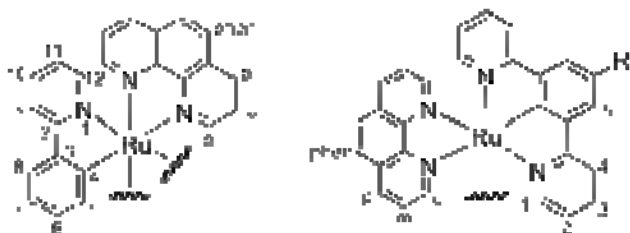


Synthesis of the compounds not described in the paper.

numeration used for the assignments of NMR spectra.



1b

The same procedure as that used for **1a** starting with 4-*N,N*-dimethylaminophenyl-2-pyridine instead of 2-phenylpyridine afforded **1b** as a yellow solid (96 % yield).

Anal. Calc. for $C_{25}H_{30}N_3F_6PRu$: C, 48.54; H, 4.89; N, 6.79; Found: C, 48.32; H, 5.00; N, 6.98

1H NMR (400 MHz, CD_3CN) : δ = 9.09 (d, 1H, $^3J_{HH}$ = 6.8, H₁₂), 7.78 (ddd, 1H, $^3J_{HH}$ = 8.1, $^3J_{HH}$ = 7.3, $^4J_{HH}$ = 1.6, H₁₀), 7.69 (dd, 1H, $^3J_{HH}$ = 8.1, $^4J_{HH}$ = 1.6, H₉), 7.60 (d, 1H, $^3J_{HH}$ = 8.7, H₈), 7.44 (d, 1H, $^4J_{HH}$ = 2.5, H₅), 7.06 (ddd, 1H, $^3J_{HH}$ = 5.8, $^3J_{HH}$ = 7.3, $^4J_{HH}$ = 1.6, H₁₁), 6.55 (dd, 1H, $^3J_{HH}$ = 8.7, $^4J_{HH}$ = 2.5, H₇), 5.96 (dd, 1H, $^3J_{HH}$ = 6.2, $^4J_{HH}$ = 1.2, H_{arom}), 5.9 (dd, 1H, $^3J_{HH}$ = 6.2, $^4J_{HH}$ = 1.2, H_{arom}), 5.65 (dd, 1H, $^3J_{HH}$ = 6.2, $^4J_{HH}$ = 1.2, H_{arom}), 5.42 (dd, 1H, $^3J_{HH}$ = 6.2, $^4J_{HH}$ = 1.2, H_{arom}), 3.13 (s, 6H, N(CH₃)₂), 2.4 (hept, 1H, CHMe₂), 2.1 (s, 3H, CH₃CN), 2.02 (s, 3H, CH₃), 0.98 (d, 3H, $^3J_{HH}$ = 6.9, CH₃), 0.95 (d, 3H, $^3J_{HH}$ = 6.9, CH₃)

^{13}C { 1H } NMR (100 MHz, CD_3CN) : δ = 176.4, 166.0, 155.1, 151.1, 137.9, 132.3, 125.3, 123.1, 121.7, 119.9, 117.7, 108.1, 102.9, 101.9, 92.4, 91.8, 88.3, 84.7, 39.6, 39.6, 30.9, 21.6, 21.2, 17.9, 2.9

1c

The same procedure as that used for **1a** starting with 4-aminophenyl-2-pyridine instead of phenyl-2-pyridine afforded **1c** as a green-yellow solid (90% yield).

Anal. Calc. for $C_{23}H_{26}N_3F_6PRu$: C, 46.78; H, 4.4; N, 7.12; Found: C, 46.20; H, 4.24; N, 7.10

1H NMR (300 MHz, DMSO- d_6) : δ = 8.43 (d, 1H, $^3J_{HH}$ = 6.6, H₁₂), 7.94 (dd, 1H, $^3J_{HH}$ = 7.3, $^4J_{HH}$ = 1.3, H₈), 7.55 (dd, 1H, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.6, H₅), 7.22-7.17 (ddd, 1H, $^3J_{HH}$ = 7.3, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.3, H₆), 7.17 -7.14 (ddd, 1H, $^3J_{HH}$ = 7.3, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.6, H₆ or H₇), 7.12 (d, 1H, $^3J_{HH}$ = 2.6, H₉), 6.86 (s, 2H, NH₂), 6.54-6.51 (dd, 1H, $^3J_{HH}$ = 6.6, $^4J_{HH}$ = 2.4, H₁₁), 6.27-6.25 (d, 1H, $^3J_{HH}$ = 6.4, H_{arom}), 6.02-6.0 (dd, 1H, $^3J_{HH}$ = 6.2, $^4J_{HH}$ = 1.1, H_{arom}), 5.87-5.84 (d, 1H, $^3J_{HH}$ = 6.4, H_{arom}), 5.80-5.77 (d, 1H, $^3J_{HH}$ = 6.2, H_{arom}), 2.4 (m, 1H, CHMe₂), 2.22 (s, 3H, CH₃CN), 2.07 (s, 3H, CH₃), 0.96 (d, 3H, $^3J_{HH}$ = 7, CH₃), 0.77 (d, 3H, $^3J_{HH}$ = 7, CH₃)

^{13}C { 1H } NMR (78 MHz, DMSO- d_6) : δ = 172.5, 164.3, 156.9, 155.5, 145.7, 141.3, 129.7, 124.3, 123.6, 115.2, 109.8, 109.7, 104.2, 96.5, 91.0, 90.2, 88.2, 89.2, 65.4, 30.8, 22.4, 21.6, 1.6

[Ru(4-*N,N*-dimethyl(pyridin-2-yl)benzenamine- κ C,N)(NCMe)₄]PF₆

To a brown solution of [RuCl₂(η^6 -C₆H₆)]₂ (150 mg, 0.3 mmol) in CH₃CN (10 mL) was added 4-*N,N*-dimethylaminophenyl-2-pyridine *N,N*-dimethyl-4-(pyridin-2-yl)benzenamine (274 mg, 1.2 mmol), NaOH (24 mg, 0.6 mmol) and KPF₆ (220.9 mg, 1.2 mmol) and the solution was stirred for 24 hours at 45°C. The desired product was purified by column chromatography over Al₂O₃ using CH₃CN as eluent. The resulting powder was dissolved in minimum CH₃CN and after the addition of *n*-hexane, an orange solid precipitated (235 mg, 64% yield).

Anal. Calc. for C₂₁H₂₅F₆N₆PRu : C, 41.52; H, 4.15; N, 13.83; Found: C, 41.13; H, 4.25; N, 12.96

¹H NMR (400 MHz, CD₃CN) : δ = 8.76 (dt, 1H, ³J_{HH}=5.5, ⁴J_{HH}=1.2, H₁₂), 7.60 (m, 2H, H₉ + H₁₀), 7.53 (d, 1H, ³J_{HH}=8.5, H₈), 7.29 (d, 1H, ⁴J_{HH}=2.6, H₅), 6.95 (td, 1H, ³J_{HH}=6.0, ⁴J_{HH}=2.6, H₁₁), 6.37 (dd, 1H, ³J_{HH}=8.5, ⁴J_{HH}=2.6, H₇), 3.04 (s, 6H, NMe₂), 2.51 (s, 3H, CH₃CN), 2.14 (s, 3H, CH₃CN), 2.01 (s, 6H, 2 CH₃CN)

¹³C {¹H} NMR (100 MHz, DMSO-d₆) : δ = 185.6, 169.2, 152.8, 150.7, 136.1, 128.3, 125.1, 123.4, 121.5, 121.0, 119.5, 116.9, 112.9, 106.9, 40.4, 4.1, 3.6, 1.6

3a

To an orange solution of [Ru(*N,N*-dimethyl-4-(pyridin-2-yl)benzenamine- κ C,N)(NCMe)₄]PF₆ (343.0 mg, 0.57 mmol) in CH₂Cl₂ (10 mL) was added 1,10-phenanthroline (phen) (101.8 mg, 0.57 mmol) which resulted in an instant deep purple/red color change. The solution was stirred for 48 hours at 40°C. The desired product was purified by column chromatography over Al₂O₃ using CH₃CN as eluent. The resulting powder was dissolved in the minimum amount of CH₃CN and after the addition of *n*-hexane, a dark purple solid precipitated (24 mg, 6 % yield). Anal. Calc. for C₂₉H₂₇F₆N₆PRu : C, 49.36; H, 3.86; N, 11.91; Found: C, 47.73, H, 3.80, N, 11.30.

¹H NMR (500 MHz, CD₃CN) : δ = 9.70 (dd, 1H, ³J_{HH}=5.0, ⁴J_{HH}=1.5, H_o), 8.70 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=1.4, H_p), 8.27 (dd, 1H, ³J_{HH}=5.3, ⁴J_{HH}=1.4, H_o), 8.21 (dd, 1H, ³J_{HH}=8.1, ⁴J_{HH}=1.4, H_p), 8.18 (dd, 1H, ³J_{HH}=7.6, ³J_{HH}=4.9, H_m), 8.17 (d, 1H, ³J_{HH}=8.7, H_{phen}), 8.02 (d, 1H, ³J_{HH}=8.9, H_{phen}), 7.71 (d, 1H, ³J_{HH}=8.7, H₈), 7.62 (d, 1H, ⁴J_{HH}=2.7, H₅), 7.59 (d, 1H, ³J_{HH}=8.1, H₁₂), 7.39 (dd, 1H, ³J_{HH}=8.1, ⁴J_{HH}=5.3, H_m), 7.33 (ddd, 1H, ³J_{HH}=8.4, ³J_{HH}=7.2, ⁴J_{HH}=1.7, H₁₀/H₁₁), 7.16 (ddd, 1H, ³J_{HH}=5.8, ⁴J_{HH}=1.7, ⁵J_{HH}=0.8, H₉), 6.55 (dd, 1H, ³J_{HH}=8.5, ⁴J_{HH}=2.6, H₇), 6.37 (ddd, 1H, ³J_{HH}=7.2, ³J_{HH}=5.8, ⁴J_{HH}=1.4, H₁₀/H₁₁), 3.13 (s, 6H, NMe₂), 2.31 (s, 3H, CH₃CN), 2.07 (s, 3H, CH₃CN)

¹³C {¹H} NMR (125 MHz, CD₃CN) : δ = 193.6, 169.8, 156.2, 151.6, 151.5, 151.1, 147.6, 136.5, 136.1, 135.4, 135.0, 131.4, 131.2, 128.5, 128.4, 126.9, 126.0, 125.7, 125.2, 122.4, 120.8, 119.6, 117.3, 107.2, 40.7, 4.6, 4.0

[Ru(2-(3-bromophenyl)-2-pyridyl- κ C,N)(NCMe)₄]PF₆

To a brown solution of $[\text{RuCl}_2(\eta^6\text{-C}_6\text{H}_6)]_2$ (800 mg, 1.6 mmol) in CH_3CN (15 mL) was added 2-(3-bromophenyl)pyridine (748.7 mg, 3.2 mmol), NaOH (128 mg, 3.2 mmol) and KPF_6 (1178.2 mg, 6.4 mmol) and the solution was stirred for 48 hours at 45°C . The desired product was purified by column chromatography over Al_2O_3 using CH_3CN as eluent. The resulting powder was dissolved in minimum CH_3CN and after the addition of n-hexane, an orange solid precipitated (1406 mg, 68% yield).

Anal. Calc. for $\text{C}_{19}\text{H}_{19}\text{BrF}_6\text{N}_5\text{PRu}$: C, 35.47; H, 2.98; N, 10.89; Found: C, 34.36; H, 2.98; N, 10.55

^1H NMR (500 MHz, CD_3CN): δ = 8.92 (d, 1H, $^3J_{\text{HH}}=5.6$, H_{12}), 7.90-7.86 (m, 3H, H_5 , H_8 , H_9), 7.77 (ddd, 1H, $^3J_{\text{HH}}=7.6$, $^4J_{\text{HH}}=1.5$, H_{10}), 7.20 (m, 2H, H_6 , H_{11}), 2.51 (s, 3H, CH_3CN), 2.16 (s, 3H, CH_3CN), 2.01 (s, 6H, 2 CH_3CN)

^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CD_3CN): δ = 184.5, 167.6, 153.4, 140.8, 137.1, 130.4, 126.3, 122.7, 122.0, 119.0, 114.9, 4.2, 3.6, 1.6

3b

To an orange solution of $[\text{Ru}(2\text{-(3-bromophenyl)pyridine})(\text{NCMe})_4]\text{PF}_6$ (1000 mg, 1.56 mmol) in CH_2Cl_2 (50 mL), was added phenanthroline (280 mg, 1.56 mmol). The solution changed from orange to deep purple and was further stirred for 48h at 40°C . The desired product was purified by column chromatography over Al_2O_3 using CH_3CN as eluent. The resulting powder was dissolved in minimum CH_3CN and after the addition of n-hexane, a dark purple solid precipitated (964 mg, 83% yield).

MS (ES, m/z): Calcd. for $\text{C}_{27}\text{H}_{21}\text{BrN}_5^{101}\text{Ru}$: 596.00; Found: 596.03

^1H NMR (400 MHz, CD_3CN): δ = 9.71 (dd, 1H, $^3J_{\text{HH}}=4.9$, $^4J_{\text{HH}}=1.4$, H_o), 8.73 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.4$, H_o), 8.24-8.15 (m, 5H), 8.03 (d, 1H, $^3J_{\text{HH}}=9.1$, H_{phen}), 8.02 (d, 1H, $^4J_{\text{HH}}=1.7$, H_8), 7.86 (d, 2H, $^3J_{\text{HH}}=8.3$, H_{12}), 7.50 (ddd, 1H, $^3J_{\text{HH}}=7.8$, $^4J_{\text{HH}}=1.7$, $\text{H}_{10}/\text{H}_{11}$), 7.42-7.35 (m, 3H, H_5/H_6 , H_9 , H_m), 6.63 (ddd, 1H, $^3J_{\text{HH}}=7.4$, $^3J_{\text{HH}}=5.8$, $^4J_{\text{HH}}=1.4$, $\text{H}_{10}/\text{H}_{11}$), 2.28 (s, 3H, CH_3CN), 2.06 (s, 3H, CH_3CN)

^{13}C $\{^1\text{H}\}$ NMR (100 MHz, CD_3CN): δ = 191.9, 168.2, 156.3, 152.3, 151.7, 150.8, 149.4, 147.4, 141.0, 136.8, 136.7, 135.4, 131.4, 128.5, 128.4, 127.1, 126.9, 125.7, 125.3, 123.5, 122.7, 119.4, 115.02, 4.5, 4.1

3c

To a deep purple solution of $[\text{Ru}(2\text{-phenyl-2-pyridyl-}\kappa\text{C,N})(\text{phen})(\text{NCMe})_2]\text{PF}_6$ ¹ (150 mg, 0.23 mmol) in CH_2Cl_2 (10 mL) was added AgNO_3 (39.1 mg, 0.23 mmol), and PhCOCl (39.1 μL , 0.23 mmol). The solution was stirred at room temperature during 2 hours. TLC revealed only a red spot. This was collected by column chromatography over Al_2O_3 using CH_3CN as eluent and concentrated *in vacuo*.

¹ A. D. Ryabov, R. Le Lagadec, H. Estevez, R. A. Toscano, S. Hernandez, L. Alexandrova, V. S. Kurova, A. Fischer, C. Sirlin, M. Pfeffer, *Inorg. Chem.* 2005, **44**, 1626.

The resulting powder was dissolved in minimum CH₃CN and after the addition of n-hexane, a dark purple solid precipitated (0.137 mg, 84% yield).

Anal. Calc. for C₂₇H₂₁F₆N₆O₂PRu : C, 45.83; H, 2.99; N, 11.88; Found: C, 46.29; H, 3.13; N, 11.57

MS (ES, m/z) : Calcd. for C₂₇H₂₁N₆O₂¹⁰¹Ru : 563.07; Found : 563.11

¹H NMR (500 MHz, CD₃CN) : δ = 9.72 (dd, 1H, ³J_{HH}=4.9, ⁴J_{HH}=1.5, H_o), 8.78 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=1.4, H_p), 8.65 (d, 1H, ⁴J_{HH}=2.3, H₈), 8.60 (d, 1H, ³J_{HH}=8.2, H₅), 8.27 (dd, 1H, ³J_{HH}=8.1, ⁴J_{HH}=1.2, H_o), 8.23 (dd, 1H, ³J_{HH}=8.2, ³J_{HH}=4.9, H_m), 8.21 (d, 1H, ³J_{HH}=8.3, H_{phen}), 8.05 (m, 4H), 7.58 (ddd, 1H, ³J_{HH}=7.8, ⁴J_{HH}=1.5, H₁₀/H₁₁), 7.43 (ddd, 1H, ³J_{HH}=5.6, H₉), 7.36 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=5.3, H_m), 6.73 (ddd, 1H, ³J_{HH}=7.2, ³J_{HH}=5.6, ⁴J_{HH}=1.2, H₁₀/H₁₁), 2.28 (s, 3H, CH₃CN), 2.09 (s, 3H, CH₃CN)

¹³C {¹H} NMR (125MHz, CD₃CN) : δ = 167.4, 155.9, 152.3, 151.6, 150.3, 147.8, 146.9, 143.9, 139.4, 137.3, 137.1, 136.0, 131.4, 131.2, 128.5, 128.4, 126.9, 126.2, 125.4, 123.6, 123.4, 121.5, 119.8, 117.5, 4.4, 4.1

4a

Ru(phen)₂Cl₂² (70mg, 0.13mmol), 2-phenylpyridine (18.5μl, 0.13mmol), tetramethylammonium hydroxide (24mg, 0.13mmol) and AgOTf (67mg, 0.26mmol) were refluxed in dichloromethane (5 mL) for 24h at 45°C. The reaction mixture was evaporated. The desired complex was purified by column chromatography over Al₂O₃ CH₂Cl₂/MeOH (95/5) as eluent. Removal of the solvents *in vacuo* afforded **4a** as a deep purple solid (86mg, 87% yield).

Anal. Calc. for C₃₆H₂₄F₃N₅O₃RuS : C, 56.54; H, 3.16; N, 9.16; Found: C, 55.39; H, 3.31; N, 8.80

¹H NMR (500 MHz, CD₃CN) : δ = 8.49 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=1.4, H_p), 8.47 (dd, 1H, ³J_{HH}=5.3, ⁴J_{HH}=1.4, H_o), 8.41 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=1.4, H_p), 8.37 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=1.4, H_p), 8.32 (dd, 1H, ³J_{HH}=8.2, ⁴J_{HH}=1.4, H_p), 8.26 (dd, 1H, ³J_{HH}=5.3, ⁴J_{HH}=1.4, H_o), 8.16 (s, 2H, H_{phen}), 8.12 (dd, 1H, ³J_{HH}=5.3, ⁴J_{HH}=1.4, H_o), 8.10 (s, 2H, H_{phen}), 8.05 (d, 1H, ³J_{HH}=8.0, H₁₂), 7.88 (m, 2H), 7.70-7.57 (m, 5H), 7.43 (dd, 1H, ³J_{HH}=8.1, ⁴J_{HH}=5.3, H_m), 6.90-6.79 (m, 2H), 6.71 (td, 1H, ³J_{HH}=7.3, ⁴J_{HH}=1.3), 6.29 (d, 1H, ³J_{HH}=7.3)

¹³C {¹H} NMR (125 MHz, CD₃CN) : δ = 192.42, 167.55, 154.89, 150.81, 150.81, 150.47, 149.93, 148.94, 148.03, 147.82, 146.10, 145.76, 135.69, 135.53, 135.26, 134.03, 132.71, 132.62, 130.27, 130.52, 130.29, 130.29, 128.27, 127.72, 127.66, 127.52, 127.52, 125.64, 125.13, 125.13, 125.00, 124.49, 122.09, 120.78, 118.73

4b

1a (80 mg, 0.14 mmol), was dissolved in dichloromethane (5 mL) under argon and 1.10 phenanthroline (50.24mg, 0.28 mmol), was then added. The resulting reaction mixture was refluxed at 45°C for 24h.

² P. A. Lay, A. M. Sargeson, A. M. Taube, *Inorg. Synth.*, 1986, **24**, 291 ; S. Rau, B. Schäfer, A. Grüssing, S. Schebesta, K. Lamm, J. Vieth, H. Görls, D. Walther, M. Rudolph, U. W. Grummt, E. Birkner, *Inorganica Chimica Acta*, 2004, **357**, 4496.

The reaction mixture was evaporated. The complex was purified by column chromatography over Al_2O_3 $\text{CH}_2\text{Cl}_2/\text{CH}_3\text{CN}$ (90/10) as eluent. Removal of the solvents *in vacuo* afforded **4b** as a deep purple solid (110 mg, 86% yield).

4c

To an orange solution of $[\text{Ru}(\text{N,N-dimethyl-4-(pyridin-2-yl)benzenamine})(\text{NCMe})_4]\text{PF}_6$ (210 mg, 0.35 mmol) in 20 mL MeOH (20 mL) was added phenanthroline (131 mg, 0.73 mmol) which resulted in an instant deep purple color change. The solution was stirred for 48 hours at 40°C after which time the desired product was purified by column chromatography over Al_2O_3 using CH_3CN as eluent. The resulting powder was dissolved in minimum CH_3CN and after the addition of n-hexane, a dark purple solid precipitated (194 mg, 69% yield).

Anal. Calc. for $\text{C}_{37}\text{H}_{29}\text{F}_6\text{N}_6\text{PRu}$: C, 55.29; H, 3.64; N, 10.46; Found: C, 54.84; H, 3.75; N, 10.01

MS (ES, m/z): Calcd. for $\text{C}_{37}\text{H}_{29}\text{N}_6^{101}\text{Ru}$: 659.14; Found: 659.19.

^1H NMR (500 MHz, CD_3CN): δ = 8.57 (dd, 1H, $^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.4$, H_o), 8.45 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.4$, H_p), 8.35 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.4$, H_p), 8.28 (m, 3H), 8.17 (dd, 1H, $^3J_{\text{HH}}=5.0$, $^4J_{\text{HH}}=1.4$, H_o), 8.12 (d, 2H, $^3J_{\text{HH}}=2.3$, 2H, H_{phen}), 8.05 (s, 2H, 2H, H_{phen}), 7.90 (dd, 1H, $^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.2$, H_o), 7.76 (d, 1H, $^3J_{\text{HH}}=8.2$, H_{12}), 7.65 (d, 1H, $^3J_{\text{HH}}=8.7$, H_8), 7.61 (m, 2H), 7.56 (dd, 1H, $^3J_{\text{HH}}=8.1$, $^4J_{\text{HH}}=5.3$, H_m), 7.51 (ddd, 1H, $^3J_{\text{HH}}=8.3$, $^3J_{\text{HH}}=7.3$, $^4J_{\text{HH}}=1.6$, $\text{H}_{10}/\text{H}_{11}$), 7.41 (d, 1H, $^3J_{\text{HH}}=5.7$, H_9), 7.40 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^3J_{\text{HH}}=5.4$, H_m), 6.61 (ddd, 1H, $^3J_{\text{HH}}=7.2$, $^3J_{\text{HH}}=5.8$, $^4J_{\text{HH}}=1.3$, $\text{H}_{10}/\text{H}_{11}$), 6.26 (dd, 1H, $^3J_{\text{HH}}=8.6$, $^4J_{\text{HH}}=2.6$, H_7), 5.52 (d, 1H, $^3J_{\text{HH}}=2.7$, H_5), 2.50 (s, 6H, NMe_2)

^{13}C { ^1H } NMR (125 MHz, CD_3CN): δ = 194.2, 168.5, 155.5, 151.5, 151.4, 151.0, 150.6, 149.8, 149.2, 148.8, 147.0, 136.0, 135.9, 134.6, 133.1, 131.5, 131.3, 131.1, 130.9, 128.5, 128.4, 128.2, 126.4, 125.9, 125.8, 125.7, 120.4, 117.9, 117.8, 106.9, 39.7

4d

To an orange solution of $[\text{Ru}(2\text{-(3-bromophenyl)pyridine})(\text{NCMe})_4]\text{PF}_6$ (249 mg, 0.39 mmol) in MeOH (20 mL) was added phenanthroline (139.5 mg, 0.77 mmol). The solution changed from orange to deep purple and was further stirred for 48h at 40°C . The desired product was purified by column chromatography over Al_2O_3 using CH_3CN as eluent. The resulting powder was dissolved in minimum CH_3CN and after the addition of n-hexane, a dark purple solid precipitated (137 mg, 42% yield).

Anal. Calc. for $\text{C}_{35}\text{H}_{23}\text{BrF}_6\text{N}_5\text{PRu}$: C, 50.07; H, 2.76; N, 8.34; Found: C, 49.39; H, 3.16; N, 7.99

^1H NMR (500 MHz, CD_3CN): δ = 8.47 (dd, 1H, $^3J_{\text{HH}}=8.1$, $^4J_{\text{HH}}=1.4$, H_p), 8.45 (dd, 1H, $^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.4$, H_o), 8.40 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.4$, H_p), 8.35 (dd, 1H, $^3J_{\text{HH}}=8.1$, $^4J_{\text{HH}}=1.2$, H_p), 8.31 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.2$, H_p), 8.20 (dd, 1H, $^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.2$, H_o), 8.14 (d, 2H, $^4J_{\text{HH}}=2.0$, 2H, H_{phen}), 8.09 (m, 3H, H_o , 2H, H_{phen}), 8.04 (d, 1H, $^3J_{\text{HH}}=8.4$, H_{12}), 8.00 (d, 1H, $^4J_{\text{HH}}=2.1$, H_8), 7.84 (dd, 1H,

$^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.2$, H_o), 7.67 (ddd, 1H, $^3J_{\text{HH}}=8.1$, $^3J_{\text{HH}}=7.6$, $^4J_{\text{HH}}=1.7$, $\text{H}_{10}/\text{H}_{11}$), 7.60 (m, 4H, H_9 , 3H_m), 7.40 (dd, 1H, $^3J_{\text{HH}}=8.0$, $^3J_{\text{HH}}=5.3$, H_m), 6.85 (ddd, 1H, $^3J_{\text{HH}}=7.2$, $^3J_{\text{HH}}=5.6$, $^4J_{\text{HH}}=1.4$, $\text{H}_{10}/\text{H}_{11}$), 6.80 (dd, 1H, $^3J_{\text{HH}}=7.9$, $^4J_{\text{HH}}=2.1$, H_6), 6.24 (d, 1H, $^3J_{\text{HH}}=7.9$, H_5)

^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CD_3CN): δ = 192.4, 167.0, 155.8, 151.9, 151.7, 151.4, 150.6, 138.3, 136.7, 136.3, 135.1, 133.9, 131.2, 128.6, 128.5, 128.4, 128.4, 127.2, 126.5, 126.1, 127.0, 125.9, 123.6, 120.1

4e

To a deep purple solution of **4a** (175mg, 0.23mmol) in CH_2Cl_2 (10 mL), was added AgNO_3 (39.11mg, 0.23mmol), and PhCOCl (39 μl , 0.23mmol). The solution was stirred at room temperature for 2 hours. TLC revealed only a red spot which was collected by column chromatography over Al_2O_3 using CH_3CN as eluent and the solvents were removed *in vacuo*. The resulting powder was dissolved in minimum $\text{CH}_3\text{CN}/\text{Et}_2\text{O}$ and after the addition of n-hexane, a dark red solid precipitated (177mg, 95% yield).

Anal. Calc. for $\text{C}_{36}\text{H}_{23}\text{F}_3\text{N}_6\text{O}_5\text{RuS}$: C, 53.40; H, 2.86; N, 10.38; Found: C, 52.47; H, 2.98; N, 10.13

MS (ES, m/z): Calcd. for $\text{C}_{35}\text{H}_{23}\text{N}_6\text{O}_2^{101}\text{Ru}$: 661.09. Found: 661.13.

^1H NMR (500 MHz, CD_3CN): δ = 8.64 (d, 1H, $^4J_{\text{HH}}=2.3$, H_8), 8.52 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.4$, H_p), 8.44 (dd, 2H, $^3J_{\text{HH}}=8.1$, $^4J_{\text{HH}}=1.1$, H_p), 8.38 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.2$, H_p), 8.33 (dd, 1H, $^3J_{\text{HH}}=5.2$, $^4J_{\text{HH}}=1.2$, H_o), 8.24 (d, 1H, $^3J_{\text{HH}}=8.4$, H_{12}), 8.18 (m, 1H), 8.16 (d, 2H, $^3J_{\text{HH}}=4.0$, 2H, H_phen), 8.12 (d, 2H, $^4J_{\text{HH}}=1.1$, 2H, H_phen), 8.06 (dd, 1H, $^3J_{\text{HH}}=5.0$, $^4J_{\text{HH}}=1.4$, H_o), 7.86 (dd, 1H, $^3J_{\text{HH}}=5.2$, $^4J_{\text{HH}}=1.1$, H_o), 7.75 (t, 1H, $^3J_{\text{HH}}=7.8$, H_{10}), 7.66-7.62 (m, 3H, H_9), 7.60 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=5.3$, H_m), 7.48 (dd, 1H, $^3J_{\text{HH}}=8.4$, $^4J_{\text{HH}}=2.4$, H_6), 7.45 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=5.5$, H_m), 6.94 (ddd, 1H, $^3J_{\text{HH}}=7.2$, $^3J_{\text{HH}}=5.6$, $^4J_{\text{HH}}=1.2$, H_{11}), 6.64 (d, 1H, $^3J_{\text{HH}}=8.4$, H_5)

^{13}C $\{^1\text{H}\}$ NMR (125 MHz, CD_3CN): δ = 167.1, 156.3, 152.7, 152.7, 152.4, 151.3, 150.0, 149.3, 149.1, 148.4, 147.1, 144.3, 137.7, 137.6, 137.4, 136.5, 135.7, 135.3, 132.3, 132.1, 132.0, 131.9, 129.3, 129.2, 129.1, 127.2, 126.9, 126.8, 124.9, 122.1, 121.2, 118.3

4g

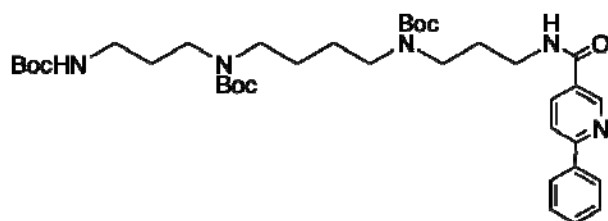
2,3,4,5,6-Penta-O-benzyl-D-gluconic acid (91 mg, 0.141 mmol) was dissolved in dry DMF/ CH_2Cl_2 (1:2, 6 ml) and then EDAC (32.40 mg, 0.169 mmol) and HOBt (22.83 mg, 0.169 mmol) were added at 0°C under argon. After half an hour, diisopropylethylamine (43.68 μL , 0.338 mmol) and **4f** (137 mg, 0.176 mmol) were added and the reaction mixture was stirred for 22h. The solution was concentrated *in vacuo*. The solid was purified by preparative TLC using $\text{CH}_2\text{Cl}_2/\text{MeOH}$ (9:1) as eluent to give **4g** (134 mg, 67% yield).

Anal. Calc. for $\text{C}_{77}\text{H}_{65}\text{F}_3\text{N}_6\text{O}_9\text{RuS}$: C, 65.66; H, 4.65; N, 5.97; Found: C, 65.62; H, 4.78; N, 6.09

MS (ES, m/z): Calcd. for $\text{C}_{76}\text{H}_{65}\text{N}_6\text{O}_6^{101}\text{Ru}$: 1259.43; Found: 1259.41

^1H NMR (400 MHz, CD_3CN) : δ = 8.48 (m, 3H), 8.40 (d, 1H, $^3J_{\text{HH}}=8.0$), 8.35 (d, 1H, $^3J_{\text{HH}}=8.1$), 8.33 (d, 1H, $^3J_{\text{HH}}=8.3$), 8.24 (d, 1H, $^3J_{\text{HH}}=5.2$), 8.15 (s, 2H), 7.68-7.55 (m, 6H), 7.43 (dd, 1H, $^3J_{\text{HH}}=8.0$, $^3J_{\text{HH}}=5.3$, H_m), 7.41 (dd, 1H, $^3J_{\text{HH}}=8.0$, $^3J_{\text{HH}}=5.3$, H_m), 7.37-7.25 (m, 13H), 7.23 (s, 2H), 7.23 (s, 2H), 7.15-7.05 (m, 4H), 6.98 (m, 1H), 6.83 (m, 2H), 6.23 (dd, 1H, $^3J_{\text{HH}}=8.0$, $^3J_{\text{HH}}=5.7$, H_m), 4.74-4.46 (m, 10H), 4.23 (dd, 1H, $^3J_{\text{HH}}=4.2$, $^4J_{\text{HH}}=1.2$), 4.08 (m, 1H), 4.02 (m, 1H), 3.87 (dd, 1H, $^3J_{\text{HH}}=10.4$, $^3J_{\text{HH}}=3.5$), 3.77 (m, 1H), 3.69 (dd, 1H, $^3J_{\text{HH}}=10.4$, $^3J_{\text{HH}}=4.7$)

^{13}C NMR $\{^1\text{H}\}$ (100 MHz, CD_3CN) : δ = 188.53, 169.64, 168.20, 155.93, 151.95, 151.87, 151.55, 150.87, 149.96, 149.06, 148.86, 147.19, 146.59, 140.01, 139.83, 139.67, 139.64, 138.51, 136.83, 136.32, 135.06, 133.82, 133.68, 133.03, 131.77, 131.57, 131.35, 129.50, 129.42, 129.34, 129.28, 129.18, 129.09, 129.02, 128.97, 128.82, 128.77, 128.70, 128.57, 128.45, 128.39, 126.68, 126.17, 126.07, 123.32, 122.35, 122.28, 119.89, 117.33, 117.30, 82.69, 82.00, 80.16, 79.89, 76.40, 75.36, 74.40, 73.90, 72.52, 69.77



Boc₃SperPhNic

A mixture of ($\text{N}^1, \text{N}^4, \text{N}^9$ -tri-*tert*-butoxycarbonyl)-1,12-diamino-4,9-diazadodecane ³ (3.45 g, 6.9 mmol), 6-phenylnicotinic acid (1.1 g, 5.7 mmol), dicyclohexylcarbodiimide (1.8 g, 8.5 mmol), and hydroxybenzotriazole (154 mg, 1.1 mmol) in CH_2Cl_2 was stirred at r.t. for 24h. The reaction mixture was filtered, concentrated, and then dissolved in ether. A white precipitate was filtered off and the filtrate was concentrated *in vacuo*. The oil obtained was purified by column chromatography over silica using $\text{CH}_2\text{Cl}_2/\text{AcOEt}$ (5/5) as eluent to give (3.7 g, 95% yield).

^1H NMR (400 MHz, $\text{C}_6\text{D}_5\text{CD}_3$) : δ = 9.29 (s, 1H), 8.17 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=2.2$), 8.02 (m, 2H), 7.38 (dd, 1H, $^3J_{\text{HH}}=8.4$, $^4J_{\text{HH}}=0.7$), 7.21 (m, 2H), 7.15 (m, 1H), 3.41 (m/q, 2H, 1- CH_2), 3.17 (m/q, 2H, 3- CH_2), 3.07 (m/t, 2H, 10- CH_2), 3.03-2.91 (m, 6H, 5,8,12- CH_2), 1.64-1.55 (m, 2H, 2- CH_2), 1.49 (qn, 2H, 11- CH_2), 1.44-1.32 (3s+m, 31H, 6,7- CH_2 , 3 Boc)

^{13}C $\{^1\text{H}\}$ NMR (100 MHz, $\text{C}_6\text{D}_5\text{CD}_3$) : δ = 165.06, 159.61, 156.76, 156.03, 155.91, 148.90, 139.40, 136.13, 119.66, 79.88, 79.43, 78.63, 47.47, 47.25, 44.96, 44.56, 38.58, 36.90, 29.70, 28.80, 28.60, 26.62, 26.57

³ A. J. Geall, I. S. Blackburn, *Tetrahedron*, 2000, **56**, 2449.

$\text{Ru(phen)}_2\text{Cl}_2$ (150mg, 0.28 mmol), 8-quinolinol (40.6 mg, 0.28 mmol), tetramethylamonium hydroxide (51mg, 0.28 mmol) and AgOTf (143.5mg, 0.56 mmol) were refluxed in CH_2Cl_2 (7 mL) for 24h at 45°C. The reaction mixture was cooled at r.t. and the solvents were removed *in vacuo*. The complex was purified by column chromatography over Al_2O_3 using $\text{CH}_2\text{Cl}_2/\text{MeOH}$ (95/5) as eluent and the solvents were removed *in vacuo* affording **6** as a deep purple solid (90 mg, 53% yield). Anal. calculated for $\text{C}_{34}\text{H}_{22}\text{F}_3\text{N}_5\text{O}_4\text{RuS} + 1/2 \text{CH}_2\text{Cl}_2$: C, 51.98; H, 2.91; N, 8.79. Found: C, 52.51; H, 3.26; N, 8.65. MS (ES, m/z): calcd for $\text{C}_{33}\text{H}_{22}\text{N}_5\text{ORu}$: 606.08; found: 606.07.

^1H NMR (500MHz, CD_3CN): δ = 9.17 (dd, 1H, $^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.2$, H_o), 8.55 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=1.2$, H_p), 8.52 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=1.2$, H_p), 8.4 (dd, 1H, $^3J_{\text{HH}}=5.2$, $^4J_{\text{HH}}=1.2$, H_o), 8.37 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.2$, H_p), 8.35 (dd, 1H, $^3J_{\text{HH}}=8.2$, $^4J_{\text{HH}}=1.1$, H_p), 8.2-8.11 (m, 5H), 8.02 (dd, 1H, $^3J_{\text{HH}}=8.7$, H_1), 7.90 (dd, 1H, $^3J_{\text{HH}}=5.3$, $^4J_{\text{HH}}=1.1$, H_o), 7.88 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^3J_{\text{HH}}=5.3$, H_m), 7.71 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=5.2$, H_m), 7.45 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=5.3$, H_m), 7.43 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=5.3$, H_m), 7.40 (dd, 1H, $^3J_{\text{HH}}=5.0$, $^4J_{\text{HH}}=1.2$, H_3), 7.32 (t, 1H, $^3J_{\text{HH}}=8.0$, H_6), 7.02 (dd, 1H, $^3J_{\text{HH}}=8.4$, $^4J_{\text{HH}}=5.0$, H_2), 6.88 (dd, 1H, $^3J_{\text{HH}}=8.0$, $^4J_{\text{HH}}=1.0$, $\text{H}_{5/7}$), 6.78 (dd, 1H, $^3J_{\text{HH}}=8.0$, $^4J_{\text{HH}}=1.0$, $\text{H}_{5/7}$)

^{13}C NMR (125 MHz, CD_3CN): 170.74, 154.84, 153.55, 152.29, 151.07, 149.81, 149.59, 149.53, 147.74, 146.68, 136.51, 135.96, 135.91, 135.68, 134.87, 131.68, 131.53, 131.50, 131.40, 131.18, 130.67, 128.60, 128.53, 126.30, 126.20, 126.00, 125.64, 122.63, 115.92, 111.15.

[Ru (Me-N⁺C⁺N) (NCMe)₃] PF₆

To a suspension of $[(\eta^6\text{-bz})\text{RuCl}_2]_2$ (110 mg, 0.215 mmol), NaOH (17 mg, 0.430 mmol) and KPF_6 (154 mg, 0.840 mmol) in acetonitrile (10 mL) was added 3,5-di(2-pyridyl)toluene (53 mg, 0.215 mmol). The mixture was refluxed for 72 h under the light of an incandescent lamp irradiation. The solvent was removed *in vacuo*, and the dark residue was dissolved in CH_2Cl_2 (10 mL). The solution was filtered through Al_2O_3 , using a 10:1 $\text{CH}_2\text{Cl}_2/\text{NCMe}$ mixture as eluent. The dark yellow fraction was collected and concentrated to about 1 mL. Addition of diethyl ether (10 mL) caused the precipitation of a dark yellow solid (151 mg, 73% yield).

HRMS (ES, m/z): Calcd. for $\text{C}_{23}\text{H}_{22}\text{N}_5^{101}\text{Ru}$: 470.0918; Found: 470.0922

^1H NMR (300 MHz, CD_3CN , 300 K): δ = 8.99 (d, 2H, $^3J_{\text{HH}}=5.5$, H_1), 8.00 (d, 2H, $^3J_{\text{HH}}=8.2$, H_4), 7.76 (td, 2H, $^3J_{\text{HH}}=8.0$, $^4J_{\text{HH}}=1.5$, H_3), 7.74 (s, 2H, H_5), 7.24 (td, 2H, $^3J_{\text{HH}}=5.5$, $^4J_{\text{HH}}=1.5$, H_2), 2.59 (s, 3H, Me), 2.00 (s, 3H, NCMe), 1.96 (s, 6H, NCMe).

^{13}C { ^1H } NMR (78 MHz, CD_3CN , 300 K): δ = 171.2, 155.3, 151.9, 145.6, 140.0, 135.8, 128.7, 123.4, 122.7, 120.0, 118.7, 112.2, 20.8, 2.61

7b

A solution of $[\text{Ru}(\text{MeO}_2\text{C}-\text{N}^+\text{C}(\text{H})\text{N})(\text{NCMe})_3]\text{PF}_6$ ⁴ (18 mg, 0.027) with 1,10 phenanthroline (5.4 mg, 0.027 mmol) in methanol (2 mL) was refluxed for 12h. The solvent was evaporated under vacuum, and the dark brown residue was dissolved in 5 mL of MeCN and filtered through Al_2O_3 using NCMe as eluent. The purple fraction was collected and evaporated to dryness under vacuum. Crystallization from CH_2Cl_2 /pentane or acetone/pentane (slow diffusion) gave dark purple crystals, which were washed with diethyl ether and dried under vacuum (18 mg, 88% yield).

Anal. calcd. for $\text{C}_{32}\text{H}_{24}\text{F}_6\text{N}_5\text{O}_2\text{PRu}$: C, 50.80; H, 3.20; N, 9.26. Found: C, 50.32; H, 3.25; N, 9.26%.

MS (ES, m/z) : Calcd. for $\text{C}_{32}\text{H}_{24}\text{O}_2^{101}\text{Ru}$: 612.09; Found : 612.09

^1H NMR (400 MHz, CD_3CN , 300 K) : δ = 10.02 (dd, 1H, $^3J_{\text{HH}}=5.1$, $^4J_{\text{HH}}=1.5$, H_o), 8.81 (dd, 1H, $^3J_{\text{HH}}=7.5$, $^4J_{\text{HH}}=1.5$, H_p), 8.62 (s, 2H, H_5), 8.35 (dd, 1H, $^3J_{\text{HH}}=7.5$, $^3J_{\text{HH}}=5.1$, H_m), 8.21 (d, 1H, $^3J_{\text{HH}}=8.8$, H_phen), 8.20 (d, 2H, $^3J_{\text{HH}}=8.0$, H_1), 8.06 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^4J_{\text{HH}}=1.5$, H_o), 7.99 (d, 1H, $^3J_{\text{HH}}=8.8$, H_phen), 7.70 (td, 2H, $^3J_{\text{HH}}=7.5$, $^4J_{\text{HH}}=1.5$, H_2), 7.57 (d, 2H, $^3J_{\text{HH}}=7.5$, H_4), 7.32 (dd, 1H, $^3J_{\text{HH}}=5.1$, $^4J_{\text{HH}}=1.5$, H_p), 7.11 (dd, 1H, $^3J_{\text{HH}}=8.3$, $^3J_{\text{HH}}=5.1$, H_m), 6.81 (td, 2H, $^3J_{\text{HH}}=7.5$, $^4J_{\text{HH}}=1.5$, H_3), 4.05 (s, 3H, CH_3), 2.10 (s, 3H, NCCH_3).

^{13}C NMR (100 MHz, CD_3CN , 300 K) : δ = 230.9, 169.1, 168.5, 155.3, 153.8, 151.2, 150.0, 146.2, 145.4, 137.2, 136.1, 134.8, 131.7, 131.1, 128.8, 128.4, 127.0, 126.4, 125.2, 124.4, 123.4, 122.8, 120.7, 50.6, 4.43

8c

1,3-dipyridylbenzene (14 mg, 60 μmoles) and N-ethylmorpholine (1 drop) were added to a suspension of $\text{Ru}(\text{N,Ndimethylamino})\text{-}2,2':6',2''\text{-terpyridineCl}_3$ ⁵ (29 mg, 60 μmoles) in ethanol (5 mL) and the mixture was heated at reflux temperature for 1 hour. The resulting violet solution was filtered through celite and then aqueous KPF_6 solution was added to the filtrate to precipitate the product. This was collected by filtration, washed with water, air dried and purified by chromatography on silica gel using a CH_2Cl_2 -MeOH (98:2) mixture. Yield: 34 mg, 75%. HRMS (ES, m/z): calc. for M^+ : 609.1344; found: 609.1376. ^1H NMR (300 MHz, CD_3CN): δ = 8.39 (d, 2H, 9Hz), 8.24 (d, 2H, 7.7 Hz), 8.13 (d, 2H, 7.3 Hz), 7.98 (s, 2H), 7.58 (m, 4H), 7.37 (t, 1H, 7.7 Hz), 7.26 (d, 2H, 4.9 Hz), 6.93 (d, 2H; 5.5 Hz), 6.83 (dd, 2H, 7.3 and 1.3 Hz), 6.73 (dd, 2H, 5.7 and 1.4 Hz), 3.48 (s, 6H).

⁴ S.H. Wadman, M. Lutz, S. M. Tooke, A. L. Spek, F. Hartl, R. W. A. Havenith, G. van Klink and G. van Koten, *Inorg. Chem.*, 2009, **48**, 5685.

⁵ E. C.; Constable, A. M. W. Cargill Thompson, D. A. Tocher, M. A. M. Daniels *New J. Chem.* 1992, **16**, 855.

X-ray diffraction study of **1c**.

ORTEP view of the cationic part of **1c**, H atoms are omitted for clarity.

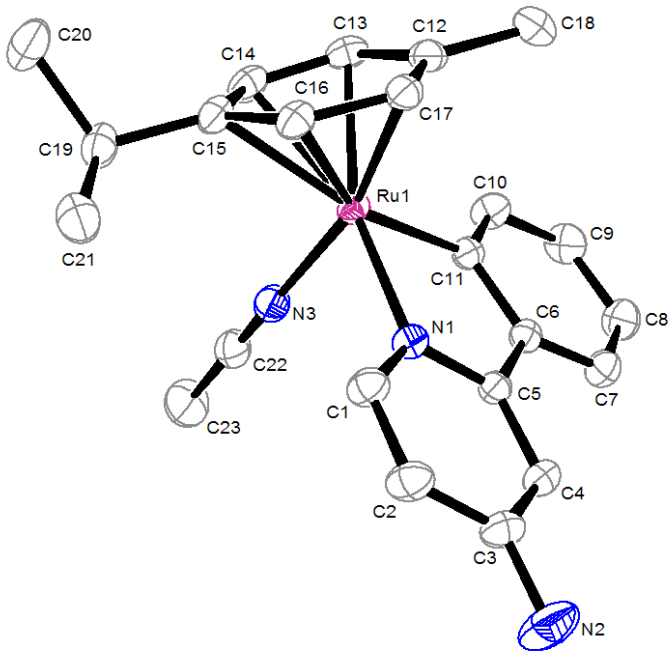


Table 1. Crystal data and structure refinement for mpam100325.

Identification code	1c
Empirical formula	C ₂₃ H ₂₆ F ₆ N ₃ P Ru
Formula weight	590.51
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 2 ₁ /c
Unit cell dimensions	a = 9.3585(3) Å alpha = 90 deg. b = 10.3118(3) Å beta = 105.7030(10) deg. c = 26.0322(8) Å gamma = 90 deg.
Volume	2418.42(13) Å ³
Z, Calculated density	4, 1.622 Mg/m ³
Absorption coefficient	0.777 mm ⁻¹
F(000)	1192
Crystal size	0.35 x 0.28 x 0.18 mm

Theta range for data collection	1.63 to 32.53 deg.
Limiting indices	-14<=h<=14, -11<=k<=15, -34<=l<=39
Reflections collected / unique	24784 / 8733 [R(int) = 0.0153]
Completeness to theta = 32.53	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8733 and 0.7734
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8733 / 0 / 319
Goodness-of-fit on F ²	1.240
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0648
R indices (all data)	R1 = 0.0379, wR2 = 0.0677
Largest diff. peak and hole	0.799 and -1.700 e.A ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (A² x 10³) for mpam100325.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	3294(1)	-264(1)	8338(1)	18(1)
N(1)	4977(2)	946(1)	8777(1)	21(1)
N(2)	8370(2)	3395(2)	9579(1)	46(1)
N(3)	4493(2)	-1796(2)	8743(1)	26(1)
C(1)	4953(2)	1535(2)	9237(1)	26(1)
C(2)	6042(2)	2352(2)	9514(1)	29(1)
C(3)	7264(2)	2604(2)	9315(1)	27(1)
C(4)	7302(2)	1991(2)	8840(1)	25(1)
C(5)	6161(2)	1173(2)	8580(1)	20(1)
C(6)	6087(2)	459(2)	8088(1)	20(1)
C(7)	7189(2)	518(2)	7816(1)	27(1)
C(8)	7049(2)	-217(2)	7357(1)	32(1)
C(9)	5832(2)	-1028(2)	7178(1)	31(1)
C(10)	4747(2)	-1101(2)	7452(1)	27(1)
C(11)	4828(2)	-340(2)	7905(1)	20(1)
C(12)	1603(2)	464(2)	7632(1)	25(1)
C(13)	1377(2)	-894(2)	7696(1)	26(1)
C(14)	1230(2)	-1372(2)	8187(1)	26(1)
C(15)	1174(2)	-534(2)	8621(1)	23(1)
C(16)	1405(2)	784(2)	8554(1)	23(1)
C(17)	1653(2)	1277(2)	8071(1)	24(1)
C(18)	1824(2)	991(2)	7122(1)	34(1)
C(19)	946(2)	-1105(2)	9131(1)	28(1)
C(20)	-689(2)	-1463(2)	9048(1)	39(1)
C(21)	1458(3)	-221(3)	9615(1)	42(1)
C(22)	5144(2)	-2695(2)	8923(1)	30(1)
C(23)	5980(3)	-3858(2)	9139(1)	46(1)
P(1)	1794(1)	4545(1)	9116(1)	27(1)
F(1)	1779(2)	3359(2)	9510(1)	53(1)
F(2)	2971(2)	3807(1)	8886(1)	41(1)

F(3)	3095(2)	5220(2)	9564(1)	52(1)
F(4)	587(2)	5292(2)	9343(1)	52(1)
F(5)	473(2)	3861(1)	8680(1)	48(1)
F(6)	1791(2)	5724(1)	8725(1)	49(1)

Table 3. Bond lengths [Å] and angles [deg] for mpam100325.

Ru(1)-C(11)	2.0543(16)
Ru(1)-N(3)	2.0553(16)
Ru(1)-N(1)	2.0899(15)
Ru(1)-C(14)	2.1863(18)
Ru(1)-C(17)	2.1888(17)
Ru(1)-C(13)	2.1942(18)
Ru(1)-C(12)	2.2083(18)
Ru(1)-C(16)	2.2683(17)
Ru(1)-C(15)	2.3123(17)
N(1)-C(1)	1.348(2)
N(1)-C(5)	1.362(2)
N(2)-C(3)	1.350(3)
N(2)-H(2N)	0.86(3)
N(2)-H(1N)	0.85(3)
N(3)-C(22)	1.138(3)
C(1)-C(2)	1.368(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.401(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.399(3)
C(4)-C(5)	1.386(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.463(2)
C(6)-C(7)	1.402(2)
C(6)-C(11)	1.410(2)
C(7)-C(8)	1.390(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.388(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.392(3)
C(9)-H(9)	0.9500
C(10)-C(11)	1.401(2)
C(10)-H(10)	0.9500
C(12)-C(17)	1.408(3)
C(12)-C(13)	1.432(3)
C(12)-C(18)	1.500(3)
C(13)-C(14)	1.412(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.435(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.395(2)
C(15)-C(19)	1.519(3)
C(16)-C(17)	1.432(3)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(21)	1.522(3)
C(19)-C(20)	1.532(3)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800

C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.459(3)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
P(1)-F(2)	1.5841(14)
P(1)-F(6)	1.5863(15)
P(1)-F(1)	1.5977(15)
P(1)-F(5)	1.5982(15)
P(1)-F(3)	1.5998(15)
P(1)-F(4)	1.6068(15)
C(11)-Ru(1)-N(3)	83.51(6)
C(11)-Ru(1)-N(1)	77.76(6)
N(3)-Ru(1)-N(1)	87.29(6)
C(11)-Ru(1)-C(14)	126.58(7)
N(3)-Ru(1)-C(14)	91.35(7)
N(1)-Ru(1)-C(14)	155.32(7)
C(11)-Ru(1)-C(17)	112.78(7)
N(3)-Ru(1)-C(17)	163.70(7)
N(1)-Ru(1)-C(17)	95.78(6)
C(14)-Ru(1)-C(17)	79.18(7)
C(11)-Ru(1)-C(13)	96.80(7)
N(3)-Ru(1)-C(13)	112.55(7)
N(1)-Ru(1)-C(13)	158.93(7)
C(14)-Ru(1)-C(13)	37.61(7)
C(17)-Ru(1)-C(13)	67.27(7)
C(11)-Ru(1)-C(12)	90.28(7)
N(3)-Ru(1)-C(12)	148.97(7)
N(1)-Ru(1)-C(12)	121.11(6)
C(14)-Ru(1)-C(12)	68.19(7)
C(17)-Ru(1)-C(12)	37.35(7)
C(13)-Ru(1)-C(12)	37.96(7)
C(11)-Ru(1)-C(16)	149.47(7)
N(3)-Ru(1)-C(16)	126.39(7)
N(1)-Ru(1)-C(16)	95.89(6)
C(14)-Ru(1)-C(16)	65.42(7)
C(17)-Ru(1)-C(16)	37.43(7)
C(13)-Ru(1)-C(16)	78.38(7)
C(12)-Ru(1)-C(16)	67.25(7)
C(11)-Ru(1)-C(15)	163.32(7)
N(3)-Ru(1)-C(15)	98.09(6)
N(1)-Ru(1)-C(15)	118.84(6)
C(14)-Ru(1)-C(15)	37.06(7)
C(17)-Ru(1)-C(15)	66.41(6)
C(13)-Ru(1)-C(15)	67.17(7)
C(12)-Ru(1)-C(15)	79.78(7)
C(16)-Ru(1)-C(15)	35.44(6)
C(1)-N(1)-C(5)	117.95(15)
C(1)-N(1)-Ru(1)	124.29(12)
C(5)-N(1)-Ru(1)	117.75(11)
C(3)-N(2)-H(2N)	119(2)
C(3)-N(2)-H(1N)	119(2)
H(2N)-N(2)-H(1N)	121(3)
C(22)-N(3)-Ru(1)	173.81(18)
N(1)-C(1)-C(2)	123.80(17)
N(1)-C(1)-H(1)	118.1
C(2)-C(1)-H(1)	118.1
C(1)-C(2)-C(3)	119.06(18)
C(1)-C(2)-H(2)	120.5
C(3)-C(2)-H(2)	120.5
N(2)-C(3)-C(4)	121.51(19)

N(2) - C(3) - C(2)	120.95 (19)
C(4) - C(3) - C(2)	117.54 (17)
C(5) - C(4) - C(3)	120.42 (17)
C(5) - C(4) - H(4)	119.8
C(3) - C(4) - H(4)	119.8
N(1) - C(5) - C(4)	121.22 (16)
N(1) - C(5) - C(6)	113.18 (15)
C(4) - C(5) - C(6)	125.59 (16)
C(7) - C(6) - C(11)	121.06 (16)
C(7) - C(6) - C(5)	123.62 (16)
C(11) - C(6) - C(5)	115.30 (14)
C(8) - C(7) - C(6)	119.95 (18)
C(8) - C(7) - H(7)	120.0
C(6) - C(7) - H(7)	120.0
C(9) - C(8) - C(7)	119.66 (17)
C(9) - C(8) - H(8)	120.2
C(7) - C(8) - H(8)	120.2
C(8) - C(9) - C(10)	120.42 (18)
C(8) - C(9) - H(9)	119.8
C(10) - C(9) - H(9)	119.8
C(9) - C(10) - C(11)	121.35 (18)
C(9) - C(10) - H(10)	119.3
C(11) - C(10) - H(10)	119.3
C(10) - C(11) - C(6)	117.50 (15)
C(10) - C(11) - Ru(1)	126.67 (13)
C(6) - C(11) - Ru(1)	115.84 (12)
C(17) - C(12) - C(13)	117.46 (17)
C(17) - C(12) - C(18)	121.35 (18)
C(13) - C(12) - C(18)	121.16 (18)
C(17) - C(12) - Ru(1)	70.57 (10)
C(13) - C(12) - Ru(1)	70.48 (11)
C(18) - C(12) - Ru(1)	128.40 (13)
C(14) - C(13) - C(12)	120.03 (17)
C(14) - C(13) - Ru(1)	70.89 (10)
C(12) - C(13) - Ru(1)	71.55 (10)
C(14) - C(13) - H(13)	120.0
C(12) - C(13) - H(13)	120.0
Ru(1) - C(13) - H(13)	130.1

C(13) - C(14) - C(15)	122.42 (17)
C(13) - C(14) - Ru(1)	71.50 (10)
C(15) - C(14) - Ru(1)	76.25 (10)
C(13) - C(14) - H(14)	118.8
C(15) - C(14) - H(14)	118.8
Ru(1) - C(14) - H(14)	125.2
C(16) - C(15) - C(14)	116.64 (17)
C(16) - C(15) - C(19)	123.39 (17)
C(14) - C(15) - C(19)	119.89 (16)
C(16) - C(15) - Ru(1)	70.56 (10)
C(14) - C(15) - Ru(1)	66.69 (9)
C(19) - C(15) - Ru(1)	131.30 (13)
C(15) - C(16) - C(17)	121.55 (17)
C(15) - C(16) - Ru(1)	74.00 (10)
C(17) - C(16) - Ru(1)	68.27 (10)
C(15) - C(16) - H(16)	119.2
C(17) - C(16) - H(16)	119.2
Ru(1) - C(16) - H(16)	131.4
C(12) - C(17) - C(16)	121.59 (17)
C(12) - C(17) - Ru(1)	72.07 (10)
C(16) - C(17) - Ru(1)	74.30 (10)
C(12) - C(17) - H(17)	119.2
C(16) - C(17) - H(17)	119.2
Ru(1) - C(17) - H(17)	126.4
C(12) - C(18) - H(18A)	109.5
C(12) - C(18) - H(18B)	109.5

H(18A)-C(18)-H(18B)	109.5
C(12)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(15)-C(19)-C(21)	113.82(17)
C(15)-C(19)-C(20)	109.89(17)
C(21)-C(19)-C(20)	109.89(18)
C(15)-C(19)-H(19)	107.7
C(21)-C(19)-H(19)	107.7
C(20)-C(19)-H(19)	107.7
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(23)	178.4(2)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
F(2)-P(1)-F(6)	90.32(8)
F(2)-P(1)-F(1)	90.16(9)
F(6)-P(1)-F(1)	179.40(10)
F(2)-P(1)-F(5)	90.18(8)
F(6)-P(1)-F(5)	90.91(9)
F(1)-P(1)-F(5)	88.73(9)
F(2)-P(1)-F(3)	90.88(9)
F(6)-P(1)-F(3)	90.21(9)
F(1)-P(1)-F(3)	90.14(9)
F(5)-P(1)-F(3)	178.45(9)
F(2)-P(1)-F(4)	179.34(9)
F(6)-P(1)-F(4)	89.40(9)
F(1)-P(1)-F(4)	90.11(9)
F(5)-P(1)-F(4)	89.22(9)
F(3)-P(1)-F(4)	89.72(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mpam100325.
The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ru(1)	17(1)	16(1)	21(1)	0(1)	5(1)	-1(1)
N(1)	19(1)	21(1)	22(1)	-1(1)	5(1)	0(1)
N(2)	36(1)	56(1)	47(1)	-24(1)	14(1)	-22(1)
N(3)	24(1)	25(1)	30(1)	3(1)	8(1)	0(1)
C(1)	23(1)	29(1)	26(1)	-5(1)	8(1)	-3(1)

C (2)	26 (1)	33 (1)	26 (1)	-9 (1)	6 (1)	-3 (1)
C (3)	24 (1)	26 (1)	29 (1)	-5 (1)	3 (1)	-5 (1)
C (4)	21 (1)	27 (1)	27 (1)	-1 (1)	6 (1)	-6 (1)
C (5)	18 (1)	19 (1)	21 (1)	2 (1)	4 (1)	1 (1)
C (6)	20 (1)	19 (1)	22 (1)	1 (1)	6 (1)	1 (1)
C (7)	24 (1)	30 (1)	29 (1)	1 (1)	10 (1)	-1 (1)
C (8)	29 (1)	40 (1)	30 (1)	-1 (1)	16 (1)	2 (1)
C (9)	33 (1)	36 (1)	27 (1)	-6 (1)	12 (1)	3 (1)
C (10)	26 (1)	28 (1)	28 (1)	-7 (1)	8 (1)	-2 (1)
C (11)	20 (1)	19 (1)	21 (1)	0 (1)	5 (1)	0 (1)
C (12)	20 (1)	25 (1)	26 (1)	1 (1)	1 (1)	0 (1)
C (13)	20 (1)	27 (1)	30 (1)	-7 (1)	2 (1)	-3 (1)
C (14)	21 (1)	20 (1)	37 (1)	-3 (1)	8 (1)	-5 (1)
C (15)	19 (1)	20 (1)	33 (1)	2 (1)	10 (1)	0 (1)
C (16)	19 (1)	19 (1)	30 (1)	0 (1)	9 (1)	2 (1)
C (17)	20 (1)	20 (1)	31 (1)	4 (1)	5 (1)	1 (1)
C (18)	33 (1)	40 (1)	25 (1)	6 (1)	2 (1)	2 (1)
C (19)	27 (1)	24 (1)	37 (1)	7 (1)	15 (1)	2 (1)
C (20)	34 (1)	44 (1)	44 (1)	-4 (1)	20 (1)	-12 (1)
C (21)	44 (1)	49 (1)	30 (1)	6 (1)	8 (1)	-11 (1)
C (22)	28 (1)	28 (1)	34 (1)	7 (1)	8 (1)	0 (1)
C (23)	41 (1)	35 (1)	60 (2)	20 (1)	11 (1)	11 (1)
P (1)	34 (1)	22 (1)	28 (1)	-2 (1)	12 (1)	-2 (1)
F (1)	75 (1)	43 (1)	44 (1)	15 (1)	24 (1)	-5 (1)
F (2)	44 (1)	39 (1)	44 (1)	-1 (1)	20 (1)	11 (1)
F (3)	50 (1)	61 (1)	43 (1)	-17 (1)	8 (1)	-16 (1)
F (4)	53 (1)	44 (1)	72 (1)	-20 (1)	37 (1)	-4 (1)
F (5)	44 (1)	37 (1)	54 (1)	-14 (1)	-3 (1)	-1 (1)
F (6)	71 (1)	28 (1)	53 (1)	12 (1)	26 (1)	7 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for mpam100325.

	x	y	z	U(eq)
H (1)	4132	1373	9377	31
H (2)	5971	2744	9837	35
H (4)	8116	2138	8694	30
H (7)	8031	1060	7944	32
H (8)	7783	-165	7167	38
H (9)	5739	-1537	6866	38
H (10)	3935	-1678	7329	33
H (13)	1326	-1473	7407	32
H (14)	1166	-2283	8232	31
H (16)	1399	1369	8835	27
H (17)	1856	2174	8046	28
H (18A)	856	1150	6868	50
H (18B)	2380	362	6969	50
H (18C)	2381	1806	7194	50
H (19)	1540	-1923	9210	34
H (20A)	-1293	-673	8989	58
H (20B)	-810	-1915	9364	58
H (20C)	-1011	-2031	8736	58
H (21A)	2517	-32	9677	62
H (21B)	1293	-653	9929	62
H (21C)	892	590	9550	62
H (23A)	5375	-4627	9010	68
H (23B)	6236	-3834	9530	68
H (23C)	6892	-3894	9023	68
H (2N)	9090 (30)	3560 (30)	9443 (12)	51 (8)
H (1N)	8330 (30)	3730 (30)	9873 (13)	55 (9)

Table 6. Torsion angles [deg] for mpam100325.

C(11)-Ru(1)-N(1)-C(1)	-177.83(16)
N(3)-Ru(1)-N(1)-C(1)	-93.88(16)
C(14)-Ru(1)-N(1)-C(1)	-6.6(3)
C(17)-Ru(1)-N(1)-C(1)	70.06(16)
C(13)-Ru(1)-N(1)-C(1)	105.2(2)
C(12)-Ru(1)-N(1)-C(1)	99.36(16)
C(16)-Ru(1)-N(1)-C(1)	32.43(16)
C(15)-Ru(1)-N(1)-C(1)	3.86(17)
C(11)-Ru(1)-N(1)-C(5)	3.53(12)
N(3)-Ru(1)-N(1)-C(5)	87.48(13)
C(14)-Ru(1)-N(1)-C(5)	174.81(15)
C(17)-Ru(1)-N(1)-C(5)	-108.57(13)
C(13)-Ru(1)-N(1)-C(5)	-73.4(2)
C(12)-Ru(1)-N(1)-C(5)	-79.28(14)
C(16)-Ru(1)-N(1)-C(5)	-146.21(13)
C(15)-Ru(1)-N(1)-C(5)	-174.78(12)
C(5)-N(1)-C(1)-C(2)	0.4(3)
Ru(1)-N(1)-C(1)-C(2)	-178.19(16)
N(1)-C(1)-C(2)-C(3)	-0.1(3)
C(1)-C(2)-C(3)-N(2)	-179.4(2)
C(1)-C(2)-C(3)-C(4)	-0.2(3)
N(2)-C(3)-C(4)-C(5)	179.4(2)
C(2)-C(3)-C(4)-C(5)	0.2(3)
C(1)-N(1)-C(5)-C(4)	-0.5(3)
Ru(1)-N(1)-C(5)-C(4)	178.24(13)
C(1)-N(1)-C(5)-C(6)	178.54(16)
Ru(1)-N(1)-C(5)-C(6)	-2.74(19)
C(3)-C(4)-C(5)-N(1)	0.2(3)
C(3)-C(4)-C(5)-C(6)	-178.72(17)
N(1)-C(5)-C(6)-C(7)	-178.84(16)
C(4)-C(5)-C(6)-C(7)	0.1(3)
N(1)-C(5)-C(6)-C(11)	-0.4(2)
C(4)-C(5)-C(6)-C(11)	178.56(17)
C(11)-C(6)-C(7)-C(8)	0.1(3)
C(5)-C(6)-C(7)-C(8)	178.42(18)
C(6)-C(7)-C(8)-C(9)	-1.4(3)
C(7)-C(8)-C(9)-C(10)	0.6(3)
C(8)-C(9)-C(10)-C(11)	1.6(3)
C(9)-C(10)-C(11)-C(6)	-2.9(3)
C(9)-C(10)-C(11)-Ru(1)	177.31(15)
C(7)-C(6)-C(11)-C(10)	2.0(3)
C(5)-C(6)-C(11)-C(10)	-176.46(16)
C(7)-C(6)-C(11)-Ru(1)	-178.15(14)
C(5)-C(6)-C(11)-Ru(1)	3.38(19)
N(3)-Ru(1)-C(11)-C(10)	87.58(17)
N(1)-Ru(1)-C(11)-C(10)	176.19(17)
C(14)-Ru(1)-C(11)-C(10)	0.7(2)
C(17)-Ru(1)-C(11)-C(10)	-92.62(17)
C(13)-Ru(1)-C(11)-C(10)	-24.46(17)
C(12)-Ru(1)-C(11)-C(10)	-61.95(17)
C(16)-Ru(1)-C(11)-C(10)	-103.07(19)
C(15)-Ru(1)-C(11)-C(10)	-9.0(3)
N(3)-Ru(1)-C(11)-C(6)	-92.24(13)
N(1)-Ru(1)-C(11)-C(6)	-3.62(12)
C(14)-Ru(1)-C(11)-C(6)	-179.10(12)
C(17)-Ru(1)-C(11)-C(6)	87.57(14)
C(13)-Ru(1)-C(11)-C(6)	155.72(13)
C(12)-Ru(1)-C(11)-C(6)	118.23(13)
C(16)-Ru(1)-C(11)-C(6)	77.11(18)
C(15)-Ru(1)-C(11)-C(6)	171.22(18)

C(11)-Ru(1)-C(12)-C(17)	-129.19(11)
N(3)-Ru(1)-C(12)-C(17)	153.00(12)
N(1)-Ru(1)-C(12)-C(17)	-53.35(12)
C(14)-Ru(1)-C(12)-C(17)	101.02(12)
C(13)-Ru(1)-C(12)-C(17)	130.08(16)
C(16)-Ru(1)-C(12)-C(17)	29.57(10)
C(15)-Ru(1)-C(12)-C(17)	64.27(11)
C(11)-Ru(1)-C(12)-C(13)	100.73(11)
N(3)-Ru(1)-C(12)-C(13)	22.92(18)
N(1)-Ru(1)-C(12)-C(13)	176.57(10)
C(14)-Ru(1)-C(12)-C(13)	-29.06(11)
C(17)-Ru(1)-C(12)-C(13)	-130.08(16)
C(16)-Ru(1)-C(12)-C(13)	-100.51(12)
C(15)-Ru(1)-C(12)-C(13)	-65.81(11)
C(11)-Ru(1)-C(12)-C(18)	-14.08(18)
N(3)-Ru(1)-C(12)-C(18)	-91.9(2)
N(1)-Ru(1)-C(12)-C(18)	61.8(2)
C(14)-Ru(1)-C(12)-C(18)	-143.9(2)
C(17)-Ru(1)-C(12)-C(18)	115.1(2)
C(13)-Ru(1)-C(12)-C(18)	-114.8(2)
C(16)-Ru(1)-C(12)-C(18)	144.7(2)
C(15)-Ru(1)-C(12)-C(18)	179.38(19)
C(17)-C(12)-C(13)-C(14)	-0.7(3)
C(18)-C(12)-C(13)-C(14)	177.51(17)
Ru(1)-C(12)-C(13)-C(14)	53.74(15)
C(17)-C(12)-C(13)-Ru(1)	-54.41(14)
C(18)-C(12)-C(13)-Ru(1)	123.77(17)
C(11)-Ru(1)-C(13)-C(14)	145.96(11)
N(3)-Ru(1)-C(13)-C(14)	60.18(12)
N(1)-Ru(1)-C(13)-C(14)	-140.57(17)
C(17)-Ru(1)-C(13)-C(14)	-102.15(12)
C(12)-Ru(1)-C(13)-C(14)	-132.37(16)
C(16)-Ru(1)-C(13)-C(14)	-64.60(11)
C(15)-Ru(1)-C(13)-C(14)	-29.27(11)
C(11)-Ru(1)-C(13)-C(12)	-81.67(11)
N(3)-Ru(1)-C(13)-C(12)	-167.45(10)
N(1)-Ru(1)-C(13)-C(12)	-8.2(2)
C(14)-Ru(1)-C(13)-C(12)	132.37(16)
C(17)-Ru(1)-C(13)-C(12)	30.22(11)
C(16)-Ru(1)-C(13)-C(12)	67.77(11)
C(15)-Ru(1)-C(13)-C(12)	103.10(12)
C(12)-C(13)-C(14)-C(15)	5.3(3)
Ru(1)-C(13)-C(14)-C(15)	59.37(16)
C(12)-C(13)-C(14)-Ru(1)	-54.05(15)
C(11)-Ru(1)-C(14)-C(13)	-43.80(14)
N(3)-Ru(1)-C(14)-C(13)	-126.73(12)
N(1)-Ru(1)-C(14)-C(13)	146.84(15)
C(17)-Ru(1)-C(14)-C(13)	66.63(12)
C(12)-Ru(1)-C(14)-C(13)	29.31(11)
C(16)-Ru(1)-C(14)-C(13)	103.35(12)
C(15)-Ru(1)-C(14)-C(13)	131.60(16)
C(11)-Ru(1)-C(14)-C(15)	-175.41(10)
N(3)-Ru(1)-C(14)-C(15)	101.67(11)
N(1)-Ru(1)-C(14)-C(15)	15.2(2)
C(17)-Ru(1)-C(14)-C(15)	-64.97(11)
C(13)-Ru(1)-C(14)-C(15)	-131.60(16)
C(12)-Ru(1)-C(14)-C(15)	-102.29(12)
C(16)-Ru(1)-C(14)-C(15)	-28.26(10)
C(13)-C(14)-C(15)-C(16)	-5.6(3)
Ru(1)-C(14)-C(15)-C(16)	51.56(15)
C(13)-C(14)-C(15)-C(19)	177.31(17)
Ru(1)-C(14)-C(15)-C(19)	-125.54(16)
C(13)-C(14)-C(15)-Ru(1)	-57.15(15)
C(11)-Ru(1)-C(15)-C(16)	-119.1(2)
N(3)-Ru(1)-C(15)-C(16)	146.49(11)
N(1)-Ru(1)-C(15)-C(16)	55.13(13)

C(14)-Ru(1)-C(15)-C(16)	-132.06(17)
C(17)-Ru(1)-C(15)-C(16)	-28.26(11)
C(13)-Ru(1)-C(15)-C(16)	-102.38(13)
C(12)-Ru(1)-C(15)-C(16)	-64.88(12)
C(11)-Ru(1)-C(15)-C(14)	13.0(3)
N(3)-Ru(1)-C(15)-C(14)	-81.45(12)
N(1)-Ru(1)-C(15)-C(14)	-172.81(10)
C(17)-Ru(1)-C(15)-C(14)	103.80(12)
C(13)-Ru(1)-C(15)-C(14)	29.68(11)
C(12)-Ru(1)-C(15)-C(14)	67.18(12)
C(16)-Ru(1)-C(15)-C(14)	132.06(17)
C(11)-Ru(1)-C(15)-C(19)	123.1(2)
N(3)-Ru(1)-C(15)-C(19)	28.66(18)
N(1)-Ru(1)-C(15)-C(19)	-62.69(18)
C(14)-Ru(1)-C(15)-C(19)	110.1(2)
C(17)-Ru(1)-C(15)-C(19)	-146.09(19)
C(13)-Ru(1)-C(15)-C(19)	139.79(19)
C(12)-Ru(1)-C(15)-C(19)	177.30(18)
C(16)-Ru(1)-C(15)-C(19)	-117.8(2)
C(14)-C(15)-C(16)-C(17)	1.4(3)
C(19)-C(15)-C(16)-C(17)	178.37(16)
Ru(1)-C(15)-C(16)-C(17)	51.10(15)
C(14)-C(15)-C(16)-Ru(1)	-49.72(14)
C(19)-C(15)-C(16)-Ru(1)	127.27(17)
C(11)-Ru(1)-C(16)-C(15)	150.42(13)
N(3)-Ru(1)-C(16)-C(15)	-42.76(14)
N(1)-Ru(1)-C(16)-C(15)	-133.73(11)
C(14)-Ru(1)-C(16)-C(15)	29.48(11)
C(17)-Ru(1)-C(16)-C(15)	134.44(17)
C(13)-Ru(1)-C(16)-C(15)	66.79(12)
C(12)-Ru(1)-C(16)-C(15)	104.93(12)
C(11)-Ru(1)-C(16)-C(17)	15.98(18)
N(3)-Ru(1)-C(16)-C(17)	-177.21(10)
N(1)-Ru(1)-C(16)-C(17)	91.82(11)
C(14)-Ru(1)-C(16)-C(17)	-104.97(12)
C(13)-Ru(1)-C(16)-C(17)	-67.65(11)
C(12)-Ru(1)-C(16)-C(17)	-29.51(11)
C(15)-Ru(1)-C(16)-C(17)	-134.44(17)
C(13)-C(12)-C(17)-C(16)	-3.4(3)
C(18)-C(12)-C(17)-C(16)	178.39(17)
Ru(1)-C(12)-C(17)-C(16)	-57.80(15)
C(13)-C(12)-C(17)-Ru(1)	54.37(14)
C(18)-C(12)-C(17)-Ru(1)	-123.81(17)
C(15)-C(16)-C(17)-C(12)	3.1(3)
Ru(1)-C(16)-C(17)-C(12)	56.75(15)
C(15)-C(16)-C(17)-Ru(1)	-53.64(15)
C(11)-Ru(1)-C(17)-C(12)	57.20(12)
N(3)-Ru(1)-C(17)-C(12)	-123.5(2)
N(1)-Ru(1)-C(17)-C(12)	136.34(11)
C(14)-Ru(1)-C(17)-C(12)	-68.09(11)
C(13)-Ru(1)-C(17)-C(12)	-30.69(11)
C(16)-Ru(1)-C(17)-C(12)	-131.52(16)
C(15)-Ru(1)-C(17)-C(12)	-104.66(12)
C(11)-Ru(1)-C(17)-C(16)	-171.28(10)
N(3)-Ru(1)-C(17)-C(16)	8.0(3)
N(1)-Ru(1)-C(17)-C(16)	-92.14(11)
C(14)-Ru(1)-C(17)-C(16)	63.43(11)
C(13)-Ru(1)-C(17)-C(16)	100.83(12)
C(12)-Ru(1)-C(17)-C(16)	131.52(16)
C(15)-Ru(1)-C(17)-C(16)	26.85(10)
C(16)-C(15)-C(19)-C(21)	-18.0(3)
C(14)-C(15)-C(19)-C(21)	158.93(18)
Ru(1)-C(15)-C(19)-C(21)	74.8(2)
C(16)-C(15)-C(19)-C(20)	105.8(2)
C(14)-C(15)-C(19)-C(20)	-77.3(2)
Ru(1)-C(15)-C(19)-C(20)	-161.46(15)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for mpam100325 [Å and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2N)...F(4)#1	0.86(3)	2.33(3)	3.032(3)	139(3)
N(2)-H(2N)...F(1)#1	0.86(3)	2.48(3)	3.244(3)	148(3)
N(2)-H(1N)...F(4)#2	0.85(3)	2.25(3)	3.030(3)	151(3)
N(2)-H(1N)...F(3)#2	0.85(3)	2.48(3)	3.249(3)	151(3)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 -x+1,-y+1,-z+2