(48A)	87(5)	106(6)	90(5)	-11(5)	11(5)	-7(5)
C(49A)	87(7)	106(7)	94(7)	-7(7)	8(6)	-7(7)
C(50A)	88(7)	106(8)	95(7)	-7(7)	10(6)	-6(7)
C(51A)	87(7)	106(7)	95(7)	-6(7)	11(6)	-6(7)
C(52A)	85(7)	106(7)	92(7)	-4(6)	9(6)	-4(6)
C(53A)	85(7)	105(7)	88(7)	-4(6)	10(6)	-3(6)
C(54)	43(9)	115(17)	64(10)	-1(10)	-14(7)	-14(9)
C(55)	69(12)	106(17)	75(12)	0(12)	-15(10)	-8(11)
C(56)	94(16)	120(20)	80(14)	-27(13)	-2(12)	22(14)
C(57)	86(15)	120(20)	80(13)	-7(13)	-1(11)	18(14)
C(58)	51(9)	102(15)	63(10)	-13(10)	-6(8)	-1(10)
C(59)	49(9)	98(14)	70(10)	3(10)	-16(8)	-6(10)
C(60)	81(15)	89(16)	96(15)	1(13)	-13(12)	6(12)
C(61)	59(11)	118(19)	92(14)	7(13)	-24(11)	-8(12)
C(62)	53(10)	116(17)	67(10)	-1(11)	-6(9)	-20(10)
C(63)	77(15)	160(30)	83(15)	9(16)	-6(12)	7(16)
C(64)	69(13)	130(20)	87(15)	26(15)	-17(11)	-4(13)

C(65)	150(30)	130(20)	90(15)	31(15)	-13(17)	-50(20)
C(66)	134(15)	141(15)	136(15)	17(12)	-15(12)	-14(12)
C(67)	121(14)	132(14)	124(14)	18(11)	-5(11)	-4(11)
C(68)	146(17)	153(17)	139(16)	0(12)	1(12)	6(12)
N(6)	114(12)	133(13)	109(11)	9(10)	3(10)	2(10)
C(69)	170(30)	180(40)	120(20)	30(20)	-10(20)	70(30)
C(70)	50(10)	82(12)	69(10)	-8(8)	7(8)	16(9)
N(1)	44(7)	79(9)	43(6)	3(6)	7(5)	14(6)
N(2)	29(6)	161(17)	40(6)	12(8)	4(5)	-13(8)
N(3)	73(10)	99(13)	67(9)	16(9)	-26(8)	-4(9)
N(4)	40(7)	87(11)	63(8)	-16(7)	-4(6)	-9(7)
P(1)	38(2)	85(3)	61(2)	-7(2)	0(2)	3(2)
P(2)	49(3)	177(7)	67(3)	-30(4)	16(2)	-28(3)
Au(1)	39(1)	95(1)	46(1)	-2(1)	-1(1)	-2(1)
Au(2)	49(1)	144(1)	65(1)	-11(1)	-1(1)	-13(1)
P(3)	74(5)	152(7)	119(6)	9(6)	-17(4)	-29(5)
F(1)	89(11)	151(14)	96(10)	4(11)	-16(9)	-22(11)
F(2)	171(16)	161(16)	184(16)	13(14)	-41(15)	11(14)
F(3)	83(11)	154(15)	181(15)	14(13)	-43(11)	-36(11)
F(4)	176(15)	182(15)	170(14)	25(14)	-52(13)	-50(14)
F(5)	121(13)	194(14)	203(14)	-13(13)	19(12)	-10(12)
F(6)	156(16)	205(18)	197(17)	-46(16)	0(15)	-8(15)
P(3A)	146(11)	164(12)	149(11)	-4(9)	2(9)	-11(9)
F(1A)	151(18)	187(18)	169(18)	-5(16)	11(16)	-6(16)
F(2A)	170(20)	180(20)	170(20)	-3(19)	-6(19)	1(19)
F(3A)	160(20)	170(20)	150(20)	8(19)	4(19)	-4(19)
F(4A)	116(17)	150(18)	116(16)	1(16)	-3(15)	-5(16)
F(5A)	129(15)	165(16)	147(15)	-19(14)	-4(14)	-26(14)
F(6A)	150(20)	160(20)	140(20)	-16(18)	-5(18)	-8(19)
P(4)	176(9)	168(9)	200(9)	9(7)	-4(7)	4(7)
F(7)	180(20)	210(20)	230(20)	5(18)	-22(18)	27(18)
F(8)	180(13)	171(12)	200(13)	11(10)	-3(10)	7(10)
F(9)	164(19)	166(19)	190(19)	-9(17)	7(17)	19(17)
F(10)	179(13)	170(12)	198(13)	9(10)	-2(10)	5(10)
F(11)	191(13)	181(13)	195(13)	9(10)	5(10)	-3(10)
F(12)	166(12)	165(12)	184(12)	6(10)	-5(10)	8(10)
P(5)	94(6)	102(7)	122(7)	-9(6)	7(5)	2(6)
F(13)	92(15)	128(17)	163(18)	-19(16)	3(15)	24(14)

F(14)	120(11)	111(11)	137(11)	7(9)	5(9)	2(9)
F(15)	108(11)	142(11)	126(11)	-10(10)	4(9)	0(9)
F(16)	126(11)	119(11)	143(11)	-4(9)	17(9)	-2(9)
F(17)	112(17)	159(18)	152(18)	25(16)	-4(15)	3(16)
F(18)	84(10)	102(10)	117(10)	6(9)	6(9)	10(9)

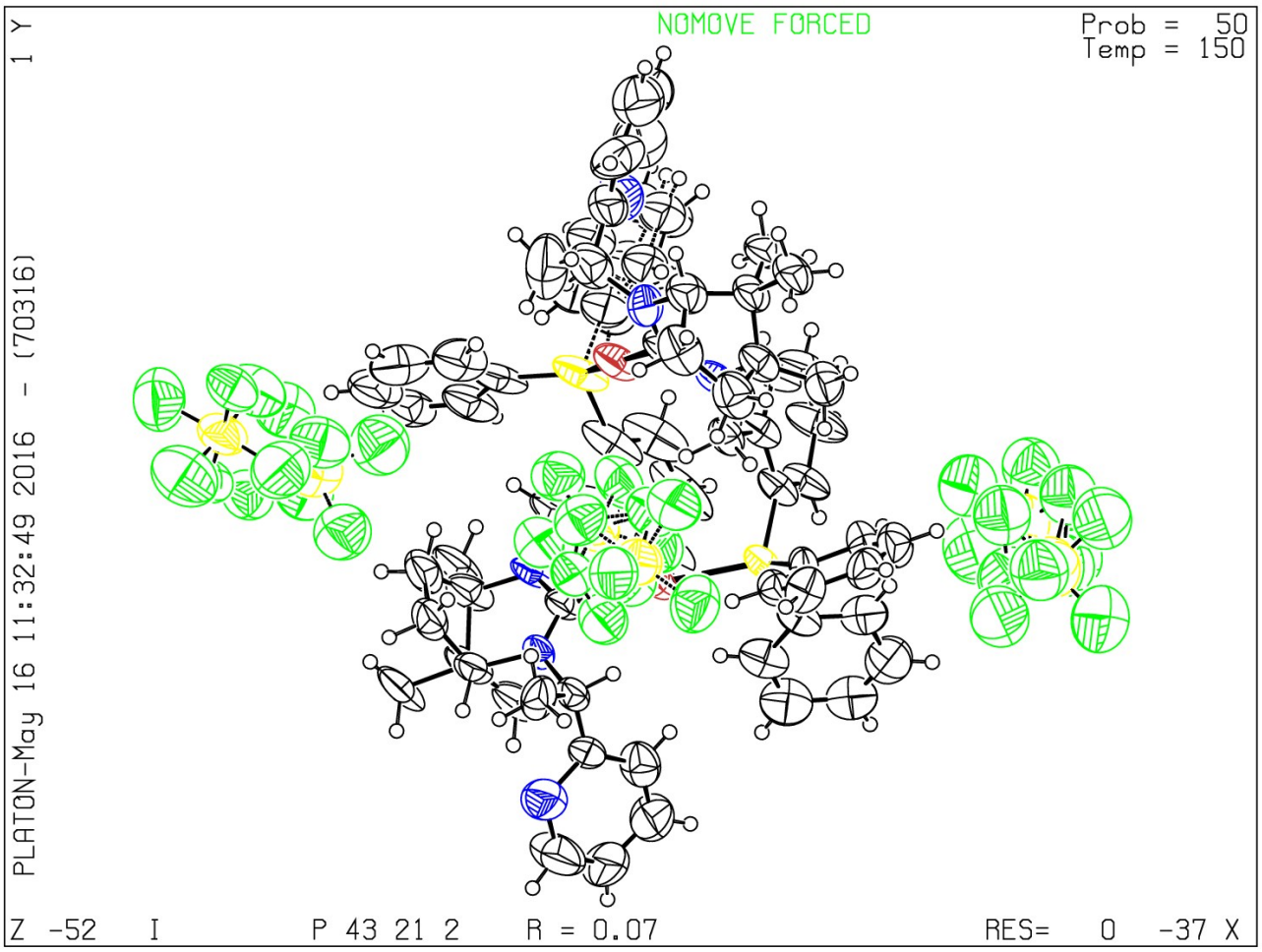

Table 9. Crystal data and structure refinement for cmpd8.

Identification code	cmpd8	
Empirical formula	C73.09 H84.19 Au F6 N6 O0.77 P3	
Formula weight	1462.93	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 10.5073(4) Å	α= 73.907(4)°.
	b = 12.4401(5) Å	β= 71.633(4)°.
	c = 14.0349(6) Å	γ = 87.024(3)°.
Volume	1671.58(13) $Å^3$	
Z	1	
Density (calculated)	1.453 Mg/m^3	
Absorption coefficient	2.338 mm^{-1}	
F(000)	749	
Crystal size	0.443 x 0.151 x 0.082 mm^3	
Theta range for data collection	3.344 to 29.913°.	
Index ranges	-13<=h<=14, -17<=k<=15, -17<=l<=19	
Reflections collected	15352	
Independent reflections	11433 [R(int) = 0.0365]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.997 and 0.987	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11433 / 55 / 829	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0412, wR2 = 0.0910	
R indices (all data)	R1 = 0.0419, wR2 = 0.0923	
Absolute structure parameter	-0.004(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.289 and -1.141 $e.Å^{-3}$	

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cmpd8. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	12120(30)	599(16)	4215(16)	157(10)
C(71)	10689(18)	1235(14)	4472(12)	92(6)
C(72)	9720(30)	140(30)	5180(50)	280(20)
C(73)	10670(20)	-792(17)	5510(14)	117(8)
C(74)	12010(20)	-410(20)	4977(19)	230(20)
C(1)	-733(10)	7845(10)	1814(9)	29(2)
C(2)	-1665(13)	8619(13)	1662(12)	42(3)
C(3)	-2355(14)	9092(13)	2471(13)	48(3)
C(4)	-2133(14)	8851(13)	3391(12)	54(4)
C(5)	-1195(13)	8075(12)	3550(10)	51(3)
C(6)	-489(12)	7577(11)	2784(10)	44(3)
C(7)	-539(11)	7563(10)	-200(10)	25(2)
C(8)	-321(13)	8595(11)	-893(10)	31(3)
C(9)	-908(16)	8932(13)	-1704(13)	42(3)
C(10)	-1713(14)	8181(14)	-1780(13)	53(4)
C(11)	-1931(15)	7095(13)	-1094(12)	72(5)
C(12)	-1379(12)	6808(11)	-287(10)	48(4)
C(13)	1830(10)	7892(10)	267(9)	27(2)
C(14)	2872(11)	7482(8)	-442(8)	26(2)
C(15)	4113(11)	8052(9)	-909(10)	32(3)
C(16)	4329(11)	9028(10)	-679(10)	35(3)
C(17)	3322(12)	9441(10)	-12(11)	38(3)
C(18)	2090(12)	8866(10)	470(11)	37(3)
C(19)	2617(10)	6409(9)	-679(9)	28(2)
C(20)	4471(13)	5320(11)	-1345(10)	27(3)
C(21)	3385(13)	6568(11)	-2647(11)	32(3)
C(22)	2486(9)	5682(9)	-2697(7)	45(2)
C(23)	3393(10)	4726(10)	-2956(9)	40(2)
C(24)	4828(9)	5180(8)	-3149(8)	31(2)
C(25)	4749(8)	6449(8)	-3468(6)	31(2)
C(26)	2885(11)	7737(8)	-2802(7)	48(2)
C(27)	4672(10)	6838(9)	-4589(6)	46(2)
C(28)	5963(10)	7114(8)	-3479(7)	39(2)

C(29)	6115(9)	3983(9)	-2012(7)	37(2)
C(30)	7424(9)	4378(9)	-2830(7)	42(2)
C(31)	8034(12)	5155(12)	-2658(12)	39(3)
C(32)	9196(12)	5628(12)	-3394(15)	89(5)
C(33)	9731(12)	5293(14)	-4328(12)	87(5)
C(34)	9102(11)	4471(13)	-4479(9)	74(4)
C(35)	5548(15)	2832(13)	-2003(13)	49(3)
C(36)	10912(11)	2298(11)	-1813(11)	36(3)
C(37)	11821(13)	1461(12)	-1657(11)	39(3)
C(38)	12552(14)	979(13)	-2419(11)	51(4)
C(39)	12398(13)	1362(13)	-3398(11)	59(4)
C(40)	11525(16)	2224(15)	-3580(12)	82(5)
C(41)	10783(13)	2684(12)	-2801(11)	58(4)
C(42)	10694(12)	2463(11)	210(10)	29(3)
C(43)	11760(11)	3062(11)	239(11)	45(3)
C(44)	12382(12)	2680(12)	974(11)	53(3)
C(45)	11964(14)	1737(14)	1727(13)	47(3)
C(46)	10866(15)	1095(13)	1738(13)	40(3)
C(47)	10256(15)	1448(12)	1014(12)	41(3)
C(48)	8332(10)	2268(9)	-295(9)	25(2)
C(49)	7225(10)	2716(8)	389(8)	20(2)
C(50)	6005(11)	2147(9)	779(9)	27(2)
C(51)	5804(11)	1167(10)	554(11)	38(3)
C(52)	6848(12)	741(10)	-109(11)	35(3)
C(53)	8095(11)	1288(10)	-537(10)	32(2)
C(54)	7436(11)	3807(9)	588(9)	26(2)
C(55)	5293(12)	4524(10)	1429(8)	24(3)
C(56)	6685(14)	3613(11)	2563(10)	33(3)
C(57)	5839(12)	2575(8)	3190(7)	49(3)
C(58)	4441(13)	2999(10)	3665(8)	52(3)
C(59)	4629(11)	4277(9)	3302(7)	40(2)
C(60)	6108(10)	4490(9)	3161(6)	38(2)
C(61)	8203(10)	3438(10)	2424(8)	55(3)
C(62)	6679(13)	5700(9)	2603(9)	50(3)
C(63)	6289(12)	4158(9)	4261(7)	56(3)
C(64)	3207(9)	5345(8)	2216(7)	35(2)
C(65)	3319(9)	6443(8)	2487(7)	35(2)
C(66)	4227(18)	7214(13)	1820(15)	60(4)

C(67)	4388(15)	8211(10)	2070(12)	76(4)
C(68)	3569(14)	8325(11)	2991(11)	70(3)
C(69)	2629(12)	7471(11)	3659(9)	65(3)
C(70)	1905(16)	4637(15)	2867(14)	55(4)
N(1)	3627(9)	6129(8)	-1571(8)	26(2)
N(2)	5115(8)	4850(7)	-2136(7)	26(2)
N(3)	7901(10)	3958(12)	-3696(8)	74(3)
N(4)	6466(10)	4027(8)	1516(8)	27(2)
N(5)	4425(9)	4689(7)	2250(7)	32(2)
N(6)	2534(10)	6536(8)	3404(8)	55(2)
P(1)	202(3)	7107(3)	872(3)	29(1)
P(2)	9967(3)	3016(3)	-843(3)	30(1)
Au(1)	4948(1)	4975(1)	-2(1)	26(1)
F(1)	5796(10)	239(9)	5388(8)	122(3)
F(2)	7612(10)	1379(11)	4873(8)	160(5)
F(3)	7692(11)	925(8)	6533(8)	127(4)
F(4)	5885(10)	-223(9)	6973(7)	127(3)
F(5)	5807(10)	1604(8)	6113(9)	124(3)
F(6)	7577(16)	-388(10)	5789(11)	131(5)
P(3)	6770(4)	619(3)	5961(2)	62(1)

Table 11. Bond lengths [Å] and angles [°] for cmpd8.

O(1)-C(74)	1.38(3)
O(1)-C(71)	1.65(2)
C(71)-C(72)	1.62(3)
C(72)-C(73)	1.56(3)
C(73)-C(74)	1.410(15)
C(1)-C(2)	1.361(18)
C(1)-C(6)	1.411(16)
C(1)-P(1)	1.821(13)
C(2)-C(3)	1.40(2)
C(3)-C(4)	1.33(2)
C(4)-C(5)	1.37(2)
C(5)-C(6)	1.381(18)
C(7)-C(8)	1.358(19)
C(7)-C(12)	1.375(14)
C(7)-P(1)	1.847(12)
C(8)-C(9)	1.415(18)
C(9)-C(10)	1.340(19)
C(10)-C(11)	1.41(2)
C(11)-C(12)	1.384(16)
C(13)-C(18)	1.378(15)
C(13)-C(14)	1.410(16)
C(13)-P(1)	1.844(10)
C(14)-C(15)	1.390(14)
C(14)-C(19)	1.517(14)
C(15)-C(16)	1.386(16)
C(16)-C(17)	1.359(18)
C(17)-C(18)	1.386(15)
C(19)-N(1)	1.476(14)
C(20)-N(1)	1.344(16)
C(20)-N(2)	1.370(15)
C(20)-Au(1)	2.029(12)
C(21)-C(26)	1.501(15)
C(21)-C(22)	1.519(15)
C(21)-N(1)	1.554(15)
C(21)-C(25)	1.561(17)
C(22)-C(23)	1.536(15)

C(23)-C(24)	1.553(13)
C(24)-N(2)	1.488(12)
C(24)-C(25)	1.521(13)
C(25)-C(27)	1.540(11)
C(25)-C(28)	1.550(11)
C(29)-N(2)	1.480(12)
C(29)-C(30)	1.487(13)
C(29)-C(35)	1.575(18)
C(30)-C(31)	1.302(16)
C(30)-N(3)	1.394(13)
C(31)-C(32)	1.36(2)
C(32)-C(33)	1.42(2)
C(33)-C(34)	1.34(2)
C(34)-N(3)	1.425(16)
C(36)-C(41)	1.384(19)
C(36)-C(37)	1.395(19)
C(36)-P(2)	1.835(14)
C(37)-C(38)	1.372(19)
C(38)-C(39)	1.38(2)
C(39)-C(40)	1.40(2)
C(40)-C(41)	1.376(19)
C(42)-C(43)	1.395(15)
C(42)-C(47)	1.42(2)
C(42)-P(2)	1.826(13)
C(43)-C(44)	1.356(17)
C(44)-C(45)	1.33(2)
C(45)-C(46)	1.430(18)
C(46)-C(47)	1.331(19)
C(48)-C(53)	1.406(15)
C(48)-C(49)	1.453(16)
C(48)-P(2)	1.829(10)
C(49)-C(50)	1.371(12)
C(49)-C(54)	1.500(13)
C(50)-C(51)	1.384(16)
C(51)-C(52)	1.385(19)
C(52)-C(53)	1.382(14)
C(54)-N(4)	1.464(15)
C(55)-N(5)	1.285(15)

C(55)-N(4)	1.375(15)
C(55)-Au(1)	2.071(10)
C(56)-C(57)	1.493(16)
C(56)-N(4)	1.503(15)
C(56)-C(60)	1.543(16)
C(56)-C(61)	1.555(16)
C(57)-C(58)	1.542(16)
C(58)-C(59)	1.531(16)
C(59)-N(5)	1.503(12)
C(59)-C(60)	1.530(14)
C(60)-C(62)	1.544(14)
C(60)-C(63)	1.553(11)
C(64)-N(5)	1.488(12)
C(64)-C(65)	1.535(13)
C(64)-C(70)	1.540(18)
C(65)-C(66)	1.319(19)
C(65)-N(6)	1.325(13)
C(66)-C(67)	1.41(2)
C(67)-C(68)	1.348(18)
C(68)-C(69)	1.399(18)
C(69)-N(6)	1.325(14)
F(1)-P(3)	1.642(9)
F(2)-P(3)	1.563(10)
F(3)-P(3)	1.558(8)
F(4)-P(3)	1.557(9)
F(5)-P(3)	1.566(9)
F(6)-P(3)	1.508(12)

C(74)-O(1)-C(71)	109.1(18)
C(72)-C(71)-O(1)	98.2(17)
C(73)-C(72)-C(71)	105.6(19)
C(74)-C(73)-C(72)	108.9(18)
O(1)-C(74)-C(73)	113(2)
C(2)-C(1)-C(6)	117.6(12)
C(2)-C(1)-P(1)	125.1(10)
C(6)-C(1)-P(1)	117.4(9)
C(1)-C(2)-C(3)	119.2(13)
C(4)-C(3)-C(2)	123.9(14)

C(3)-C(4)-C(5)	117.1(13)
C(4)-C(5)-C(6)	121.6(12)
C(5)-C(6)-C(1)	120.5(13)
C(8)-C(7)-C(12)	118.4(11)
C(8)-C(7)-P(1)	124.1(8)
C(12)-C(7)-P(1)	117.4(10)
C(7)-C(8)-C(9)	123.3(12)
C(10)-C(9)-C(8)	117.3(15)
C(9)-C(10)-C(11)	120.8(13)
C(12)-C(11)-C(10)	120.2(12)
C(7)-C(12)-C(11)	119.8(12)
C(18)-C(13)-C(14)	117.7(10)
C(18)-C(13)-P(1)	123.5(10)
C(14)-C(13)-P(1)	118.8(8)
C(15)-C(14)-C(13)	120.2(10)
C(15)-C(14)-C(19)	120.9(10)
C(13)-C(14)-C(19)	118.9(9)
C(16)-C(15)-C(14)	120.0(12)
C(17)-C(16)-C(15)	120.1(10)
C(16)-C(17)-C(18)	120.1(11)
C(13)-C(18)-C(17)	121.8(13)
N(1)-C(19)-C(14)	117.0(9)
N(1)-C(20)-N(2)	115.4(10)
N(1)-C(20)-Au(1)	121.9(9)
N(2)-C(20)-Au(1)	122.1(9)
C(26)-C(21)-C(22)	116.5(9)
C(26)-C(21)-N(1)	111.3(10)
C(22)-C(21)-N(1)	105.7(9)
C(26)-C(21)-C(25)	114.4(10)
C(22)-C(21)-C(25)	102.6(9)
N(1)-C(21)-C(25)	105.2(8)
C(21)-C(22)-C(23)	106.5(8)
C(22)-C(23)-C(24)	104.0(8)
N(2)-C(24)-C(25)	107.8(7)
N(2)-C(24)-C(23)	108.1(8)
C(25)-C(24)-C(23)	105.0(8)
C(24)-C(25)-C(27)	109.2(7)
C(24)-C(25)-C(28)	115.6(7)

C(27)-C(25)-C(28)	105.7(7)
C(24)-C(25)-C(21)	99.1(8)
C(27)-C(25)-C(21)	111.8(7)
C(28)-C(25)-C(21)	115.5(8)
N(2)-C(29)-C(30)	109.3(8)
N(2)-C(29)-C(35)	109.4(8)
C(30)-C(29)-C(35)	114.7(9)
C(31)-C(30)-N(3)	124.9(11)
C(31)-C(30)-C(29)	113.2(10)
N(3)-C(30)-C(29)	121.9(10)
C(30)-C(31)-C(32)	118.0(14)
C(31)-C(32)-C(33)	121.3(13)
C(34)-C(33)-C(32)	119.7(12)
C(33)-C(34)-N(3)	118.9(12)
C(41)-C(36)-C(37)	117.7(12)
C(41)-C(36)-P(2)	116.7(10)
C(37)-C(36)-P(2)	125.4(10)
C(38)-C(37)-C(36)	123.5(13)
C(37)-C(38)-C(39)	118.1(14)
C(38)-C(39)-C(40)	119.3(13)
C(41)-C(40)-C(39)	121.7(14)
C(40)-C(41)-C(36)	119.5(13)
C(43)-C(42)-C(47)	116.7(12)
C(43)-C(42)-P(2)	118.7(10)
C(47)-C(42)-P(2)	124.6(9)
C(44)-C(43)-C(42)	121.9(13)
C(45)-C(44)-C(43)	121.2(11)
C(44)-C(45)-C(46)	119.1(13)
C(47)-C(46)-C(45)	120.5(15)
C(46)-C(47)-C(42)	120.6(13)
C(53)-C(48)-C(49)	118.6(9)
C(53)-C(48)-P(2)	122.3(9)
C(49)-C(48)-P(2)	119.1(7)
C(50)-C(49)-C(48)	118.0(9)
C(50)-C(49)-C(54)	122.8(10)
C(48)-C(49)-C(54)	119.1(8)
C(49)-C(50)-C(51)	122.4(11)
C(50)-C(51)-C(52)	120.0(10)

C(53)-C(52)-C(51)	120.1(11)
C(52)-C(53)-C(48)	120.9(12)
N(4)-C(54)-C(49)	115.7(9)
N(5)-C(55)-N(4)	118.6(9)
N(5)-C(55)-Au(1)	121.4(8)
N(4)-C(55)-Au(1)	120.0(8)
C(57)-C(56)-N(4)	109.8(9)
C(57)-C(56)-C(60)	104.6(10)
N(4)-C(56)-C(60)	106.7(9)
C(57)-C(56)-C(61)	112.6(10)
N(4)-C(56)-C(61)	110.3(10)
C(60)-C(56)-C(61)	112.6(9)
C(56)-C(57)-C(58)	104.6(9)
C(59)-C(58)-C(57)	104.5(9)
N(5)-C(59)-C(60)	108.1(8)
N(5)-C(59)-C(58)	108.5(8)
C(60)-C(59)-C(58)	104.2(9)
C(59)-C(60)-C(56)	97.0(8)
C(59)-C(60)-C(62)	116.5(9)
C(56)-C(60)-C(62)	115.6(9)
C(59)-C(60)-C(63)	107.9(8)
C(56)-C(60)-C(63)	111.5(8)
C(62)-C(60)-C(63)	107.9(8)
N(5)-C(64)-C(65)	109.8(7)
N(5)-C(64)-C(70)	112.0(9)
C(65)-C(64)-C(70)	114.9(10)
C(66)-C(65)-N(6)	123.8(12)
C(66)-C(65)-C(64)	118.5(11)
N(6)-C(65)-C(64)	117.6(8)
C(65)-C(66)-C(67)	119.6(17)
C(68)-C(67)-C(66)	116.9(14)
C(67)-C(68)-C(69)	120.3(12)
N(6)-C(69)-C(68)	120.7(11)
C(20)-N(1)-C(19)	116.9(10)
C(20)-N(1)-C(21)	124.9(10)
C(19)-N(1)-C(21)	116.3(9)
C(20)-N(2)-C(29)	121.3(9)
C(20)-N(2)-C(24)	121.4(9)

C(29)-N(2)-C(24)	117.3(7)
C(30)-N(3)-C(34)	117.1(12)
C(55)-N(4)-C(54)	118.6(9)
C(55)-N(4)-C(56)	120.6(10)
C(54)-N(4)-C(56)	120.5(9)
C(55)-N(5)-C(64)	122.8(8)
C(55)-N(5)-C(59)	121.2(9)
C(64)-N(5)-C(59)	116.0(8)
C(65)-N(6)-C(69)	118.6(10)
C(1)-P(1)-C(13)	103.1(5)
C(1)-P(1)-C(7)	103.8(6)
C(13)-P(1)-C(7)	100.7(5)
C(42)-P(2)-C(48)	101.3(5)
C(42)-P(2)-C(36)	101.7(6)
C(48)-P(2)-C(36)	102.9(5)
C(20)-Au(1)-C(55)	175.0(6)
F(6)-P(3)-F(4)	84.6(7)
F(6)-P(3)-F(3)	91.4(7)
F(4)-P(3)-F(3)	92.7(6)
F(6)-P(3)-F(2)	92.2(8)
F(4)-P(3)-F(2)	173.3(7)
F(3)-P(3)-F(2)	93.2(7)
F(6)-P(3)-F(5)	173.7(7)
F(4)-P(3)-F(5)	93.3(6)
F(3)-P(3)-F(5)	94.6(6)
F(2)-P(3)-F(5)	89.3(7)
F(6)-P(3)-F(1)	86.8(6)
F(4)-P(3)-F(1)	85.4(6)
F(3)-P(3)-F(1)	177.5(6)
F(2)-P(3)-F(1)	88.7(6)
F(5)-P(3)-F(1)	87.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cmpd8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	300(20)	89(12)	155(15)	-27(10)	-186(16)	24(13)
C(71)	106(13)	118(14)	51(9)	-35(9)	-7(9)	-49(11)
C(72)	300(30)	260(30)	270(30)	-60(20)	-100(20)	-20(20)
C(73)	123(15)	170(18)	68(11)	-47(11)	-48(11)	97(14)
C(74)	320(30)	230(30)	200(30)	-120(20)	-100(20)	10(20)
C(1)	24(5)	34(5)	26(5)	-7(4)	-4(4)	7(4)
C(2)	36(6)	52(7)	39(7)	-18(5)	-11(5)	12(5)
C(3)	42(7)	47(7)	63(8)	-28(6)	-21(6)	20(5)
C(4)	52(7)	69(8)	50(7)	-39(7)	-9(6)	2(6)
C(5)	62(8)	73(8)	31(6)	-28(5)	-21(6)	4(6)
C(6)	43(6)	58(7)	35(6)	-12(5)	-21(5)	0(5)
C(7)	19(4)	27(5)	35(6)	-16(4)	-10(4)	4(4)
C(8)	34(5)	41(6)	24(5)	-12(5)	-18(4)	5(5)
C(9)	52(8)	34(7)	44(9)	-15(6)	-22(7)	13(6)
C(10)	46(8)	71(9)	45(7)	0(6)	-29(6)	-13(6)
C(11)	88(11)	76(10)	69(9)	-3(7)	-57(10)	-34(9)
C(12)	68(9)	48(6)	39(6)	-1(5)	-36(7)	-22(6)
C(13)	19(4)	37(6)	35(5)	-14(4)	-16(4)	5(4)
C(14)	35(5)	23(5)	31(5)	-12(4)	-22(4)	7(4)
C(15)	28(5)	36(6)	37(6)	-9(5)	-17(5)	4(4)
C(16)	31(5)	40(6)	42(6)	-12(5)	-19(5)	-6(4)
C(17)	34(6)	26(5)	66(8)	-15(5)	-30(6)	5(4)
C(18)	40(7)	35(6)	46(7)	-17(5)	-25(6)	9(5)
C(19)	16(4)	44(6)	28(5)	-14(5)	-8(4)	7(4)
C(20)	27(3)	29(3)	29(3)	-9(2)	-10(2)	0(2)
C(21)	38(6)	34(6)	30(6)	-6(5)	-23(5)	13(5)
C(22)	39(5)	73(7)	33(5)	-17(5)	-22(4)	6(5)
C(23)	44(5)	45(7)	42(6)	-18(5)	-25(5)	2(5)
C(24)	30(5)	41(6)	25(5)	-9(4)	-14(4)	9(4)
C(25)	30(4)	43(5)	21(4)	-5(4)	-12(4)	4(4)
C(26)	61(6)	52(6)	41(5)	-17(5)	-31(5)	30(5)
C(27)	58(6)	58(6)	24(4)	-8(4)	-21(4)	18(5)
C(28)	39(5)	42(5)	31(5)	-1(4)	-10(4)	-3(4)

C(29)	37(5)	52(6)	26(5)	-15(5)	-15(4)	20(4)
C(30)	30(4)	65(7)	32(5)	-11(4)	-15(4)	19(4)
C(31)	22(5)	47(7)	60(8)	-28(6)	-16(5)	5(5)
C(32)	43(7)	78(9)	151(15)	-29(10)	-43(9)	15(6)
C(33)	40(6)	105(12)	75(10)	19(8)	-2(7)	11(7)
C(34)	35(5)	129(12)	50(7)	-22(7)	-8(5)	22(7)
C(35)	52(7)	50(8)	47(7)	-21(6)	-14(6)	20(6)
C(36)	27(5)	41(6)	37(6)	-8(5)	-9(4)	-2(4)
C(37)	35(6)	45(7)	33(6)	-8(5)	-10(5)	17(5)
C(38)	44(7)	72(9)	34(6)	-19(6)	-10(5)	27(6)
C(39)	52(8)	81(10)	34(6)	-17(7)	-1(6)	19(7)
C(40)	82(11)	127(15)	44(8)	-39(9)	-22(8)	41(10)
C(41)	57(8)	75(9)	45(7)	-21(7)	-21(6)	36(7)
C(42)	25(5)	31(5)	33(6)	-13(4)	-8(4)	8(4)
C(43)	37(6)	42(6)	57(7)	-11(5)	-17(5)	-9(5)
C(44)	46(7)	60(7)	58(7)	-6(6)	-30(6)	-15(6)
C(45)	38(7)	65(8)	53(7)	-24(6)	-27(6)	3(6)
C(46)	42(7)	35(7)	41(9)	-3(6)	-19(6)	6(6)
C(47)	43(6)	29(6)	58(9)	-13(6)	-24(6)	5(5)
C(48)	26(5)	21(4)	31(5)	-8(4)	-14(4)	2(4)
C(49)	22(4)	13(4)	24(4)	0(3)	-10(3)	-2(3)
C(50)	24(5)	26(5)	29(5)	-3(4)	-8(4)	-2(4)
C(51)	25(5)	29(6)	58(7)	-4(5)	-17(5)	-3(4)
C(52)	35(6)	30(6)	47(6)	-13(5)	-18(5)	-4(4)
C(53)	27(5)	28(5)	46(6)	-15(5)	-15(4)	5(4)
C(54)	30(5)	25(5)	27(5)	-10(4)	-13(4)	0(4)
C(55)	31(5)	31(5)	9(4)	0(3)	-11(4)	4(4)
C(56)	48(7)	37(6)	18(5)	-8(4)	-16(5)	17(5)
C(57)	91(8)	33(5)	27(5)	1(4)	-32(5)	13(5)
C(58)	57(7)	57(7)	30(6)	10(5)	-17(6)	-1(6)
C(59)	47(6)	59(7)	14(4)	-9(5)	-11(4)	16(5)
C(60)	53(6)	43(5)	19(4)	-11(4)	-14(4)	16(5)
C(61)	60(6)	78(7)	43(6)	-26(5)	-36(5)	39(6)
C(62)	78(8)	41(6)	46(7)	-16(5)	-36(6)	9(6)
C(63)	86(8)	62(7)	31(5)	-18(5)	-34(5)	22(6)
C(64)	33(5)	46(6)	25(5)	-8(4)	-13(4)	17(4)
C(65)	35(4)	39(5)	28(4)	-4(4)	-13(4)	13(4)
C(66)	72(9)	38(7)	66(10)	0(6)	-28(8)	7(7)

C(67)	87(9)	45(7)	93(11)	4(7)	-44(9)	11(6)
C(68)	87(9)	66(8)	79(9)	-24(7)	-55(8)	21(7)
C(69)	73(8)	83(9)	54(7)	-39(7)	-21(6)	3(7)
C(70)	45(8)	59(9)	60(9)	-17(7)	-16(7)	13(7)
N(1)	27(4)	37(5)	21(4)	-14(4)	-13(3)	9(3)
N(2)	25(4)	35(5)	21(4)	-14(3)	-10(3)	14(3)
N(3)	53(6)	141(11)	42(6)	-44(7)	-25(5)	40(7)
N(4)	30(4)	31(4)	25(4)	-12(3)	-14(4)	15(3)
N(5)	42(5)	41(5)	16(4)	-6(4)	-14(4)	13(4)
N(6)	48(5)	62(6)	55(6)	-22(5)	-10(5)	-1(4)
P(1)	31(1)	31(2)	30(1)	-11(1)	-15(1)	8(1)
P(2)	23(1)	26(1)	38(2)	-8(1)	-8(1)	5(1)
Au(1)	27(1)	31(1)	21(1)	-7(1)	-10(1)	3(1)
F(1)	131(8)	132(8)	141(8)	-59(7)	-81(7)	25(6)
F(2)	103(7)	195(12)	103(8)	73(8)	-24(6)	-8(8)
F(3)	158(9)	122(8)	139(8)	-42(6)	-92(8)	-5(7)
F(4)	125(8)	128(8)	81(6)	13(5)	-4(6)	-15(6)
F(5)	129(8)	93(7)	169(10)	-61(7)	-55(8)	43(6)
F(6)	218(13)	65(6)	151(11)	-45(7)	-111(10)	58(7)
P(3)	85(2)	52(2)	44(2)	-4(1)	-22(2)	17(2)

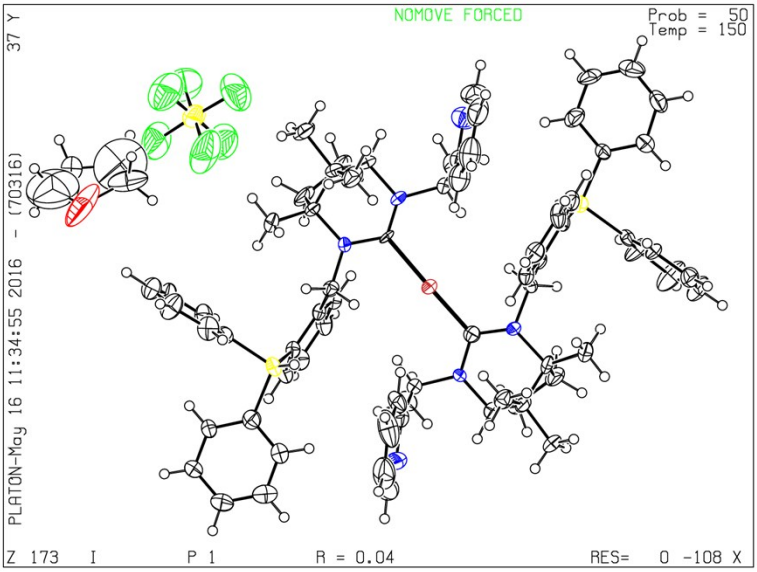

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Table 13. Crystal data and structure refinement details.

Identification code	**2015NCS0429 / NiMeNCP_all**	
Empirical formula	$C_{35}H_{38}ClF_6N_3NiP_2$	
Formula weight	770.78	
Temperature	100(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	*P*21	
Unit cell dimensions	*a* = 10.9383(3) Å	α = 90°
	b = 19.4448(3) Å	β = 108.045(3)°
	c = 17.0362(4) Å	γ = 90°
Volume	3445.25(15) Å^3	
Z	4	
Density (calculated)	1.484 Mg / m^3	
Absorption coefficient	0.797 mm^{-1}	
F(000)	1592	
Crystal	Leaf; yellow	
Crystal size	0.276 × 0.034 × 0.030 mm^3	
θ range for data collection	1.636 – 29.615°	

Index ranges	$-14 \le h \le 14$, $-15 \le k \le 26$, $-23 \le l \le 22$
Reflections collected	32767
Independent reflections	13427 [R_{int} = 0.0322]
Completeness to θ = 25.242°	100.0 %
Absorption correction	Semi–empirical from equivalents
Max. and min. transmission	1.00000 and 0.82472
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13427 / 1 / 840
Goodness-of-fit on F^2	1.022
Final R indices [$F^2 > 2\sigma(F^2)$]	$R1$ = 0.0600, $wR2$ = 0.1573
R indices (all data)	$R1$ = 0.0755, $wR2$ = 0.1694
Absolute structure parameter	0.001(9)
Extinction coefficient	n/a
Largest diff. peak and hole	0.819 and –0.847 e Å^{-3}

Diffractometer: *Rigaku AFC12* goniometer equipped with an enhanced sensitivity (HG) *Saturn724+* detector mounted at the window of an *FR-E+ SuperBright* molybdenum rotating anode generator with HF *Varimax* optics (100μm focus). **Cell determination and Data collection**: CrystalClear-SM Expert 2.0 r7 (Rigaku, 2011). **Data reduction and cell refinement & Absorption correction:** CrysalisPRO 171.37.35 (Rigaku Oxford Diffraction 2015). **Structure solution**: SHELXST (G. M. Sheldrick, Acta Cryst. (2008) A**64** 112–122). S**tructure refinement**: SHELXL97 (G. M. Sheldrick (1997), University of Göttingen, Germany). **Graphics:** Mercury 3.5.1 (CCDC 2014). **Publication material:** WinGX: Farrugia, L. J. (2012). J. Appl. Cryst. 45, 849-854.

Special details:

Table 14. Atomic coordinates [× 10^4], equivalent isotropic displacement parameters [Å² × 10^3] and site occupancy factors. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	*x*	*y*	*z*	U_{eq}	*S.o.f.*
C1	3663(6)	5878(3)	834(4)	28(1)	1
C2	3650(6)	6512(3)	439(4)	31(1)	1
C3	4316(7)	6603(4)	−128(4)	37(2)	1
C4	5014(7)	6054(4)	−303(4)	39(2)	1
C5	4998(7)	5420(4)	72(4)	37(2)	1
C6	4352(6)	5330(4)	638(4)	31(1)	1
C7	4025(6)	6183(3)	2545(4)	32(1)	1
C8	5021(7)	6608(4)	2516(5)	43(2)	1
C9	5819(8)	6891(4)	3249(5)	51(2)	1
C10	5622(8)	6762(4)	3976(5)	49(2)	1
C11	4662(7)	6335(4)	4015(4)	44(2)	1
C12	3847(7)	6046(4)	3303(4)	41(2)	1
C13	2839(6)	4912(3)	1885(4)	29(1)	1
C14	4018(6)	4600(4)	2305(4)	32(1)	1
C15	4049(7)	3917(4)	2553(4)	37(2)	1
C16	2940(7)	3564(4)	2447(4)	39(2)	1
C17	1748(7)	3867(4)	2018(4)	37(2)	1
C18	1693(6)	4541(3)	1721(4)	30(1)	1
C19	412(6)	4839(4)	1252(4)	31(1)	1
C20	−422(7)	3877(4)	−115(4)	38(2)	1
C21	36(6)	4581(3)	−315(4)	31(1)	1
C22	1253(6)	4529(3)	−592(4)	33(1)	1
C23	1174(7)	5151(4)	−1178(4)	36(2)	1
C24	−52(7)	5541(3)	−1173(4)	34(1)	1
C25	−949(6)	4966(4)	−1046(4)	33(1)	1
C26	−2127(6)	5230(4)	−865(5)	44(2)	1

C27	−1369(7)	4523(4)	−1821(4)	42(2)	1
C28	509(6)	5743(3)	315(4)	29(1)	1
C29	203(7)	7039(4)	−1329(4)	41(2)	1
C30	274(7)	6772(4)	−488(4)	34(2)	1
C31	−794(7)	7019(3)	−152(4)	34(1)	1
C32	−1890(7)	7368(4)	−594(5)	40(2)	1
C33	−2757(7)	7565(4)	−198(5)	47(2)	1
C34	−2502(7)	7429(5)	640(5)	49(2)	1
C35	−1399(7)	7067(4)	1046(5)	44(2)	1
C36	13819(7)	3929(3)	7422(4)	34(2)	1
C37	13546(8)	4037(4)	8150(5)	44(2)	1
C38	14378(9)	3802(4)	8897(4)	49(2)	1
C39	15465(9)	3450(4)	8913(5)	51(2)	1
C40	15735(8)	3325(4)	8184(5)	44(2)	1
C41	14920(6)	3567(4)	7440(4)	37(2)	1
C42	13612(6)	4237(4)	5738(4)	29(1)	1
C43	14264(6)	4786(4)	5554(4)	34(2)	1
C44	15040(7)	4688(4)	5040(4)	39(2)	1
C45	15127(7)	4057(5)	4718(4)	44(2)	1
C46	14446(7)	3503(4)	4888(5)	44(2)	1
C47	13694(6)	3597(4)	5403(4)	35(2)	1
C48	12638(7)	5178(3)	6769(4)	31(1)	1
C49	13790(7)	5501(4)	7182(4)	34(1)	1
C50	13813(7)	6159(4)	7493(4)	37(2)	1
C51	12673(7)	6502(4)	7424(4)	36(2)	1
C52	11518(7)	6177(4)	7007(4)	34(2)	1
C53	11474(6)	5527(3)	6660(4)	28(1)	1
C54	10185(6)	5203(3)	6205(4)	30(1)	1
C55	9705(8)	6293(4)	4995(4)	43(2)	1
C56	9383(6)	5565(4)	4678(4)	33(1)	1

C57	7935(7)	5395(4)	4394(4)	41(2)	1
C58	7762(7)	4843(4)	3723(5)	43(2)	1
C59	9114(6)	4708(3)	3683(4)	31(1)	1
C60	9809(7)	5395(4)	3903(4)	34(1)	1
C61	9238(8)	5912(4)	3202(4)	46(2)	1
C62	11239(7)	5350(4)	4064(5)	40(2)	1
C63	10170(6)	4390(4)	5138(4)	30(1)	1
C64	10704(8)	3081(4)	4098(6)	49(2)	1
C65	9520(7)	3471(4)	4114(4)	39(2)	1
C66	8804(7)	3132(3)	4642(5)	39(2)	1
C67	7691(8)	2737(4)	4285(5)	46(2)	1
C68	7065(8)	2437(4)	4779(5)	47(2)	1
C69	7537(8)	2542(5)	5614(6)	54(2)	1
C70	8612(8)	2928(4)	5950(5)	46(2)	1
N1	336(5)	5070(3)	404(3)	27(1)	1
N2	304(5)	5996(3)	–428(3)	29(1)	1
N3	–553(6)	6864(3)	656(4)	35(1)	1
N4	10047(5)	5050(3)	5330(3)	27(1)	1
N5	9760(5)	4210(3)	4351(3)	33(1)	1
N6	9260(6)	3210(3)	5464(4)	37(1)	1
F1	6796(5)	4326(3)	1927(3)	62(1)	1
F2	6829(5)	3203(3)	2205(4)	83(2)	1
F3	7211(5)	2993(3)	977(4)	74(2)	1
F4	7192(4)	4117(3)	746(3)	54(1)	1
F5	5493(4)	3627(3)	988(3)	53(1)	1
F6	8528(4)	3667(3)	1928(3)	50(1)	1
F7	5399(5)	6486(3)	6180(3)	67(1)	1
F8	6990(5)	6067(3)	5766(3)	67(1)	1
F9	8417(5)	6320(3)	6967(3)	67(1)	1
F10	6855(5)	6779(3)	7419(3)	67(1)	1

F11	7079(5)	7154(3)	6208(3)	67(1)	1
F12	6703(5)	5718(3)	6960(3)	67(1)	1
P1	2863(2)	5826(1)	1616(1)	27(1)	1
P2	12691(2)	4276(1)	6467(1)	29(1)	1
P3	6999(2)	3643(1)	1466(1)	31(1)	1
P4	6915(2)	6439(1)	6584(1)	32(1)	1
Ni1	1014(1)	6371(1)	1201(1)	31(1)	1
Ni2	10844(1)	3713(1)	5959(1)	32(1)	1
Cl1	1573(2)	7161(1)	2170(1)	56(1)	1
Cl2	11495(2)	2897(1)	6870(2)	71(1)	1

Table 15. Bond lengths [Å] and angles [°].

C1–C2	1.402(9)
C1–C6	1.405(9)
C1–P1	1.809(7)
C2–C3	1.389(10)
C2–H2	0.9300
C3–C4	1.396(10)
C3–H3	0.9300
C4–C5	1.392(11)
C4–H4	0.9300
C5–C6	1.372(10)
C5–H5	0.9300
C6–H6	0.9300
C7–C8	1.381(10)
C7–C12	1.390(10)
C7–P1	1.832(7)
C8–C9	1.396(10)
C8–H8	0.9300
C9–C10	1.344(13)
C9–H9	0.9300
C10–C11	1.357(12)
C10–H10	0.9300
C11–C12	1.384(10)
C11–H11	0.9300
C12–H12	0.9300
C13–C18	1.398(9)
C13–C14	1.404(9)
C13–P1	1.838(7)
C14–C15	1.391(9)
C14–H14	0.9300
C15–C16	1.356(11)
C15–H15	0.9300
C16–C17	1.412(10)
C16–H16	0.9300
C17–C18	1.399(9)
C17–H17	0.9300
C18–C19	1.498(9)
C19–N1	1.491(8)
C19–H19A	0.9700
C19–H19B	0.9700
C20–C21	1.532(9)
C20–H20A	0.9600
C20–H20B	0.9600
C20–H20C	0.9600
C21–N1	1.505(8)
C21–C22	1.547(9)
C21–C25	1.562(8)
C22–C23	1.555(9)
C22–H22A	0.9700
C22–H22B	0.9700
C23–C24	1.542(10)
C23–H23A	0.9700
C23–H23B	0.9700
C24–N2	1.497(8)
C24–C25	1.546(9)
C24–H24	0.9800
C25–C26	1.505(10)
C25–C27	1.523(10)

C26–H26A	0.9600	C37–C38	1.392(11)
C26–H26B	0.9600	C37–H37	0.9300
C26–H26C	0.9600	C38–C39	1.364(13)
C27–H27A	0.9600	C38–H38	0.9300
C27–H27B	0.9600	C39–C40	1.384(12)
C27–H27C	0.9600	C39–H39	0.9300
C28–N2	1.310(8)	C40–C41	1.386(10)
C28–N1	1.338(8)	C40–H40	0.9300
C28–Ni1	1.887(7)	C41–H41	0.9300
C29–C30	1.504(9)	C42–C43	1.373(10)
C29–H29A	0.9600	C42–C47	1.383(9)
C29–H29B	0.9600	C42–P2	1.826(7)
C29–H29C	0.9600	C43–C44	1.409(10)
C30–N2	1.510(8)	C43–H43	0.9300
C30–C31	1.530(10)	C44–C45	1.360(11)
C30–H30	0.9800	C44–H44	0.9300
C31–N3	1.352(9)	C45–C46	1.389(11)
C31–C32	1.380(10)	C45–H45	0.9300
C32–C33	1.378(11)	C46–C47	1.389(10)
C32–H32	0.9300	C46–H46	0.9300
C33–C34	1.392(12)	C47–H47	0.9300
C33–H33	0.9300	C48–C49	1.390(9)
C34–C35	1.383(11)	C48–C53	1.404(10)
C34–H34	0.9300	C48–P2	1.834(7)
C35–N3	1.355(9)	C49–C50	1.381(10)
C35–H35	0.9300	C49–H49	0.9300
C36–C37	1.380(10)	C50–C51	1.387(11)
C36–C41	1.386(10)	C50–H50	0.9300
C36–P2	1.839(7)	C51–C52	1.394(10)

C51–H51	0.9300	C62–H62B	0.9600
C52–C53	1.390(9)	C62–H62C	0.9600
C52–H52	0.9300	C63–N5	1.324(8)
C53–C54	1.520(9)	C63–N4	1.340(8)
C54–N4	1.482(8)	C63–Ni2	1.895(7)
C54–H54A	0.9700	C64–C65	1.508(11)
C54–H54B	0.9700	C64–H64A	0.9600
C55–C56	1.516(10)	C64–H64B	0.9600
C55–H55A	0.9600	C64–H64C	0.9600
C55–H55B	0.9600	C65–N5	1.493(8)
C55–H55C	0.9600	C65–C66	1.514(10)
C56–N4	1.505(8)	C65–H65	0.9800
C56–C57	1.543(10)	C66–N6	1.341(10)
C56–C60	1.566(9)	C66–C67	1.409(10)
C57–C58	1.537(10)	C67–C68	1.369(11)
C57–H57A	0.9700	C67–H67	0.9300
C57–H57B	0.9700	C68–C69	1.371(12)
C58–C59	1.525(9)	C68–H68	0.9300
C58–H58A	0.9700	C69–C70	1.362(11)
C58–H58B	0.9700	C69–H69	0.9300
C59–N5	1.495(9)	C70–N6	1.362(10)
C59–C60	1.525(9)	C70–H70	0.9300
C59–H59	0.9800	N3–Ni1	1.932(6)
C60–C62	1.504(10)	N6–Ni2	1.940(6)
C60–C61	1.538(10)	F1–P3	1.593(5)
C61–H61A	0.9600	F2–P3	1.580(5)
C61–H61B	0.9600	F3–P3	1.570(5)
C61–H61C	0.9600	F4–P3	1.599(5)
C62–H62A	0.9600	F5–P3	1.597(4)

F6–P3	1.613(4)	C1–C6–H6	120.0
F7–P4	1.590(6)	C8–C7–C12	119.2(7)
F8–P4	1.594(5)	C8–C7–P1	122.6(5)
F9–P4	1.586(5)	C12–C7–P1	118.1(5)
F10–P4	1.589(6)	C7–C8–C9	119.0(8)
F11–P4	1.564(6)	C7–C8–H8	120.5
F12–P4	1.589(6)	C9–C8–H8	120.5
P1–Ni1	2.1970(18)	C10–C9–C8	121.1(8)
P2–Ni2	2.2242(18)	C10–C9–H9	119.4
Ni1–Cl1	2.198(2)	C8–C9–H9	119.4
Ni2–Cl2	2.180(2)	C9–C10–C11	120.5(7)
		C9–C10–H10	119.8
C2–C1–C6	118.7(6)	C11–C10–H10	119.8
C2–C1–P1	117.9(5)	C10–C11–C12	120.3(7)
C6–C1–P1	123.4(5)	C10–C11–H11	119.9
C3–C2–C1	121.1(6)	C12–C11–H11	119.9
C3–C2–H2	119.5	C11–C12–C7	119.9(7)
C1–C2–H2	119.5	C11–C12–H12	120.1
C2–C3–C4	119.4(6)	C7–C12–H12	120.1
C2–C3–H3	120.3	C18–C13–C14	120.2(6)
C4–C3–H3	120.3	C18–C13–P1	122.1(5)
C5–C4–C3	119.6(6)	C14–C13–P1	117.6(5)
C5–C4–H4	120.2	C15–C14–C13	120.0(6)
C3–C4–H4	120.2	C15–C14–H14	120.0
C6–C5–C4	121.2(7)	C13–C14–H14	120.0
C6–C5–H5	119.4	C16–C15–C14	120.5(7)
C4–C5–H5	119.4	C16–C15–H15	119.8
C5–C6–C1	120.1(7)	C14–C15–H15	119.8
C5–C6–H6	120.0	C15–C16–C17	120.1(6)

C15–C16–H16	120.0	C21–C22–H22B	110.7
C17–C16–H16	120.0	C23–C22–H22B	110.7
C18–C17–C16	120.5(7)	H22A–C22–H22B	108.8
C18–C17–H17	119.7	C24–C23–C22	104.7(5)
C16–C17–H17	119.7	C24–C23–H23A	110.8
C13–C18–C17	118.5(6)	C22–C23–H23A	110.8
C13–C18–C19	122.7(6)	C24–C23–H23B	110.8
C17–C18–C19	118.9(6)	C22–C23–H23B	110.8
N1–C19–C18	113.4(5)	H23A–C23–H23B	108.9
N1–C19–H19A	108.9	N2–C24–C23	107.3(5)
C18–C19–H19A	108.9	N2–C24–C25	108.6(5)
N1–C19–H19B	108.9	C23–C24–C25	103.7(5)
C18–C19–H19B	108.9	N2–C24–H24	112.3
H19A–C19–H19B	107.7	C23–C24–H24	112.3
C21–C20–H20A	109.5	C25–C24–H24	112.3
C21–C20–H20B	109.5	C26–C25–C27	108.8(6)
H20A–C20–H20B	109.5	C26–C25–C24	113.7(6)
C21–C20–H20C	109.5	C27–C25–C24	108.8(6)
H20A–C20–H20C	109.5	C26–C25–C21	115.1(6)
H20B–C20–H20C	109.5	C27–C25–C21	111.6(6)
N1–C21–C20	112.8(5)	C24–C25–C21	98.4(5)
N1–C21–C22	107.4(5)	C25–C26–H26A	109.5
C20–C21–C22	112.4(5)	C25–C26–H26B	109.5
N1–C21–C25	105.6(5)	H26A–C26–H26B	109.5
C20–C21–C25	114.4(5)	C25–C26–H26C	109.5
C22–C21–C25	103.6(5)	H26A–C26–H26C	109.5
C21–C22–C23	105.3(5)	H26B–C26–H26C	109.5
C21–C22–H22A	110.7	C25–C27–H27A	109.5
C23–C22–H22A	110.7	C25–C27–H27B	109.5

H27A–C27–H27B	109.5	C35–C34–H34	120.8
C25–C27–H27C	109.5	C33–C34–H34	120.8
H27A–C27–H27C	109.5	N3–C35–C34	121.7(7)
H27B–C27–H27C	109.5	N3–C35–H35	119.2
N2–C28–N1	119.3(6)	C34–C35–H35	119.2
N2–C28–Ni1	116.7(5)	C37–C36–C41	119.0(7)
N1–C28–Ni1	124.0(5)	C37–C36–P2	117.8(6)
C30–C29–H29A	109.5	C41–C36–P2	123.1(5)
C30–C29–H29B	109.5	C36–C37–C38	120.6(8)
H29A–C29–H29B	109.5	C36–C37–H37	119.7
C30–C29–H29C	109.5	C38–C37–H37	119.7
H29A–C29–H29C	109.5	C39–C38–C37	120.1(7)
H29B–C29–H29C	109.5	C39–C38–H38	119.9
C29–C30–N2	113.8(6)	C37–C38–H38	119.9
C29–C30–C31	115.4(6)	C38–C39–C40	119.8(7)
N2–C30–C31	107.0(5)	C38–C39–H39	120.1
C29–C30–H30	106.7	C40–C39–H39	120.1
N2–C30–H30	106.7	C39–C40–C41	120.3(8)
C31–C30–H30	106.7	C39–C40–H40	119.8
N3–C31–C32	121.8(7)	C41–C40–H40	119.8
N3–C31–C30	112.4(6)	C36–C41–C40	120.1(7)
C32–C31–C30	125.8(7)	C36–C41–H41	120.0
C33–C32–C31	118.9(7)	C40–C41–H41	120.0
C33–C32–H32	120.6	C43–C42–C47	120.0(6)
C31–C32–H32	120.6	C43–C42–P2	123.9(5)
C32–C33–C34	119.9(7)	C47–C42–P2	115.9(5)
C32–C33–H33	120.0	C42–C43–C44	119.6(7)
C34–C33–H33	120.0	C42–C43–H43	120.2
C35–C34–C33	118.5(8)	C44–C43–H43	120.2

C45–C44–C43	120.2(7)	C48–C53–C54	121.8(6)
C45–C44–H44	119.9	N4–C54–C53	112.7(5)
C43–C44–H44	119.9	N4–C54–H54A	109.1
C44–C45–C46	120.5(7)	C53–C54–H54A	109.1
C44–C45–H45	119.8	N4–C54–H54B	109.1
C46–C45–H45	119.8	C53–C54–H54B	109.1
C47–C46–C45	119.3(7)	H54A–C54–H54B	107.8
C47–C46–H46	120.3	C56–C55–H55A	109.5
C45–C46–H46	120.3	C56–C55–H55B	109.5
C42–C47–C46	120.4(7)	H55A–C55–H55B	109.5
C42–C47–H47	119.8	C56–C55–H55C	109.5
C46–C47–H47	119.8	H55A–C55–H55C	109.5
C49–C48–C53	119.4(6)	H55B–C55–H55C	109.5
C49–C48–P2	118.2(5)	N4–C56–C55	110.7(5)
C53–C48–P2	122.2(5)	N4–C56–C57	107.6(6)
C50–C49–C48	121.3(7)	C55–C56–C57	114.5(6)
C50–C49–H49	119.4	N4–C56–C60	106.2(5)
C48–C49–H49	119.4	C55–C56–C60	113.7(6)
C49–C50–C51	120.3(7)	C57–C56–C60	103.6(5)
C49–C50–H50	119.9	C58–C57–C56	105.1(5)
C51–C50–H50	119.9	C58–C57–H57A	110.7
C50–C51–C52	118.3(7)	C56–C57–H57A	110.7
C50–C51–H51	120.8	C58–C57–H57B	110.7
C52–C51–H51	120.8	C56–C57–H57B	110.7
C53–C52–C51	122.4(7)	H57A–C57–H57B	108.8
C53–C52–H52	118.8	C59–C58–C57	104.8(6)
C51–C52–H52	118.8	C59–C58–H58A	110.8
C52–C53–C48	118.2(6)	C57–C58–H58A	110.8
C52–C53–C54	119.9(6)	C59–C58–H58B	110.8

C57–C58–H58B	110.8	C65–C64–H64A	109.5
H58A–C58–H58B	108.9	C65–C64–H64B	109.5
N5–C59–C58	108.3(6)	H64A–C64–H64B	109.5
N5–C59–C60	107.3(5)	C65–C64–H64C	109.5
C58–C59–C60	104.8(6)	H64A–C64–H64C	109.5
N5–C59–H59	112.0	H64B–C64–H64C	109.5
C58–C59–H59	112.0	N5–C65–C64	114.1(6)
C60–C59–H59	112.0	N5–C65–C66	109.7(6)
C62–C60–C59	113.9(6)	C64–C65–C66	113.4(6)
C62–C60–C61	109.2(6)	N5–C65–H65	106.3
C59–C60–C61	109.3(6)	C64–C65–H65	106.3
C62–C60–C56	115.0(6)	C66–C65–H65	106.3
C59–C60–C56	97.9(5)	N6–C66–C67	120.3(7)
C61–C60–C56	111.1(6)	N6–C66–C65	118.6(6)
C60–C61–H61A	109.5	C67–C66–C65	121.2(7)
C60–C61–H61B	109.5	C68–C67–C66	119.8(7)
H61A–C61–H61B	109.5	C68–C67–H67	120.1
C60–C61–H61C	109.5	C66–C67–H67	120.1
H61A–C61–H61C	109.5	C67–C68–C69	118.4(8)
H61B–C61–H61C	109.5	C67–C68–H68	120.8
C60–C62–H62A	109.5	C69–C68–H68	120.8
C60–C62–H62B	109.5	C70–C69–C68	121.2(8)
H62A–C62–H62B	109.5	C70–C69–H69	119.4
C60–C62–H62C	109.5	C68–C69–H69	119.4
H62A–C62–H62C	109.5	C69–C70–N6	120.7(8)
H62B–C62–H62C	109.5	C69–C70–H70	119.7
N5–C63–N4	118.2(6)	N6–C70–H70	119.7
N5–C63–Ni2	119.7(5)	C28–N1–C19	116.0(5)
N4–C63–Ni2	122.0(5)	C28–N1–C21	121.9(5)

C19–N1–C21	122.0(5)	F3–P3–F1	177.2(4)
C28–N2–C24	121.2(5)	F2–P3–F1	89.4(4)
C28–N2–C30	115.7(5)	F3–P3–F5	90.7(3)
C24–N2–C30	122.6(5)	F2–P3–F5	92.2(3)
C31–N3–C35	119.1(6)	F1–P3–F5	89.3(3)
C31–N3–Ni1	117.7(5)	F3–P3–F4	88.9(3)
C35–N3–Ni1	123.2(5)	F2–P3–F4	177.4(4)
C63–N4–C54	116.8(5)	F1–P3–F4	88.3(3)
C63–N4–C56	121.3(5)	F5–P3–F4	88.9(3)
C54–N4–C56	118.9(5)	F3–P3–F6	88.9(3)
C63–N5–C65	120.4(6)	F2–P3–F6	89.2(3)
C63–N5–C59	122.1(6)	F1–P3–F6	91.0(3)
C65–N5–C59	114.6(5)	F5–P3–F6	178.5(3)
C66–N6–C70	119.7(6)	F4–P3–F6	89.7(3)
C66–N6–Ni2	120.2(5)	F11–P4–F9	93.6(3)
C70–N6–Ni2	120.1(5)	F11–P4–F12	178.2(3)
C1–P1–C7	104.5(3)	F9–P4–F12	88.1(3)
C1–P1–C13	106.6(3)	F11–P4–F10	92.2(3)
C7–P1–C13	102.1(3)	F9–P4–F10	91.0(3)
C1–P1–Ni1	110.1(2)	F12–P4–F10	87.3(3)
C7–P1–Ni1	114.7(2)	F11–P4–F7	90.5(3)
C13–P1–Ni1	117.6(2)	F9–P4–F7	174.8(4)
C42–P2–C48	107.6(3)	F12–P4–F7	87.8(3)
C42–P2–C36	103.0(3)	F10–P4–F7	92.0(3)
C48–P2–C36	100.0(3)	F11–P4–F8	90.1(3)
C42–P2–Ni2	110.0(2)	F9–P4–F8	88.1(3)
C48–P2–Ni2	118.4(2)	F12–P4–F8	90.4(3)
C36–P2–Ni2	116.3(2)	F10–P4–F8	177.6(3)
F3–P3–F2	93.4(4)	F7–P4–F8	88.7(3)

C28–Ni1–N3	86.5(3)
C28–Ni1–P1	87.56(19)
N3–Ni1–P1	170.06(19)
C28–Ni1–Cl1	176.0(2)
N3–Ni1–Cl1	90.78(19)
P1–Ni1–Cl1	94.67(7)
C63–Ni2–N6	86.5(3)
C63–Ni2–Cl2	176.1(2)
N6–Ni2–Cl2	89.62(19)
C63–Ni2–P2	92.53(19)
N6–Ni2–P2	176.9(2)
Cl2–Ni2–P2	91.36(8)

Symmetry transformations used to generate equivalent atoms:

Table 16. Anisotropic displacement parameters [Å^2× 10^3]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \cdots + 2\,h\,k\,a^*\,b^*\,U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C1	29(3)	24(3)	30(3)	1(2)	6(2)	−1(3)
C2	27(3)	27(4)	36(3)	3(3)	6(2)	3(3)
C3	39(4)	30(4)	40(4)	12(3)	9(3)	−1(3)
C4	36(4)	47(4)	38(3)	4(3)	15(3)	3(3)
C5	42(4)	34(4)	38(3)	0(3)	16(3)	6(3)
C6	28(3)	26(3)	37(3)	1(3)	8(3)	−1(3)
C7	32(3)	23(3)	38(3)	1(3)	6(3)	9(3)
C8	51(4)	32(4)	41(4)	2(3)	4(3)	2(3)
C9	54(5)	29(4)	56(5)	4(3)	−4(4)	−13(3)
C10	59(5)	27(4)	47(4)	−5(3)	−5(4)	12(4)
C11	52(4)	42(4)	35(3)	0(3)	9(3)	15(4)
C12	49(4)	41(4)	35(3)	−3(3)	16(3)	7(3)
C13	34(3)	21(3)	34(3)	5(2)	13(3)	1(3)
C14	33(3)	30(4)	33(3)	0(3)	8(3)	2(3)
C15	41(4)	29(3)	36(3)	7(3)	7(3)	7(3)
C16	61(4)	23(3)	29(3)	5(3)	8(3)	2(3)
C17	45(4)	29(4)	34(3)	3(3)	10(3)	−8(3)
C18	37(3)	27(3)	27(3)	4(2)	13(2)	1(3)
C19	28(3)	37(4)	30(3)	9(3)	11(2)	−2(3)
C20	41(4)	32(4)	38(3)	3(3)	8(3)	−5(3)
C21	34(3)	30(3)	28(3)	6(3)	8(2)	2(3)
C22	39(3)	22(3)	36(3)	3(3)	10(3)	3(3)
C23	42(4)	29(3)	38(3)	3(3)	14(3)	−3(3)
C24	45(4)	23(3)	34(3)	6(3)	10(3)	−2(3)
C25	33(3)	33(4)	31(3)	4(3)	5(3)	0(3)
C26	27(3)	51(5)	50(4)	16(4)	5(3)	0(3)

C27	44(4)	34(4)	38(4)	6(3)	−1(3)	−3(3)
C28	26(3)	24(3)	40(3)	5(3)	13(3)	8(2)
C29	46(4)	29(4)	43(4)	6(3)	10(3)	−3(3)
C30	34(3)	30(3)	38(4)	6(3)	11(3)	−3(3)
C31	34(3)	23(3)	44(4)	4(3)	11(3)	1(3)
C32	40(4)	21(3)	55(4)	1(3)	8(3)	−1(3)
C33	29(4)	32(4)	69(5)	4(4)	1(3)	3(3)
C34	37(4)	47(5)	65(5)	−5(4)	19(4)	5(3)
C35	40(4)	47(5)	49(4)	−4(4)	20(3)	5(3)
C36	45(4)	22(3)	37(3)	3(3)	12(3)	1(3)
C37	56(5)	32(4)	46(4)	1(3)	20(3)	−1(3)
C38	84(6)	32(4)	31(3)	−1(3)	17(3)	−16(4)
C39	66(5)	32(4)	41(4)	3(3)	−1(4)	−12(4)
C40	44(4)	34(4)	47(4)	−1(3)	2(3)	−1(3)
C41	41(4)	31(4)	35(3)	−2(3)	7(3)	−3(3)
C42	24(3)	30(3)	33(3)	−1(3)	7(2)	−1(3)
C43	33(3)	29(4)	41(3)	1(3)	13(3)	−2(3)
C44	38(4)	41(4)	41(4)	5(3)	18(3)	−5(3)
C45	41(4)	56(5)	39(4)	−1(3)	18(3)	1(4)
C46	51(4)	40(4)	43(4)	−10(3)	19(3)	−1(4)
C47	37(3)	25(4)	44(3)	−5(3)	15(3)	−5(3)
C48	41(3)	23(3)	32(3)	−1(2)	16(3)	−9(3)
C49	32(3)	29(4)	41(3)	0(3)	12(3)	0(3)
C50	47(4)	32(4)	31(3)	0(3)	9(3)	−10(3)
C51	48(4)	30(4)	30(3)	−7(3)	13(3)	−2(3)
C52	51(4)	25(3)	30(3)	−1(2)	18(3)	−1(3)
C53	37(3)	24(3)	26(3)	1(2)	14(2)	−1(3)
C54	36(3)	25(3)	29(3)	−2(2)	12(3)	5(3)
C55	66(5)	22(3)	36(3)	1(3)	9(3)	2(3)
C56	37(3)	33(4)	28(3)	−2(3)	10(3)	2(3)

C57	39(4)	46(4)	36(3)	0(3)	9(3)	11(3)
C58	34(4)	46(4)	45(4)	−10(3)	8(3)	−9(3)
C59	41(4)	24(3)	30(3)	−6(3)	15(3)	1(3)
C60	40(4)	29(3)	32(3)	0(3)	10(3)	−1(3)
C61	59(5)	42(4)	35(4)	3(3)	13(3)	2(4)
C62	43(4)	36(4)	44(4)	4(3)	17(3)	−5(3)
C63	27(3)	30(3)	33(3)	−2(3)	9(2)	−3(3)
C64	55(5)	30(4)	68(5)	−8(4)	26(4)	−4(4)
C65	50(4)	23(3)	40(4)	−5(3)	10(3)	−3(3)
C66	42(4)	17(3)	61(5)	0(3)	18(3)	−2(3)
C67	49(4)	35(4)	47(4)	−5(3)	7(3)	−1(3)
C68	41(4)	30(4)	69(5)	3(4)	16(4)	−8(3)
C69	43(4)	51(5)	62(5)	11(4)	10(4)	−13(4)
C70	49(4)	29(4)	61(5)	6(3)	18(4)	−5(3)
N1	27(3)	24(3)	29(2)	4(2)	8(2)	2(2)
N2	39(3)	21(3)	26(2)	2(2)	12(2)	−1(2)
N3	35(3)	31(3)	37(3)	−1(2)	8(2)	6(2)
N4	33(3)	20(3)	29(2)	−1(2)	12(2)	−3(2)
N5	40(3)	23(3)	36(3)	−6(2)	12(2)	−6(2)
N6	37(3)	21(3)	50(3)	4(2)	13(3)	−2(2)
F1	64(3)	62(3)	50(3)	−22(2)	4(2)	22(3)
F2	61(3)	97(5)	93(4)	68(4)	28(3)	15(3)
F3	54(3)	39(3)	109(4)	−41(3)	−5(3)	13(2)
F4	57(3)	62(3)	45(2)	14(2)	18(2)	−4(2)
F5	26(2)	61(3)	61(3)	−3(2)	0(2)	1(2)
F6	33(2)	62(3)	48(2)	−4(2)	2(2)	6(2)
F7	63(1)	78(2)	57(1)	−3(1)	16(1)	1(1)
F8	63(1)	78(2)	57(1)	−3(1)	16(1)	1(1)
F9	63(1)	78(2)	57(1)	−3(1)	16(1)	1(1)
F10	63(1)	78(2)	57(1)	−3(1)	16(1)	1(1)

F11	63(1)	78(2)	57(1)	−3(1)	16(1)	1(1)
F12	63(1)	78(2)	57(1)	−3(1)	16(1)	1(1)
P1	29(1)	20(1)	32(1)	1(1)	10(1)	3(1)
P2	31(1)	21(1)	37(1)	−1(1)	13(1)	−1(1)
P3	29(1)	27(1)	34(1)	1(1)	4(1)	1(1)
P4	33(1)	31(1)	31(1)	−1(1)	8(1)	0(1)
Ni1	33(1)	29(1)	34(1)	1(1)	13(1)	8(1)
Ni2	33(1)	21(1)	43(1)	0(1)	12(1)	−2(1)
Cl1	51(1)	56(1)	55(1)	−16(1)	9(1)	15(1)
Cl2	44(1)	44(1)	112(2)	25(1)	4(1)	−3(1)

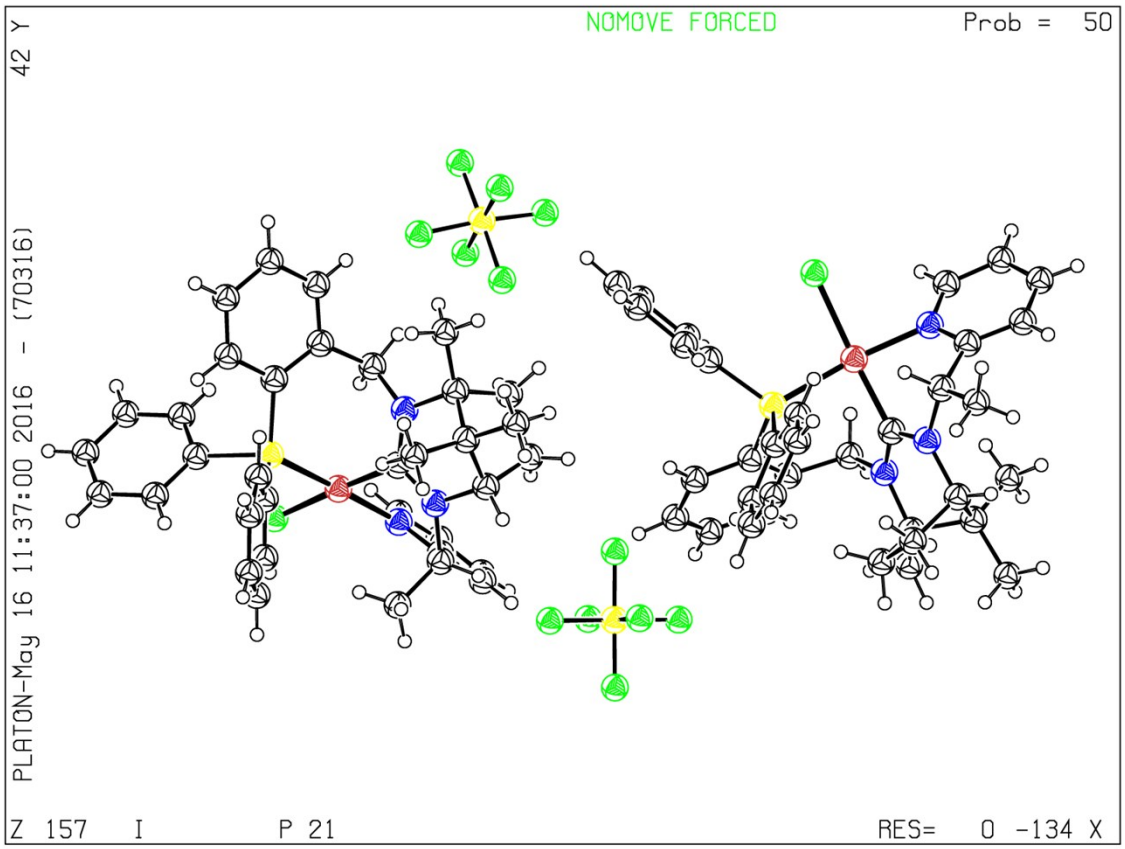


Table 17. Crystal data and structure refinement for cmpd11.

Identification code	cmpd11	
Empirical formula	C74 H84 Cl2 F12 N8 P4 Pt	
Formula weight	1703.36	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.0849(2) Å	α= 90°.
	b = 15.7236(4) Å	β= 100.252(2)°.
	c = 25.0744(6) Å	γ = 90°.
Volume	3912.59(16) $Å^3$	
Z	2	
Density (calculated)	1.446 Mg/m^3	
Absorption coefficient	2.018 mm^{-1}	
F(000)	1728	
Crystal size	0.468 x 0.290 x 0.149 mm^3	
Theta range for data collection	3.487 to 29.626°.	
Index ranges	-13<=h<=12, -20<=k<=19, -24<=l<=34	
Reflections collected	21921	
Independent reflections	14918 [R(int) = 0.0310]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.997 and 0.993	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14918 / 665 / 1016	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1086	
R indices (all data)	R1 = 0.0515, wR2 = 0.1123	
Absolute structure parameter	0.001(4)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.991 and -1.374 e.$Å^{-3}$	

Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cmpd11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	5635(2)	980(2)	3297(1)	25(1)
P(2)	3377(2)	1163(2)	1530(1)	28(1)
Cl(1)	6396(2)	1509(2)	2094(1)	34(1)
Cl(2)	2643(2)	580(1)	2731(1)	31(1)
Pt(1)	4509(1)	1060(1)	2413(1)	24(1)
N(1)	8665(7)	-775(5)	3075(3)	36(2)
N(2)	9151(10)	-1643(6)	3837(4)	55(2)
N(3)	11092(13)	-643(9)	4579(5)	90(4)
N(4)	335(8)	2888(6)	1844(4)	57(3)
N(5)	-1137(10)	3618(8)	1193(5)	83(4)
C(1)	4828(9)	1725(7)	3688(4)	40(2)
C(2)	4639(12)	2548(7)	3486(5)	54(3)
C(3)	3960(13)	3157(9)	3751(5)	71(4)
C(4)	3475(12)	2909(11)	4201(5)	75(5)
C(5)	3607(12)	2101(10)	4393(5)	68(4)
C(6)	4298(9)	1511(8)	4138(4)	48(2)
C(7)	5635(8)	-45(6)	3632(3)	32(2)
C(8)	6249(10)	-122(8)	4169(4)	46(2)
C(9)	6237(12)	-913(9)	4421(4)	63(4)
C(10)	5650(11)	-1611(9)	4143(5)	61(3)
C(11)	5078(10)	-1526(7)	3608(4)	46(2)
C(12)	5044(9)	-757(6)	3362(4)	34(2)
C(13)	7434(8)	1270(5)	3425(3)	28(2)
C(14)	8379(8)	764(5)	3216(3)	29(2)
C(15)	9720(7)	1024(12)	3317(3)	45(2)
C(16)	10133(10)	1720(8)	3628(5)	55(3)
C(17)	9221(11)	2197(7)	3832(4)	52(3)
C(18)	7868(10)	1987(6)	3736(4)	40(2)
C(19)	8003(9)	4(6)	2849(3)	33(2)
C(20)	8793(10)	-921(7)	3597(4)	45(2)
C(21)	8895(11)	-1503(7)	2701(4)	44(2)
C(22)	7754(12)	-2126(7)	2691(5)	58(3)
C(23)	8163(12)	-2709(7)	3174(6)	66(3)

C(24)	9478(12)	-2361(8)	3481(6)	67(4)
C(25)	10162(11)	-1992(8)	3042(6)	61(3)
C(26)	9107(15)	-1162(8)	2163(5)	64(3)
C(27)	10548(17)	-2732(9)	2689(8)	101(6)
C(28)	11370(12)	-1438(10)	3242(7)	85(5)
C(29)	9442(12)	-1670(10)	4449(5)	69(4)
C(30)	10866(12)	-1459(11)	4633(6)	81(5)
C(31)	11856(14)	-2009(12)	4863(5)	85(5)
C(32)	13154(14)	-1711(16)	5052(6)	99(6)
C(33)	13414(18)	-862(19)	5013(7)	119(8)
C(34)	12400(20)	-362(18)	4780(9)	141(9)
C(35)	9020(17)	-2543(11)	4639(6)	97(5)
C(36)	4152(8)	424(6)	1123(3)	33(2)
C(37)	4279(9)	567(7)	589(4)	44(2)
C(38)	4845(12)	-60(9)	309(4)	61(3)
C(39)	5333(12)	-802(9)	563(5)	58(3)
C(40)	5219(13)	-939(8)	1088(5)	59(3)
C(41)	4624(12)	-343(8)	1367(4)	54(3)
C(42)	3354(8)	2230(6)	1229(4)	37(2)
C(43)	4056(9)	2889(7)	1506(4)	41(2)
C(44)	4038(10)	3703(7)	1279(5)	59(3)
C(45)	3296(12)	3821(10)	763(6)	74(4)
C(46)	2553(12)	3181(9)	485(5)	61(3)
C(47)	2582(9)	2370(7)	714(4)	44(2)
C(48)	1578(7)	872(7)	1398(3)	35(3)
C(49)	647(9)	1328(7)	1631(4)	50(3)
C(50)	-711(8)	1072(16)	1506(4)	65(3)
C(51)	-1124(11)	390(12)	1170(5)	83(5)
C(52)	-218(12)	-63(11)	955(5)	78(5)
C(53)	1157(10)	185(9)	1072(4)	58(3)
C(54)	1041(9)	2067(7)	2011(4)	45(3)
C(55)	-267(11)	3014(9)	1355(6)	72(4)
C(56)	134(11)	3507(7)	2272(6)	64(4)
C(57)	-1244(10)	3279(7)	2432(6)	52(3)
C(58)	-2300(10)	3677(8)	1962(5)	59(3)
C(59)	-1468(12)	4158(8)	1623(7)	80(5)
C(60)	-163(13)	4390(10)	2009(8)	102(6)
C(61)	1343(12)	3471(9)	2733(7)	78(4)

C(62)	-420(17)	5080(9)	2427(9)	130(10)
C(63)	1002(14)	4678(11)	1722(10)	140(10)
C(64)	-1780(9)	3736(7)	617(4)	106(6)
C(65)	-1892(9)	2984(7)	354(4)	130(8)
C(66)	-3139(9)	2582(7)	282(4)	156(9)
C(67)	-3354(9)	1842(7)	-24(4)	239(17)
C(68)	-2322(9)	1504(7)	-260(4)	190(12)
C(69)	-1075(9)	1906(7)	-188(4)	176(11)
N(6)	-860(9)	2646(7)	119(4)	131(6)
C(70)	-980(20)	4488(12)	392(8)	125(8)
P(3)	6790(10)	6537(5)	1087(3)	68(3)
F(1)	6570(20)	6778(11)	480(4)	124(8)
F(2)	5415(14)	6903(10)	1146(8)	125(8)
F(3)	7073(19)	6274(11)	1697(4)	133(9)
F(4)	8204(15)	6168(12)	1041(9)	160(9)
F(5)	7458(19)	7422(8)	1235(8)	118(8)
F(6)	6151(19)	5647(7)	942(7)	90(7)
P(3A)	7626(10)	6838(4)	931(3)	104(3)
F(1A)	8170(16)	6509(9)	431(4)	129(7)
F(2A)	8218(17)	7735(6)	858(6)	150(8)
F(3A)	7009(18)	7169(11)	1418(5)	147(8)
F(4A)	7005(17)	5941(8)	995(6)	121(6)
F(5A)	8920(14)	6574(9)	1316(5)	155(8)
F(6A)	6287(13)	7113(10)	546(6)	131(7)
N(7)	3978(16)	7947(14)	2255(6)	122(6)
C(71)	3220(30)	7873(18)	1880(9)	146(9)
C(72)	2330(30)	7710(20)	1330(11)	224(15)
N(8)	-4940(30)	4414(19)	2670(12)	199(10)
C(73)	-3930(40)	4470(40)	2991(17)	290(20)
C(74)	-2950(40)	4580(30)	3499(16)	330(30)
P(4)	11561(13)	-4685(7)	4225(4)	161(4)
F(7)	12010(20)	-3759(8)	4091(8)	170(6)
F(8)	13057(15)	-4936(13)	4421(9)	192(7)
F(9)	11088(19)	-5585(8)	4367(7)	156(8)
F(10)	10070(16)	-4408(12)	4035(8)	197(9)
F(11)	11480(20)	-4373(11)	4807(5)	167(9)
F(12)	11660(20)	-4970(12)	3642(5)	173(7)
P(4A)	13208(12)	-4092(7)	4035(4)	152(4)

F(7A)	14768(14)	-4168(16)	4107(9)	238(12)
F(8A)	13320(20)	-3709(12)	4612(5)	192(7)
F(9A)	11642(14)	-3989(16)	3946(9)	180(6)
F(10A)	13080(20)	-4479(12)	3460(5)	183(8)
F(11A)	13130(30)	-4996(9)	4270(8)	187(7)
F(12A)	13300(20)	-3185(9)	3801(8)	192(9)

Table 19. Bond lengths [Å] and angles [°] for cmpd11.

P(1)-C(1)	1.811(9)
P(1)-C(7)	1.816(10)
P(1)-C(13)	1.842(8)
P(1)-Pt(1)	2.3068(17)
P(2)-C(36)	1.812(9)
P(2)-C(42)	1.837(10)
P(2)-C(48)	1.843(8)
P(2)-Pt(1)	2.3102(17)
Cl(1)-Pt(1)	2.3026(19)
Cl(2)-Pt(1)	2.2983(19)
N(1)-C(20)	1.311(12)
N(1)-C(19)	1.460(11)
N(1)-C(21)	1.524(12)
N(2)-C(20)	1.306(12)
N(2)-C(29)	1.510(15)
N(2)-C(24)	1.511(16)
N(3)-C(30)	1.31(2)
N(3)-C(34)	1.40(2)
N(4)-C(55)	1.285(16)
N(4)-C(56)	1.489(18)
N(4)-C(54)	1.496(12)
N(5)-C(55)	1.307(14)
N(5)-C(59)	1.46(2)
N(5)-C(64)	1.486(14)
C(1)-C(6)	1.374(14)
C(1)-C(2)	1.391(16)
C(2)-C(3)	1.409(16)
C(3)-C(4)	1.37(2)
C(4)-C(5)	1.36(2)
C(5)-C(6)	1.383(15)
C(7)-C(8)	1.384(12)
C(7)-C(12)	1.387(14)
C(8)-C(9)	1.396(16)
C(9)-C(10)	1.376(18)
C(10)-C(11)	1.369(16)
C(11)-C(12)	1.355(14)

C(13)-C(18)	1.396(12)
C(13)-C(14)	1.413(11)
C(14)-C(15)	1.393(11)
C(14)-C(19)	1.513(12)
C(15)-C(16)	1.37(2)
C(16)-C(17)	1.356(16)
C(17)-C(18)	1.383(14)
C(21)-C(26)	1.503(16)
C(21)-C(22)	1.508(16)
C(21)-C(25)	1.601(15)
C(22)-C(23)	1.517(18)
C(23)-C(24)	1.512(18)
C(24)-C(25)	1.516(18)
C(25)-C(28)	1.510(19)
C(25)-C(27)	1.552(19)
C(29)-C(30)	1.466(18)
C(29)-C(35)	1.537(19)
C(30)-C(31)	1.369(18)
C(31)-C(32)	1.39(2)
C(32)-C(33)	1.37(3)
C(33)-C(34)	1.34(3)
C(36)-C(37)	1.387(12)
C(36)-C(41)	1.396(15)
C(37)-C(38)	1.392(15)
C(38)-C(39)	1.378(17)
C(39)-C(40)	1.359(16)
C(40)-C(41)	1.369(16)
C(42)-C(43)	1.372(15)
C(42)-C(47)	1.401(13)
C(43)-C(44)	1.399(14)
C(44)-C(45)	1.386(18)
C(45)-C(46)	1.368(19)
C(46)-C(47)	1.398(16)
C(48)-C(53)	1.376(16)
C(48)-C(49)	1.391(13)
C(49)-C(50)	1.408(14)
C(49)-C(54)	1.510(15)
C(50)-C(51)	1.38(2)

C(51)-C(52)	1.34(2)
C(52)-C(53)	1.419(14)
C(56)-C(61)	1.525(19)
C(56)-C(60)	1.543(17)
C(56)-C(57)	1.557(16)
C(57)-C(58)	1.572(15)
C(58)-C(59)	1.500(17)
C(59)-C(60)	1.53(2)
C(60)-C(63)	1.55(2)
C(60)-C(62)	1.56(3)
C(64)-C(65)	1.3491
C(64)-C(70)	1.59(2)
C(65)-C(66)	1.3900
C(65)-N(6)	1.3900
C(66)-C(67)	1.3900
C(67)-C(68)	1.3900
C(68)-C(69)	1.3900
C(69)-N(6)	1.3900
P(3)-F(2)	1.533(10)
P(3)-F(1)	1.546(10)
P(3)-F(6)	1.556(9)
P(3)-F(3)	1.560(9)
P(3)-F(5)	1.562(10)
P(3)-F(4)	1.562(10)
P(3A)-F(5A)	1.536(9)
P(3A)-F(1A)	1.545(9)
P(3A)-F(3A)	1.555(10)
P(3A)-F(2A)	1.555(9)
P(3A)-F(4A)	1.563(10)
P(3A)-F(6A)	1.575(9)
N(7)-C(71)	1.108(19)
C(71)-C(72)	1.53(2)
N(8)-C(73)	1.189(13)
C(73)-C(74)	1.476(13)
P(4)-F(12)	1.548(10)
P(4)-F(8)	1.553(10)
P(4)-F(9)	1.554(10)
P(4)-F(11)	1.554(10)

P(4)-F(10)	1.557(10)
P(4)-F(7)	1.579(10)
P(4A)-F(11A)	1.545(10)
P(4A)-F(8A)	1.550(10)
P(4A)-F(10A)	1.550(10)
P(4A)-F(12A)	1.552(10)
P(4A)-F(7A)	1.556(10)
P(4A)-F(9A)	1.564(10)

C(1)-P(1)-C(7)	106.7(5)
C(1)-P(1)-C(13)	105.6(4)
C(7)-P(1)-C(13)	102.8(4)
C(1)-P(1)-Pt(1)	107.0(3)
C(7)-P(1)-Pt(1)	116.9(3)
C(13)-P(1)-Pt(1)	117.0(2)
C(36)-P(2)-C(42)	109.3(4)
C(36)-P(2)-C(48)	104.4(4)
C(42)-P(2)-C(48)	102.3(4)
C(36)-P(2)-Pt(1)	107.8(3)
C(42)-P(2)-Pt(1)	115.2(3)
C(48)-P(2)-Pt(1)	117.2(3)
Cl(2)-Pt(1)-Cl(1)	178.66(9)
Cl(2)-Pt(1)-P(1)	86.68(7)
Cl(1)-Pt(1)-P(1)	93.15(7)
Cl(2)-Pt(1)-P(2)	93.46(7)
Cl(1)-Pt(1)-P(2)	86.73(7)
P(1)-Pt(1)-P(2)	179.09(17)
C(20)-N(1)-C(19)	119.4(8)
C(20)-N(1)-C(21)	118.9(8)
C(19)-N(1)-C(21)	120.0(7)
C(20)-N(2)-C(29)	118.7(10)
C(20)-N(2)-C(24)	116.7(9)
C(29)-N(2)-C(24)	123.8(9)
C(30)-N(3)-C(34)	116.2(17)
C(55)-N(4)-C(56)	119.0(10)
C(55)-N(4)-C(54)	121.4(11)
C(56)-N(4)-C(54)	118.8(9)
C(55)-N(5)-C(59)	115.0(12)

C(55)-N(5)-C(64)	123.0(13)
C(59)-N(5)-C(64)	122.0(9)
C(6)-C(1)-C(2)	118.6(10)
C(6)-C(1)-P(1)	124.4(8)
C(2)-C(1)-P(1)	116.8(8)
C(1)-C(2)-C(3)	120.5(13)
C(4)-C(3)-C(2)	118.1(13)
C(5)-C(4)-C(3)	122.3(12)
C(4)-C(5)-C(6)	119.3(13)
C(1)-C(6)-C(5)	121.1(12)
C(8)-C(7)-C(12)	118.9(9)
C(8)-C(7)-P(1)	119.4(8)
C(12)-C(7)-P(1)	121.8(7)
C(7)-C(8)-C(9)	118.8(11)
C(10)-C(9)-C(8)	121.2(10)
C(11)-C(10)-C(9)	119.1(10)
C(12)-C(11)-C(10)	120.4(11)
C(11)-C(12)-C(7)	121.6(9)
C(18)-C(13)-C(14)	119.8(7)
C(18)-C(13)-P(1)	119.9(7)
C(14)-C(13)-P(1)	120.3(6)
C(15)-C(14)-C(13)	117.7(10)
C(15)-C(14)-C(19)	118.2(9)
C(13)-C(14)-C(19)	123.9(7)
C(16)-C(15)-C(14)	121.8(12)
C(17)-C(16)-C(15)	120.1(9)
C(16)-C(17)-C(18)	121.1(10)
C(17)-C(18)-C(13)	119.5(9)
N(1)-C(19)-C(14)	112.2(7)
N(2)-C(20)-N(1)	125.6(10)
C(26)-C(21)-C(22)	116.6(10)
C(26)-C(21)-N(1)	110.3(8)
C(22)-C(21)-N(1)	107.4(8)
C(26)-C(21)-C(25)	115.0(9)
C(22)-C(21)-C(25)	103.4(9)
N(1)-C(21)-C(25)	103.1(8)
C(21)-C(22)-C(23)	106.3(10)
C(24)-C(23)-C(22)	106.1(9)

N(2)-C(24)-C(25)	108.6(9)
N(2)-C(24)-C(23)	107.9(10)
C(25)-C(24)-C(23)	103.9(11)
C(28)-C(25)-C(24)	115.1(12)
C(28)-C(25)-C(27)	110.6(11)
C(24)-C(25)-C(27)	108.7(11)
C(28)-C(25)-C(21)	114.9(10)
C(24)-C(25)-C(21)	98.5(8)
C(27)-C(25)-C(21)	108.3(11)
C(30)-C(29)-N(2)	108.4(10)
C(30)-C(29)-C(35)	114.5(11)
N(2)-C(29)-C(35)	109.0(12)
N(3)-C(30)-C(31)	122.2(15)
N(3)-C(30)-C(29)	111.5(12)
C(31)-C(30)-C(29)	126.1(16)
C(30)-C(31)-C(32)	120.1(18)
C(33)-C(32)-C(31)	119.1(17)
C(34)-C(33)-C(32)	117.7(18)
C(33)-C(34)-N(3)	125(2)
C(37)-C(36)-C(41)	118.7(9)
C(37)-C(36)-P(2)	124.2(8)
C(41)-C(36)-P(2)	117.1(7)
C(36)-C(37)-C(38)	119.3(10)
C(39)-C(38)-C(37)	120.7(10)
C(40)-C(39)-C(38)	119.9(11)
C(39)-C(40)-C(41)	120.4(12)
C(40)-C(41)-C(36)	121.0(10)
C(43)-C(42)-C(47)	119.9(9)
C(43)-C(42)-P(2)	121.0(7)
C(47)-C(42)-P(2)	119.1(8)
C(42)-C(43)-C(44)	121.1(10)
C(45)-C(44)-C(43)	117.9(12)
C(46)-C(45)-C(44)	122.1(11)
C(45)-C(46)-C(47)	119.5(10)
C(42)-C(47)-C(46)	119.4(11)
C(53)-C(48)-C(49)	119.7(8)
C(53)-C(48)-P(2)	119.5(7)
C(49)-C(48)-P(2)	120.9(7)

C(48)-C(49)-C(50)	117.5(12)
C(48)-C(49)-C(54)	122.7(8)
C(50)-C(49)-C(54)	119.8(12)
C(51)-C(50)-C(49)	122.2(13)
C(52)-C(51)-C(50)	120.2(11)
C(51)-C(52)-C(53)	118.7(14)
C(48)-C(53)-C(52)	121.7(12)
N(4)-C(54)-C(49)	115.4(8)
N(4)-C(55)-N(5)	125.9(14)
N(4)-C(56)-C(61)	109.2(9)
N(4)-C(56)-C(60)	108.8(13)
C(61)-C(56)-C(60)	115.2(11)
N(4)-C(56)-C(57)	106.1(10)
C(61)-C(56)-C(57)	115.2(12)
C(60)-C(56)-C(57)	101.7(9)
C(56)-C(57)-C(58)	103.3(10)
C(59)-C(58)-C(57)	104.7(9)
N(5)-C(59)-C(58)	110.5(11)
N(5)-C(59)-C(60)	108.8(12)
C(58)-C(59)-C(60)	105.4(13)
C(59)-C(60)-C(56)	97.7(11)
C(59)-C(60)-C(63)	114.3(17)
C(56)-C(60)-C(63)	110.8(12)
C(59)-C(60)-C(62)	111.3(12)
C(56)-C(60)-C(62)	112.4(15)
C(63)-C(60)-C(62)	109.8(15)
C(65)-C(64)-N(5)	110.5(7)
C(65)-C(64)-C(70)	118.8(9)
N(5)-C(64)-C(70)	106.0(11)
C(64)-C(65)-C(66)	117.1
C(64)-C(65)-N(6)	122.6
C(66)-C(65)-N(6)	120.0
C(67)-C(66)-C(65)	120.0
C(68)-C(67)-C(66)	120.0
C(67)-C(68)-C(69)	120.0
N(6)-C(69)-C(68)	120.0
C(69)-N(6)-C(65)	120.0
F(2)-P(3)-F(1)	91.5(7)

F(2)-P(3)-F(6)	90.9(7)
F(1)-P(3)-F(6)	90.5(7)
F(2)-P(3)-F(3)	90.9(7)
F(1)-P(3)-F(3)	177.6(9)
F(6)-P(3)-F(3)	89.3(7)
F(2)-P(3)-F(5)	90.1(7)
F(1)-P(3)-F(5)	89.8(7)
F(6)-P(3)-F(5)	178.9(8)
F(3)-P(3)-F(5)	90.3(7)
F(2)-P(3)-F(4)	178.7(8)
F(1)-P(3)-F(4)	89.7(7)
F(6)-P(3)-F(4)	89.7(6)
F(3)-P(3)-F(4)	87.9(7)
F(5)-P(3)-F(4)	89.3(7)
F(5A)-P(3A)-F(1A)	92.0(7)
F(5A)-P(3A)-F(3A)	90.6(6)
F(1A)-P(3A)-F(3A)	177.2(8)
F(5A)-P(3A)-F(2A)	91.0(7)
F(1A)-P(3A)-F(2A)	90.5(7)
F(3A)-P(3A)-F(2A)	90.3(6)
F(5A)-P(3A)-F(4A)	90.2(6)
F(1A)-P(3A)-F(4A)	89.3(6)
F(3A)-P(3A)-F(4A)	89.8(7)
F(2A)-P(3A)-F(4A)	178.8(8)
F(5A)-P(3A)-F(6A)	178.9(8)
F(1A)-P(3A)-F(6A)	89.1(6)
F(3A)-P(3A)-F(6A)	88.3(7)
F(2A)-P(3A)-F(6A)	89.0(6)
F(4A)-P(3A)-F(6A)	89.8(6)
N(7)-C(71)-C(72)	172(3)
N(8)-C(73)-C(74)	163(6)
F(12)-P(4)-F(8)	90.2(7)
F(12)-P(4)-F(9)	91.5(7)
F(8)-P(4)-F(9)	90.9(7)
F(12)-P(4)-F(11)	178.3(9)
F(8)-P(4)-F(11)	89.7(7)
F(9)-P(4)-F(11)	90.2(7)
F(12)-P(4)-F(10)	90.7(7)

F(8)-P(4)-F(10)	178.5(9)
F(9)-P(4)-F(10)	90.3(7)
F(11)-P(4)-F(10)	89.5(7)
F(12)-P(4)-F(7)	89.9(7)
F(8)-P(4)-F(7)	90.1(7)
F(9)-P(4)-F(7)	178.3(9)
F(11)-P(4)-F(7)	88.5(7)
F(10)-P(4)-F(7)	88.6(7)
F(11A)-P(4A)-F(8A)	90.2(7)
F(11A)-P(4A)-F(10A)	89.5(7)
F(8A)-P(4A)-F(10A)	179.6(10)
F(11A)-P(4A)-F(12A)	179.5(9)
F(8A)-P(4A)-F(12A)	89.8(7)
F(10A)-P(4A)-F(12A)	90.5(7)
F(11A)-P(4A)-F(7A)	90.3(7)
F(8A)-P(4A)-F(7A)	90.8(7)
F(10A)-P(4A)-F(7A)	89.4(7)
F(12A)-P(4A)-F(7A)	89.2(7)
F(11A)-P(4A)-F(9A)	91.7(7)
F(8A)-P(4A)-F(9A)	90.0(7)
F(10A)-P(4A)-F(9A)	89.7(7)
F(12A)-P(4A)-F(9A)	88.8(7)
F(7A)-P(4A)-F(9A)	177.8(9)

Symmetry transformations used to generate equivalent atoms:

Table 20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cmpd11. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	18(1)	34(1)	24(1)	1(1)	6(1)	6(1)
P(2)	18(1)	45(2)	23(1)	8(1)	6(1)	4(1)
Cl(1)	19(1)	48(1)	34(1)	15(1)	6(1)	2(1)
Cl(2)	19(1)	42(1)	32(1)	14(1)	7(1)	6(1)
Pt(1)	17(1)	34(1)	23(1)	5(1)	6(1)	5(1)
N(1)	33(4)	42(4)	32(4)	9(3)	9(3)	15(3)
N(2)	60(6)	47(5)	56(5)	26(5)	6(4)	9(4)
N(3)	83(9)	97(10)	96(9)	20(8)	30(7)	-8(8)
N(4)	32(4)	62(6)	83(7)	44(5)	28(4)	22(4)
N(5)	50(6)	102(9)	102(9)	69(8)	28(6)	42(6)
C(1)	28(4)	50(6)	39(5)	-15(5)	0(4)	9(4)
C(2)	64(8)	46(7)	46(6)	-10(5)	-4(5)	25(6)
C(3)	76(9)	67(8)	59(7)	-17(7)	-14(7)	39(7)
C(4)	43(6)	116(12)	60(8)	-52(8)	-7(6)	27(7)
C(5)	47(6)	93(10)	66(8)	-35(8)	18(6)	-1(7)
C(6)	38(5)	64(7)	47(5)	-17(5)	17(4)	0(5)
C(7)	24(4)	42(5)	33(4)	13(4)	11(3)	12(4)
C(8)	39(5)	68(7)	31(5)	15(5)	4(4)	-2(5)
C(9)	56(7)	97(10)	36(5)	40(6)	9(5)	4(7)
C(10)	50(6)	72(8)	63(7)	40(7)	14(5)	2(6)
C(11)	35(5)	46(6)	62(6)	19(5)	19(5)	5(4)
C(12)	22(4)	39(6)	43(5)	6(4)	9(4)	6(4)
C(13)	25(4)	37(6)	21(3)	11(3)	1(3)	0(3)
C(14)	27(4)	34(5)	29(4)	14(3)	9(3)	5(3)
C(15)	22(3)	71(6)	42(4)	13(9)	3(3)	-24(7)
C(16)	27(5)	77(8)	58(7)	19(6)	-3(5)	-15(5)
C(17)	50(6)	53(7)	47(6)	-9(5)	-5(5)	-18(5)
C(18)	43(5)	46(6)	30(4)	-1(4)	5(4)	0(4)
C(19)	32(4)	39(5)	28(4)	5(4)	8(3)	11(4)
C(20)	48(6)	44(6)	44(5)	11(5)	6(4)	12(5)
C(21)	50(6)	36(5)	50(6)	3(5)	23(5)	16(5)
C(22)	57(7)	51(7)	71(8)	-13(6)	29(6)	-2(5)
C(23)	64(7)	39(6)	100(10)	4(7)	34(7)	-4(5)

C(24)	56(7)	46(7)	99(10)	25(7)	13(7)	16(6)
C(25)	37(6)	56(7)	93(9)	8(7)	23(6)	25(5)
C(26)	87(10)	54(7)	61(7)	-13(6)	42(7)	9(7)
C(27)	108(13)	45(8)	168(17)	21(9)	71(13)	38(8)
C(28)	41(7)	86(10)	132(13)	34(10)	26(8)	21(7)
C(29)	46(6)	100(10)	60(7)	33(7)	8(5)	8(6)
C(30)	41(6)	122(13)	84(9)	52(9)	23(6)	26(7)
C(31)	63(8)	130(14)	61(8)	4(8)	11(6)	26(9)
C(32)	43(8)	170(20)	78(10)	-7(12)	-2(7)	0(10)
C(33)	54(10)	210(30)	92(12)	-24(15)	15(8)	-48(13)
C(34)	89(14)	200(30)	148(19)	-10(18)	73(14)	-51(16)
C(35)	110(12)	114(13)	65(8)	51(9)	11(8)	-5(10)
C(36)	22(4)	48(5)	29(4)	1(4)	7(3)	1(4)
C(37)	40(5)	64(7)	31(4)	6(5)	12(4)	8(5)
C(38)	68(8)	87(9)	35(5)	-8(6)	26(5)	-2(7)
C(39)	55(7)	74(8)	49(6)	-20(6)	17(5)	-5(6)
C(40)	74(8)	52(7)	51(6)	-10(6)	13(6)	4(6)
C(41)	70(8)	56(7)	40(6)	3(5)	19(5)	9(6)
C(42)	24(4)	49(6)	39(5)	28(4)	11(4)	9(4)
C(43)	26(4)	45(6)	51(6)	18(5)	6(4)	4(4)
C(44)	35(5)	48(6)	93(9)	30(7)	9(5)	6(5)
C(45)	45(6)	89(10)	91(9)	60(9)	24(6)	10(7)
C(46)	45(6)	92(9)	49(6)	37(7)	14(5)	6(6)
C(47)	32(5)	59(6)	41(5)	23(5)	10(4)	4(4)
C(48)	17(3)	59(9)	26(3)	10(4)	1(3)	0(4)
C(49)	27(4)	89(10)	35(4)	33(5)	7(3)	9(5)
C(50)	25(4)	122(10)	51(5)	28(12)	13(4)	8(10)
C(51)	28(6)	161(15)	58(7)	35(9)	-2(5)	-19(8)
C(52)	43(7)	146(14)	41(6)	14(7)	-3(5)	-40(8)
C(53)	31(5)	100(10)	40(6)	5(6)	2(4)	-19(6)
C(54)	35(5)	59(6)	46(5)	30(5)	20(4)	22(5)
C(55)	49(7)	95(10)	81(9)	56(8)	36(6)	43(7)
C(56)	28(5)	40(6)	126(12)	27(7)	19(6)	8(5)
C(57)	39(6)	43(6)	75(8)	7(6)	11(6)	14(5)
C(58)	30(5)	67(8)	82(8)	8(7)	13(5)	12(5)
C(59)	44(7)	52(7)	147(14)	53(9)	25(8)	25(6)
C(60)	47(7)	70(10)	185(18)	66(11)	14(9)	9(7)
C(61)	36(6)	57(8)	136(13)	15(9)	4(7)	4(5)

C(62)	87(12)	32(7)	250(30)	16(11)	-23(15)	20(7)
C(63)	45(8)	94(12)	280(30)	117(16)	10(12)	5(8)
C(64)	77(9)	136(14)	110(12)	81(11)	25(8)	51(10)
C(65)	107(13)	102(13)	153(16)	53(12)	-54(12)	-11(11)
C(66)	123(15)	152(17)	167(17)	64(15)	-44(13)	-23(13)
C(67)	240(30)	240(30)	220(20)	30(20)	30(20)	-10(20)
C(68)	200(20)	140(17)	200(20)	1(15)	-48(16)	-75(16)
C(69)	176(19)	136(17)	190(19)	10(16)	-33(16)	24(15)
N(6)	79(9)	183(16)	118(11)	1(11)	-17(8)	34(10)
C(70)	136(15)	122(14)	133(14)	95(13)	68(12)	70(12)
P(3)	111(7)	33(5)	52(5)	-11(4)	-9(4)	21(5)
F(1)	221(18)	98(15)	40(9)	-16(10)	-8(12)	-1(15)
F(2)	155(17)	84(13)	136(16)	6(12)	23(14)	66(13)
F(3)	184(18)	103(17)	86(11)	20(11)	-46(12)	14(14)
F(4)	193(18)	99(15)	180(17)	-38(15)	13(16)	89(15)
F(5)	177(17)	67(12)	106(15)	-9(12)	17(14)	19(13)
F(6)	116(16)	66(12)	85(13)	3(10)	12(12)	2(12)
P(3A)	188(9)	46(4)	58(4)	2(3)	-30(5)	26(5)
F(1A)	199(17)	88(10)	86(10)	-13(9)	-16(11)	39(11)
F(2A)	240(20)	68(10)	112(13)	-1(10)	-44(14)	18(12)
F(3A)	232(18)	118(14)	80(11)	-30(11)	-2(12)	46(14)
F(4A)	174(15)	92(13)	86(9)	15(11)	-5(11)	-10(14)
F(5A)	211(17)	94(12)	120(13)	-10(10)	-76(12)	60(12)
F(6A)	191(15)	86(11)	100(12)	15(10)	-17(11)	59(11)
N(7)	84(9)	216(19)	69(8)	-10(10)	24(7)	-28(11)
C(71)	162(18)	154(17)	135(16)	-7(15)	57(14)	-33(15)
C(72)	220(30)	260(30)	180(30)	-10(20)	0(20)	-10(30)
P(4)	224(8)	130(7)	119(6)	9(6)	4(6)	84(6)
F(7)	227(11)	123(10)	152(10)	-23(9)	9(10)	102(9)
F(8)	258(12)	154(11)	156(11)	2(10)	12(11)	84(11)
F(9)	206(16)	127(13)	128(13)	15(12)	16(13)	87(13)
F(10)	220(15)	165(14)	183(14)	-13(12)	-21(13)	93(13)
F(11)	217(16)	158(15)	112(12)	-14(12)	-9(12)	77(13)
F(12)	238(12)	153(11)	119(10)	-22(10)	13(11)	59(11)
P(4A)	201(7)	127(7)	111(5)	-28(5)	-19(5)	114(6)
F(7A)	260(18)	212(18)	226(17)	-25(16)	-5(16)	79(16)
F(8A)	256(13)	162(13)	143(11)	-59(11)	-10(11)	81(11)
F(9A)	231(11)	140(10)	155(10)	1(10)	-6(10)	67(11)

F(10A)	256(15)	164(14)	115(12)	-36(11)	-10(12)	71(13)
F(11A)	258(12)	147(11)	149(11)	2(10)	19(11)	76(11)
F(12A)	219(15)	146(14)	191(15)	-10(13)	-15(13)	52(13)

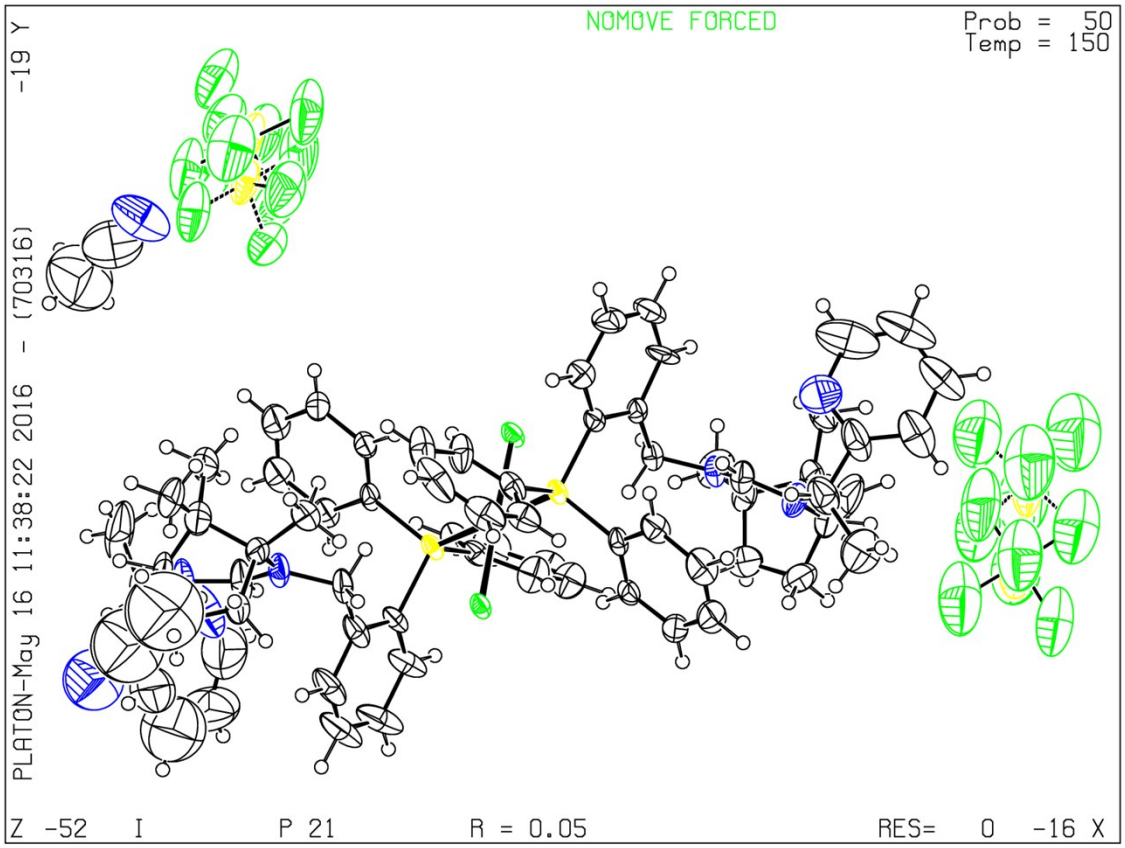


Table 21. Crystal data and structure refinement for cmpd12.

Identification code	cmpd12	
Empirical formula	C43 H53 Cl F6 N3 O2 P2 Pt	
Formula weight	1050.36	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I4	
Unit cell dimensions	a = 21.4948(3) Å	α= 90°.
	b = 21.4948(3) Å	β= 90°.
	c = 19.2489(5) Å	γ = 90°.
Volume	8893.5(3) $Å^3$	
Z	8	
Density (calculated)	1.569 Mg/m^3	
Absorption coefficient	3.352 mm^{-1}	
F(000)	4216	
Crystal size	0.357 x 0.218 x 0.127 mm^3	
Theta range for data collection	3.578 to 29.807°.	
Index ranges	-29<=h<=28, -29<=k<=24, -26<=l<=26	
Reflections collected	24546	
Independent reflections	10665 [R(int) = 0.0297]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.999 and 0.999	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10665 / 17 / 534	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0561	
R indices (all data)	R1 = 0.0480, wR2 = 0.0634	
Absolute structure parameter	-0.013(3)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.855 and -1.178 $e.Å^{-3}$	

Table 22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cmpd12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8331(3)	1872(3)	5784(4)	51(2)
C(2)	8857(3)	1669(4)	6140(4)	57(2)
C(3)	9205(3)	1205(4)	5857(4)	59(2)
C(4)	9034(3)	952(3)	5247(4)	53(2)
C(5)	8505(3)	1164(3)	4893(3)	39(2)
C(6)	8292(3)	907(3)	4216(4)	45(2)
C(7)	8430(3)	1327(4)	3605(4)	57(2)
C(8)	7184(2)	1057(2)	4493(3)	32(1)
C(9)	7523(3)	21(3)	4105(4)	46(2)
C(10)	7460(3)	-329(3)	4802(5)	57(2)
C(11)	6771(3)	-264(3)	5003(4)	59(2)
C(12)	6484(3)	133(3)	4422(4)	46(2)
C(13)	6879(3)	-34(3)	3777(4)	48(2)
C(14)	6779(4)	-718(3)	3554(5)	70(2)
C(15)	6785(4)	373(4)	3148(4)	68(2)
C(16)	5784(3)	49(3)	4315(5)	66(2)
C(17)	6213(3)	1117(3)	5096(3)	36(1)
C(18)	5683(2)	1489(2)	4800(3)	36(2)
C(19)	5764(3)	1995(3)	4359(3)	37(1)
C(20)	5239(3)	2335(3)	4142(4)	49(2)
C(21)	4650(3)	2179(3)	4357(4)	57(2)
C(22)	4572(3)	1696(3)	4813(5)	55(2)
C(23)	5077(3)	1354(3)	5037(4)	49(2)
C(24)	6601(3)	2087(3)	3166(3)	48(2)
C(25)	6132(4)	1783(3)	2802(4)	59(2)
C(26)	6247(5)	1611(4)	2110(4)	78(3)
C(27)	6797(6)	1732(5)	1799(5)	83(3)
C(28)	7260(5)	2029(4)	2153(5)	81(3)
C(29)	7162(4)	2218(4)	2842(4)	61(2)
C(30)	6397(3)	3117(3)	4101(4)	44(2)
C(31)	6342(4)	3475(3)	3520(5)	67(2)
C(32)	6200(4)	4106(4)	3574(7)	90(3)
C(33)	6124(4)	4367(4)	4208(8)	94(4)

C(34)	6185(4)	4028(4)	4772(9)	91(4)
C(35)	6328(3)	3393(3)	4722(7)	67(2)
N(1)	8165(2)	1629(2)	5177(3)	37(1)
N(2)	7637(2)	694(2)	4248(3)	40(1)
N(3)	6619(2)	807(2)	4598(4)	37(1)
P(1)	6529(1)	2279(1)	4083(1)	36(1)
Cl(1)	7765(1)	2958(1)	4843(1)	61(1)
Pt(1)	7378(1)	1949(1)	4667(1)	31(1)
C(37)	5532(12)	2501(9)	6402(9)	178(7)
C(36)	5913(9)	2854(11)	6842(12)	199(9)
O(1)	5592(12)	3427(10)	6909(12)	327(12)
C(39)	5010(14)	3442(12)	6558(16)	320(20)
C(38)	4970(12)	2832(11)	6261(12)	219(11)
C(40)	7590(9)	491(9)	6629(8)	180(7)
C(41)	7478(10)	499(10)	7343(8)	209(9)
C(42)	6982(9)	898(13)	7546(9)	238(13)
C(43)	6819(9)	1193(9)	6919(10)	194(8)
O(2)	7238(6)	990(8)	6387(6)	218(7)
F(1)	0	0	6358(5)	62(2)
F(2)	-21(3)	-738(2)	7189(3)	85(2)
F(3)	0	0	8024(5)	73(2)
P(2)	0	0	3452(3)	56(1)
F(4)	-105(3)	722(2)	3472(4)	117(2)
F(5)	0	0	2662(7)	149(6)
F(6)	0	0	4260(7)	155(6)
P(3)	0	0	7196(2)	51(1)
F(7)	5102(4)	510(4)	2381(5)	151(3)
F(8)	5714(3)	-118(5)	1802(4)	142(3)
F(9)	5070(4)	506(4)	1235(4)	146(3)
P(4)	5000	0	1809(2)	72(1)

Table 23. Bond lengths [Å] and angles [°] for cmpd12.

C(1)-N(1)	1.329(8)
C(1)-C(2)	1.392(10)
C(2)-C(3)	1.361(11)
C(3)-C(4)	1.345(11)
C(4)-C(5)	1.402(8)
C(5)-N(1)	1.353(8)
C(5)-C(6)	1.488(9)
C(6)-N(2)	1.481(8)
C(6)-C(7)	1.512(9)
C(8)-N(2)	1.333(7)
C(8)-N(3)	1.344(6)
C(8)-Pt(1)	1.991(5)
C(9)-N(2)	1.494(8)
C(9)-C(13)	1.527(9)
C(9)-C(10)	1.544(11)
C(10)-C(11)	1.537(10)
C(11)-C(12)	1.536(9)
C(12)-N(3)	1.515(7)
C(12)-C(16)	1.529(9)
C(12)-C(13)	1.548(10)
C(13)-C(15)	1.508(10)
C(13)-C(14)	1.546(9)
C(17)-N(3)	1.458(8)
C(17)-C(18)	1.502(8)
C(18)-C(19)	1.391(8)
C(18)-C(23)	1.411(8)
C(19)-C(20)	1.408(8)
C(19)-P(1)	1.834(6)
C(20)-C(21)	1.374(9)
C(21)-C(22)	1.369(10)
C(22)-C(23)	1.380(9)
C(24)-C(29)	1.388(10)
C(24)-C(25)	1.390(10)
C(24)-P(1)	1.819(7)
C(25)-C(26)	1.405(11)
C(26)-C(27)	1.352(13)

C(27)-C(28)	1.365(14)
C(28)-C(29)	1.403(12)
C(30)-C(35)	1.343(13)
C(30)-C(31)	1.361(10)
C(30)-P(1)	1.824(6)
C(31)-C(32)	1.395(12)
C(32)-C(33)	1.353(15)
C(33)-C(34)	1.313(17)
C(34)-C(35)	1.403(10)
N(1)-Pt(1)	2.072(5)
P(1)-Pt(1)	2.2579(15)
Cl(1)-Pt(1)	2.3472(15)
C(37)-C(36)	1.402(12)
C(37)-C(38)	1.428(12)
C(36)-O(1)	1.417(12)
O(1)-C(39)	1.423(12)
C(39)-C(38)	1.432(12)
C(40)-O(2)	1.392(11)
C(40)-C(41)	1.395(12)
C(41)-C(42)	1.422(12)
C(42)-C(43)	1.408(12)
C(43)-O(2)	1.432(11)
F(1)-P(3)	1.613(10)
F(2)-P(3)	1.586(4)
F(3)-P(3)	1.595(10)
P(2)-F(5)	1.521(14)
P(2)-F(6)	1.555(14)
P(2)-F(4)	1.568(5)
P(2)-F(4)#1	1.568(5)
P(2)-F(4)#2	1.568(5)
P(2)-F(4)#3	1.568(5)
P(3)-F(2)#1	1.586(4)
P(3)-F(2)#2	1.586(4)
P(3)-F(2)#3	1.586(4)
F(7)-P(4)	1.570(8)
F(8)-P(4)	1.555(7)
F(9)-P(4)	1.558(6)
P(4)-F(8)#4	1.555(7)

P(4)-F(9)#4	1.558(6)
P(4)-F(7)#4	1.570(8)

N(1)-C(1)-C(2)	121.9(7)
C(3)-C(2)-C(1)	118.6(7)
C(4)-C(3)-C(2)	119.7(7)
C(3)-C(4)-C(5)	121.0(7)
N(1)-C(5)-C(4)	118.8(6)
N(1)-C(5)-C(6)	117.6(5)
C(4)-C(5)-C(6)	123.6(6)
N(2)-C(6)-C(5)	111.7(5)
N(2)-C(6)-C(7)	113.8(6)
C(5)-C(6)-C(7)	113.5(5)
N(2)-C(8)-N(3)	118.6(5)
N(2)-C(8)-Pt(1)	118.0(4)
N(3)-C(8)-Pt(1)	123.3(4)
N(2)-C(9)-C(13)	107.4(5)
N(2)-C(9)-C(10)	109.1(6)
C(13)-C(9)-C(10)	104.0(5)
C(11)-C(10)-C(9)	105.0(6)
C(12)-C(11)-C(10)	104.8(6)
N(3)-C(12)-C(16)	109.4(5)
N(3)-C(12)-C(11)	106.9(6)
C(16)-C(12)-C(11)	115.3(6)
N(3)-C(12)-C(13)	107.3(5)
C(16)-C(12)-C(13)	113.8(6)
C(11)-C(12)-C(13)	103.5(5)
C(15)-C(13)-C(9)	114.2(6)
C(15)-C(13)-C(14)	108.1(6)
C(9)-C(13)-C(14)	108.3(5)
C(15)-C(13)-C(12)	115.8(6)
C(9)-C(13)-C(12)	98.5(5)
C(14)-C(13)-C(12)	111.5(6)
N(3)-C(17)-C(18)	116.7(5)
C(19)-C(18)-C(23)	118.2(5)
C(19)-C(18)-C(17)	123.6(5)
C(23)-C(18)-C(17)	118.0(5)
C(18)-C(19)-C(20)	119.2(5)

C(18)-C(19)-P(1)	123.3(4)
C(20)-C(19)-P(1)	117.4(5)
C(21)-C(20)-C(19)	121.5(6)
C(22)-C(21)-C(20)	119.4(6)
C(21)-C(22)-C(23)	120.5(6)
C(22)-C(23)-C(18)	121.1(6)
C(29)-C(24)-C(25)	120.0(7)
C(29)-C(24)-P(1)	117.6(6)
C(25)-C(24)-P(1)	122.3(6)
C(24)-C(25)-C(26)	118.3(8)
C(27)-C(26)-C(25)	121.6(9)
C(26)-C(27)-C(28)	120.5(9)
C(27)-C(28)-C(29)	119.9(9)
C(24)-C(29)-C(28)	119.8(8)
C(35)-C(30)-C(31)	118.2(7)
C(35)-C(30)-P(1)	118.0(5)
C(31)-C(30)-P(1)	123.7(6)
C(30)-C(31)-C(32)	120.5(9)
C(33)-C(32)-C(31)	119.7(10)
C(34)-C(33)-C(32)	120.3(9)
C(33)-C(34)-C(35)	120.3(13)
C(30)-C(35)-C(34)	120.9(12)
C(1)-N(1)-C(5)	120.0(5)
C(1)-N(1)-Pt(1)	120.4(5)
C(5)-N(1)-Pt(1)	119.7(4)
C(8)-N(2)-C(6)	121.9(5)
C(8)-N(2)-C(9)	120.8(5)
C(6)-N(2)-C(9)	116.5(5)
C(8)-N(3)-C(17)	117.2(5)
C(8)-N(3)-C(12)	121.5(5)
C(17)-N(3)-C(12)	118.0(5)
C(24)-P(1)-C(30)	104.9(3)
C(24)-P(1)-C(19)	106.3(3)
C(30)-P(1)-C(19)	100.6(3)
C(24)-P(1)-Pt(1)	110.1(2)
C(30)-P(1)-Pt(1)	115.3(2)
C(19)-P(1)-Pt(1)	118.4(2)
C(8)-Pt(1)-N(1)	86.1(2)

C(8)-Pt(1)-P(1)	92.84(16)
N(1)-Pt(1)-P(1)	178.21(15)
C(8)-Pt(1)-Cl(1)	171.30(16)
N(1)-Pt(1)-Cl(1)	87.12(14)
P(1)-Pt(1)-Cl(1)	93.85(6)
C(36)-C(37)-C(38)	110.0(16)
C(37)-C(36)-O(1)	103.8(15)
C(36)-O(1)-C(39)	113.9(16)
O(1)-C(39)-C(38)	102.8(16)
C(37)-C(38)-C(39)	109.2(17)
O(2)-C(40)-C(41)	103.1(12)
C(40)-C(41)-C(42)	114.0(15)
C(43)-C(42)-C(41)	102.8(14)
C(42)-C(43)-O(2)	108.7(13)
C(40)-O(2)-C(43)	109.7(11)
F(5)-P(2)-F(6)	180.0
F(5)-P(2)-F(4)	91.4(3)
F(6)-P(2)-F(4)	88.6(3)
F(5)-P(2)-F(4)#1	91.4(3)
F(6)-P(2)-F(4)#1	88.6(3)
F(4)-P(2)-F(4)#1	89.966(17)
F(5)-P(2)-F(4)#2	91.4(3)
F(6)-P(2)-F(4)#2	88.6(3)
F(4)-P(2)-F(4)#2	89.965(17)
F(4)#1-P(2)-F(4)#2	177.2(7)
F(5)-P(2)-F(4)#3	91.4(3)
F(6)-P(2)-F(4)#3	88.6(3)
F(4)-P(2)-F(4)#3	177.2(7)
F(4)#1-P(2)-F(4)#3	89.966(17)
F(4)#2-P(2)-F(4)#3	89.966(17)
F(2)-P(3)-F(2)#1	89.995(5)
F(2)-P(3)-F(2)#2	89.997(5)
F(2)#1-P(3)-F(2)#2	179.0(5)
F(2)-P(3)-F(2)#3	179.0(5)
F(2)#1-P(3)-F(2)#3	89.996(5)
F(2)#2-P(3)-F(2)#3	89.996(5)
F(2)-P(3)-F(3)	90.5(2)
F(2)#1-P(3)-F(3)	90.5(2)

F(2)#2-P(3)-F(3)	90.5(2)
F(2)#3-P(3)-F(3)	90.5(2)
F(2)-P(3)-F(1)	89.5(2)
F(2)#1-P(3)-F(1)	89.5(2)
F(2)#2-P(3)-F(1)	89.5(2)
F(2)#3-P(3)-F(1)	89.5(2)
F(3)-P(3)-F(1)	180.0
F(8)#4-P(4)-F(8)	179.1(7)
F(8)#4-P(4)-F(9)#4	90.8(5)
F(8)-P(4)-F(9)#4	88.6(5)
F(8)#4-P(4)-F(9)	88.6(5)
F(8)-P(4)-F(9)	90.8(5)
F(9)#4-P(4)-F(9)	89.6(7)
F(8)#4-P(4)-F(7)#4	89.0(5)
F(8)-P(4)-F(7)#4	91.7(5)
F(9)#4-P(4)-F(7)#4	89.8(5)
F(9)-P(4)-F(7)#4	177.5(5)
F(8)#4-P(4)-F(7)	91.7(5)
F(8)-P(4)-F(7)	89.0(5)
F(9)#4-P(4)-F(7)	177.4(5)
F(9)-P(4)-F(7)	89.8(5)
F(7)#4-P(4)-F(7)	90.9(7)

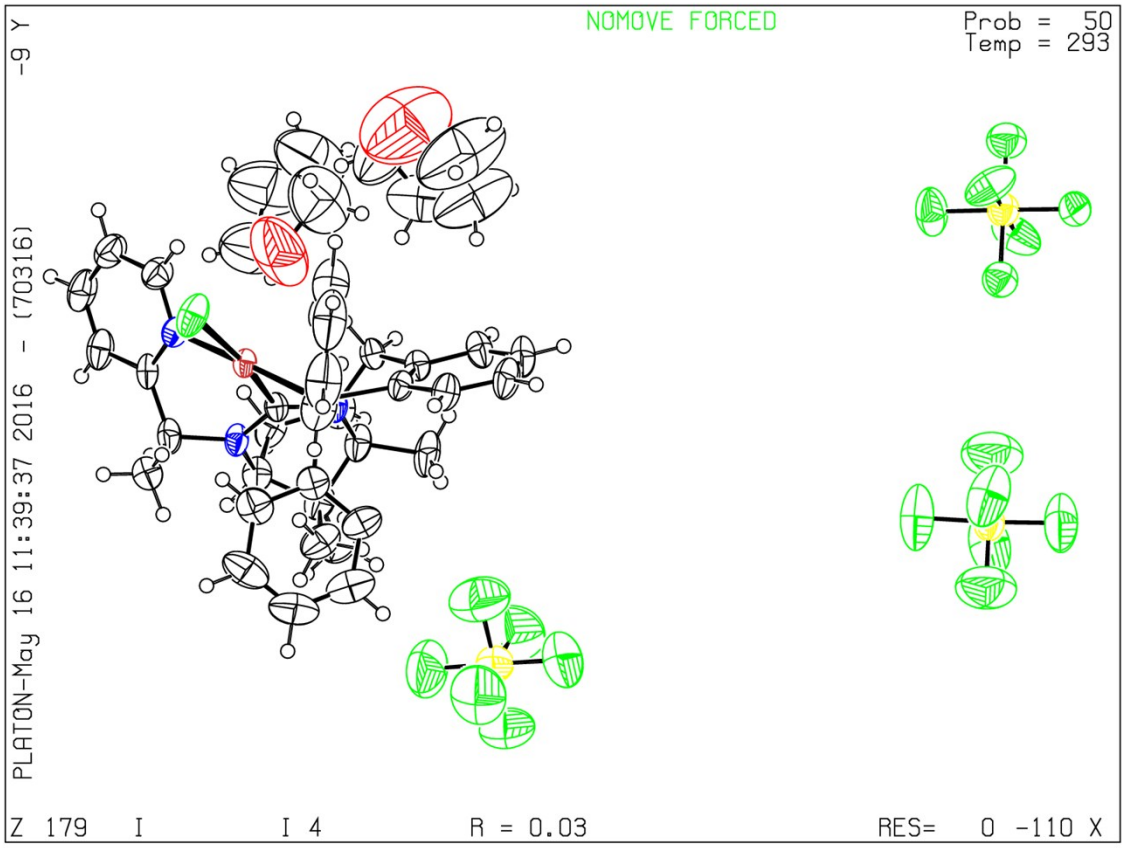
Symmetry transformations used to generate equivalent atoms:

#1 y,-x,z #2 -y,x,z #3 -x,-y,z #4 -x+1,-y,z

Table 24. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for cmpd12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	48(4)	55(4)	51(4)	-1(4)	-7(3)	0(3)
C(2)	52(5)	68(5)	51(4)	6(4)	-15(4)	-6(4)
C(3)	42(4)	66(5)	71(5)	27(4)	-21(4)	-1(4)
C(4)	34(4)	43(4)	82(5)	8(4)	-9(4)	5(3)
C(5)	22(3)	36(3)	59(4)	8(3)	0(3)	0(2)
C(6)	26(3)	42(4)	68(5)	-3(3)	3(3)	4(3)
C(7)	45(4)	71(5)	55(4)	-4(4)	4(3)	1(4)
C(8)	27(3)	28(3)	41(4)	4(2)	1(2)	3(2)
C(9)	42(4)	27(3)	71(4)	-9(3)	2(3)	2(3)
C(10)	49(4)	39(3)	82(7)	7(4)	-20(4)	5(3)
C(11)	58(5)	37(4)	81(5)	14(4)	-1(4)	2(3)
C(12)	35(3)	26(3)	78(5)	-3(3)	-4(3)	-2(2)
C(13)	46(4)	31(3)	66(4)	-5(3)	-8(3)	-1(3)
C(14)	71(5)	47(5)	93(6)	-23(4)	-10(5)	-3(4)
C(15)	78(6)	55(5)	71(5)	-11(4)	-19(4)	-2(4)
C(16)	37(4)	37(4)	124(7)	-13(4)	-5(4)	-14(3)
C(17)	32(3)	32(3)	45(3)	7(3)	4(3)	0(2)
C(18)	33(3)	28(3)	48(5)	1(3)	3(3)	-1(2)
C(19)	30(3)	35(3)	47(3)	-1(3)	-5(3)	2(2)
C(20)	38(4)	44(4)	66(4)	10(3)	-9(3)	5(3)
C(21)	32(4)	47(4)	92(5)	-2(4)	-12(3)	7(3)
C(22)	29(3)	47(4)	91(8)	-3(4)	4(4)	0(2)
C(23)	38(4)	39(4)	71(4)	0(3)	13(3)	-3(3)
C(24)	51(4)	47(4)	47(4)	12(3)	-2(3)	4(3)
C(25)	76(5)	49(4)	51(4)	6(3)	-17(4)	1(4)
C(26)	117(8)	59(6)	58(5)	-2(4)	-20(5)	-3(5)
C(27)	122(8)	78(6)	48(5)	-1(4)	5(5)	17(6)
C(28)	105(7)	84(6)	55(5)	19(5)	28(5)	13(5)
C(29)	67(5)	60(5)	55(4)	18(4)	2(4)	3(4)
C(30)	33(3)	33(3)	66(4)	11(3)	-9(3)	1(3)
C(31)	61(5)	43(4)	98(6)	28(4)	-17(5)	5(3)
C(32)	61(6)	58(6)	150(10)	52(7)	-19(6)	7(4)
C(33)	53(5)	36(5)	195(13)	5(7)	-11(7)	5(4)

C(34)	64(5)	45(4)	162(12)	-27(7)	-3(8)	6(4)
C(35)	61(4)	42(3)	99(7)	0(6)	-23(7)	-7(3)
N(1)	34(3)	33(3)	44(3)	3(2)	-5(2)	-2(2)
N(2)	27(3)	30(3)	61(3)	-9(2)	0(2)	-1(2)
N(3)	28(2)	24(2)	58(3)	0(3)	0(3)	-2(2)
P(1)	32(1)	30(1)	45(1)	7(1)	-3(1)	0(1)
Cl(1)	52(1)	32(1)	98(2)	2(1)	-22(1)	-8(1)
Pt(1)	27(1)	25(1)	42(1)	2(1)	-1(1)	-1(1)
C(37)	270(30)	151(16)	114(12)	-12(12)	17(14)	-3(19)
C(36)	159(17)	180(20)	260(30)	-23(17)	-92(17)	19(14)
O(1)	400(30)	210(20)	370(30)	-86(18)	-100(20)	54(19)
C(39)	320(40)	260(30)	360(40)	-150(30)	-210(30)	180(30)
C(38)	300(30)	170(20)	190(20)	-21(16)	-120(20)	13(19)
C(40)	206(19)	215(19)	120(13)	-2(13)	-24(13)	84(15)
C(41)	290(30)	220(20)	109(14)	41(13)	-4(15)	41(19)
C(42)	200(20)	400(40)	113(12)	21(18)	-5(13)	170(20)
C(43)	172(18)	210(20)	200(20)	40(17)	8(16)	65(15)
O(2)	156(11)	360(20)	139(9)	116(12)	40(8)	31(11)
F(1)	62(4)	62(4)	62(6)	0	0	0
F(2)	124(4)	48(3)	84(3)	4(2)	46(3)	-2(3)
F(3)	79(4)	79(4)	60(5)	0	0	0
P(2)	47(1)	47(1)	74(3)	0	0	0
F(4)	90(4)	54(3)	209(7)	-9(4)	-35(4)	3(3)
F(5)	186(10)	186(10)	77(9)	0	0	0
F(6)	189(9)	189(9)	87(9)	0	0	0
P(3)	48(1)	48(1)	55(2)	0	0	0
F(7)	190(9)	141(7)	122(6)	-39(5)	-12(6)	-14(6)
F(8)	78(5)	192(8)	157(7)	9(6)	-18(5)	9(5)
F(9)	154(6)	160(6)	123(5)	72(5)	1(5)	-7(5)
P(4)	69(2)	88(2)	60(2)	0	0	-1(2)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