Electronic Supplementary Information for Dalton Transactions

List of Supplementary Information

Synthesis of Pd complexes directly linked to the light-absorbing $[(bpy)_3Ru]^{2+}$ unit and their photochemical reactions toward styrenes.

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Experimental procedures for X-ray crystallography (***Ru^{Me}-PB***).

Data Collection

An red platelet crystal of $C_{54}H_{53}N_9F_{12}RuO_2P_2$ having approximate dimensions of 0.20 x 0.20 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS IV imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 360 seconds. The crystal-to-detector distance was 110.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	= 13.285(10) Å	α	= 109.13(2)°
b	= 14.900(10) Å	β	= 104.13(3)°
c	= 16.506(9) Å	γ	= 106.40(3)°
V	= 2749.4(31) Å^3		

For Z = 2 and F.W. = 1244.08, the calculated density is 1.503 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -60 ± 1°C to a maximum 2θ value of 54.9°. A total of 36 oscillation images were collected. A sweep of data was done using ω oscillations from 0.0 to 180.0° in 5.0° steps. The exposure rate was 900.0 [sec./°]. The crystal-to-detector distance was 110.00 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 18534 reflections that were collected, 10855 were unique (R_{int} = 0.095).

The linear absorption coefficient, μ, for Mo-Kα radiation is 4.348 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The

final cycle of full-matrix least-squares refinement[3] on F^2 was based on 10855 observed reflections and 678 variable parameters and converged with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0761$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.2112$$

The standard deviation of an observation of unit weight[4] was 0.924. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.727 and -0.716 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) SHELX97: Sheldrick, G.M. (1997).

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

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

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

(7) 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).

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

(9) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical

Crystallography Laboratory, Oxford, UK. (1996)
(11) SHELX97: Sheldrick, G.M. (1997).

Experimental procedures for X-ray crystallography (***Ru^{H}-PB -Pd^{C3}***).

Data Collection

An orange prism crystal of $C_{53}H_{47}N_{12}F_{18}P_3PdRu$ having approximate dimensions of 0.30 x 0.10 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS IV imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 360 seconds. The crystal-to-detector distance was 110.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a C-centered monoclinic cell with dimensions:

a = 32.970(9) Å
b = 21.782(7) Å β = 114.948(12)°
c = 18.688(3) Å
V = 12168.7(56) Å^3

For Z = 8 and F.W. = 1378.23, the calculated density is 1.504 g/cm^3. Based on the systematic absences of:

hkl: h+k ± 2n
h0l: l ± 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

C2/c (#15)

The data were collected at a temperature of -60 ± 1°C to a maximum 2θ value of 55.0°. A total of 45 oscillation images were collected. A sweep of data was done using ω oscillations from 0.0 to 180.0° in 4.0° steps. The exposure rate was 720.0 [sec./°]. The crystal-to-detector distance was 110.00 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 43273 reflections that were collected, 13470 were unique (R_{int} = 0.1725).

The linear absorption coefficient, μ, for Mo-Kα radiation is 7.25 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 13470 observed reflections and 739 variable parameters and converged with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0788$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2181$$

The standard deviation of an observation of unit weight[4] was 0.94. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.773 and -0.709 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) SHELX97: Sheldrick, G.M. (1997).

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

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

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

(7) 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).
(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
(9) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.
(10) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)
(11) SHELX97: Sheldrick, G.M. (1997).

Table 1. Crystallographic Data for ***Ru^{Me}-PB*** and ***Ru^{H}-PB -Pd^{C3}***.

	Ru^{Me}-PB	***Ru^{H}-PB -Pd^{C3}***
formula	$C_{54}H_{53}N_9F_{12}RuO_2P_2$	$C_{53}H_{47}F_{18}N_{12}P_3PdRu$
formula weight	1251.06	1494.41
crystal system	triclinic	monoclinic
space group	*P*-1(#2)	*C*2/*c* (#15)
a/Å	13.285(10)	32.970(9)
b/Å	14.900(10)	21.782(7)
c/Å	16.507(9)	18.688(3)
α/deg	109.13(2)	90
β/deg	104.13(3)	114.948(12)
γ/deg	106.40(3)	90
V/Å^3	2749(3)	12169(6)
Z	2	8
d_{calc}/g·cm^{-3}	1.511	1.631
temp	-60	-60
radiation	MoKα (λ = 0.71069 Å)	MoKα (λ = 0.71069 Å)
μ/cm^{-1}	4.35	7.25
diffractometer	Rigaku RAXIS IV	Rigaku RAXIS IV
max 2θ/deg	55.0	55.0
reflections collected	18534	43273
independent reflections	10855 [R(int) = 0.0949]	13470 [R(int) = 0.1725]
no. of parameters refined	678	739
R1 (I > 2σ)	0.0761	0.0788
wR_2 (All)	0.2112	0.2181
goodness of fit	0.924	0.940

Table S4. Bond lengths [Å] for *Ru^{Me}-PB*.

Ru(1)-N(4),2.056(5)	C(21)-C(22),1.401(11)
Ru(1)-N(3),2.062(5)	C(22)-C(23),1.359(10)
Ru(1)-N(2),2.064(6)	C(23)-C(24),1.415(10)
Ru(1)-N(1),2.078(5)	C(24)-C(32),1.407(10)
Ru(1)-N(6),2.083(6)	C(24)-C(25),1.420(9)
Ru(1)-N(5),2.088(6)	C(25)-C(26),1.390(10)
N(1)-C(1),1.339(9)	C(26)-C(27),1.442(11)
N(1)-C(5),1.363(9)	C(26)-C(35),1.504(10)
N(2)-C(10),1.362(8)	C(27)-C(31),1.422(9)
N(2)-C(6),1.387(8)	C(27)-C(28),1.431(10)
N(3)-C(15),1.353(8)	C(28)-C(29),1.368(11)
N(3)-C(11),1.367(7)	C(29)-C(30),1.414(9)
N(4)-C(16),1.353(7)	C(31)-C(32),1.432(9)
N(4)-C(20),1.358(7)	C(33)-C(34),1.355(11)
N(5)-C(21),1.348(8)	C(34)-C(35),1.373(10)
N(5)-C(32),1.375(8)	C(35)-C(36),1.430(11)
N(6)-C(30),1.336(8)	C(36)-C(37),1.393(10)
N(6)-C(31),1.379(9)	C(37)-C(38),1.459(12)
N(7)-C(33),1.341(12)	C(38)-C(39),1.387(11)
N(7)-C(37),1.344(11)	C(39)-C(40),1.370(14)
N(8)-C(38),1.310(12)	C(40)-C(41),1.372(15)
N(8)-C(42),1.331(14)	C(41)-C(42),1.372(15)
C(1)-C(2),1.399(9)	P(1)-F(103),1.49(2)
C(2)-C(3),1.402(11)	P(1)-F(5),1.547(11)
C(3)-C(4),1.384(10)	P(1)-F(105),1.568(18)
C(3)-C(43),1.503(10)	P(1)-F(6),1.569(11)
C(4)-C(5),1.418(9)	P(1)-F(106),1.582(19)
C(5)-C(6),1.479(9)	P(1)-F(1),1.586(7)
C(6)-C(7),1.377(10)	P(1)-F(2),1.595(7)
C(7)-C(8),1.396(10)	P(1)-F(4),1.596(10)
C(8)-C(9),1.400(10)	P(1)-F(3),1.620(10)
C(8)-C(44),1.509(11)	P(1)-F(104),1.662(16)
C(9)-C(10),1.386(10)	P(2)-F(22),1.50(3)
C(11)-C(12),1.345(9)	P(2)-F(24),1.510(19)
C(12)-C(13),1.417(11)	P(2)-F(17),1.54(2)
C(13)-C(14),1.390(9)	P(2)-F(11),1.545(18)
C(13)-C(45),1.488(10)	P(2)-F(15),1.56(3)
C(14)-C(15),1.402(8)	P(2)-F(16),1.585(17)
C(15)-C(16),1.479(8)	P(2)-F(14),1.591(17)
C(16)-C(17),1.404(9)	P(2)-F(19),1.61(2)
C(17)-C(18),1.390(9)	P(2)-F(20),1.618(18)
C(18)-C(19),1.405(9)	P(2)-F(9),1.623(19)
C(18)-C(46),1.516(9)	P(2)-F(18),1.63(2)
C(19)-C(20),1.366(8)	P(2)-F(13),1.63(3)

F(7)-F(14),0.70(2)
F(7)-F(15),0.80(3)
F(7)-F(23),1.59(3)
F(8)-F(16),0.54(2)
F(8)-F(22),1.13(3)
F(8)-F(13),1.60(4)
F(9)-F(22),1.19(3)
F(9)-F(10),1.58(4)
F(9)-F(15),1.63(4)
F(10)-F(18),0.76(3)
F(10)-F(19),1.16(3)
F(10)-F(24),1.29(4)
F(11)-F(20),0.76(2)
F(11)-F(21),1.09(2)
F(11)-F(17),1.69(3)
F(12)-F(17),0.71(3)
F(12)-F(22),1.39(3)
F(12)-F(15),1.58(3)
F(12)-F(20),1.74(2)
F(13)-F(16),1.09(3)
F(13)-F(24),1.17(3)
F(13)-F(21),1.51(4)
F(14)-F(23),0.92(2)
F(14)-F(15),1.42(3)
F(15)-F(19),1.61(3)
F(15)-F(17),1.74(3)
F(16)-F(22),1.56(3)
F(17)-F(20),1.05(2)
F(17)-F(22),1.73(4)
F(18)-F(24),0.70(3)
F(18)-F(23),1.64(3)
F(18)-F(19),1.77(3)
F(19)-F(22),1.60(3)
F(21)-F(23),1.29(3)
F(21)-F(24),1.63(3)
F(23)-F(24),1.67(3)
O(01)-C(48),1.33(2)
C(47)-C(48),1.63(2)
C(48)-C(49),1.38(2)
C(101)-C(103),1.73(4)
C(102)-C(103),1.58(4)
C(103)-O(02),1.73(5)
C(201)-C(202),1.39(5)
C(201)-N(201),1.52(3)
C(201)-C(201)#1,1.59(5)

Table S5. Bond angles [deg] for ***Ru^{Me}-PB***.

N(4)-Ru(1)-N(3),78.4(2)
N(4)-Ru(1)-N(2),94.5(2)
N(3)-Ru(1)-N(2),90.1(2)
N(4)-Ru(1)-N(1),171.9(2)
N(3)-Ru(1)-N(1),96.9(2)
N(2)-Ru(1)-N(1),78.9(2)
N(4)-Ru(1)-N(6),96.08(19)
N(3)-Ru(1)-N(6),169.6(2)
N(2)-Ru(1)-N(6),99.2(2)
N(1)-Ru(1)-N(6),89.6(2)
N(4)-Ru(1)-N(5),91.3(2)
N(3)-Ru(1)-N(5),91.6(2)
N(2)-Ru(1)-N(5),174.2(2)
N(1)-Ru(1)-N(5),95.4(2)
N(6)-Ru(1)-N(5),79.6(2)
C(1)-N(1)-C(5),118.9(6)
C(1)-N(1)-Ru(1),126.4(5)
C(5)-N(1)-Ru(1),114.7(4)
C(10)-N(2)-C(6),117.0(6)
C(10)-N(2)-Ru(1),126.3(5)
C(6)-N(2)-Ru(1),116.5(4)
C(15)-N(3)-C(11),117.0(5)
C(15)-N(3)-Ru(1),116.2(4)
C(11)-N(3)-Ru(1),126.6(5)
C(16)-N(4)-C(20),117.0(5)
C(16)-N(4)-Ru(1),116.1(4)
C(20)-N(4)-Ru(1),126.9(4)
C(21)-N(5)-C(32),117.9(7)
C(21)-N(5)-Ru(1),128.8(5)
C(32)-N(5)-Ru(1),113.3(5)
C(30)-N(6)-C(31),118.6(6)
C(30)-N(6)-Ru(1),127.8(5)
C(31)-N(6)-Ru(1),113.7(4)
C(33)-N(7)-C(37),117.3(7)
C(38)-N(8)-C(42),117.1(9)
N(1)-C(1)-C(2),122.3(8)
C(1)-C(2)-C(3),119.7(7)
C(4)-C(3)-C(2),118.1(7)
C(4)-C(3)-C(43),120.1(8)
C(2)-C(3)-C(43),121.8(7)
C(3)-C(4)-C(5),119.7(7)
N(1)-C(5)-C(4),121.3(6)
N(1)-C(5)-C(6),116.9(6)
C(4)-C(5)-C(6),121.8(7)
C(7)-C(6)-N(2),122.3(6)
C(7)-C(6)-C(5),125.1(6)
N(2)-C(6)-C(5),112.6(6)
C(6)-C(7)-C(8),121.3(7)
C(7)-C(8)-C(9),115.6(7)
C(7)-C(8)-C(44),120.6(7)
C(9)-C(8)-C(44),123.7(8)
C(10)-C(9)-C(8),122.0(7)
N(2)-C(10)-C(9),121.7(7)
C(12)-C(11)-N(3),124.3(7)
C(11)-C(12)-C(13),120.2(6)
C(14)-C(13)-C(12),115.8(6)
C(14)-C(13)-C(45),121.6(8)
C(12)-C(13)-C(45),122.6(7)
C(13)-C(14)-C(15),121.5(6)
N(3)-C(15)-C(14),121.2(5)
N(3)-C(15)-C(16),114.2(5)
C(14)-C(15)-C(16),124.6(6)
N(4)-C(16)-C(17),122.0(5)
N(4)-C(16)-C(15),114.8(5)
C(17)-C(16)-C(15),123.1(5)
C(18)-C(17)-C(16),120.2(6)
C(17)-C(18)-C(19),117.1(6)
C(17)-C(18)-C(46),121.8(6)
C(19)-C(18)-C(46),121.1(6)
C(20)-C(19)-C(18),119.7(6)
N(4)-C(20)-C(19),123.9(6)
N(5)-C(21)-C(22),122.6(7)
C(23)-C(22)-C(21),119.4(7)
C(22)-C(23)-C(24),120.5(8)
C(32)-C(24)-C(23),117.1(6)
C(32)-C(24)-C(25),119.0(7)
C(23)-C(24)-C(25),124.0(7)
C(26)-C(25)-C(24),122.3(8)
C(25)-C(26)-C(27),119.0(7)
C(25)-C(26)-C(35),120.6(8)
C(27)-C(26)-C(35),120.4(7)
C(31)-C(27)-C(28),115.6(7)
C(31)-C(27)-C(26),119.5(6)
C(28)-C(27)-C(26),124.9(7)
C(29)-C(28)-C(27),119.9(7)
C(28)-C(29)-C(30),121.0(7)
N(6)-C(30)-C(29),121.2(8)
N(6)-C(31)-C(27),123.8(6)

N(6)-C(31)-C(32),116.4(6)
C(27)-C(31)-C(32),119.9(7)
N(5)-C(32)-C(24),122.6(6)
N(5)-C(32)-C(31),117.1(7)
C(24)-C(32)-C(31),120.2(6)
N(7)-C(33)-C(34),124.4(9)
C(33)-C(34)-C(35),120.3(9)
C(34)-C(35)-C(36),116.7(7)
C(34)-C(35)-C(26),123.2(8)
C(36)-C(35)-C(26),120.1(7)
C(37)-C(36)-C(35),119.1(8)
N(7)-C(37)-C(36),122.2(8)
N(7)-C(37)-C(38),116.1(7)
C(36)-C(37)-C(38),121.8(8)
N(8)-C(38)-C(39),121.0(9)
N(8)-C(38)-C(37),116.1(8)
C(39)-C(38)-C(37),122.9(9)
C(40)-C(39)-C(38),121.1(10)
C(39)-C(40)-C(41),118.3(10)
C(42)-C(41)-C(40),116.2(12)
N(8)-C(42)-C(41),126.2(13)
F(103)-P(1)-F(5),123.0(11)
F(103)-P(1)-F(105),171.1(12)
F(5)-P(1)-F(105),54.6(7)
F(103)-P(1)-F(6),129.6(12)
F(5)-P(1)-F(6),97.4(7)
F(105)-P(1)-F(6),47.3(7)
F(103)-P(1)-F(106),89.4(13)
F(5)-P(1)-F(106),144.7(9)
F(105)-P(1)-F(106),91.2(10)
F(6)-P(1)-F(106),47.5(7)
F(103)-P(1)-F(1),109.1(10)
F(5)-P(1)-F(1),93.9(5)
F(105)-P(1)-F(1),79.9(7)
F(6)-P(1)-F(1),95.5(5)
F(106)-P(1)-F(1),87.2(7)
F(103)-P(1)-F(2),72.8(10)
F(5)-P(1)-F(2),85.2(5)
F(105)-P(1)-F(2),98.3(7)
F(6)-P(1)-F(2),83.1(5)
F(106)-P(1)-F(2),92.6(7)
F(1)-P(1)-F(2),178.2(4)
F(103)-P(1)-F(4),41.1(10)
F(5)-P(1)-F(4),91.6(6)
F(105)-P(1)-F(4),142.3(9)
F(6)-P(1)-F(4),170.4(6)
F(106)-P(1)-F(4),123.7(9)
F(1)-P(1)-F(4),87.4(5)
F(2)-P(1)-F(4),94.3(5)
F(103)-P(1)-F(3),52.9(10)
F(5)-P(1)-F(3),175.8(6)
F(105)-P(1)-F(3),129.5(8)
F(6)-P(1)-F(3),86.1(5)
F(106)-P(1)-F(3),39.0(7)
F(1)-P(1)-F(3),88.0(4)
F(2)-P(1)-F(3),93.0(4)
F(4)-P(1)-F(3),84.8(5)
F(103)-P(1)-F(104),94.5(12)
F(5)-P(1)-F(104),31.0(5)
F(105)-P(1)-F(104),84.7(9)
F(6)-P(1)-F(104),128.2(8)
F(106)-P(1)-F(104),175.7(10)
F(1)-P(1)-F(104),93.0(6)
F(2)-P(1)-F(104),87.1(6)
F(4)-P(1)-F(104),60.6(7)
F(3)-P(1)-F(104),145.3(7)
F(22)-P(2)-F(24),116.6(14)
F(22)-P(2)-F(17),69.4(13)
F(24)-P(2)-F(17),163.0(15)
F(22)-P(2)-F(11),118.9(14)
F(24)-P(2)-F(11),97.9(13)
F(17)-P(2)-F(11),66.3(12)
F(22)-P(2)-F(15),85.3(18)
F(24)-P(2)-F(15),126.6(15)
F(17)-P(2)-F(15),68.2(13)
F(11)-P(2)-F(15),113.4(14)
F(22)-P(2)-F(16),60.6(12)
F(24)-P(2)-F(16),74.8(11)
F(17)-P(2)-F(16),96.6(11)
F(11)-P(2)-F(16),85.1(9)
F(15)-P(2)-F(16),145.9(15)
F(22)-P(2)-F(14),138.8(16)
F(24)-P(2)-F(14),92.4(13)
F(17)-P(2)-F(14),91.7(11)
F(11)-P(2)-F(14),82.2(10)
F(15)-P(2)-F(14),53.5(12)
F(16)-P(2)-F(14),160.5(13)
F(22)-P(2)-F(19),61.7(13)
F(24)-P(2)-F(19),86.4(12)
F(17)-P(2)-F(19),109.8(14)
F(11)-P(2)-F(19),174.3(11)
F(15)-P(2)-F(19),60.9(13)

F(16)-P(2)-F(19),99.7(10)
F(14)-P(2)-F(19),94.0(11)
F(22)-P(2)-F(20),97.9(13)
F(24)-P(2)-F(20),125.2(13)
F(17)-P(2)-F(20),38.6(9)
F(11)-P(2)-F(20),27.7(8)
F(15)-P(2)-F(20),95.6(13)
F(16)-P(2)-F(20),88.8(9)
F(14)-P(2)-F(20),86.7(9)
F(19)-P(2)-F(20),148.4(12)
F(22)-P(2)-F(9),44.7(11)
F(24)-P(2)-F(9),99.4(11)
F(17)-P(2)-F(9),95.5(14)
F(11)-P(2)-F(9),160.8(12)
F(15)-P(2)-F(9),61.4(14)
F(16)-P(2)-F(9),91.5(10)
F(14)-P(2)-F(9),105.2(12)
F(19)-P(2)-F(9),17.7(10)
F(20)-P(2)-F(9),133.6(11)
F(22)-P(2)-F(18),114.5(14)
F(24)-P(2)-F(18),25.3(9)
F(17)-P(2)-F(18),169.4(12)
F(11)-P(2)-F(18),116.8(14)
F(15)-P(2)-F(18),101.9(14)
F(16)-P(2)-F(18),93.8(10)
F(14)-P(2)-F(18),79.1(11)
F(19)-P(2)-F(18),66.3(12)
F(20)-P(2)-F(18),144.1(14)
F(9)-P(2)-F(18),82.2(12)
F(22)-P(2)-F(13),98.9(17)
F(24)-P(2)-F(13),43.5(12)
F(17)-P(2)-F(13),121.6(17)
F(11)-P(2)-F(13),72.5(15)
F(15)-P(2)-F(13),170.1(18)
F(16)-P(2)-F(13),39.5(12)
F(14)-P(2)-F(13),121.9(18)
F(19)-P(2)-F(13),113.2(15)
F(20)-P(2)-F(13),92.7(15)
F(9)-P(2)-F(13),115.8(15)
F(18)-P(2)-F(13),68.2(14)
F(14)-F(7)-F(15),141(4)
F(14)-F(7)-F(23),14(2)
F(15)-F(7)-F(23),128(3)
F(14)-F(7)-P(2),73(2)
F(15)-F(7)-P(2),69(3)
F(23)-F(7)-P(2),60.6(10)
F(16)-F(8)-F(22),134(4)
F(16)-F(8)-F(13),14(3)
F(22)-F(8)-F(13),120(2)
F(16)-F(8)-P(2),73(3)
F(22)-F(8)-P(2),61.5(15)
F(13)-F(8)-P(2),60.0(13)
F(22)-F(9)-F(10),113(2)
F(22)-F(9)-P(2),62.1(16)
F(10)-F(9)-P(2),64.9(13)
F(22)-F(9)-F(15),93(2)
F(10)-F(9)-F(15),90.4(18)
P(2)-F(9)-F(15),57.4(12)
F(18)-F(10)-F(19),134(5)
F(18)-F(10)-F(24),26(2)
F(19)-F(10)-F(24),121(3)
F(18)-F(10)-F(9),129(4)
F(19)-F(10)-F(9),11.4(16)
F(24)-F(10)-F(9),112(2)
F(18)-F(10)-P(2),71(3)
F(19)-F(10)-P(2),64.7(18)
F(24)-F(10)-P(2),58.1(14)
F(9)-F(10)-P(2),58.8(12)
F(20)-F(11)-F(21),157(4)
F(20)-F(11)-P(2),81(2)
F(21)-F(11)-P(2),77.6(18)
F(20)-F(11)-F(17),25(2)
F(21)-F(11)-F(17),133(2)
P(2)-F(11)-F(17),56.8(10)
F(17)-F(12)-F(22),107(3)
F(17)-F(12)-F(15),91(3)
F(22)-F(12)-F(15),88.5(18)
F(17)-F(12)-P(2),64(2)
F(22)-F(12)-P(2),56.5(12)
F(15)-F(12)-P(2),56.3(11)
F(17)-F(12)-F(20),10(2)
F(22)-F(12)-F(20),97.1(15)
F(15)-F(12)-F(20),90.4(14)
P(2)-F(12)-F(20),55.9(7)
F(16)-F(13)-F(24),113(3)
F(16)-F(13)-F(21),121(3)
F(24)-F(13)-F(21),74(3)
F(16)-F(13)-F(8),7.1(15)
F(24)-F(13)-F(8),106(3)
F(21)-F(13)-F(8),118(2)
F(16)-F(13)-P(2),68(2)
F(24)-F(13)-P(2),62.7(18)

F(21)-F(13)-P(2),64.9(16)
F(8)-F(13)-P(2),61.7(12)
F(7)-F(14)-F(23),156(4)
F(7)-F(14)-F(15),21(2)
F(23)-F(14)-F(15),136(3)
F(7)-F(14)-P(2),83(2)
F(23)-F(14)-P(2),76(2)
F(15)-F(14)-P(2),62.1(13)
F(7)-F(15)-F(14),18(2)
F(7)-F(15)-P(2),82(3)
F(14)-F(15)-P(2),64.4(13)
F(7)-F(15)-F(12),123(3)
F(14)-F(15)-F(12),114(2)
P(2)-F(15)-F(12),66.3(13)
F(7)-F(15)-F(19),114(3)
F(14)-F(15)-F(19),101.2(19)
P(2)-F(15)-F(19),61.1(13)
F(12)-F(15)-F(19),91(2)
F(7)-F(15)-F(9),129(3)
F(14)-F(15)-F(9),114(2)
P(2)-F(15)-F(9),61.2(13)
F(12)-F(15)-F(9),74.8(18)
F(19)-F(15)-F(9),17.7(10)
F(7)-F(15)-F(17),99(3)
F(14)-F(15)-F(17),90.2(18)
P(2)-F(15)-F(17),55.4(12)
F(12)-F(15)-F(17),23.9(10)
F(19)-F(15)-F(17),100.8(19)
F(9)-F(15)-F(17),88.2(19)
F(8)-F(16)-F(13),159(5)
F(8)-F(16)-F(22),32(3)
F(13)-F(16)-F(22),127(3)
F(8)-F(16)-P(2),88(3)
F(13)-F(16)-P(2),73(2)
F(22)-F(16)-P(2),56.9(11)
F(12)-F(17)-F(20),163(4)
F(12)-F(17)-P(2),92(3)
F(20)-F(17)-P(2),74.5(17)
F(12)-F(17)-F(11),148(3)
F(20)-F(17)-F(11),17.7(14)
P(2)-F(17)-F(11),56.9(10)
F(12)-F(17)-F(22),50(2)
F(20)-F(17)-F(22),113(2)
P(2)-F(17)-F(22),54.0(11)
F(11)-F(17)-F(22),100.0(16)
F(12)-F(17)-F(15),65(2)
F(20)-F(17)-F(15),113(2)
P(2)-F(17)-F(15),56.3(12)
F(11)-F(17)-F(15),98.3(16)
F(22)-F(17)-F(15),73.3(18)
F(24)-F(18)-F(10),125(5)
F(24)-F(18)-P(2),68(3)
F(10)-F(18)-P(2),83(3)
F(24)-F(18)-F(23),80(3)
F(10)-F(18)-F(23),124(4)
P(2)-F(18)-F(23),59.9(11)
F(24)-F(18)-F(19),112(3)
F(10)-F(18)-F(19),28(3)
P(2)-F(18)-F(19),56.3(10)
F(23)-F(18)-F(19),99.9(16)
F(10)-F(19)-F(22),114(2)
F(10)-F(19)-F(15),109(3)
F(22)-F(19)-F(15),80.6(18)
F(10)-F(19)-P(2),75(2)
F(22)-F(19)-P(2),55.7(12)
F(15)-F(19)-P(2),58.0(12)
F(10)-F(19)-F(18),17.9(19)
F(22)-F(19)-F(18),102.7(16)
F(15)-F(19)-F(18),94.2(16)
P(2)-F(19)-F(18),57.4(10)
F(11)-F(20)-F(17),138(3)
F(11)-F(20)-P(2),71(2)
F(17)-F(20)-P(2),66.9(16)
F(11)-F(20)-F(12),132(3)
F(17)-F(20)-F(12),6.8(16)
P(2)-F(20)-F(12),61.5(8)
F(11)-F(21)-F(23),102(2)
F(11)-F(21)-F(13),91(2)
F(23)-F(21)-F(13),109(3)
F(11)-F(21)-F(24),114(2)
F(23)-F(21)-F(24),68.7(19)
F(13)-F(21)-F(24),43.5(15)
F(11)-F(21)-P(2),63.2(15)
F(23)-F(21)-P(2),64.9(15)
F(13)-F(21)-P(2),61.0(15)
F(24)-F(21)-P(2),54.1(10)
F(8)-F(22)-F(9),123(3)
F(8)-F(22)-F(12),118(3)
F(9)-F(22)-F(12),98(2)
F(8)-F(22)-P(2),76.8(17)
F(9)-F(22)-P(2),73.2(17)
F(12)-F(22)-P(2),72.9(14)

F(8)-F(22)-F(16),14.6(12)
F(9)-F(22)-F(16),113(2)
F(12)-F(22)-F(16),113(2)
P(2)-F(22)-F(16),62.5(11)
F(8)-F(22)-F(19),113(2)
F(9)-F(22)-F(19),12.0(14)
F(12)-F(22)-F(19),99(2)
P(2)-F(22)-F(19),62.6(11)
F(16)-F(22)-F(19),101.5(16)
F(8)-F(22)-F(17),97(2)
F(9)-F(22)-F(17),105(2)
F(12)-F(22)-F(17),22.9(11)
P(2)-F(22)-F(17),56.6(12)
F(16)-F(22)-F(17),90.3(17)
F(19)-F(22)-F(17),101.6(18)
F(14)-F(23)-F(21),124(3)
F(14)-F(23)-F(7),10.5(17)
F(21)-F(23)-F(7),121(2)
F(14)-F(23)-P(2),70.9(18)
F(21)-F(23)-P(2),69.6(16)
F(7)-F(23)-P(2),61.8(10)
F(14)-F(23)-F(18),103(3)
F(21)-F(23)-F(18),90(2)
F(7)-F(23)-F(18),92.9(17)
P(2)-F(23)-F(18),59.7(11)
F(14)-F(23)-F(24),117(3)
F(21)-F(23)-F(24),65.4(19)
F(7)-F(23)-F(24),106.3(16)
P(2)-F(23)-F(24),54.4(10)
F(18)-F(23)-F(24),24.3(10)
F(18)-F(24)-F(13),156(4)
F(18)-F(24)-F(10),29(3)
F(13)-F(24)-F(10),129(3)
F(18)-F(24)-P(2),87(3)
F(13)-F(24)-P(2),74(2)
F(10)-F(24)-P(2),75.2(16)
F(18)-F(24)-F(21),122(4)
F(13)-F(24)-F(21),63(2)
F(10)-F(24)-F(21),133(2)
P(2)-F(24)-F(21),65.1(12)
F(18)-F(24)-F(23),76(3)
F(13)-F(24)-F(23),106(2)
F(10)-F(24)-F(23),93(2)
P(2)-F(24)-F(23),61.6(11)
F(21)-F(24)-F(23),45.9(11)
O(01)-C(48)-C(49),128(2)
O(01)-C(48)-C(47),102.7(17)
C(49)-C(48)-C(47),128.5(18)
C(102)-C(103)-C(101),89(3)
C(102)-C(103)-O(02),95(3)
C(101)-C(103)-O(02),142(4)
C(202)-C(201)-N(201),119(3)
C(202)-C(201)-C(201)#1,157(4)
N(201)-C(201)-C(201)#1,83(3)

Symmetry transformations used to generate equivalent atoms:

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

Table S6. Bond lengths [Å] for ***Ru^{H}-PB -Pd^{C3}***.

Table 3. Bond lengths [Agst] and angles [deg] for 1.

PPd(2)-N(8),2.081(7)	C(15)-C(16),1.440(12)
Pd(2)-N(7),2.083(7)	C(16)-C(17),1.377(12)
Pd(2)-C(43),2.102(11)	C(17)-C(18),1.399(13)
Pd(2)-C(44),2.118(10)	C(18)-C(19),1.350(13)
Pd(2)-C(45),2.137(10)	C(19)-C(20),1.378(12)
Ru(1)-N(1),2.031(8)	C(21)-C(22),1.393(12)
Ru(1)-N(4),2.044(7)	C(22)-C(23),1.367(11)
Ru(1)-N(2),2.047(8)	C(23)-C(24),1.406(11)
Ru(1)-N(5),2.052(7)	C(24)-C(31),1.405(12)
Ru(1)-N(6),2.063(7)	C(24)-C(25),1.413(11)
Ru(1)-N(3),2.067(7)	C(25)-C(26),1.372(12)
N(1)-C(1),1.342(11)	C(26)-C(27),1.413(12)
N(1)-C(5),1.373(12)	C(26)-C(35),1.520(11)
N(2)-C(10),1.321(11)	C(27)-C(32),1.403(11)
N(2)-C(6),1.368(12)	C(27)-C(28),1.405(13)
N(3)-C(11),1.326(11)	C(28)-C(29),1.370(14)
N(3)-C(15),1.358(11)	C(29)-C(30),1.387(12)
N(4)-C(20),1.351(10)	C(31)-C(32),1.417(12)
N(4)-C(16),1.390(11)	C(33)-C(34),1.378(12)
N(5)-C(21),1.327(10)	C(34)-C(35),1.361(11)
N(5)-C(31),1.385(9)	C(35)-C(36),1.375(11)
N(6)-C(30),1.351(11)	C(36)-C(37),1.362(11)
N(6)-C(32),1.373(11)	C(37)-C(38),1.493(11)
N(7)-C(37),1.344(10)	C(38)-C(39),1.385(12)
N(7)-C(33),1.345(10)	C(39)-C(40),1.374(12)
N(8)-C(38),1.328(10)	C(40)-C(41),1.344(14)
N(8)-C(42),1.358(12)	C(41)-C(42),1.347(14)
C(1)-C(2),1.378(14)	C(43)-C(44),1.438(15)
C(2)-C(3),1.378(14)	C(44)-C(45),1.406(17)
C(3)-C(4),1.339(14)	P(1)-F(112),1.49(2)
C(4)-C(5),1.449(15)	P(1)-F(101),1.49(3)
C(5)-C(6),1.432(14)	P(1)-F(4),1.53(3)
C(6)-C(7),1.404(14)	P(1)-F(3),1.56(2)
C(7)-C(8),1.370(17)	P(1)-F(1),1.57(3)
C(8)-C(9),1.349(17)	P(1)-F(5),1.57(3)
C(9)-C(10),1.380(14)	P(1)-F(115),1.58(3)
C(11)-C(12),1.408(14)	P(1)-F(106),1.587(19)
C(12)-C(13),1.360(14)	P(1)-F(114),1.60(3)
C(13)-C(14),1.370(13)	P(1)-F(105),1.61(2)
C(14)-C(15),1.400(13)	P(1)-F(104),1.63(2)

P(1)-F(111),1.64(3)
F(1)-F(113),0.71(4)
F(2)-F(112),0.59(4)
F(3)-F(115),0.65(3)
F(3)-F(103),0.75(3)
F(3)-F(101),1.58(4)
F(4)-F(116),0.60(4)
F(4)-F(104),0.68(3)
F(4)-F(105),1.64(4)
F(4)-F(111),1.72(4)
F(5)-F(102),0.58(4)
F(5)-F(105),0.90(3)
F(5)-F(103),1.47(3)
F(6)-F(106),0.55(3)
F(6)-F(101),1.18(3)
F(101)-F(106),0.73(3)
F(101)-F(115),1.43(4)
F(101)-F(112),1.70(4)
F(103)-F(115),1.36(4)
F(104)-F(116),0.52(4)
F(111)-F(113),1.06(4)
F(112)-F(114),0.63(3)
F(113)-F(115),1.48(3)
P(2)-F(9),1.523(19)
P(2)-F(206),1.55(2)
P(2)-F(202),1.563(15)
P(2)-F(12),1.58(2)
P(2)-F(7),1.596(15)
P(2)-F(10),1.597(17)
P(2)-F(201),1.598(17)
P(2)-F(8),1.606(19)
P(2)-F(11),1.614(15)
P(2)-F(205),1.653(16)
P(2)-F(203),1.69(2)
P(2)-F(204),1.69(3)
F(7)-F(204),0.87(3)
F(7)-F(205),1.67(2)
F(8)-F(206),1.29(2)
F(8)-F(201),1.40(2)
F(9)-F(203),0.96(2)
F(9)-F(201),1.35(2)
F(10)-F(206),1.18(2)
F(11)-F(202),1.126(16)
F(11)-F(204),1.61(3)
F(12)-F(205),0.98(2)
F(12)-F(202),1.64(2)
F(12)-F(201),1.69(3)
P(3)-F(16),1.52(2)
P(3)-F(316),1.558(14)
P(3)-F(14),1.566(7)
P(3)-F(13),1.570(7)
P(3)-F(317),1.574(14)
P(3)-F(315),1.593(12)
P(3)-F(15),1.60(2)
P(3)-F(318),1.608(13)
P(3)-F(17),1.617(16)
P(3)-F(18),1.65(2)
C(46)-C(47),1.41(2)
C(47)-N(9),1.20(2)
C(49)-C(48A),1.15(5)
C(49)-C(48),1.70(3)
C(48)-N(10),1.33(2)
C(48)-C(48A),1.99(5)
N(10)-C(48)#1,1.33(2)
N(10A)-C(48A),1.25(5)
N(10A)-N(10A)#1,1.32(6)
C(50)-N(11),1.05(2)
C(50)-C(51),1.53(3)
C(52)-N(12),1.25(4)
C(52)-C(53),1.30(4)

Table S7. Bond angles [deg] for ***Ru^{H}-PB -Pd^{C3}***.

N(8)-Pd(2)-N(7),77.8(3)
N(8)-Pd(2)-C(43),171.8(5)
N(7)-Pd(2)-C(43),104.1(4)
N(8)-Pd(2)-C(44),140.2(4)
N(7)-Pd(2)-C(44),141.2(4)
C(43)-Pd(2)-C(44),39.8(4)
N(8)-Pd(2)-C(45),105.9(4)
N(7)-Pd(2)-C(45),167.5(5)
C(43)-Pd(2)-C(45),70.5(4)
C(44)-Pd(2)-C(45),38.6(5)
N(1)-Ru(1)-N(4),94.1(3)
N(1)-Ru(1)-N(2),79.5(3)
N(4)-Ru(1)-N(2),170.6(3)
N(1)-Ru(1)-N(5),175.0(3)
N(4)-Ru(1)-N(5),88.3(3)
N(2)-Ru(1)-N(5),98.6(3)
N(1)-Ru(1)-N(6),95.5(3)
N(4)-Ru(1)-N(6),97.6(3)
N(2)-Ru(1)-N(6),89.9(3)
N(5)-Ru(1)-N(6),79.8(3)
N(1)-Ru(1)-N(3),90.5(3)
N(4)-Ru(1)-N(3),79.0(3)
N(2)-Ru(1)-N(3),94.1(3)
N(5)-Ru(1)-N(3),94.3(3)
N(6)-Ru(1)-N(3),173.3(3)
C(1)-N(1)-C(5),117.7(9)
C(1)-N(1)-Ru(1),126.6(7)
C(5)-N(1)-Ru(1),115.8(7)
C(10)-N(2)-C(6),119.0(9)
C(10)-N(2)-Ru(1),127.1(7)
C(6)-N(2)-Ru(1),113.8(7)
C(11)-N(3)-C(15),119.6(9)
C(11)-N(3)-Ru(1),125.5(7)
C(15)-N(3)-Ru(1),114.9(6)
C(20)-N(4)-C(16),116.4(8)
C(20)-N(4)-Ru(1),128.2(6)
C(16)-N(4)-Ru(1),115.4(6)
C(21)-N(5)-C(31),117.2(8)
C(21)-N(5)-Ru(1),129.2(6)
C(31)-N(5)-Ru(1),113.7(6)
C(30)-N(6)-C(32),115.6(8)
C(30)-N(6)-Ru(1),130.3(6)
C(32)-N(6)-Ru(1),114.0(6)
C(37)-N(7)-C(33),117.2(8)
C(37)-N(7)-Pd(2),115.5(6)
C(33)-N(7)-Pd(2),126.6(6)
C(38)-N(8)-C(42),117.2(9)
C(38)-N(8)-Pd(2),116.3(6)
C(42)-N(8)-Pd(2),126.4(7)
N(1)-C(1)-C(2),123.3(10)
C(3)-C(2)-C(1),120.2(11)
C(4)-C(3)-C(2),118.5(12)
C(3)-C(4)-C(5),120.7(12)
N(1)-C(5)-C(6),114.0(10)
N(1)-C(5)-C(4),119.6(10)
C(6)-C(5)-C(4),126.5(11)
N(2)-C(6)-C(7),119.8(11)
N(2)-C(6)-C(5),116.9(9)
C(7)-C(6)-C(5),123.0(12)
C(8)-C(7)-C(6),118.7(13)
C(9)-C(8)-C(7),121.0(12)
C(8)-C(9)-C(10),118.3(11)
N(2)-C(10)-C(9),123.0(11)
N(3)-C(11)-C(12),122.2(10)
C(13)-C(12)-C(11),120.2(11)
C(12)-C(13)-C(14),116.2(12)
C(13)-C(14)-C(15),123.6(11)
N(3)-C(15)-C(14),118.1(9)
N(3)-C(15)-C(16),116.2(8)
C(14)-C(15)-C(16),125.6(10)
C(17)-C(16)-N(4),120.3(8)
C(17)-C(16)-C(15),125.2(9)
N(4)-C(16)-C(15),114.4(8)
C(16)-C(17)-C(18),122.1(9)
C(19)-C(18)-C(17),116.5(10)
C(18)-C(19)-C(20),121.0(10)
N(4)-C(20)-C(19),123.6(9)
N(5)-C(21)-C(22),123.6(8)
C(23)-C(22)-C(21),118.8(9)
C(22)-C(23)-C(24),120.9(9)
C(31)-C(24)-C(23),116.2(8)
C(31)-C(24)-C(25),119.6(8)
C(23)-C(24)-C(25),124.2(9)
C(26)-C(25)-C(24),120.2(9)
C(25)-C(26)-C(27),121.0(8)
C(25)-C(26)-C(35),118.3(9)
C(27)-C(26)-C(35),120.6(9)
C(32)-C(27)-C(28),118.0(10)

C(32)-C(27)-C(26),119.7(9)
C(28)-C(27)-C(26),122.3(9)
C(29)-C(28)-C(27),116.7(9)
C(28)-C(29)-C(30),122.8(10)
N(6)-C(30)-C(29),122.0(10)
N(5)-C(31)-C(24),123.3(8)
N(5)-C(31)-C(32),116.5(8)
C(24)-C(31)-C(32),120.2(8)
N(6)-C(32)-C(27),124.6(9)
N(6)-C(32)-C(31),116.1(8)
C(27)-C(32)-C(31),119.3(9)
N(7)-C(33)-C(34),123.4(9)
C(35)-C(34)-C(33),119.1(8)
C(34)-C(35)-C(36),117.3(8)
C(34)-C(35)-C(26),121.5(8)
C(36)-C(35)-C(26),121.2(8)
C(37)-C(36)-C(35),121.8(8)
N(7)-C(37)-C(36),121.1(8)
N(7)-C(37)-C(38),114.7(8)
C(36)-C(37)-C(38),124.2(8)
N(8)-C(38)-C(39),122.4(9)
N(8)-C(38)-C(37),114.9(8)
C(39)-C(38)-C(37),122.7(8)
C(40)-C(39)-C(38),119.0(10)
C(41)-C(40)-C(39),118.0(11)
C(40)-C(41)-C(42),121.4(11)
C(41)-C(42)-N(8),121.9(11)
C(44)-C(43)-Pd(2),70.7(7)
C(45)-C(44)-C(43),118.7(15)
C(45)-C(44)-Pd(2),71.4(6)
C(43)-C(44)-Pd(2),69.5(6)
C(44)-C(45)-Pd(2),70.0(6)
F(112)-P(1)-F(101),69.3(14)
F(112)-P(1)-F(4),108.4(16)
F(101)-P(1)-F(4),130(2)
F(112)-P(1)-F(3),80.1(14)
F(101)-P(1)-F(3),62.1(16)
F(4)-P(1)-F(3),166.7(15)
F(112)-P(1)-F(1),168.9(14)
F(101)-P(1)-F(1),99.6(16)
F(4)-P(1)-F(1),77.5(18)
F(3)-P(1)-F(1),96.0(17)
F(112)-P(1)-F(5),100.0(16)
F(101)-P(1)-F(5),134.5(17)
F(4)-P(1)-F(5),95.5(17)
F(3)-P(1)-F(5),72.6(14)
F(1)-P(1)-F(5),88.6(17)
F(112)-P(1)-F(115),98.1(14)
F(101)-P(1)-F(115),55.4(14)
F(4)-P(1)-F(115),153.0(17)
F(3)-P(1)-F(115),23.9(12)
F(1)-P(1)-F(115),75.5(16)
F(5)-P(1)-F(115),84.6(15)
F(112)-P(1)-F(106),75.1(13)
F(101)-P(1)-F(106),27.3(12)
F(4)-P(1)-F(106),102.7(17)
F(3)-P(1)-F(106),89.2(13)
F(1)-P(1)-F(106),94.6(13)
F(5)-P(1)-F(106),161.8(14)
F(115)-P(1)-F(106),78.9(12)
F(112)-P(1)-F(114),23.4(11)
F(101)-P(1)-F(114),88.6(18)
F(4)-P(1)-F(114),86.0(16)
F(3)-P(1)-F(114),100.8(14)
F(1)-P(1)-F(114),163.2(16)
F(5)-P(1)-F(114),96.0(16)
F(115)-P(1)-F(114),120.9(14)
F(106)-P(1)-F(114),86.0(14)
F(112)-P(1)-F(105),105.9(13)
F(101)-P(1)-F(105),166.8(16)
F(4)-P(1)-F(105),62.9(15)
F(3)-P(1)-F(105),105.3(13)
F(1)-P(1)-F(105),85.1(13)
F(5)-P(1)-F(105),32.7(12)
F(115)-P(1)-F(105),115.0(13)
F(106)-P(1)-F(105),165.4(12)
F(114)-P(1)-F(105),90.1(15)
F(112)-P(1)-F(104),96.2(15)
F(101)-P(1)-F(104),106.0(16)
F(4)-P(1)-F(104),24.6(13)
F(3)-P(1)-F(104),168.2(14)
F(1)-P(1)-F(104),85.6(18)
F(5)-P(1)-F(104),119.2(14)
F(115)-P(1)-F(104),149.5(15)
F(106)-P(1)-F(104),78.9(12)
F(114)-P(1)-F(104),78.0(13)
F(105)-P(1)-F(104),86.5(11)
F(112)-P(1)-F(111),165.4(15)
F(101)-P(1)-F(111),103.3(18)
F(4)-P(1)-F(111),66.0(16)
F(3)-P(1)-F(111),108.2(15)
F(1)-P(1)-F(111),12(2)

F(5)-P(1)-F(111),94.1(16)
F(115)-P(1)-F(111),87.1(15)
F(106)-P(1)-F(111),92.7(14)
F(114)-P(1)-F(111),150.9(14)
F(105)-P(1)-F(111),83.9(15)
F(104)-P(1)-F(111),73.2(15)
F(113)-F(1)-P(1),83(4)
F(112)-F(2)-P(1),57(3)
F(115)-F(3)-F(103),153(6)
F(115)-F(3)-P(1),80(4)
F(103)-F(3)-P(1),88(3)
F(115)-F(3)-F(101),65(4)
F(103)-F(3)-F(101),127(4)
P(1)-F(3)-F(101),56.8(14)
F(116)-F(4)-F(104),47(4)
F(116)-F(4)-P(1),93(4)
F(104)-F(4)-P(1),87(3)
F(116)-F(4)-F(105),113(7)
F(104)-F(4)-F(105),143(4)
P(1)-F(4)-F(105),61.1(14)
F(116)-F(4)-F(111),140(7)
F(104)-F(4)-F(111),99(6)
P(1)-F(4)-F(111),60.2(16)
F(105)-F(4)-F(111),80(2)
F(102)-F(5)-F(105),26(4)
F(102)-F(5)-F(103),133(6)
F(105)-F(5)-F(103),139(3)
F(102)-F(5)-P(1),89(5)
F(105)-F(5)-P(1),76(2)
F(103)-F(5)-P(1),68.2(17)
F(106)-F(6)-F(101),27(3)
F(106)-F(6)-P(1),74(4)
F(101)-F(6)-P(1),61.0(18)
F(106)-F(101)-F(6),20(3)
F(106)-F(101)-F(115),135(5)
F(6)-F(101)-F(115),116(3)
F(106)-F(101)-P(1),84(4)
F(6)-F(101)-P(1),75.4(19)
F(115)-F(101)-P(1),65.5(19)
F(106)-F(101)-F(3),144(5)
F(6)-F(101)-F(3),130(3)
F(115)-F(101)-F(3),24.4(15)
P(1)-F(101)-F(3),61.0(16)
F(106)-F(101)-F(112),93(4)
F(6)-F(101)-F(112),102(3)
F(115)-F(101)-F(112),96(2)
P(1)-F(101)-F(112),55.4(14)
F(3)-F(101)-F(112),74(2)
F(5)-F(102)-P(1),71(5)
F(3)-F(103)-F(115),13(3)
F(3)-F(103)-F(5),109(4)
F(115)-F(103)-F(5),97(2)
F(3)-F(103)-P(1),66(3)
F(115)-F(103)-P(1),60.9(14)
F(5)-F(103)-P(1),58.8(15)
F(116)-F(104)-F(4),58(4)
F(116)-F(104)-P(1),85(4)
F(4)-F(104)-P(1),69(3)
F(113)-F(111)-P(1),71.5(18)
F(113)-F(111)-F(4),119(3)
P(1)-F(111)-F(4),53.9(14)
F(2)-F(112)-F(114),42(3)
F(2)-F(112)-P(1),104(4)
F(114)-F(112)-P(1),87(3)
F(2)-F(112)-F(101),159(5)
F(114)-F(112)-F(101),130(5)
P(1)-F(112)-F(101),55.4(13)
F(1)-F(113)-F(111),4(4)
F(1)-F(113)-F(115),119(4)
F(111)-F(113)-F(115),121(2)
F(1)-F(113)-P(1),71(3)
F(111)-F(113)-P(1),70.8(19)
F(115)-F(113)-P(1),60.6(14)
F(112)-F(114)-P(1),69(4)
F(3)-F(115)-F(103),15(3)
F(3)-F(115)-F(101),90(4)
F(103)-F(115)-F(101),99(2)
F(3)-F(115)-F(113),119(5)
F(103)-F(115)-F(113),105(2)
F(101)-F(115)-F(113),106(2)
F(3)-F(115)-P(1),76(4)
F(103)-F(115)-P(1),70.4(15)
F(101)-F(115)-P(1),59.1(16)
F(113)-F(115)-P(1),64.8(14)
F(104)-F(116)-F(4),75(5)
F(104)-F(116)-P(1),77(4)
F(4)-F(116)-P(1),66(4)
F(5)-F(105)-P(1),71(2)
F(5)-F(105)-F(4),127(3)
P(1)-F(105)-F(4),56.0(14)
F(6)-F(106)-F(101),134(6)
F(6)-F(106)-P(1),87(4)

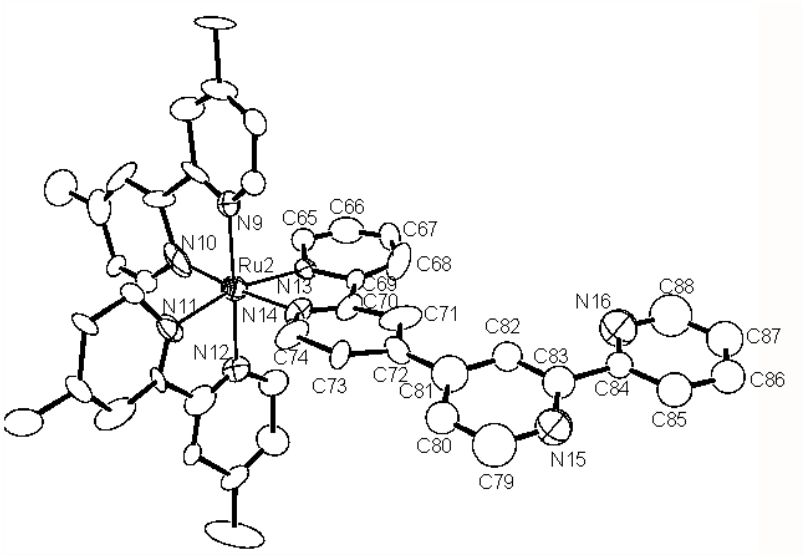
F(101)-F(106)-P(1),69(3)
F(9)-P(2)-F(206),98.5(11)
F(9)-P(2)-F(202),147.0(11)
F(206)-P(2)-F(202),89.9(10)
F(9)-P(2)-F(12),90.2(11)
F(206)-P(2)-F(12),136.8(13)
F(202)-P(2)-F(12),63.1(9)
F(9)-P(2)-F(7),96.0(10)
F(206)-P(2)-F(7),125.1(11)
F(202)-P(2)-F(7),105.0(8)
F(12)-P(2)-F(7),95.5(10)
F(9)-P(2)-F(10),84.3(10)
F(206)-P(2)-F(10),44.1(8)
F(202)-P(2)-F(10),121.8(8)
F(12)-P(2)-F(10),174.4(10)
F(7)-P(2)-F(10),85.8(9)
F(9)-P(2)-F(201),51.3(8)
F(206)-P(2)-F(201),88.5(11)
F(202)-P(2)-F(201),97.6(9)
F(12)-P(2)-F(201),64.6(9)
F(7)-P(2)-F(201),138.6(9)
F(10)-P(2)-F(201),111.1(9)
F(9)-P(2)-F(8),93.2(11)
F(206)-P(2)-F(8),48.2(9)
F(202)-P(2)-F(8),69.0(8)
F(12)-P(2)-F(8),89.4(12)
F(7)-P(2)-F(8),169.6(9)
F(10)-P(2)-F(8),90.3(9)
F(201)-P(2)-F(8),51.8(8)
F(9)-P(2)-F(11),171.3(11)
F(206)-P(2)-F(11),77.6(9)
F(202)-P(2)-F(11),41.5(6)
F(12)-P(2)-F(11),98.0(10)
F(7)-P(2)-F(11),80.3(8)
F(10)-P(2)-F(11),87.6(8)
F(201)-P(2)-F(11),135.6(9)
F(8)-P(2)-F(11),89.9(9)
F(9)-P(2)-F(205),83.4(9)
F(206)-P(2)-F(205),172.1(12)
F(202)-P(2)-F(205),84.4(8)
F(12)-P(2)-F(205),35.3(8)
F(7)-P(2)-F(205),62.0(8)
F(10)-P(2)-F(205),143.8(9)
F(201)-P(2)-F(205),86.7(9)
F(8)-P(2)-F(205),124.2(10)
F(11)-P(2)-F(205),101.6(8)
F(9)-P(2)-F(203),34.5(9)
F(206)-P(2)-F(203),101.6(12)
F(202)-P(2)-F(203),168.1(10)
F(12)-P(2)-F(203),108.8(11)
F(7)-P(2)-F(203),66.0(9)
F(10)-P(2)-F(203),66.7(9)
F(201)-P(2)-F(203),85.7(9)
F(8)-P(2)-F(203),121.1(11)
F(11)-P(2)-F(203),138.1(10)
F(205)-P(2)-F(203),84.4(9)
F(9)-P(2)-F(204),115.2(13)
F(206)-P(2)-F(204),97.2(13)
F(202)-P(2)-F(204),95.0(11)
F(12)-P(2)-F(204),117.0(14)
F(7)-P(2)-F(204),30.5(9)
F(10)-P(2)-F(204),66.3(11)
F(201)-P(2)-F(204),166.2(12)
F(8)-P(2)-F(204),139.6(12)
F(11)-P(2)-F(204),58.2(10)
F(205)-P(2)-F(204),88.8(12)
F(203)-P(2)-F(204),80.8(12)
F(204)-F(7)-P(2),81(2)
F(204)-F(7)-F(205),131(3)
P(2)-F(7)-F(205),60.7(8)
F(206)-F(8)-F(201),109.6(18)
F(206)-F(8)-P(2),63.7(13)
F(201)-F(8)-P(2),63.8(11)
F(203)-F(9)-F(201),149(3)
F(203)-F(9)-P(2),82(2)
F(201)-F(9)-P(2),67.2(12)
F(206)-F(10)-P(2),66.0(14)
F(202)-F(11)-F(204),121.9(17)
F(202)-F(11)-P(2),66.9(11)
F(204)-F(11)-P(2),63.4(11)
F(205)-F(12)-P(2),76.7(18)
F(205)-F(12)-F(202),108(2)
P(2)-F(12)-F(202),58.1(9)
F(205)-F(12)-F(201),110(2)
P(2)-F(12)-F(201),58.4(10)
F(202)-F(12)-F(201),90.9(14)
F(9)-F(201)-F(8),111.5(16)
F(9)-F(201)-P(2),61.5(11)
F(8)-F(201)-P(2),64.4(10)
F(9)-F(201)-F(12),91.5(15)
F(8)-F(201)-F(12),92.1(15)
P(2)-F(201)-F(12),57.1(9)

F(11)-F(202)-P(2),71.6(12)
F(11)-F(202)-F(12),119.6(16)
P(2)-F(202)-F(12),58.8(9)
F(9)-F(203)-P(2),63.4(18)
F(7)-F(204)-F(11),109(3)
F(7)-F(204)-P(2),68(2)
F(11)-F(204)-P(2),58.4(11)
F(12)-F(205)-P(2),68.0(17)
F(12)-F(205)-F(7),122(2)
P(2)-F(205)-F(7),57.3(7)
F(10)-F(206)-F(8),133(2)
F(10)-F(206)-P(2),70.0(14)
F(8)-F(206)-P(2),68.1(14)
F(16)-P(3)-F(316),157.4(13)
F(16)-P(3)-F(14),103.7(15)
F(316)-P(3)-F(14),92.0(6)
F(16)-P(3)-F(13),75.6(14)
F(316)-P(3)-F(13),88.6(7)
F(14)-P(3)-F(13),179.1(4)
F(16)-P(3)-F(317),104.2(10)
F(316)-P(3)-F(317),92.6(8)
F(14)-P(3)-F(317),87.4(6)
F(13)-P(3)-F(317),93.3(7)
F(16)-P(3)-F(315),72.7(9)
F(316)-P(3)-F(315),90.9(7)
F(14)-P(3)-F(315),91.4(5)
F(13)-P(3)-F(315),87.8(5)
F(317)-P(3)-F(315),176.3(9)
F(16)-P(3)-F(15),90.2(12)
F(316)-P(3)-F(15),104.8(10)
F(14)-P(3)-F(15),95.1(10)
F(13)-P(3)-F(15),85.5(10)
F(317)-P(3)-F(15),14.7(10)
F(315)-P(3)-F(15),162.8(10)
F(16)-P(3)-F(318),22.4(12)
F(316)-P(3)-F(318),175.1(8)
F(14)-P(3)-F(318),85.1(7)
F(13)-P(3)-F(318),94.3(7)
F(317)-P(3)-F(318),91.2(7)
F(315)-P(3)-F(318),85.3(8)
F(15)-P(3)-F(318),79.4(10)
F(16)-P(3)-F(17),94.5(10)
F(316)-P(3)-F(17),69.0(8)
F(14)-P(3)-F(17),89.5(6)
F(13)-P(3)-F(17),89.9(6)
F(317)-P(3)-F(17),161.2(9)
F(315)-P(3)-F(17),22.1(6)
F(15)-P(3)-F(17),172.4(11)
F(318)-P(3)-F(17),107.0(9)
F(16)-P(3)-F(18),170.6(15)
F(316)-P(3)-F(18),18.4(10)
F(14)-P(3)-F(18),85.7(9)
F(13)-P(3)-F(18),95.1(9)
F(317)-P(3)-F(18),75.0(10)
F(315)-P(3)-F(18),108.3(9)
F(15)-P(3)-F(18),88.1(11)
F(318)-P(3)-F(18),163.7(10)
F(17)-P(3)-F(18),86.2(10)
N(9)-C(47)-C(46),171(2)
C(48A)-C(49)-C(48),86(3)
N(10)-C(48)-C(49),165(2)
N(10)-C(48)-C(48A),131(2)
C(49)-C(48)-C(48A),35.2(13)
C(48)#1-N(10)-C(48),119(3)
C(48A)-N(10A)-N(10A)#1,131(3)
C(49)-C(48A)-N(10A),173(5)
C(49)-C(48A)-C(48),59(2)
N(10A)-C(48A)-C(48),127(4)
N(11)-C(50)-C(51),164(3)
N(12)-C(52)-C(53),166(4)

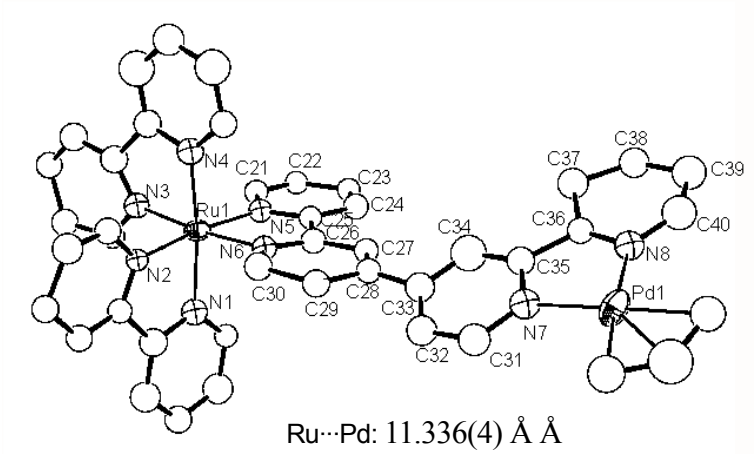
Symmetry transformations used to generate equivalent atoms:

#1 -x y -z+1/2

Ortep diagram of the cationic part of ***Ru^{Me}-QP***.

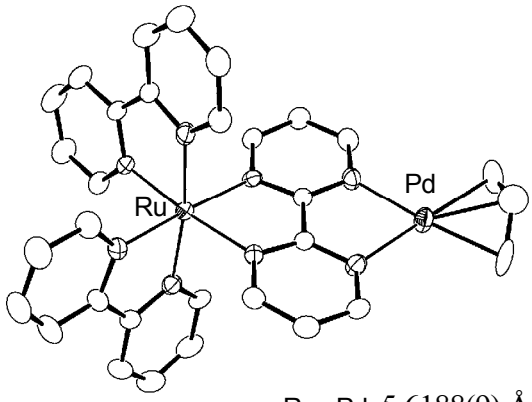


Ortep diagram of the cationic part of ***Ru^{H}-QP-Pd^{C3}***.



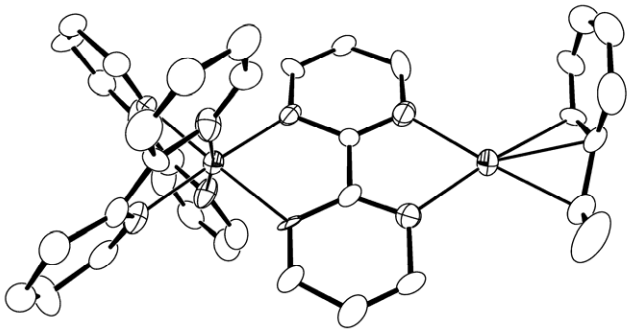
Ru···Pd: 11.336(4) Å Å

Ortep diagram of the cationic part of ***Ru^{H}-bpm-Pd^{C3}***.



Ru···Pd: 5.6188(9) Å

Ortep diagram of the cationic part of ***Ru^{H}-bpm-Pd(η^3-CH$_3$CHPh)***.

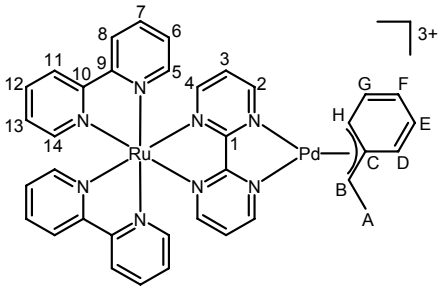


^{1}H-NMR (400 MHz, CD_3NO_2, -25 ºC, δ/ppm): δ1.45, 1.49 (3H, d, J = 6.48 Hz, H_A), 4.22 (1H, m, H_B), 6.48 (1H, bdd, J = 6.96 Hz, H_H), 7.43-8.60 (26H, bpy, bpm, H_D-H_G).

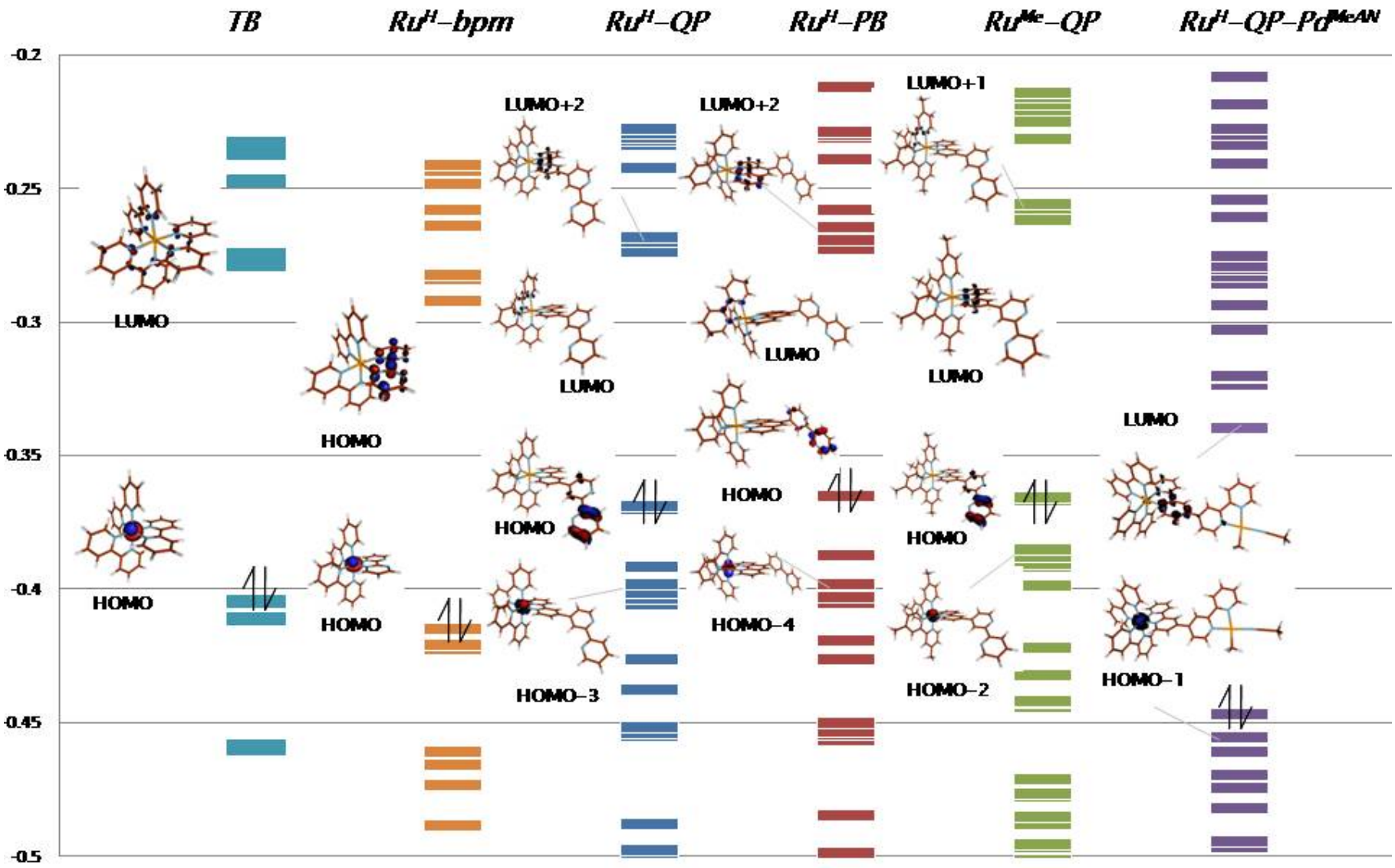
^{13}C-NMR (100 MHz, CD_3NO_2, -25 ºC, δ/ppm): δ15.4 (q, J_{CH} = 126.8 Hz, C_A), 94.8 (d, J_{CH} = 165.0 Hz, C_B), 118.1 (d, J_{CH} = 168.3 Hz, C_H), 120.5 (s, C_C), 125.6 (d, J_{CH} = 167.5 Hz, C8, C11), 128.0 (d, J_{CH} = 177.4 Hz, C3), 128.9 (d, J_{CH} = 170.8 Hz, C6, C13), 133.7, 135.0, 136.2 (d, J_{CH} =163.3, 164.2, 161.7 Hz, C_D-C_G), 139.9, 140.0 (d, J_{CH} = 169.1 Hz, C7, C12), 153.0, 153.9 (d, J_{CH} = 183.1, 180.7 Hz, C5, C14), 157.9, 158.1 (s, C9, C10), 162.6 (d, J_{CH} = 190.6 Hz, C2, C4), 165.5 (bs, C1).

ESI-MS : m/z = 954.9; [{(bpy)$_2$^{101}Ru(bpm)^{106}Pd(η^3-CH$_3$CHPh)}(BF$_4$)$_2$]$^+$.

m/z = 1132.9; [{(bpy)$_2$^{101}Ru(bpm)^{106}Pd(η^3-CH$_3$CHPh)}(BF$_4$)$_4$]$^-$.



Energy diagram of some frontier orbitals of $[(bpy)_3Ru]^{2+}$, $[(bpy)_2Ru(bpm)]^{2+}$, ***Ru^{R}-QP*** (R = H, Me), ***Ru^{H}-PB***, ***Ru^{H}-QP-Pd^{MeAN}***.



DFT calculations were performed using the Gaussian-03 (rev. D02) quantum chemistry program package at the B3LYP/LanL2DZ level. The HOMO and LUMO energies were determined by using minimized singlet geometries to approximate the ground state.