S-1 ^{1}H and ^{13}C NMR spectrum of **5**, **6**, **7**, **9**

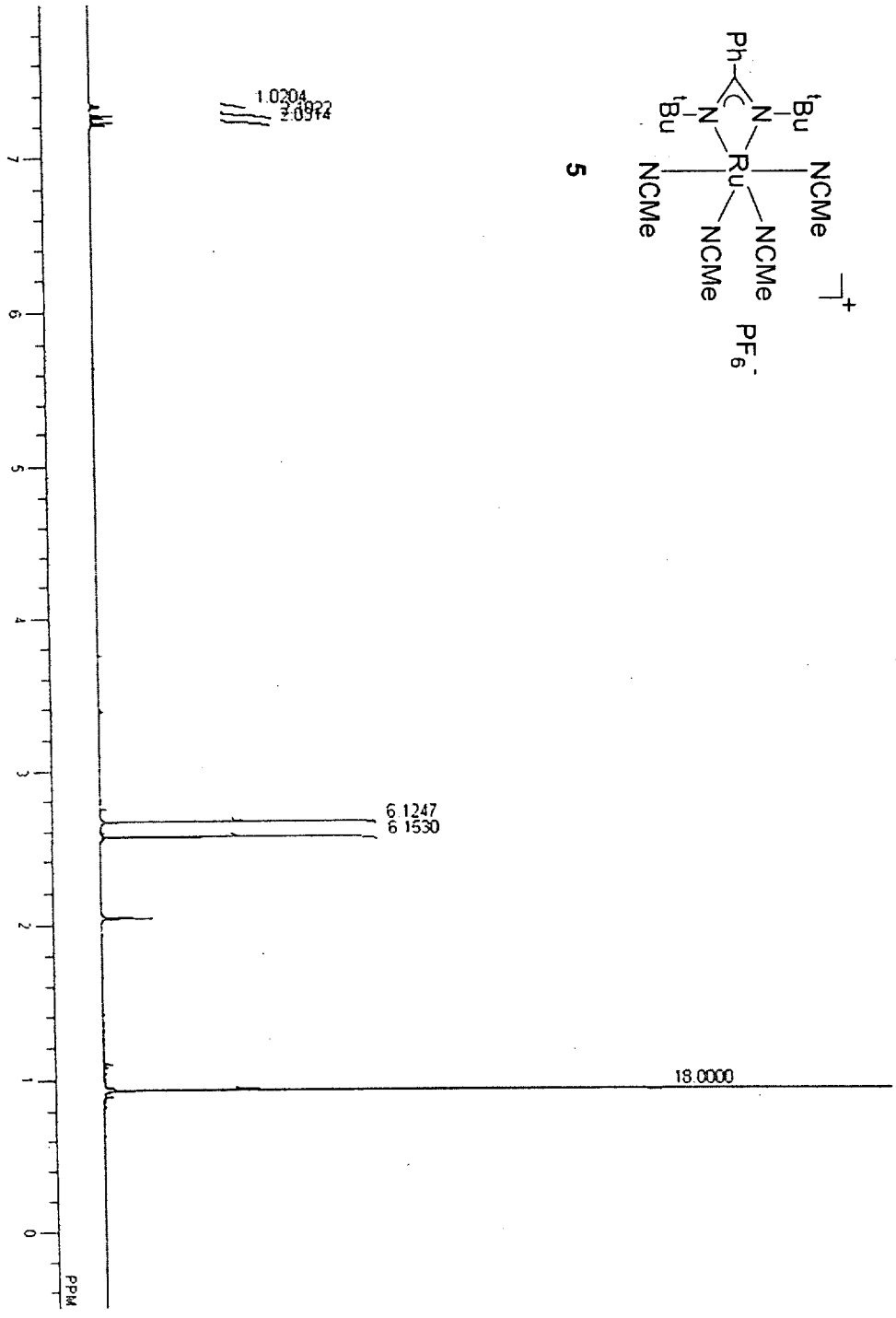

Figure S1. ^{1}H NMR spectrum of **5**

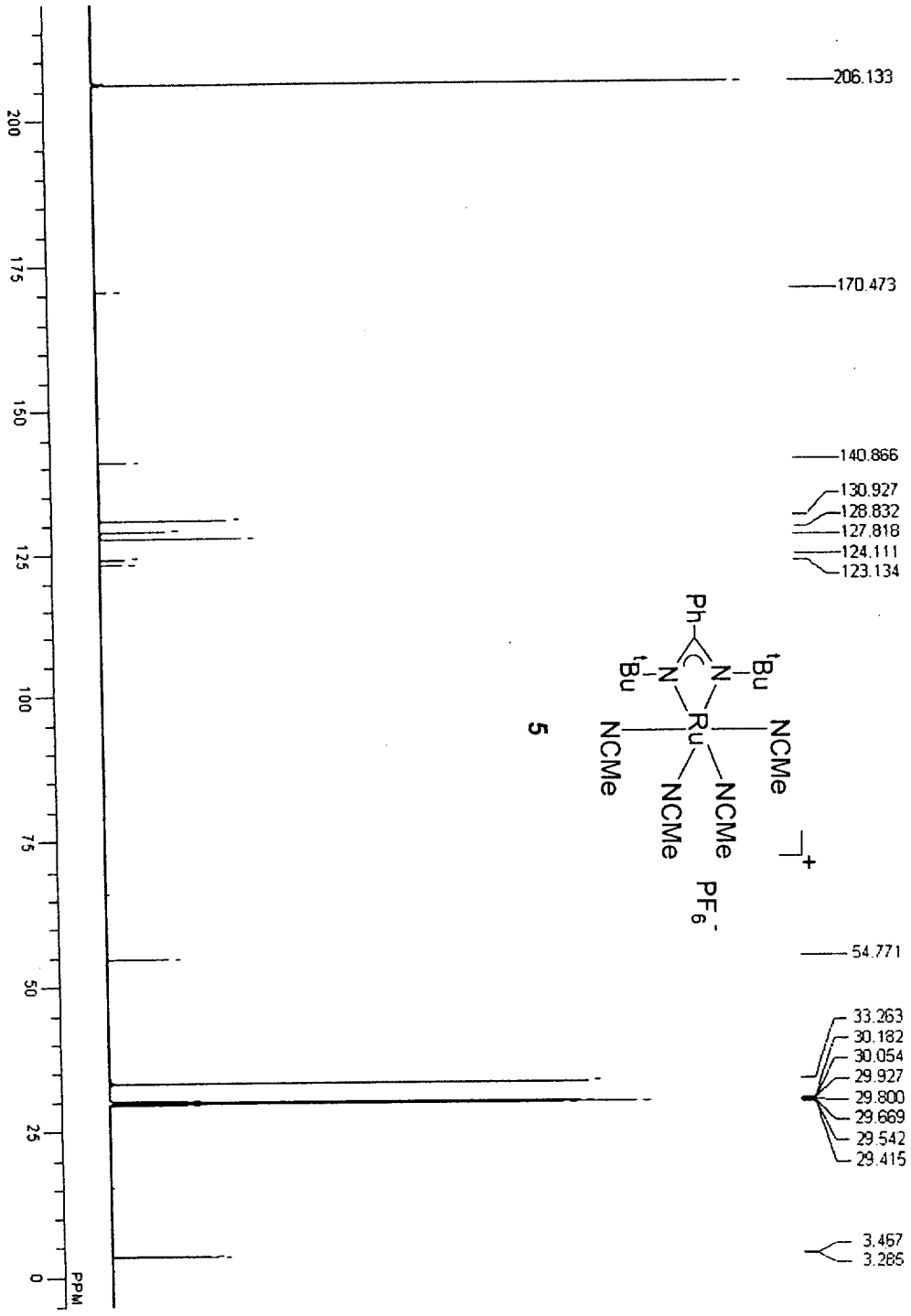

Figure S2. ^{13}C NMR spectrum of **5**

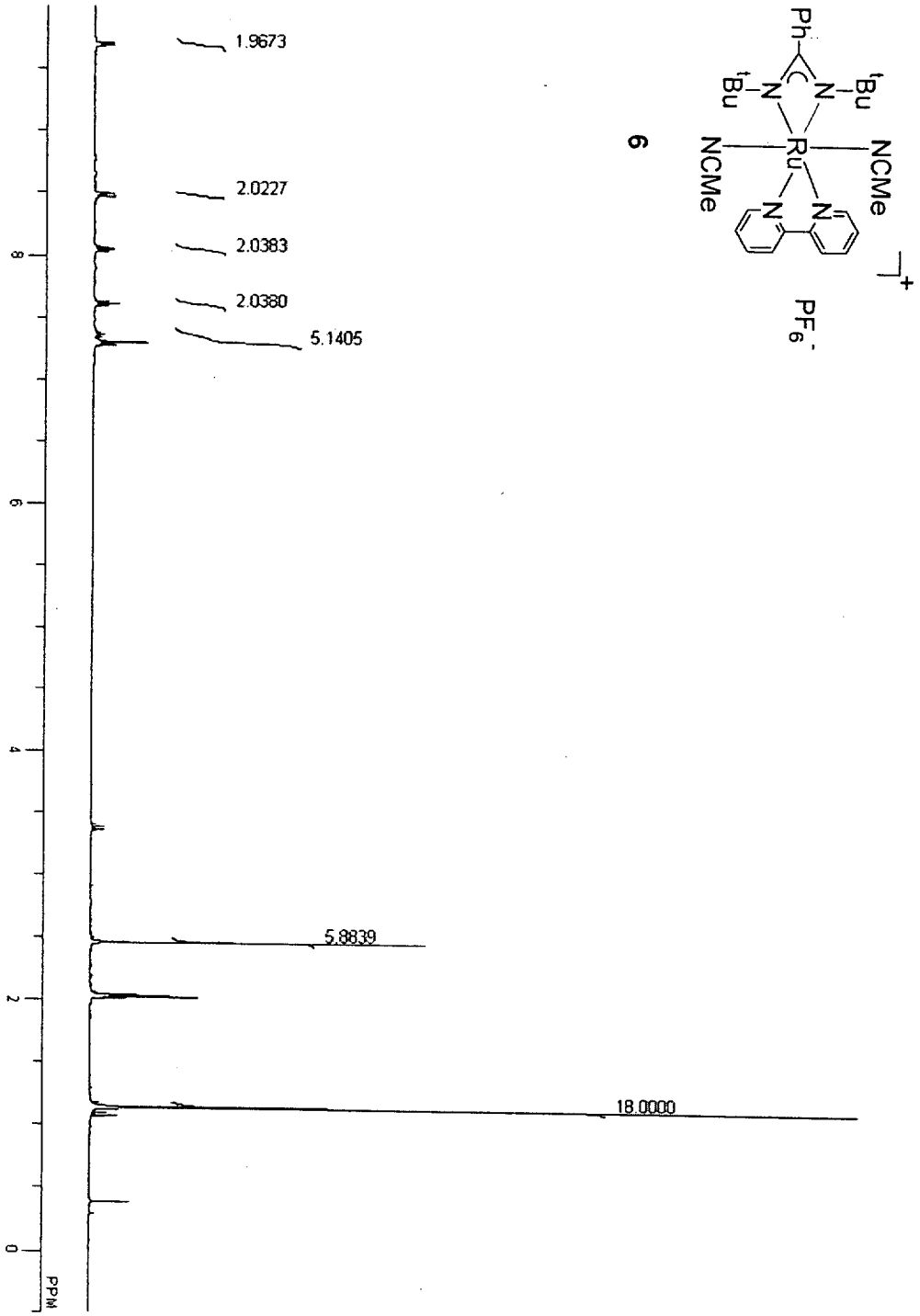

Figure S3. ^{1}H NMR spectrum of **6**

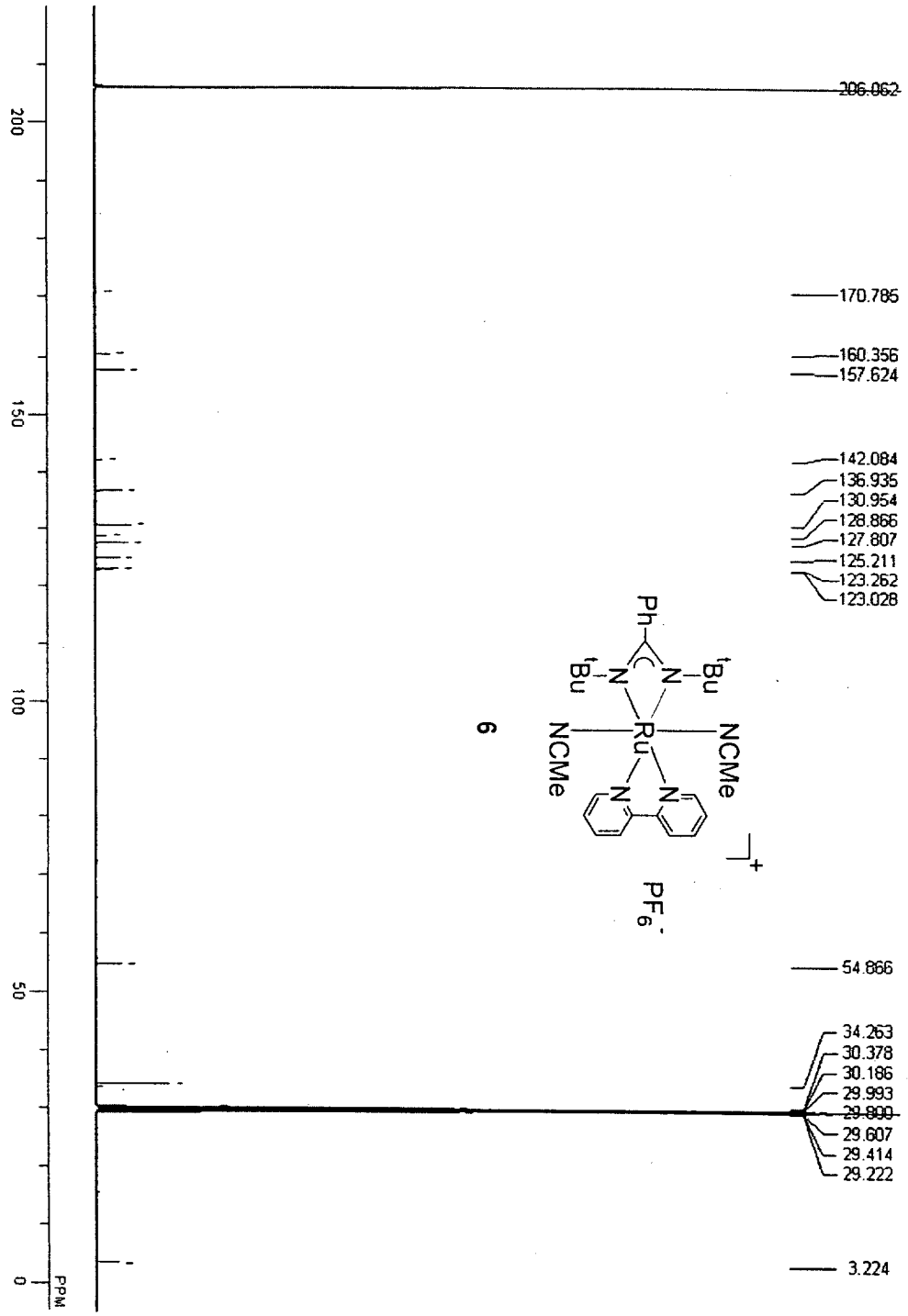

Figure S4. ^{13}C NMR spectrum of **6**

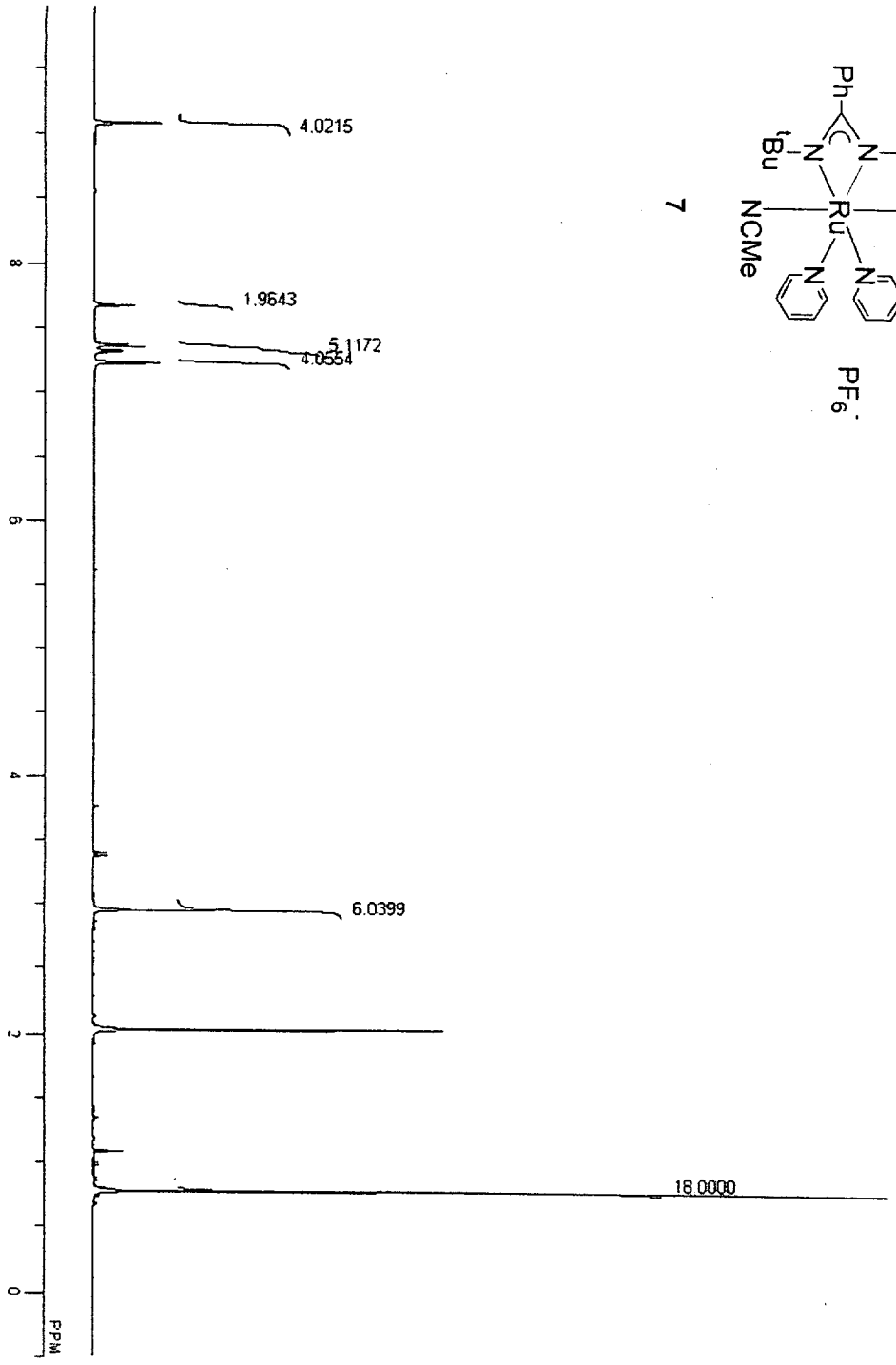

Figure S5. ^{1}H NMR spectrum of **7**

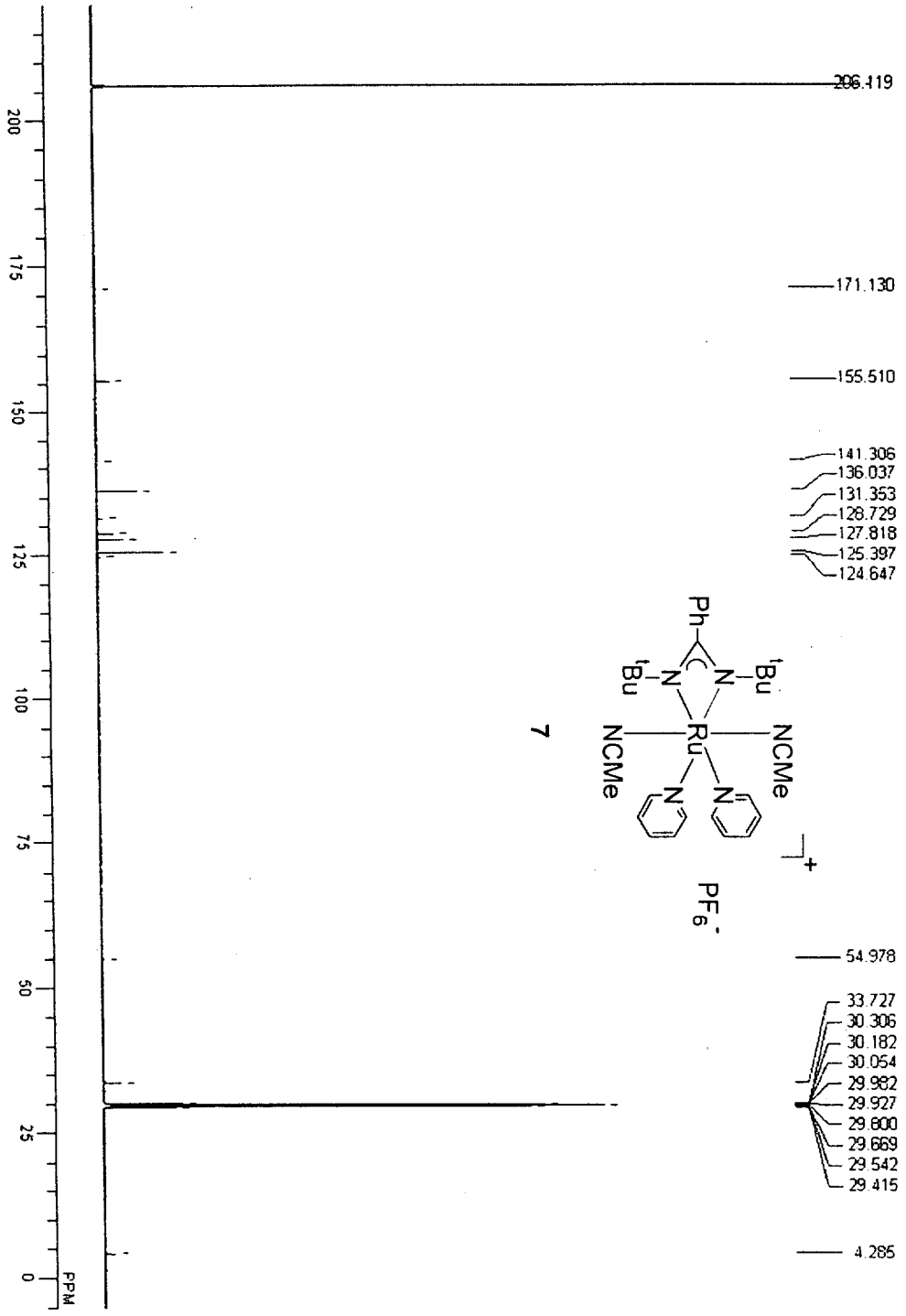

Figure S6. ^{13}C NMR spectrum of **7**

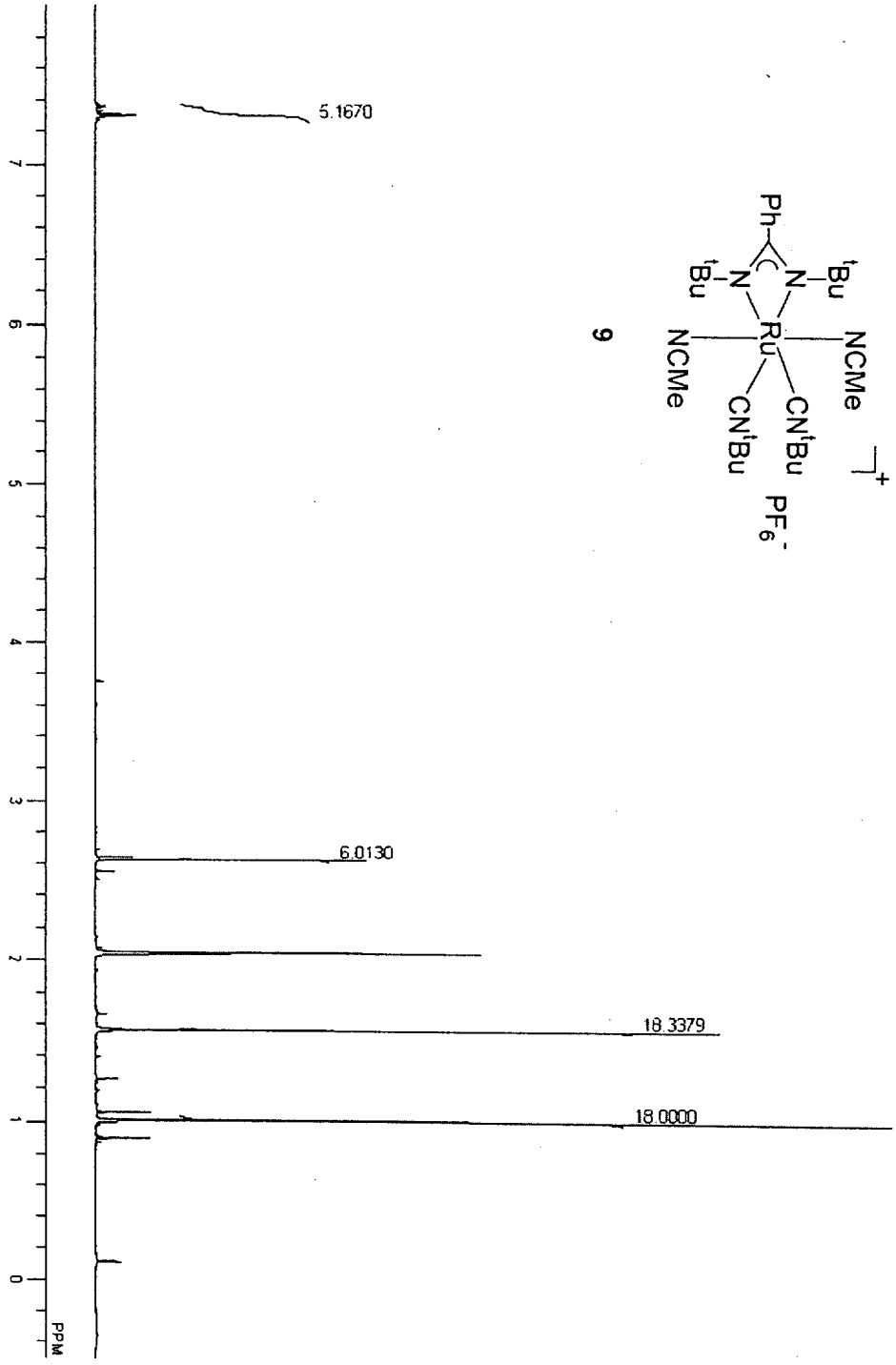

Figure S7. ^{1}H NMR spectrum of **9**

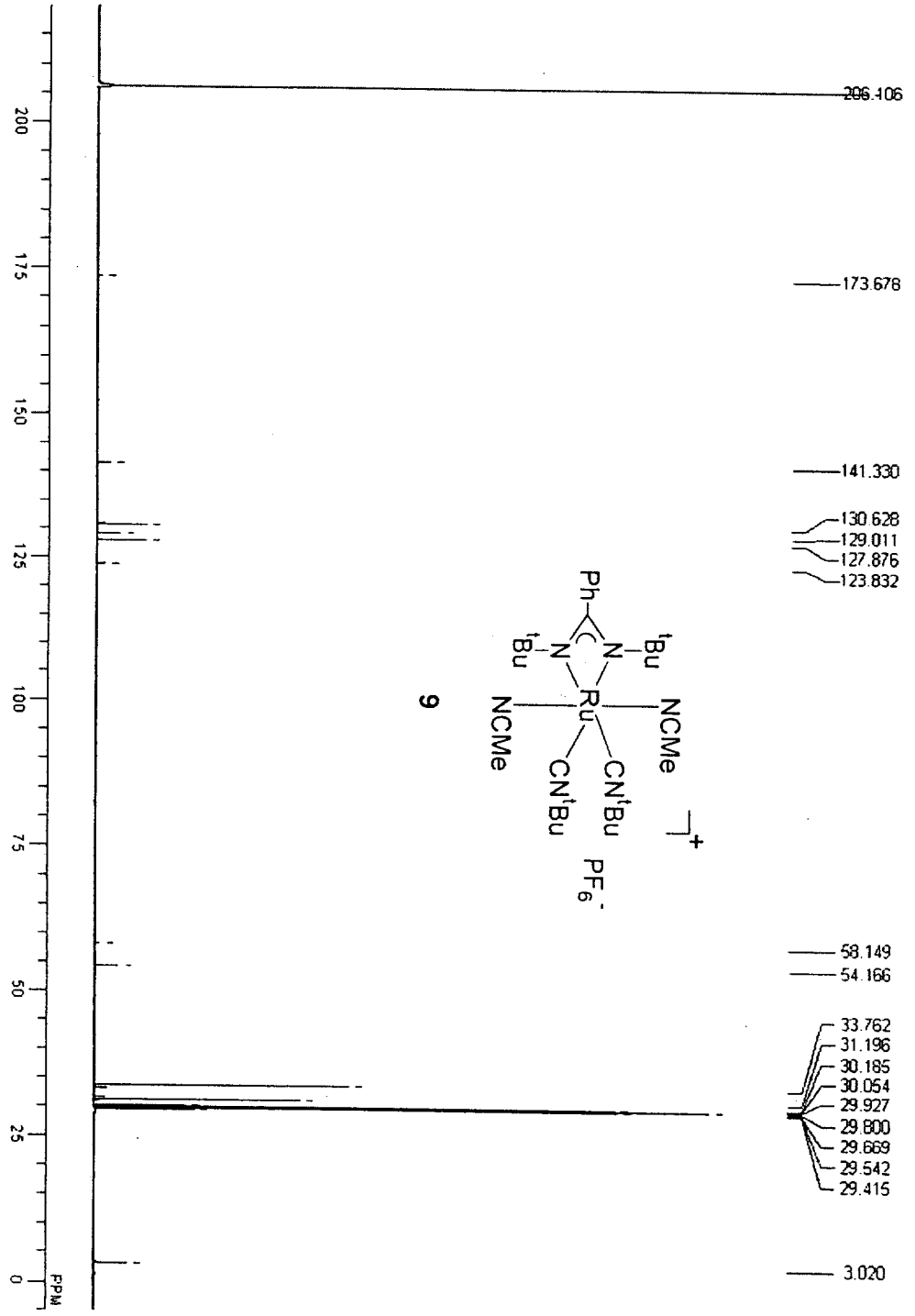

Figure S8. ^{13}C NMR spectrum of **9**

S-2 X-ray determination of $(\eta^6\text{-}C_6H_5OMe)Ru\{\eta^2\text{-}^tBuNC(Ph)=N^tBu\}Cl$, **4b** and $[Ru(\eta\text{-}^tBuNC(Ph)=N^tBu)(bipy)(MeCN)_2]^+PF_6^-$, **6**

Single crystals for X-ray diffraction were grown from a solution of toluene/n-hexane at room temperature for **4b**, and from a solution of CH_2Cl_2/n-hexane at room temperature for **7**. Diffraction data for **4b** and **7** were collected on Rigaku R-AXIS RAPID IP diffractometer (Mo-Kα, λ = 0.71069 Å) at room temperature (23 °C) and then processed with teXsan. Structure solutions were performed by the Patterson method (**4b**) with the program DIRDIF-PATTY and the direct methods (**6**) with the program SIR 92. Refinements were carried out by full-matrix least squares on F^2 with all non-hydrogen atoms refined anisotropically using the program SHELXL-97-2 PC version. The positions of all hydrogen atoms were calculated assuming idealized geometries.

X-ray data of (η^6-C_6H_5OMe)Ru{η^2-^{t}BuNC(Ph)=N^{t}Bu}Cl, **4b**

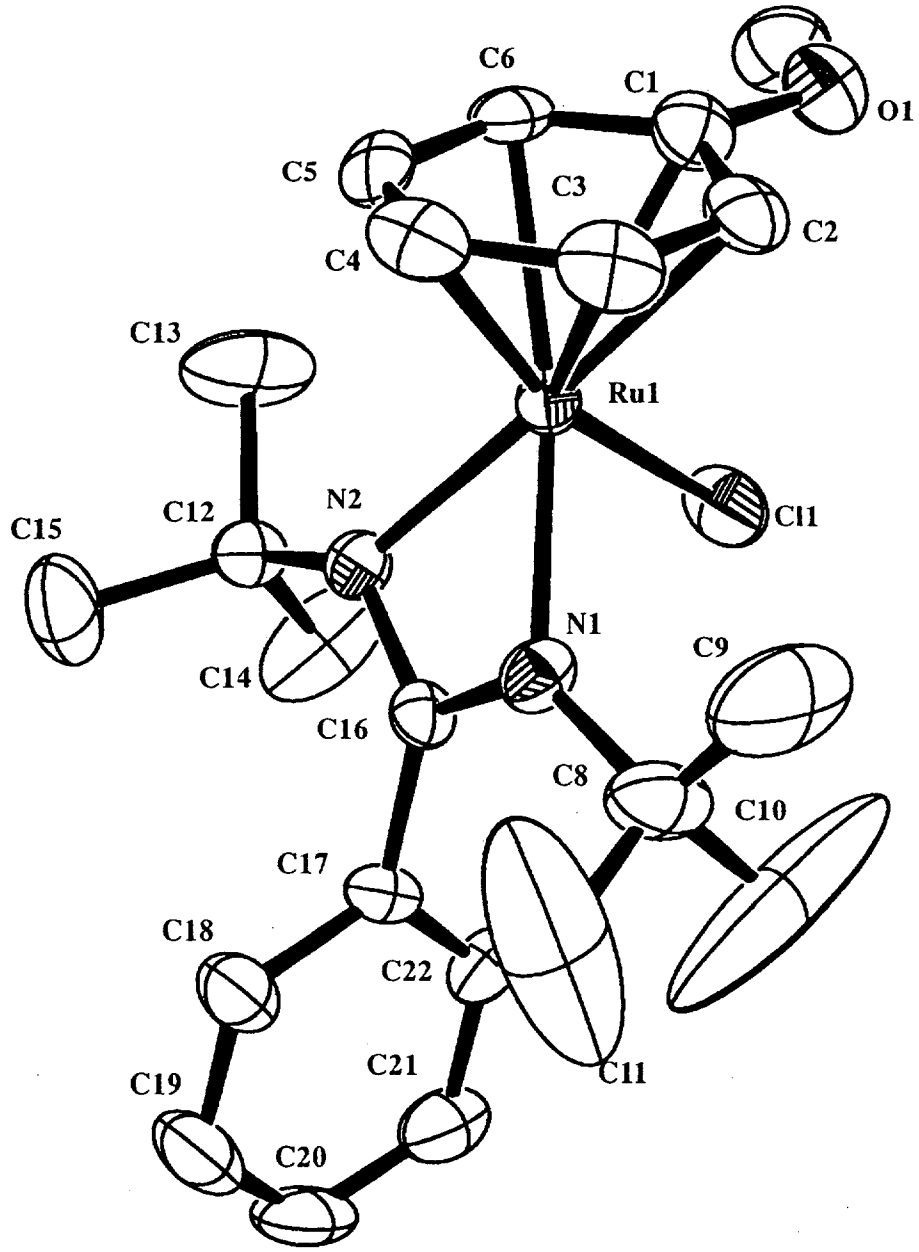

Figure S9. ORTEP drawing of **4b** (50% probability ellipsoids) showing the numbering system. All hydrogen atoms are omitted for clarity.

Table S1. Crystal data and structure refinement for **4b**

Empirical formula	$C_{22}H_{31}ClN_2ORu$
Formula weight	476.01
Crystal habits, color	prismatic, orange
Crystal size	0.20 x 0.10 x 0.05 mm
Crystal system	Monoclinic
Space group	*Cc* (#9)
Unit cell dimensions	a = 10.1667(6)Å
	b = 17.8999(11)Å β = 93.309(2)
	c = 11.9921(7)Å
Volume	2178.7(2) Å^3
Z	4
Density (calculated)	1.451 Mg/m^3
Absorption coefficient	0.856 mm^{-1}
F(000)	984
Temperature	293(2) K
θ range for data collection	2.28 to 27.48
Index ranges	0<=h<=13; 0<=k<=23; -15<=l<=15
Reflection collected	2489
Independent reflections	2489 [R(int) = 0.000]
Reflections observed (>2σ)	2053
Structure Solution	Patterson methods
	(Dir Diff 99)
Refinement method	Full-matrix
	least-squares on F^2
Data/ restraints / parameters	2489 / 2 / 244
R indices (I>2σ(I))	R_1 = 0.0413 wR_2 = 0.1021
R indices (all data)	R_1 = 0.0549 wR_2 = 0.1114
Goodness-of-fit on F^2	0.761
Largest diff. peak and hole	0.427 and -1.162 e.Å^{-3}

Refinement of F^2 against all reflections. The weighted R-factor wR and goodness of fit S are base on F^2, conventional R-factors R are based on F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on all data will be even larger.

$w = 1/[\sigma^2(F_o^2)]$

Table S2. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **4b**. Ueq is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	Ueq
Ru(1)	5(1)	1129(1)	5001(1)	25(1)
Cl(1)	684(3)	1083(2)	6958(2)	46(1)
O(1)	-2223(6)	229(4)	6407(6)	45(1)
N(1)	2038(10)	1146(4)	4715(8)	31(2)
N(2)	981(6)	2166(3)	5038(6)	30(1)
C(1)	-1863(8)	505(5)	5432(7)	36(2)
C(2)	-1031(8)	49(4)	4831(8)	37(2)
C(3)	-613(9)	280(5)	3793(8)	42(2)
C(4)	-967(10)	983(7)	3345(8)	40(2)
C(5)	-1699(8)	1464(5)	4002(8)	41(2)
C(6)	-2163(11)	1230(6)	5027(11)	34(3)
C(7)	-2808(9)	715(7)	7165(9)	53(2)
C(8)	3067(8)	568(5)	4626(10)	51(2)
C(9)	2492(14)	-134(7)	4350(20)	112(7)
C(10)	3820(30)	449(13)	5670(30)	230(20)
C(11)	4010(30)	772(10)	3840(30)	240(20)
C(12)	696(7)	2926(4)	5435(7)	31(2)
C(13)	-789(9)	2955(6)	5594(13)	72(4)
C(14)	1322(13)	3108(7)	6571(11)	76(4)
C(15)	1029(12)	3506(5)	4559(11)	62(3)
C(16)	2182(7)	1860(4)	4991(6)	26(1)
C(17)	3457(6)	2240(4)	5251(7)	29(1)
C(18)	4099(9)	2629(5)	4435(8)	41(2)
C(19)	5236(9)	3017(5)	4697(10)	52(3)
C(20)	5794(8)	3005(6)	5765(11)	54(3)
C(21)	5210(8)	2610(5)	6585(9)	47(2)
C(22)	4041(8)	2224(4)	6325(7)	36(2)

Table S3. Anisotropic displacement parameters ($Å^2x10^3$) for **4b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	27(1)	25(1)	24(1)	0(1)	-3(1)	-2(1)
Cl(1)	48(1)	62(2)	26(1)	10(1)	-6(1)	-18(1)
O(1)	48(3)	44(3)	43(4)	3(3)	9(3)	-6(3)
N(1)	32(4)	28(4)	34(5)	-4(3)	-3(3)	4(3)
N(2)	28(3)	24(3)	37(4)	1(3)	4(2)	5(2)
C(1)	36(4)	34(4)	39(4)	-5(3)	3(3)	-3(3)
C(2)	37(4)	28(4)	45(5)	-6(3)	-1(3)	-9(3)
C(3)	45(4)	44(5)	37(4)	-22(4)	2(4)	-6(4)
C(4)	41(5)	60(6)	18(4)	-10(4)	-1(3)	-17(4)
C(5)	42(4)	36(4)	42(5)	6(4)	-26(4)	-10(3)
C(6)	20(4)	40(6)	40(6)	-4(4)	-6(4)	-4(3)
C(7)	42(5)	73(7)	47(5)	6(5)	11(4)	7(5)
C(8)	33(4)	43(5)	77(7)	-13(5)	12(4)	1(4)
C(9)	64(8)	42(6)	230(20)	-26(10)	-26(11)	17(6)
C(10)	230(30)	140(18)	300(40)	-150(20)	-210(30)	150(20)
C(11)	310(40)	76(11)	360(40)	73(18)	290(40)	96(18)
C(12)	29(3)	26(3)	37(4)	-6(3)	2(3)	0(3)
C(13)	32(4)	58(7)	128(12)	-39(7)	14(5)	13(4)
C(14)	88(8)	74(8)	62(7)	-43(6)	-25(6)	39(7)
C(15)	76(7)	35(5)	78(8)	16(5)	29(6)	11(5)
C(16)	29(3)	23(3)	26(3)	-2(3)	-1(3)	-4(2)
C(17)	22(3)	30(3)	35(4)	-5(3)	5(3)	-3(3)
C(18)	38(4)	35(4)	51(5)	3(4)	14(4)	-3(3)
C(19)	45(5)	45(5)	70(7)	7(5)	25(5)	-10(4)
C(20)	22(4)	46(5)	95(9)	-10(6)	0(4)	-10(4)
C(21)	34(4)	47(5)	58(6)	-7(4)	-8(4)	4(4)
C(22)	36(4)	34(4)	39(4)	-1(3)	-5(3)	9(3)

Table S4. Bond distances (Å) and angles (deg) for **4b**.

Distances

Ru(1)-N(2)	2.103(6)	N(1)-C(16)	1.325(10)	C(8)-C(10)	1.45(3)
Ru(1)-N(1)	2.115(10)	N(1)-C(8)	1.479(12)	C(12)-C(14)	1.506(13)
Ru(1)-C(5)	2.135(8)	N(2)-C(16)	1.342(9)	C(12)-C(15)	1.529(12)
Ru(1)-C(3)	2.169(8)	N(2)-C(12)	1.476(9)	C(12)-C(13)	1.533(11)
Ru(1)-C(4)	2.183(10)	C(1)-C(2)	1.403(12)	C(16)-C(17)	1.481(9)
Ru(1)-C(2)	2.205(7)	C(1)-C(6)	1.414(13)	C(17)-C(22)	1.388(11)
Ru(1)-C(6)	2.214(11)	C(2)-C(3)	1.401(13)	C(17)-C(18)	1.394(11)
Ru(1)-C(1)	,2.288(8)	C(3)-C(4)	1.407(16)	C(18)-C(19)	1.369(13)
Ru(1)-Cl(1)	2.408(2)	C(4)-C(5)	1.408(15)	C(19)-C(20)	1.371(17)
Ru(1)-C(16)	2.571(7)	C(5)-C(6)	1.405(16)	C(20)-C(21)	1.374(15)
O(1)-C(1)	1.340(10)	C(8)-C(9)	1.417(16)	C(21)-C(22)	1.394(12)
O(1)-C(7)	1.415(12)	C(8)-C(11)	1.43(2)		

Angles

N(2)-Ru(1)-N(1)	61.7(3)	C(5)-Ru(1)-C(1)	66.8(3)
N(2)-Ru(1)-C(5)	97.5(3)	C(3)-Ru(1)-C(1)	66.2(3)
N(1)-Ru(1)-C(5)	132.3(4)	C(4)-Ru(1)-C(1)	79.0(3)
N(2)-Ru(1)-C(3)	138.7(3)	C(2)-Ru(1)-C(1)	36.3(3)
N(1)-Ru(1)-C(3)	98.6(3)	C(6)-Ru(1)-C(1)	36.6(3)
C(5)-Ru(1)-C(3)	68.1(4)	N(2)-Ru(1)-Cl(1)	84.3(2)
N(2)-Ru(1)-C(4)	108.3(3)	N(1)-Ru(1)-Cl(1)	86.0(3)
N(1)-Ru(1)-C(4)	104.4(4)	C(5)-Ru(1)-Cl(1)	137.3(3)
C(5)-Ru(1)-C(4)	38.1(4)	C(3)-Ru(1)-Cl(1)	133.1(3)
C(3)-Ru(1)-C(4)	37.7(4)	C(4)-Ru(1)-Cl(1)	166.3(3)
N(2)-Ru(1)-C(2)	175.9(3)	C(2)-Ru(1)-Cl(1)	99.7(3)
N(1)-Ru(1)-C(2)	117.6(3)	C(6)-Ru(1)-Cl(1)	102.7(3)
C(5)-Ru(1)-C(2)	80.0(3)	C(1)-Ru(1)-Cl(1)	87.6(2)
C(3)-Ru(1)-C(2)	37.3(3)	N(2)-Ru(1)-C(16)	31.4(2)
C(4)-Ru(1)-C(2)	67.8(4)	N(1)-Ru(1)-C(16)	30.9(3)
N(2)-Ru(1)-C(6)	113.4(3)	C(5)-Ru(1)-C(16)	121.7(3)
N(1)-Ru(1)-C(6)	169.8(4)	C(3)-Ru(1)-C(16)	124.7(3)
C(5)-Ru(1)-C(6)	37.7(4)	C(4)-Ru(1)-C(16)	113.7(3)
C(3)-Ru(1)-C(6)	79.4(4)	C(2)-Ru(1)-C(16)	148.4(3)
C(4)-Ru(1)-C(6)	67.9(4)	C(6)-Ru(1)-C(16)	144.7(3)
C(2)-Ru(1)-C(6)	66.6(4)	C(1)-Ru(1)-C(16)	167.3(3)
N(2)-Ru(1)-C(1)	145.4(3)	Cl(1)-Ru(1)-C(16)	79.84(17)
N(1)-Ru(1)-C(1)	151.1(3)	C(1)-O(1)-C(7)	118.7(8)

C(16)-N(1)-C(8)	128.6(9)	C(9)-C(8)-C(11)	110.8(17)
C(16)-N(1)-Ru(1)	93.9(6)	C(9)-C(8)-C(10)	105.1(16)
C(8)-N(1)-Ru(1)	134.7(6)	C(11)-C(8)-C(10)	106(2)
C(16)-N(2)-C(12)	125.9(6)	C(9)-C(8)-N(1)	110.7(8)
C(16)-N(2)-Ru(1)	93.9(4)	C(11)-C(8)-N(1)	111.9(12)
C(12)-N(2)-Ru(1)	136.0(4)	C(10)-C(8)-N(1)	112.5(12)
O(1)-C(1)-C(2)	115.9(8)	N(2)-C(12)-C(14)	114.2(7)
O(1)-C(1)-C(6)	125.0(8)	N(2)-C(12)-C(15)	110.5(7)
C(2)-C(1)-C(6)	118.8(9)	C(14)-C(12)-C(15)	112.1(9)
O(1)-C(1)-Ru(1)	130.5(6)	N(2)-C(12)-C(13)	106.5(6)
C(2)-C(1)-Ru(1)	68.6(4)	C(14)-C(12)-C(13)	104.4(9)
C(6)-C(1)-Ru(1)	68.9(6)	C(15)-C(12)-C(13)	108.7(9)
C(3)-C(2)-C(1)	120.5(8)	N(1)-C(16)-N(2)	108.5(7)
C(3)-C(2)-Ru(1)	69.9(4)	N(1)-C(16)-C(17)	125.3(7)
C(1)-C(2)-Ru(1)	75.0(4)	N(2)-C(16)-C(17)	126.2(6)
C(2)-C(3)-C(4)	121.2(8)	N(1)-C(16)-Ru(1)	55.2(5)
C(2)-C(3)-Ru(1)	72.7(5)	N(2)-C(16)-Ru(1)	54.7(4)
C(4)-C(3)-Ru(1)	71.7(5)	C(17)-C(16)-Ru(1)	167.4(5)
C(3)-C(4)-C(5)	117.7(8)	C(22)-C(17)-C(18)	118.0(7)
C(3)-C(4)-Ru(1)	70.6(6)	C(22)-C(17)-C(16)	120.6(7)
C(5)-C(4)-Ru(1)	69.1(5)	C(18)-C(17)-C(16)	121.4(8)
C(6)-C(5)-C(4)	121.5(9)	C(19)-C(18)-C(17)	121.0(9)
C(6)-C(5)-Ru(1)	74.2(6)	C(18)-C(19)-C(20)	120.3(9)
C(4)-C(5)-Ru(1)	72.8(6)	C(19)-C(20)-C(21)	120.3(8)
C(5)-C(6)-C(1)	119.8(10)	C(20)-C(21)-C(22)	119.5(9)
C(5)-C(6)-Ru(1)	68.1(6)	C(17)-C(22)-C(21)	120.8(8)
C(1)-C(6)-Ru(1)	74.6(6)		

Table S5. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **4b**.

Atom	x	y	z	U(eq)
H(1)	-647	-388	5172	45
H(2)	57	-4	3451	50
H(3)	-557	1155	2695	46
H(4)	-1800	1975	3783	47
H(5)	-2523	1579	5517	35
H(6)	-2610	553	7902	65
H(7)	-2520	1205	7058	65
H(8)	-3754	694	7015	65
H(9)	2261	-396	5001	122
H(10)	1709	-73	3868	122
H(11)	3092	-441	3958	122
H(12)	3141	541	6372	226
H(13)	3973	-95	5888	226
H(14)	4509	717	5925	226
H(15)	4896	909	4559	241
H(16)	4454	380	3583	241
H(17)	3977	1204	3578	241
H(18)	-932	2974	6387	85
H(19)	-1162	3400	5266	85
H(20)	-1221	2534	5285	85
H(21)	782	2942	7138	93
H(22)	2167	2878	6667	93
H(23)	1439	3640	6642	93
H(24)	1332	3952	4914	73
H(25)	1730	3313	4126	73
H(26)	290	3603	4072	73
H(27)	3725	2623	3667	50
H(28)	5629	3314	4139	61
H(29)	6590	3270	5927	70
H(30)	5613	2593	7337	57
H(31)	3625	1946	6894	46

X-ray data of $[Ru(\eta\text{-}^{t}BuNC(Ph)=N^{t}Bu)(bipy)(MeCN)_2]^{+}PF_6^{-}$, **6**

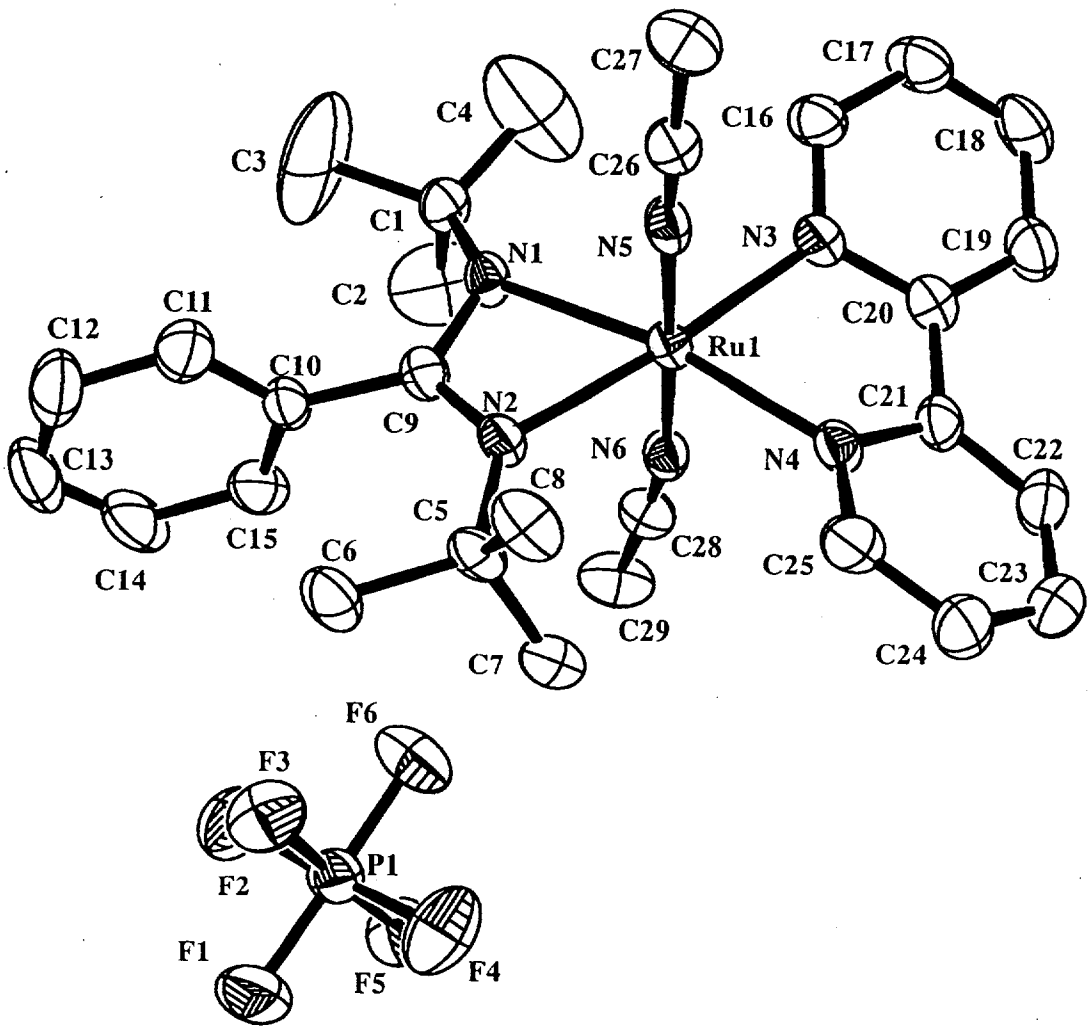

Figure S10. ORTEP drawing of **6** (50% probability ellipsoids) showing the numbering system. All hydrogen atoms are omitted for clarity.

Table S6. Crystal data and structure refinement for **6**

Empirical formula	$C_{29}H_{37}F_6N_6PRu$
Formula weight	715.69
Crystal habits, color	prismatic, black
Crystal size	0.30 x 0.20 x 0.10 mm
Crystal system	Monoclinic
Space group	$P2_1/n$ (#14))
Unit cell dimensions	a = 9.1744(5)Å
	b = 13.6993(7)Å β = 94.3950(10)°
	c = 24.8932(17)Å
Volume	3119.4(3) Å^3
Z	4
Density (calculated)	1.524 Mg/m^3
Absorption coefficient	0.620 mm^{-1}
F(000)	1464
Temperature	293(2) K
θ range for data collection	1.64 to 27.48
Index ranges	0<=h<=11; 0<=k<=17; -32<=l<=32
Reflection collected	7047
Independent reflections	7047 [R(int) = 0.000]
Reflections observed (>2σ)	4931
Structure Solution	Patterson methods
	(SIR92)
Refinement method	Full-matrix
	least-squares on F^2
Data/ restraints / parameters	7047 / 0 / 388
R indices (I>2σ(I))	R_1 = 0.0553 wR_2 = 0.1460
R indices (all data)	R_1 = 0.0874 wR_2 = 0.1671
Goodness-of-fit on F^2	1.073
Largest diff. peak and hole	1.394 and –1.079 e.Å^{-3}

Refinement of F^2 against all reflections. The weighted R-factor wR and goodness of fit S are base on F^2, conventional R-factors R are based on F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on all data will be even larger.
$w = 1/[\sigma^2(F_o^2)]$

Table S7. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **6**. Ueq is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	Ueq
Ru(1)	7149(1)	3087(1)	6693(1)	25(1)
P(1)	5735(2)	1963(1)	3870(1)	39(1)
F(1)	5735(4)	2255(4)	3247(2)	76(1)
F(2)	6760(4)	1054(3)	3761(2)	63(1)
F(3)	7156(4)	2616(3)	4001(2)	60(1)
F(4)	4717(4)	2872(3)	3979(2)	76(1)
F(5)	4317(3)	1292(3)	3736(2)	58(1)
F(6)	5748(5)	1650(3)	4484(1)	66(1)
N(1)	8984(4)	2184(3)	6501(2)	30(1)
N(2)	8116(4)	3347(3)	5968(2)	30(1)
N(3)	6369(4)	2717(3)	7433(2)	30(1)
N(4)	5231(4)	3934(3)	6721(2)	31(1)
N(5)	8451(4)	4039(3)	7102(2)	31(1)
N(6)	5898(4)	2098(3)	6277(2)	30(1)
C(1)	9613(5)	1235(3)	6671(2)	34(1)
C(2)	8761(11)	407(6)	6359(4)	93(3)
C(3)	11139(11)	1061(8)	6529(6)	149(6)
C(4)	9443(16)	1062(7)	7249(4)	133(5)
C(5)	7788(5)	4040(3)	5521(2)	33(1)
C(6)	8750(7)	3991(4)	5041(2)	46(1)
C(7)	6223(6)	3858(4)	5293(2)	41(1)
C(8)	8006(6)	5067(4)	5768(2)	44(1)
C(9)	9027(5)	2600(3)	6017(2)	30(1)
C(10)	9957(5)	2283(4)	5579(2)	33(1)
C(11)	11379(6)	2625(4)	5553(2)	45(1)
C(12)	12182(7)	2381(5)	5122(3)	61(2)
C(13)	11551(8)	1763(6)	4719(3)	67(2)
C(14)	10187(8)	1412(5)	4749(2)	60(2)
C(15)	9376(6)	1670(4)	5175(2)	42(1)
C(16)	7145(5)	2380(4)	7867(2)	38(1)
C(17)	6496(7)	2126(4)	8338(2)	47(1)
C(18)	5038(7)	2238(5)	8366(2)	51(1)
C(19)	4227(6)	2651(5)	7929(2)	46(1)
C(20)	4911(5)	2912(3)	7474(2)	34(1)
C(21)	4249(5)	3539(4)	7049(2)	35(1)

C(22)	2792(6)	3810(4)	7008(2)	48(1)
C(23)	2314(6)	4553(5)	6660(2)	53(2)
C(24)	3322(7)	5019(4)	6372(2)	52(2)
C(25)	4760(6)	4676(4)	6411(2)	41(1)
C(26)	9173(5)	4559(3)	7374(2)	32(1)
C(27)	10041(6)	5204(4)	7721(2)	44(1)
C(28)	5343(5)	1520(4)	5996(2)	35(1)
C(29)	4750(7)	765(4)	5639(2)	52(2)

Table S8. Anisotropic displacement parameters ($Å^2x10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru(1)	30(1)	24(1)	23(1)	-1(1)	6(1)	1(1)
P(1)	39(1)	40(1)	39(1)	3(1)	4(1)	-2(1)
F(1)	62(2)	116(3)	49(2)	34(2)	1(2)	-6(2)
F(2)	58(2)	57(2)	75(3)	-14(2)	5(2)	12(2)
F(3)	52(2)	54(2)	74(3)	1(2)	-3(2)	-12(2)
F(4)	59(2)	45(2)	122(4)	-6(2)	11(2)	9(2)
F(5)	47(2)	59(2)	66(2)	-6(2)	4(2)	-15(2)
F(6)	87(3)	73(3)	38(2)	5(2)	9(2)	-15(2)
N(1)	36(2)	23(2)	31(2)	-1(2)	11(2)	8(2)
N(2)	37(2)	30(2)	24(2)	3(2)	9(2)	4(2)
N(3)	38(2)	27(2)	27(2)	0(2)	7(2)	1(2)
N(4)	38(2)	29(2)	25(2)	-2(2)	7(2)	6(2)
N(5)	33(2)	33(2)	28(2)	3(2)	13(2)	1(2)
N(6)	31(2)	32(2)	29(2)	4(2)	8(2)	3(2)
C(1)	38(2)	28(2)	36(3)	0(2)	7(2)	8(2)
C(2)	114(7)	43(4)	118(8)	-7(5)	-16(6)	-1(4)
C(3)	103(7)	128(9)	229(14)	111(9)	92(8)	91(7)
C(4)	242(13)	89(7)	74(6)	34(5)	46(7)	105(8)
C(5)	46(3)	27(2)	26(2)	6(2)	7(2)	0(2)
C(6)	60(3)	43(3)	36(3)	11(2)	17(2)	7(2)
C(7)	50(3)	39(3)	32(3)	1(2)	-1(2)	1(2)
C(8)	64(3)	32(3)	38(3)	0(2)	12(3)	-8(2)
C(9)	31(2)	29(2)	29(2)	-4(2)	6(2)	-2(2)
C(10)	35(2)	36(2)	28(2)	0(2)	9(2)	8(2)
C(11)	38(3)	50(3)	48(3)	6(3)	8(2)	2(2)

C(12)	44(3)	73(4)	69(4)	25(4)	29(3)	14(3)
C(13)	80(5)	81(5)	44(3)	10(3)	35(3)	37(4)
C(14)	80(4)	69(4)	31(3)	-10(3)	8(3)	24(4)
C(15)	51(3)	40(3)	36(3)	-5(2)	1(2)	11(2)
C(16)	40(2)	42(3)	34(3)	5(2)	3(2)	-2(2)
C(17)	55(3)	53(3)	33(3)	11(2)	2(2)	-2(3)
C(18)	68(4)	55(3)	33(3)	8(3)	22(3)	0(3)
C(19)	48(3)	54(3)	40(3)	3(3)	16(2)	3(3)
C(20)	41(2)	31(2)	30(2)	-1(2)	8(2)	-1(2)
C(21)	38(2)	35(2)	33(2)	-6(2)	9(2)	6(2)
C(22)	39(3)	56(3)	50(3)	2(3)	15(2)	10(2)
C(23)	47(3)	63(4)	50(3)	5(3)	8(3)	21(3)
C(24)	60(3)	50(3)	46(3)	10(3)	12(3)	25(3)
C(25)	54(3)	33(3)	35(3)	1(2)	3(2)	9(2)
C(26)	36(2)	29(2)	31(2)	1(2)	5(2)	2(2)
C(27)	57(3)	36(3)	39(3)	-4(2)	1(2)	-7(2)
C(28)	40(2)	32(2)	33(3)	3(2)	3(2)	-4(2)
C(29)	71(4)	34(3)	47(3)	-7(3)	-11(3)	-9(3)

Table S9. Bond distances (Å) and angles (deg) for **6**.

Distances					
Ru(1)-N(5)	1.995(4)	N(2)-C(5)	1.475(6)	C(11)-C(12)	1.389(9)
Ru(1)-N(6)	2.010(4)	N(3)-C(16)	1.329(6)	C(12)-C(13)	1.404(11)
Ru(1)-N(3)	2.088(4)	N(3)-C(20)	1.376(6)	C(13)-C(14)	1.348(11)
Ru(1)-N(2)	2.102(4)	N(4)-C(25)	1.328(6)	C(14)-C(15)	1.388(8)
Ru(1)-N(4)	2.114(4)	N(4)-C(21)	1.373(6)	C(16)-C(17)	1.399(7)
Ru(1)-N(1)	2.171(4)	N(5)-C(26)	1.156(6)	C(17)-C(18)	1.353(9)
Ru(1)-C(9)	2.587(5)	N(6)-C(28)	1.150(6)	C(18)-C(19)	1.389(8)
P(1)-F(6)	1.588(4)	C(1)-C(4)	1.480(10)	C(19)-C(20)	1.385(7)
P(1)-F(4)	1.592(4)	C(1)-C(3)	1.489(9)	C(20)-C(21)	1.457(7)
P(1)-F(3)	1.594(4)	C(1)-C(2)	1.552(9)	C(21)-C(22)	1.384(7)
P(1)-F(2)	1.595(4)	C(5)-C(7)	1.523(7)	C(22)-C(23)	1.385(8)
P(1)-F(1)	1.601(4)	C(5)-C(6)	1.541(7)	C(23)-C(24)	1.370(9)
P(1)-F(5)	1.606(3)	C(5)-C(8)	1.543(7)	C(24)-C(25)	1.397(8)
N(1)-C(9)	1.337(6)	C(9)-C(10)	1.500(6)	C(26)-C(27)	1.432(7)
N(1)-C(1)	1.471(6)	C(10)-C(15)	1.384(7)	C(28)-C(29)	1.442(7)
N(2)-C(9)	1.321(6)	C(10)-C(11)	1.393(7)		

Angles

N(5)-Ru(1)-N(6)	178.02(15)	C(1)-N(1)-Ru(1)	137.3(3)
N(5)-Ru(1)-N(3)	86.59(15)	C(9)-N(2)-C(5)	131.2(4)
N(6)-Ru(1)-N(3)	94.03(15)	C(9)-N(2)-Ru(1)	95.4(3)
N(5)-Ru(1)-N(2)	92.99(15)	C(5)-N(2)-Ru(1)	133.0(3)
N(6)-Ru(1)-N(2)	86.19(15)	C(16)-N(3)-C(20)	118.0(4)
N(3)-Ru(1)-N(2)	173.74(14)	C(16)-N(3)-Ru(1)	127.1(3)
N(5)-Ru(1)-N(4)	95.24(15)	C(20)-N(3)-Ru(1)	114.8(3)
N(6)-Ru(1)-N(4)	86.73(15)	C(25)-N(4)-C(21)	116.7(4)
N(3)-Ru(1)-N(4)	76.24(15)	C(25)-N(4)-Ru(1)	129.5(3)
N(2)-Ru(1)-N(4)	110.01(15)	C(21)-N(4)-Ru(1)	112.9(3)
N(5)-Ru(1)-N(1)	92.33(15)	C(26)-N(5)-Ru(1)	174.8(4)
N(6)-Ru(1)-N(1)	85.69(15)	C(28)-N(6)-Ru(1)	170.5(4)
N(3)-Ru(1)-N(1)	112.28(15)	N(1)-C(1)-C(4)	110.7(5)
N(2)-Ru(1)-N(1)	61.48(15)	N(1)-C(1)-C(3)	115.4(5)
N(4)-Ru(1)-N(1)	168.97(15)	C(4)-C(1)-C(3)	112.1(8)
N(5)-Ru(1)-C(9)	95.65(14)	N(1)-C(1)-C(2)	109.4(5)
N(6)-Ru(1)-C(9)	82.74(14)	C(4)-C(1)-C(2)	106.4(7)
N(3)-Ru(1)-C(9)	143.27(15)	C(3)-C(1)-C(2)	102.2(7)
N(2)-Ru(1)-C(9)	30.55(15)	N(2)-C(5)-C(7)	107.9(4)
N(4)-Ru(1)-C(9)	139.52(15)	N(2)-C(5)-C(6)	117.5(4)
N(1)-Ru(1)-C(9)	31.12(14)	C(7)-C(5)-C(6)	106.4(4)
F(6)-P(1)-F(4)	90.5(3)	N(2)-C(5)-C(8)	105.9(4)
F(6)-P(1)-F(3)	90.5(2)	C(7)-C(5)-C(8)	112.8(4)
F(4)-P(1)-F(3)	90.4(2)	C(6)-C(5)-C(8)	106.5(4)
F(6)-P(1)-F(2)	89.5(2)	N(2)-C(9)-N(1)	110.6(4)
F(4)-P(1)-F(2)	179.8(3)	N(2)-C(9)-C(10)	123.2(4)
F(3)-P(1)-F(2)	89.4(2)	N(1)-C(9)-C(10)	126.2(4)
F(6)-P(1)-F(1)	178.7(3)	N(2)-C(9)-Ru(1)	54.0(2)
F(4)-P(1)-F(1)	90.8(3)	N(1)-C(9)-Ru(1)	57.0(2)
F(3)-P(1)-F(1)	89.9(2)	C(10)-C(9)-Ru(1)	172.9(3)
F(2)-P(1)-F(1)	89.3(2)	C(15)-C(10)-C(11)	118.8(5)
F(6)-P(1)-F(5)	89.5(2)	C(15)-C(10)-C(9)	119.6(4)
F(4)-P(1)-F(5)	90.4(2)	C(11)-C(10)-C(9)	121.5(5)
F(3)-P(1)-F(5)	179.2(2)	C(12)-C(11)-C(10)	120.6(6)
F(2)-P(1)-F(5)	89.8(2)	C(11)-C(12)-C(13)	118.9(6)
F(1)-P(1)-F(5)	90.1(2)	C(14)-C(13)-C(12)	120.7(5)
C(9)-N(1)-C(1)	126.6(4)	C(13)-C(14)-C(15)	120.3(6)
C(9)-N(1)-Ru(1)	91.9(3)	C(10)-C(15)-C(14)	120.7(6)

N(3)-C(16)-C(17)	122.1(5)	N(4)-C(21)-C(20)	114.1(4)
C(18)-C(17)-C(16)	120.0(5)	C(22)-C(21)-C(20)	124.0(5)
C(17)-C(18)-C(19)	118.6(5)	C(21)-C(22)-C(23)	120.1(5)
C(20)-C(19)-C(18)	119.8(5)	C(24)-C(23)-C(22)	118.3(5)
N(3)-C(20)-C(19)	120.9(5)	C(23)-C(24)-C(25)	118.6(5)
N(3)-C(20)-C(21)	114.5(4)	N(4)-C(25)-C(24)	124.1(5)
C(19)-C(20)-C(21)	123.8(5)	N(5)-C(26)-C(27)	178.6(5)
N(4)-C(21)-C(22)	121.6(5)	N(6)-C(28)-C(29)	175.9(6)

Table S10. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **6**.

Atom	x	y	z	U(eq)
H(1)	11811	3031	5838	55
H(2)	13152	2638	5097	74
H(3)	12100	1594	4422	78
H(4)	9766	992	4468	74
H(5)	8394	1412	5195	51
H(6)	8188	2311	7851	46
H(7)	7098	1868	8642	56
H(8)	4568	2033	8677	62
H(9)	3187	2759	7940	55
H(10)	2105	3479	7220	58
H(11)	1301	4738	6615	65
H(12)	3058	5575	6152	60
H(13)	5461	4995	6199	50
H(14)	8277	-9	6596	119
H(15)	8003	684	6106	119
H(16)	9380	24	6154	119
H(17)	11776	992	6851	176
H(18)	11194	500	6316	176
H(19)	11477	1616	6334	176
H(20)	9929	1559	7469	137
H(21)	8423	1075	7320	137
H(22)	9832	445	7362	137
H(23)	9753	3934	5166	57
H(24)	8480	3443	4820	57
H(25)	8622	4571	4830	57

H(26)	5590	3793	5579	49
H(27)	5886	4384	5067	49
H(28)	6167	3267	5085	49
H(29)	8018	5026	6152	55
H(30)	8913	5334	5675	55
H(31)	7231	5482	5638	55
H(32)	9888	5072	8090	54
H(33)	11054	5117	7671	54
H(34)	9782	5866	7644	54
H(35)	4334	260	5841	63
H(36)	4008	1029	5390	63
H(37)	5503	495	5441	63