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SUPPORTING INFORMATION

X-ray Crystallography

Data Collection

An air and moisture sensitive black crystal of $C_{88}H_{56}N_8PF_6Ru_2 \cdot CH_2Cl_2$ with approximate dimensions of 0.40 x 0.20 x 0.11 mm^3 grown from a solution of dichloromethane/benzene was mounted on a glass fiber in paratone oil at -80 °C using an improvised cold stage. All measurements were made on a Siemens SMART[9] diffractometer with graphite-monochromated Mo-Kα radiation. Cell constants and an orientation matrix for data collection, obtained from a least squares refinement using the setting angles of 7481 carefully centered reflections with $I > 10\ \sigma(I)$ in the range $2.20° < 2\theta < 52.10°$ corresponded to a primitive tetragonal cell (Laue class: 4/mmm) with dimensions:

$a =$ 18.5148(4) Å
$c =$ 26.4410(4) Å
$V =$ 9063.9(3) $Å^3$

For $Z = 4$ and $F.W. = 1572.57$, the calculated density is 1.15 g/cm^3.
The systematic absences of:

0kl: $k+l \neq 2n$
hk0: $h+k \neq 2n$
hhl: $l \neq 2n$

and successful solution and refinement of the structure the space group was determined to be: *P4/nnc* (#126). Wilson statistics supported a centric space group. The data were collected at a temperature of -143 ± 1_C using the ω scan technique to a maximum 2θ value of 52.1°.

Data Reduction.

Data were integrated using the program SAINT[10] with a 1.6 x 1.6 x 0.6° box. A total of 43012 reflections were collected. A correction for decay was deemed unnecessary. An empirical absorption correction, XPREP, was applied which resulted in transmission factors ranging from 0.79 to 0.90. The data were corrected for Lorentz and polarization effects. The linear absorption coefficient, μ, for Mo-K_α radiation is 4.06 cm^{-1}. Symmetry-equivalent, non-Friedel, reflections were averaged to produce 4813 unique reflections ($R_{int} = 0.07$).

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Only the Ru atom was refined anisotropically, all remaining atoms were refined isotropically. Hydrogen atoms were included at fixed positions and not refined. The $C_{22}H_{14}N_2P_{0.25}F_{1.5}Ru_{0.5} \cdot C_{0.25}H_{0.5}Cl_{0.5}$ unit (1/4 th of the full molecule) was found in the difference Fourier map. The P atom of PF_6^- was disordered over three positions with populations of 0.11, 0.09, and 0.05 (see Figures S1 and S2). The maximum and minimum peaks on the final difference Fourier map corresponded to 1.98 and -0.93 $e^-/Å^3$, respectively. The final cycle of full-matrix least-squares refinement was based on 2039 observed reflections ($I > 3\sigma(I)$) and 198 variable parameters and converged (largest parameter shift was 0.21 times its esd) with unweighted and weighted agreement factors of:

$R = \Sigma \, ||F_o| - |F_c|| \, / \, \Sigma \, |F_o| = 0.078$; $R_w = [(\Sigma_w \, (|F_o| - |F_c|)^2 \, / \, \Sigma_w \, F_o^2)]^{1/2} = 0.100$

The standard deviation of an observation of unit weight[3] was 3.00. The weighting scheme was based on counting statistics and included a factor (p = 0.03) to downweight the intense reflections. Plots of $\Sigma_w \, (|F_o| - |F_c|)^2$ versus $|F_o|$, reflection order in data collection, sin θ/λ, and various classes of indices showed no unusual trends. Neutral atom scattering factors were taken from Cromer and Waber[4]. Anomalous dispersion effects were included in F_{calc}[5]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[6]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[7]. All calculations were performed using the teXsan[8] crystallographic software package of Molecular Structure Corporation.

References:

1. SHELXS-86: Sheldrich, G. (1986).

2. DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

3. Standard deviation of an observation of unit weight: $[\Sigma \, w(|F_o| - |F_c|)^2/(N_o - N_v)]^{1/2}$ where: N_o = number of observations N_v = number of variables.

4. Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

5. Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

6. Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

7. Creagh, D. C. & Hubbell, J. H.; Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

8. teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

9. SMART: Area-Detector Software Package; Siemens Industrial Automation, Inc.: Madison, WI, (1995).

10. SAINT: SAX Area-Detector Integration Program; V4.024; Siemens Industrial Automation, Inc.: Madison, WI, (1995).

Table S-1: Summary of Crystallographic Data and Parameters for $C_{88}H_{56}N_8PF_6Ru_2 \cdot CH_2Cl_2$

Formula:	$C_{88}H_{56}N_8PF_6Ru_2 \cdot CH_2Cl_2$
FW	1572.57
Temperature (K)	130
Space Group	P4/nnc(#126); Tetragonal
a (Å)	18.5148(4)
b (Å)	18.5148(4)
c (Å)	26.4410(4)
α (deg)	90.000(1)
β (deg)	90.000(1)
γ (deg)	90.000(1)
Volume (Å^3)	9063.9(3)
Z	4
Abs. Coeff., μ_{calc} (cm^{-1})	4.06
F_{000}	3352
d_{obs}[c] (d_{calc})	(1.15) g cm^{-3}
Crystal Size (mm)	0.40 x 0.20 x 0.11
Radiation	Mo K_α (λ = 0.71069 Å)
Monochromator	Highly-oriented graphite
Diffractometer	Siemens SMART
Reflections measured	0<h<21; -22<k < 22; -30<l < 30
2θ range	2.20° < 2θ < 52.10°
Scan Type	ω
Scan width	0.3°
Scan speed	10-second frame exposure
Reflections collected	43012
Unique reflections:	4813 (R_{int} = 0.07)
Reflections with ($F_o^2 > 3\sigma(F_o^2)$)	2039
Number of Variables	198
Parameter-to-variable ratio	10.3
R (R_w)	0.078 (0.100)
Final Difference ρ_{max} (e^-/ Å^3)[d]	+1.98; -0.93

[a]Unit cell parameters and their esd's were derived by a least-squares fitting of 7481 reflections with $I > 10\ \sigma(I)$ and 2θ between 2.20° and 52.10°. [b]In this and subsequent tables, the esd's of all parameters are given in parentheses. [c]The density of the crystal was not measured. [d]Maximum negative and positive difference peaks.

Table S-2. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ru	0.1881	-0.2500	0.2500	0.99(6)	1/2
Cl(1)	-0.396(2)	-0.113(2)	0.4074(10)	3.4(6)	1/4
Cl(2)	-0.293(1)	-0.016(1)	0.3685(8)	1.3(4)	1/4
P(1)	0.2500	0.2500	-0.2500	2.8(5)	0.090
P(2)	0.2500	0.2500	0.2500	2.2(8)	0.050
P(3)	0.2500	0.2500	0.010(1)	3.7(7)	0.110
F(1)	0.2500	0.319(3)	0.2500	5(1)	0.200
F(2)	0.2500	0.2500	0.200(3)	5(2)	0.100
F(3)	0.2500	0.2500	0.058(2)	4(1)	0.110
F(4)	0.239(3)	0.164(2)	0.007(1)	4.2(9)	0.440
F(5)	0.2500	0.2500	-0.046(4)	6(2)	0.110
F(7)	0.2500	0.2500	-0.301(5)	6(3)	0.180
F(9)	0.2500	0.146(8)	-0.2500	4(2)	0.360
N(1)	0.166(1)	-0.144(1)	0.2305(7)	0.9(4)	
N(2)	0.166(1)	-0.223(1)	0.3234(7)	1.3(5)	
C(1)	0.155(1)	-0.160(1)	0.1387(9)	1.4(5)	
C(2)	0.155(1)	-0.120(1)	0.1828(10)	1.5(5)	
C(3)	0.135(1)	-0.043(1)	0.1869(9)	1.6(5)	
C(4)	0.139(1)	-0.021(1)	0.2359(8)	1.4(6)	
C(5)	0.157(1)	-0.088(1)	0.2628(8)	1.1(6)	
C(6)	0.158(1)	-0.091(1)	0.3148(8)	1.3(6)	
C(7)	0.164(2)	-0.155(2)	0.3433(9)	1.6(5)	
C(8)	0.162(1)	-0.162(2)	0.3985(8)	1.3(6)	
C(9)	0.159(1)	-0.227(1)	0.4108(8)	1.5(6)	
C(10)	0.161(1)	-0.268(1)	0.3641(8)	0.8(4)	
C(11)	0.140(2)	-0.115(2)	0.0883(10)	1.7(7)	
C(12)	0.186(1)	-0.065(1)	0.0694(9)	1.3(5)	
C(13)	0.174(2)	-0.030(2)	0.023(1)	2.2(7)	
C(14)	0.109(2)	-0.048(2)	-0.001(1)	3.3(9)	
C(15)	0.060(2)	-0.101(2)	0.017(1)	2.2(7)	
C(16)	0.073(2)	-0.132(1)	0.0603(9)	2.3(7)	
C(17)	0.147(1)	-0.020(2)	0.3420(9)	1.8(5)	
C(18)	0.199(1)	0.039(1)	0.3421(9)	1.5(6)	
C(19)	0.187(2)	0.104(2)	0.367(1)	3.3(8)	
C(20)	0.124(2)	0.107(2)	0.4014(9)	2.4(6)	
C(21)	0.072(1)	0.047(1)	0.4049(9)	1.9(6)	
C(22)	0.078(2)	-0.020(2)	0.3737(10)	2.2(5)	
C(23)	-0.3120	-0.0986	0.3842	1.6(5)	
H(1)	0.1212	-0.0148	0.1605	1.9222	
H(2)	0.1352	0.0295	0.2475	2.5152	
H(3)	0.1665	-0.1182	0.4203	1.5559	
H(4)	0.1585	-0.2467	0.4436	2.2115	
H(5)	0.0377	-0.1673	0.0733	2.4678	
H(6)	0.0201	-0.1136	-0.0037	2.4678	
H(7)	0.0930	-0.0152	-0.0311	2.4678	
H(8)	0.2065	0.0022	0.0091	2.4678	

Table S-2. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(9)	0.2266	-0.0501	0.0889	2.4678
H(10)	0.2382	0.0306	0.3200	2.4891
H(11)	0.2173	0.1416	0.3636	2.4891
H(12)	0.1175	0.1484	0.4210	2.4891
H(13)	0.0315	0.0489	0.4258	2.4891
H(14)	0.0486	-0.0569	0.3761	1.9743
H(15)	-0.2792	-0.1112	0.4104	2.0400
H(16)	-0.3046	-0.1294	0.3560	2.0400

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table S-3. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru	0.014(2)	0.016(2)	0.010(1)	0.0000	0.0000	0.0005

The general temperature factor expression:
$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S-4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ru	Ru	2.29	Ru	N(1)	2.07(2)
Ru	N(1)	2.07(2)	Ru	N(2)	2.05(2)
Ru	N(2)	2.05(2)	Cl(1)	C(23)	1.70(4)
Cl(2)	C(23)	1.62(2)	P(1)	F(7)	1.4(1)
P(1)	F(7)	1.4(1)	P(1)	F(9)	1.9(1)
P(1)	F(9)	1.9(1)	P(1)	F(9)	1.9(1)
P(1)	F(9)	1.9(1)	P(2)	F(1)	1.28(6)
P(2)	F(1)	1.28(6)	P(2)	F(1)	1.28(6)
P(2)	F(1)	1.28(6)	P(2)	F(2)	1.32(9)
P(2)	F(2)	1.32(9)	P(3)	F(3)	1.27(6)
P(3)	F(4)	1.60(4)	P(3)	F(4)	1.60(4)
P(3)	F(4)	1.60(4)	P(3)	F(4)	1.60(4)
P(3)	F(5)	1.5(1)	N(1)	C(2)	1.35(3)
N(1)	C(5)	1.35(3)	N(2)	C(7)	1.37(3)
N(2)	C(10)	1.37(3)	C(1)	C(2)	1.38(3)
C(1)	C(10)	1.34(3)	C(1)	C(11)	1.59(3)
C(2)	C(3)	1.48(4)	C(3)	C(4)	1.36(3)
C(4)	C(5)	1.46(3)	C(5)	C(6)	1.38(3)
C(6)	C(7)	1.40(3)	C(6)	C(17)	1.51(4)
C(7)	C(8)	1.47(3)	C(8)	C(9)	1.25(3)
C(9)	C(10)	1.46(3)	C(11)	C(12)	1.36(4)
C(11)	C(16)	1.49(4)	C(12)	C(13)	1.40(4)
C(13)	C(14)	1.41(5)	C(14)	C(15)	1.42(4)
C(15)	C(16)	1.30(4)	C(17)	C(18)	1.45(4)
C(17)	C(22)	1.53(4)	C(18)	C(19)	1.40(4)
C(19)	C(20)	1.46(4)	C(20)	C(21)	1.48(4)

Table S-5. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(3)	H(1)	0.91	C(4)	H(2)	0.99
C(8)	H(3)	1.00	C(9)	H(4)	0.94
C(12)	H(9)	0.94	C(13)	H(8)	0.93
C(14)	H(7)	1.03	C(15)	H(6)	0.95
C(16)	H(5)	0.98	C(18)	H(10)	0.95
C(19)	H(11)	0.90	C(20)	H(12)	0.93
C(21)	H(13)	0.93	C(22)	H(14)	0.87
C(23)	H(15)	0.95	C(23)	H(16)	0.95

Table S-6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Ru	Ru	N(1)	101.2(5)	Ru	Ru	N(1)	101.2(5)
Ru	Ru	N(2)	101.7(6)	Ru	Ru	N(2)	101.7(6)
N(1)	Ru	N(1)	157(1)	N(1)	Ru	N(2)	87.9(8)
N(1)	Ru	N(2)	87.6(8)	N(1)	Ru	N(2)	87.6(8)
N(1)	Ru	N(2)	87.9(8)	N(2)	Ru	N(2)	156(1)
F(7)	P(1)	F(7)	180.0	F(7)	P(1)	F(9)	90.0
F(7)	P(1)	F(9)	90.0	F(7)	P(1)	F(9)	90.0
F(7)	P(1)	F(9)	90.0	F(7)	P(1)	F(9)	90.0
F(7)	P(1)	F(9)	90.0	F(7)	P(1)	F(9)	90.0
F(7)	P(1)	F(9)	90.0	F(9)	P(1)	F(9)	180(1)
F(9)	P(1)	F(9)	90.0	F(9)	P(1)	F(9)	90.0
F(9)	P(1)	F(9)	90.0	F(9)	P(1)	F(9)	90.0
F(9)	P(1)	F(9)	180(1)	F(1)	P(2)	F(1)	180.0
F(1)	P(2)	F(1)	90.0	F(1)	P(2)	F(1)	90.0
F(1)	P(2)	F(2)	90.0	F(1)	P(2)	F(2)	90.0
F(1)	P(2)	F(1)	90.0	F(1)	P(2)	F(1)	90.0
F(1)	P(2)	F(2)	90.0	F(1)	P(2)	F(2)	90.0
F(1)	P(2)	F(1)	180.0	F(1)	P(2)	F(2)	90.0
F(1)	P(2)	F(2)	90.0	F(1)	P(2)	F(2)	90.0
F(1)	P(2)	F(2)	90.0	F(2)	P(2)	F(2)	180(1)
F(3)	P(3)	F(4)	92(2)	F(3)	P(3)	F(4)	92(2)
F(3)	P(3)	F(4)	92(2)	F(3)	P(3)	F(4)	92(2)
F(3)	P(3)	F(5)	180.0	F(4)	P(3)	F(4)	174(4)
F(4)	P(3)	F(4)	89.9(2)	F(4)	P(3)	F(4)	89.9(2)
F(4)	P(3)	F(5)	87(2)	F(4)	P(3)	F(4)	89.9(2)
F(4)	P(3)	F(4)	89.9(2)	F(4)	P(3)	F(5)	87(2)
F(4)	P(3)	F(4)	174(4)	F(4)	P(3)	F(5)	87(2)
F(4)	P(3)	F(5)	87(2)	Ru	N(1)	C(2)	124(1)
Ru	N(1)	C(5)	126(1)	C(2)	N(1)	C(5)	108(2)
Ru	N(2)	C(7)	126(1)	Ru	N(2)	C(10)	127(1)
C(7)	N(2)	C(10)	105(1)	C(2)	C(1)	C(10)	125(2)
C(2)	C(1)	C(11)	115(2)	C(10)	C(1)	C(11)	119(2)
N(1)	C(2)	C(1)	127(2)	N(1)	C(2)	C(3)	106(2)
C(1)	C(2)	C(3)	125(2)	C(2)	C(3)	C(4)	109(2)
C(3)	C(4)	C(5)	103(2)	N(1)	C(5)	C(4)	111(1)
N(1)	C(5)	C(6)	126(2)	C(4)	C(5)	C(6)	121(2)
C(5)	C(6)	C(7)	125(2)	C(5)	C(6)	C(17)	115(2)
C(7)	C(6)	C(17)	118(2)	N(2)	C(7)	C(6)	124(2)
N(2)	C(7)	C(8)	107(2)	C(6)	C(7)	C(8)	127(2)
C(7)	C(8)	C(9)	110(2)	C(8)	C(9)	C(10)	106(2)
N(2)	C(10)	C(1)	125(2)	N(2)	C(10)	C(9)	109(1)
C(1)	C(10)	C(9)	124(2)	C(1)	C(11)	C(12)	124(2)
C(1)	C(11)	C(16)	116(2)	C(12)	C(11)	C(16)	119(2)
C(11)	C(12)	C(13)	122(2)	C(12)	C(13)	C(14)	115(2)
C(13)	C(14)	C(15)	123(2)	C(14)	C(15)	C(16)	119(3)
C(11)	C(16)	C(15)	119(2)	C(6)	C(17)	C(18)	124(2)

Table S-6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	C(17)	C(22)	112(2)	C(18)	C(17)	C(22)	122(2)
C(17)	C(18)	C(19)	123(2)	C(18)	C(19)	C(20)	116(2)
C(19)	C(20)	C(21)	121(2)	C(20)	C(21)	C(22)	122(2)
C(17)	C(22)	C(21)	111(2)	Cl(1)	C(23)	Cl(2)	116(1)

Table S-7. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(3)	H(1)	124.5	C(4)	C(3)	H(1)	125.5
C(3)	C(4)	H(2)	124.7	C(5)	C(4)	H(2)	131.7
C(7)	C(8)	H(3)	119.8	C(9)	C(8)	H(3)	129.5
C(8)	C(9)	H(4)	127.9	C(10)	C(9)	H(4)	125.4
C(11)	C(12)	H(9)	119.5	C(13)	C(12)	H(9)	118.4
C(12)	C(13)	H(8)	122.5	C(14)	C(13)	H(8)	121.6
C(13)	C(14)	H(7)	117.1	C(15)	C(14)	H(7)	119.3
C(14)	C(15)	H(6)	118.0	C(16)	C(15)	H(6)	122.4
C(11)	C(16)	H(5)	121.4	C(15)	C(16)	H(5)	118.9
C(17)	C(18)	H(10)	112.2	C(19)	C(18)	H(10)	123.8
C(18)	C(19)	H(11)	120.8	C(20)	C(19)	H(11)	122.4
C(19)	C(20)	H(12)	119.1	C(21)	C(20)	H(12)	119.3
C(20)	C(21)	H(13)	122.6	C(22)	C(21)	H(13)	114.7
C(17)	C(22)	H(14)	124.6	C(21)	C(22)	H(14)	123.5
Cl(1)	C(23)	H(15)	106.5	Cl(1)	C(23)	H(16)	108.6
Cl(2)	C(23)	H(15)	106.5	Cl(2)	C(23)	H(16)	109.5
H(15)	C(23)	H(16)	109.5				

Table S-8. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru	Ru	N(1)	C(2)	93(2)	Ru	Ru	N(1)	C(5)	-90(2)
Ru	Ru	N(1)	C(2)	93(2)	Ru	Ru	N(1)	C(5)	-90(2)
Ru	Ru	N(2)	C(7)	83(2)	Ru	Ru	N(2)	C(10)	-85(2)
Ru	Ru	N(2)	C(7)	83(2)	Ru	Ru	N(2)	C(10)	-85(2)
Ru	N(1)	C(2)	C(1)	0(4)	Ru	N(1)	C(2)	C(3)	175(1)
Ru	N(1)	C(5)	C(4)	-176(1)	Ru	N(1)	C(5)	C(6)	-2(4)
Ru	N(1)	C(2)	C(1)	0(4)	Ru	N(1)	C(2)	C(3)	175(1)
Ru	N(1)	C(5)	C(4)	-176(1)	Ru	N(1)	C(5)	C(6)	-2(4)
Ru	N(2)	C(7)	C(6)	16(4)	Ru	N(2)	C(7)	C(8)	-167(1)
Ru	N(2)	C(10)	C(1)	-15(3)	Ru	N(2)	C(10)	C(9)	168(1)
Ru	N(2)	C(7)	C(6)	16(4)	Ru	N(2)	C(7)	C(8)	-167(1)
Ru	N(2)	C(10)	C(1)	-15(3)	Ru	N(2)	C(10)	C(9)	168(1)
N(1)	Ru	Ru	N(1)	29(1)	N(1)	Ru	Ru	N(1)	-150(1)
N(1)	Ru	Ru	N(2)	-60.7(8)	N(1)	Ru	Ru	N(2)	119.3(8)
N(1)	Ru	N(1)	C(2)	-86(2)	N(1)	Ru	N(1)	C(5)	89(2)
N(1)	Ru	N(2)	C(7)	-17(2)	N(1)	Ru	N(2)	C(10)	173(2)
N(1)	Ru	N(2)	C(7)	-175(2)	N(1)	Ru	N(2)	C(10)	15(2)
N(1)	C(2)	C(1)	C(10)	5(4)	N(1)	C(2)	C(1)	C(11)	-178(2)
N(1)	C(2)	C(3)	C(4)	2(3)	N(1)	C(5)	C(4)	C(3)	1(2)
N(1)	C(5)	C(6)	C(7)	-5(4)	N(1)	C(5)	C(6)	C(17)	179(2)
N(2)	Ru	Ru	N(2)	-150(1)	N(2)	Ru	Ru	N(2)	29(1)
N(2)	Ru	N(1)	C(2)	-164(2)	N(2)	Ru	N(1)	C(5)	10(2)
N(2)	Ru	N(1)	C(2)	-7(2)	N(2)	Ru	N(1)	C(5)	167(2)
N(2)	Ru	N(2)	C(7)	-96(2)	N(2)	Ru	N(2)	C(10)	94(2)
N(2)	C(7)	C(6)	C(5)	-2(4)	N(2)	C(7)	C(6)	C(17)	172(2)
N(2)	C(7)	C(8)	C(9)	-3(3)	N(2)	C(10)	C(1)	C(2)	3(4)
N(2)	C(10)	C(1)	C(11)	-172(2)	N(2)	C(10)	C(9)	C(8)	0(3)
C(1)	C(2)	N(1)	C(5)	-176(2)	C(1)	C(2)	C(3)	C(4)	178(2)
C(1)	C(10)	N(2)	C(7)	173(2)	C(1)	C(10)	C(9)	C(8)	-175(2)
C(1)	C(11)	C(12)	C(13)	175(2)	C(1)	C(11)	C(16)	C(15)	-175(2)
C(2)	N(1)	C(5)	C(4)	0(3)	C(2)	N(1)	C(5)	C(6)	173(2)
C(2)	C(1)	C(10)	C(9)	178(2)	C(2)	C(1)	C(11)	C(12)	66(3)
C(2)	C(1)	C(11)	C(16)	-115(2)	C(2)	C(3)	C(4)	C(5)	-2(2)
C(3)	C(2)	N(1)	C(5)	-1(2)	C(3)	C(2)	C(1)	C(10)	-169(2)
C(3)	C(2)	C(1)	C(11)	6(4)	C(3)	C(4)	C(5)	C(6)	-172(2)
C(4)	C(5)	C(6)	C(7)	168(2)	C(4)	C(5)	C(6)	C(17)	-6(3)
C(5)	C(6)	C(7)	C(8)	-177(2)	C(5)	C(6)	C(17)	C(18)	-68(3)
C(5)	C(6)	C(17)	C(22)	116(2)	C(6)	C(7)	N(2)	C(10)	-172(2)
C(6)	C(7)	C(8)	C(9)	172(3)	C(6)	C(17)	C(18)	C(19)	179(2)
C(6)	C(17)	C(22)	C(21)	173(2)	C(7)	N(2)	C(10)	C(9)	-2(2)
C(7)	C(6)	C(17)	C(18)	116(3)	C(7)	C(6)	C(17)	C(22)	-58(3)
C(7)	C(8)	C(9)	C(10)	1(3)	C(8)	C(7)	N(2)	C(10)	3(2)
C(8)	C(7)	C(6)	C(17)	-2(4)	C(9)	C(10)	C(1)	C(11)	2(4)
C(10)	C(1)	C(11)	C(12)	-117(3)	C(10)	C(1)	C(11)	C(16)	61(3)
C(11)	C(12)	C(13)	C(14)	3(4)	C(11)	C(16)	C(15)	C(14)	-3(4)
C(12)	C(11)	C(16)	C(15)	2(4)	C(12)	C(13)	C(14)	C(15)	-4(4)

Table S-8. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(18)	C(17)	C(22)	C(21)	-1(3)	C(18)	C(19)	C(20)	C(21)	-6(4)
C(19)	C(18)	C(17)	C(22)	-6(4)	C(19)	C(20)	C(21)	C(22)	0(4)
C(13)	C(12)	C(11)	C(16)	-2(4)	C(13)	C(14)	C(15)	C(16)	4(5)
C(17)	C(18)	C(19)	C(20)	9(4)	C(17)	C(22)	C(21)	C(20)	4(3)

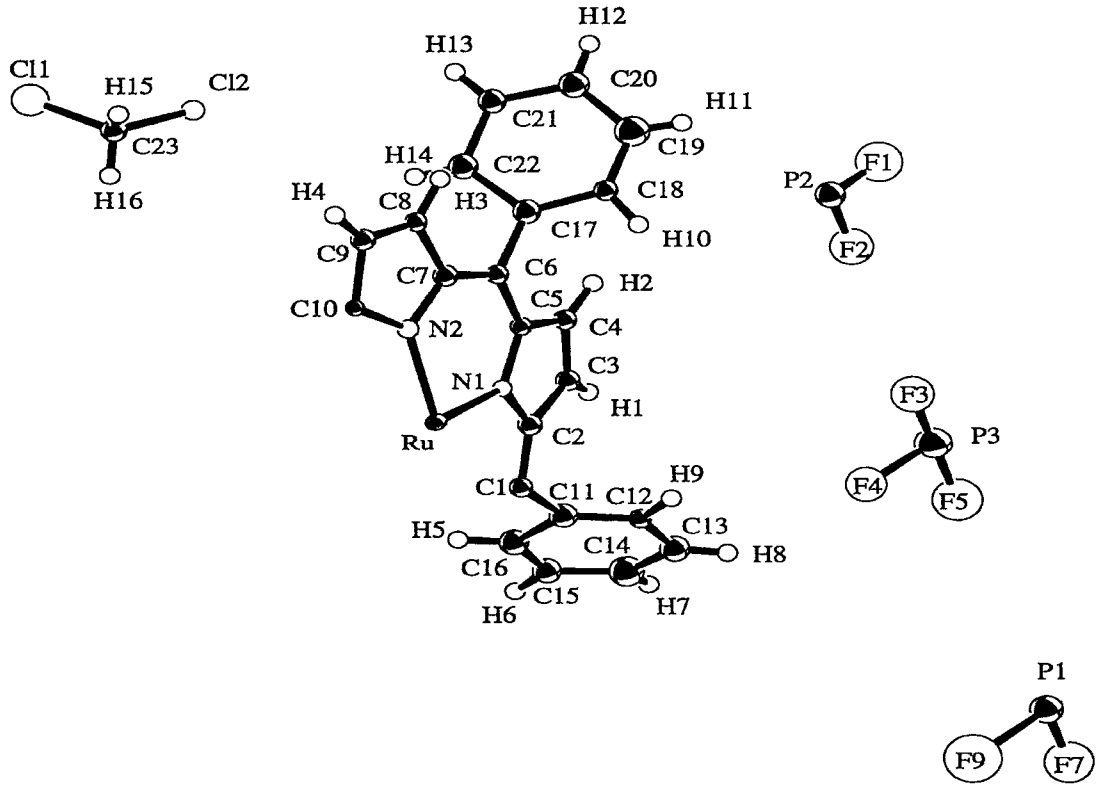

Figure S1. ORTEP drawing of the asymmetric unit (1/4 of the molecule). One Ru atom, 2 phenyl rings, 2 pyrrole rings, 3 P atoms, and 7 F atoms were found in the Fourier Map. A solvate dichloromethane molecule was also found. The three P atoms give the three locations over which the single PF_6^- counter-anion is positionally disordered. The partial occupancies are 0.09, 0.11, and 0.05 (summing to 0.25). In an analogous fashion, the 7 F atoms seen above are symmetry expanded to 22 positions over which the 6 F atoms in the PF_6^- counter-anion are positionally disordered (see Figure S2).

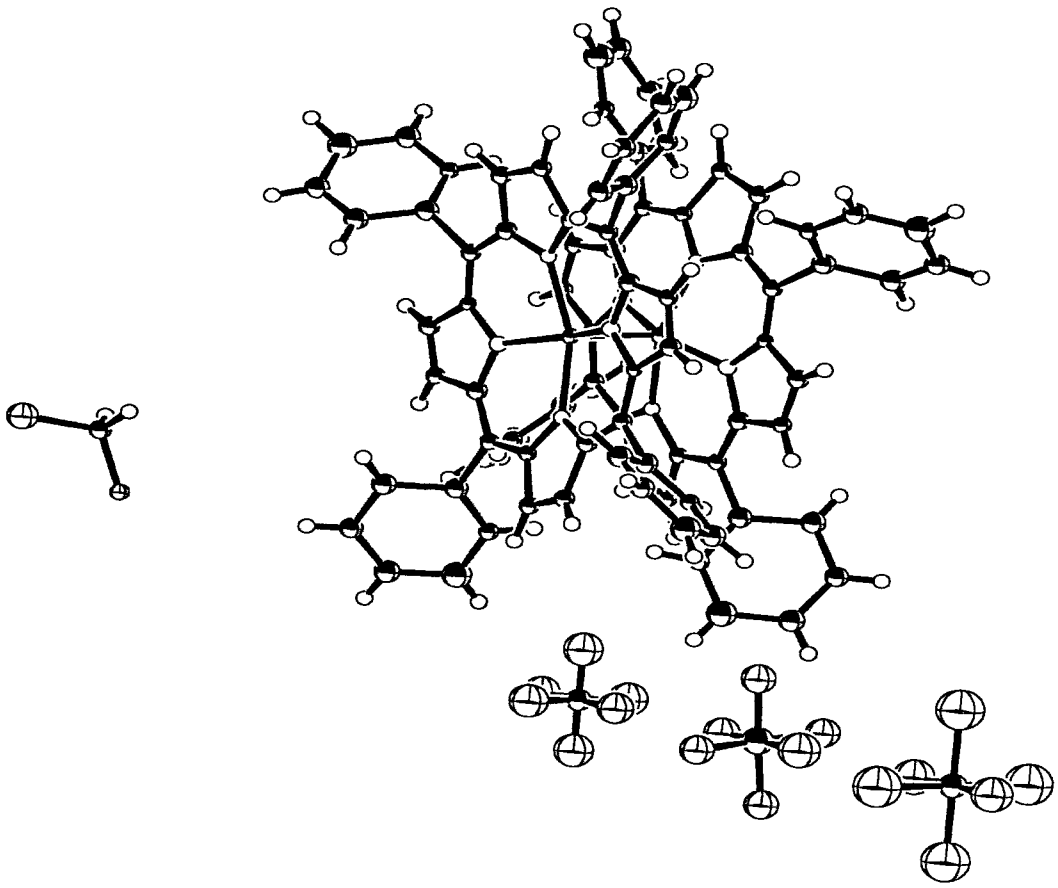

Figure S2. ORTEP drawing of the $[Ru(TPP)]^+$ unit and three PF_6^- molecules obtained by symmetry expansion of the asymmetric unit. Occupancies of the three P atoms are 0.36, 0.44, and 0.20. The 6 F atoms of $[Ru(TPP)]_2PF_6$ are positionally disordered between 22 positions, as shown.