Electronic Supplementary Information for Dalton Transactions

Supplementary Material

Synthesis, molecular structure and evaluation of new organometallic ruthenium anticancer agents

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There were some issues with the CIF files complex **7**.

Compound **7** crystallised in a monoclinic cell and the structural solution was performed in the space group $P2_1$. The asymmetric unit comprised one molecule of **7.** Compound **7** crystallised in the R_{Ru} configuration (*R* configuration at the ruthenium metal centre). The bond lengths and angles observed for **7** are comparable to those observed for compound **3**. The average Ru-C(arene) bond lengths are significantly shorter by *ca.* 0.12Å (2.194(4)Å & 2.094(4)Å for **3** & **7** respectively). This reduction in bond length may be expected owing to the reduced steric bulk of the arene ring.

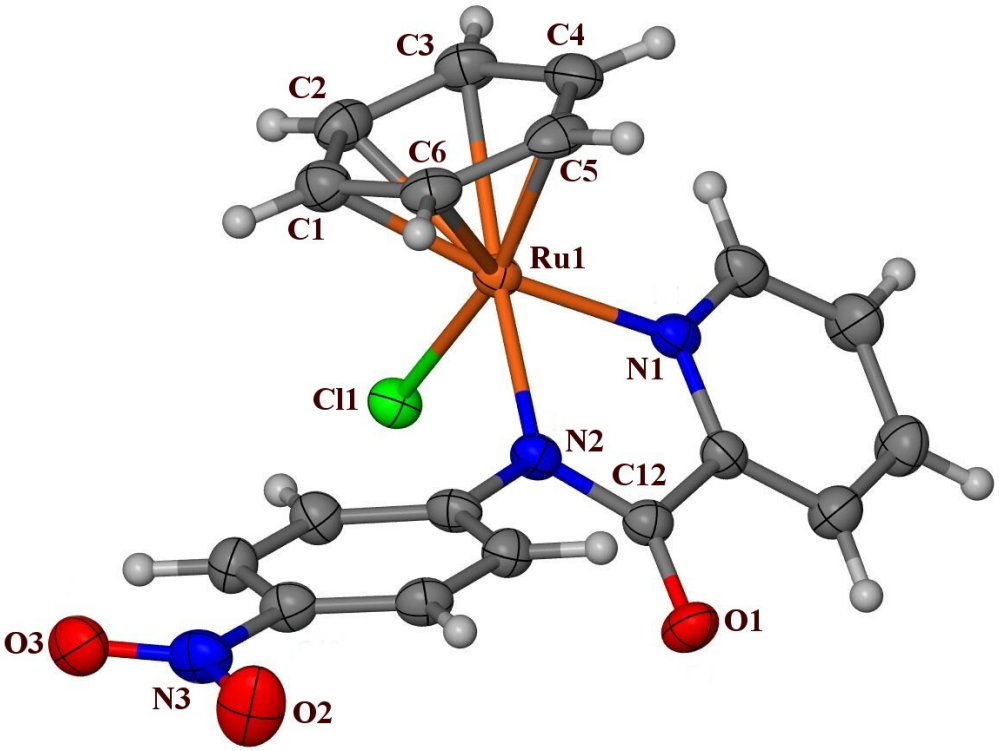

Figure S1. The molecular structure of compound **7**, with 50% probability thermal ellipsoids.

	7
Formula	$C_{18}H_{14}ClN_3O_3Ru$
Mol wt	456.84
Temperature K	150(2)
Wavelength [Mo-K_α] Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1$
a (Å)	11.374(2)
B (Å)	7.9523(16)
C (Å)	11.445(2)
α (°)	90
β (°)	104.00(3)
γ (°)	90
Volume $Å^3$	1004.5(4)
Z	2
Density (calcd) Mg/m^3	1.51
μ mm^{-1}	0.934
Crystal size mm	0.43 x 0.1 x 0.03
Reflections collected	14032

Independent reflections	4429 [R(int) = 0.1087]
Data / restraints / parameters	4429 / 1 / 262
Goodness-of-fit on F^2	1.076
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0468, wR_2 = 0.1234
R indices (all data)	R_1 = 0.0481, wR_2 = 0.1249
Largest diff. peak and hole e.Å^{-3}	1.111 and -1.342

Table S1. Selected Bond Distances Å and Bond Angles (°) for compound **7.** Estimated standard deviations are given in parentheses.

Ru(1)-N(1)	2.084(4)	Ru(1)-N(2)	2.093(4)
Ru(1)-Cl(1)	2.4271(13)	Ru(1)-C(1)	2.197(6)
Ru(1)-C(2)	2.189(5)	Ru(1)-C(3)	2.224(5)
Ru(1)-C(4)	2.171(5)	Ru(1)-C(5)	2.181(5)
Ru(1)-C(6)	2.164(5)		
O(1)-C(12)	1.232(6)	O(2)-N(3)	1.226(6)
O(3)-N(3)	1.231(7)		
C(1)-C(2)	1.426(7)	C(2)-C(3)	1.408(8)
C(3)-C(4)	1.425(8)	C(4)-C(5)	1.420(8)
C(5)-C(6)	1.414(8)	C(1)-C(6)	1.414(8)
Ru(1)-C(Arene) Average	2.074(4)		
Cg(2)-Ru(1)[a]	1.6662		
Cg(2)-Ru(1)-Cl(1)[a]	128.10	Cg(2)-Ru(1)-N(2)[a]	131.60
Cg(2)-Ru(1)-N(1)[a]	130.5	N(1)-Ru(1)-N(2)	76.87(15)
N(1)-Ru(1)-Cl(1)	84.92(14)	N(2)-Ru(1)-Cl(1)	87.15(11)
C(3)-C(2)-C(1)	120.9(5)	C(2)-C(3)-C(4)	119.1(5)
C(5)-C(4)-C(3)	120.8(5)	C(6)-C(5)-C(4)	118.9(5)
C(5)-C(6)-C(1)	121.3(4)	C(6)-C(1)-C(2)	118.8(5)

[a] Cg(4) denotes centroid of the C_6 ring C(1)-C(6).