Supplementary Material (ESI) for Chemical Communications

X-ray crystal structure determination of 3

Crystal suitable for X-ray analysis were obtained by slow concentration of a acetonitril solution of **3**. $[C_{64}H_{43}N_{10}O_4Ru_2](PF_6) \cdot 3\ CH_3CN$, Fw = 1486.36, dark red needle, 0.30 x 0.12 x 0.06 mm^3, triclinic, $P\bar{1}$ (no.2), a = 9.5350(1), b = 15.4639(2), c = 21.5139(3) Å, α = 97.2304(4), β = 96.0597(5), γ = 92.7702(6)°, V = 3123.27(7) $Å^3$, Z = 2, D_x = 1.580 g/cm^3, μ = 0.59 mm^{-1}. 57455 Reflections were measured on a Nonius Kappa CCD diffractometer with rotating anode (graphite monochromator, λ = 0.71073 Å) up to a resolution of $(\sin\theta/\lambda)_{max}$ = 0.65 $Å^{-1}$ at a temperature of 110 K. An absorption correction based on multiple measured reflections was applied (0.94-0.97 correction range). 14126 Reflections were unique (R_{int} = 0.048). The structure was solved with automated Patterson methods (program DIRDIF-99[1]) and refined with SHELXL-97[2] against F^2 of all reflections. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were introduced in calculated positions and refined with a riding model. The assignment of C11/N12 and C21/N22 was based on the refinements of the occupancies on the corresponding sites. The PF_6 anion and one acetonitrile molecule were disordered. 941 Parameters were refined with 447 restraints. R1/wR2 [$I > 2\sigma(I)$]: 0.0362/0.0878. R1/wR2 [all refl.]: 0.0500/0.0955. S = 1.035. Residual electron density between -0.83 and 1.77 e/$Å^3$. Geometry calculations and checking for higher symmetry was performed with the PLATON program[3].

References

[1] Beurskens, P. T.; Admiraal, G.; Beurskens, G.; Bosman, W. P.; Garcia-Granda, S.; Gould, R. O.; Smits, J. M. M.; Smykalla C. *The DIRDIF99 program system*, Technical Report of the Crystallography Laboratory at University of Nijmegen; University of Nijmegen: Nijmegen, The Netherlands, 1999.

[2] Sheldrick, G. M. *SHELXL-97. Program for crystal structure refinement*; Universität Göttingen: Göttingen, Germany, 1997.

[3] Spek, A. L. *J. Appl. Cryst.* **2003**, *36*, 7-13.