Supplementary material for:

"Intramolecular Addition of Stabilized Enolates to (η^6-Arene) Ruthenium Complexes: Synthesis of Ru-Coordinated Azaspirocycles"

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Full crystallographic details of cyclohexadienyl ruthenium complex **8**.

Table 1. Crystal data and structure refinement for **8**.

Empirical formula	C18 H20 Cl N O2 Ru	
Formula weight	418.87	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.4668(2) Å	α= 90°.
	b = 11.6934(2) Å	β= 105.362(1)°.
	c = 11.6686(2) Å	γ = 90°.
Volume	1640.26(5) $Å^3$	
Z	4	
Density (calculated)	1.696 Mg/m^3	
Absorption coefficient	1.127 mm^{-1}	
F(000)	848	
Crystal size	0.30 x 0.22 x 0.20 mm^3	
Theta range for data collection	2.51 to 26.43°.	
Index ranges	$-15 \leq h \leq 15$, $-14 \leq k \leq 14$, $-14 \leq l \leq 14$	
Reflections collected	22366	
Independent reflections	3386 [R(int) = 0.034]	
Completeness to theta = 26.43°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.8060 and 0.7285	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3386 / 0 / 208	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0207, wR2 = 0.0555	
R indices (all data)	R1 = 0.0257, wR2 = 0.0565	
Largest diff. peak and hole	0.554 and -0.431 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru	2815(1)	15279(1)	-4741(1)	24(1)
Cl	3901(1)	12993(1)	-2836(1)	46(1)
O(1)	229(1)	13237(1)	-1167(1)	45(1)
O(2)	3087(2)	15489(2)	-842(2)	69(1)
N	549(1)	12969(1)	-2983(1)	30(1)
C(1)	3156(2)	14306(2)	-3111(2)	26(1)
C(2)	3847(2)	15285(2)	-2930(2)	29(1)
C(3)	3340(2)	16367(2)	-3171(2)	34(1)
C(4)	2172(2)	16407(2)	-3589(2)	33(1)
C(5)	1567(2)	15376(2)	-3733(2)	29(1)
C(6)	1976(2)	14301(2)	-2995(2)	27(1)
C(7)	1318(2)	13275(2)	-3661(2)	36(1)
C(8)	767(2)	13455(2)	-1889(2)	29(1)
C(9)	1719(2)	14242(2)	-1782(2)	28(1)
C(10)	2224(2)	14805(2)	-786(2)	36(1)
C(11)	1906(2)	14767(2)	359(2)	45(1)
C(12)	3753(3)	16044(3)	134(2)	66(1)
C(13)	-246(2)	12055(2)	-3380(2)	37(1)
C(1')	3595(2)	15633(2)	-6215(2)	45(1)
C(2')	2508(3)	15994(3)	-6570(2)	59(1)
C(3')	1817(2)	15074(3)	-6580(2)	64(1)
C(4')	2500(2)	14083(2)	-6219(2)	55(1)
C(5')	3615(2)	14457(2)	-5978(2)	40(1)

Table 3. Bond lengths [Å] and angles [°] for **8**

Ru-C(1)	2.1594(18)
Ru-C(2)	2.1639(19)
Ru-C(4')	2.173(2)
Ru-C(4)	2.182(2)
Ru-C(5')	2.183(2)
Ru-C(3)	2.1835(19)
Ru-C(5)	2.188(2)
Ru-C(3')	2.190(2)
Ru-C(1')	2.228(2)
Ru-C(2')	2.228(2)
Cl-C(1)	1.7793(19)
O(1)-C(8)	1.234(2)
O(2)-C(10)	1.357(3)
O(2)-C(12)	1.381(3)
N-C(8)	1.358(2)
N-C(7)	1.440(2)
N-C(13)	1.448(2)
C(1)-C(2)	1.415(3)
C(1)-C(6)	1.513(3)
C(2)-C(3)	1.408(3)
C(3)-C(4)	1.409(3)
C(4)-C(5)	1.409(3)
C(5)-C(6)	1.533(3)
C(6)-C(9)	1.532(3)
C(6)-C(7)	1.543(3)
C(8)-C(9)	1.481(3)
C(9)-C(10)	1.340(3)
C(10)-C(11)	1.490(3)
C(1')-C(2')	1.375(4)
C(1')-C(5')	1.401(3)
C(2')-C(3')	1.376(4)
C(3')-C(4')	1.433(4)
C(4')-C(5')	1.413(4)

C(1)-Ru-C(2)	38.20(7)
C(1)-Ru-C(4')	108.16(10)
C(2)-Ru-C(4')	135.47(10)
C(1)-Ru-C(4)	78.15(7)
C(2)-Ru-C(4)	67.44(8)
C(4')-Ru-C(4)	149.22(10)
C(1)-Ru-C(5')	109.41(8)
C(2)-Ru-C(5')	112.93(8)
C(4')-Ru-C(5')	37.87(9)
C(4)-Ru-C(5')	168.62(9)
C(1)-Ru-C(3)	67.84(8)
C(2)-Ru-C(3)	37.80(7)
C(4')-Ru-C(3)	172.50(10)
C(4)-Ru-C(3)	37.65(8)
C(5')-Ru-C(3)	136.30(9)
C(1)-Ru-C(5)	63.66(7)
C(2)-Ru-C(5)	78.37(8)
C(4')-Ru-C(5)	117.06(9)
C(4)-Ru-C(5)	37.61(8)
C(5')-Ru-C(5)	153.26(8)
C(3)-Ru-C(5)	67.47(8)
C(1)-Ru-C(3')	137.18(11)
C(2)-Ru-C(3')	173.72(11)
C(4')-Ru-C(3')	38.35(12)
C(4)-Ru-C(3')	117.65(10)
C(5')-Ru-C(3')	62.90(9)
C(3)-Ru-C(3')	148.45(11)
C(5)-Ru-C(3')	103.42(9)
C(1)-Ru-C(1')	138.88(9)
C(2)-Ru-C(1')	119.04(9)
C(4')-Ru-C(1')	62.03(9)
C(4)-Ru-C(1')	132.09(8)
C(5')-Ru-C(1')	37.02(9)
C(3)-Ru-C(1')	116.39(8)
C(5)-Ru-C(1')	157.45(9)

C(3')-Ru-C(1')	60.95(10)
C(1)-Ru-C(2')	169.97(9)
C(2)-Ru-C(2')	147.24(11)
C(4')-Ru-C(2')	62.14(11)
C(4)-Ru-C(2')	111.42(9)
C(5')-Ru-C(2')	61.63(9)
C(3)-Ru-C(2')	121.47(10)
C(5)-Ru-C(2')	121.93(9)
C(3')-Ru-C(2')	36.27(12)
C(1')-Ru-C(2')	35.94(10)
C(10)-O(2)-C(12)	123.2(2)
C(8)-N-C(7)	114.65(16)
C(8)-N-C(13)	123.98(17)
C(7)-N-C(13)	120.41(17)
C(2)-C(1)-C(6)	123.87(18)
C(2)-C(1)-Cl	113.79(15)
C(6)-C(1)-Cl	117.02(14)
C(2)-C(1)-Ru	71.07(11)
C(6)-C(1)-Ru	96.42(11)
Cl-C(1)-Ru	125.83(10)
C(3)-C(2)-C(1)	118.29(19)
C(3)-C(2)-Ru	71.86(11)
C(1)-C(2)-Ru	70.72(11)
C(2)-C(3)-C(4)	117.83(18)
C(2)-C(3)-Ru	70.35(11)
C(4)-C(3)-Ru	71.11(11)
C(3)-C(4)-C(5)	119.02(18)
C(3)-C(4)-Ru	71.24(12)
C(5)-C(4)-Ru	71.42(11)
C(4)-C(5)-C(6)	123.11(18)
C(4)-C(5)-Ru	70.96(12)
C(6)-C(5)-Ru	94.66(12)
C(1)-C(6)-C(9)	121.96(16)
C(1)-C(6)-C(5)	97.65(15)
C(9)-C(6)-C(5)	115.88(16)
C(1)-C(6)-C(7)	110.95(16)
C(9)-C(6)-C(7)	102.50(16)
C(5)-C(6)-C(7)	107.51(16)
N-C(7)-C(6)	104.98(16)
O(1)-C(8)-N	123.12(19)
O(1)-C(8)-C(9)	129.75(19)
N-C(8)-C(9)	107.13(16)
C(10)-C(9)-C(8)	124.05(18)
C(10)-C(9)-C(6)	127.88(19)
C(8)-C(9)-C(6)	108.05(16)
C(9)-C(10)-O(2)	116.36(19)
C(9)-C(10)-C(11)	126.0(2)
O(2)-C(10)-C(11)	117.6(2)
C(2')-C(1')-C(5')	109.0(2)
C(2')-C(1')-Ru	72.05(14)
C(5')-C(1')-Ru	69.74(12)
C(1')-C(2')-C(3')	109.1(3)
C(1')-C(2')-Ru	72.01(13)
C(3')-C(2')-Ru	70.33(14)
C(2')-C(3')-C(4')	107.9(2)
C(2')-C(3')-Ru	73.40(15)
C(4')-C(3')-Ru	70.20(13)
C(5')-C(4')-C(3')	106.5(2)
C(5')-C(4')-Ru	71.43(13)
C(3')-C(4')-Ru	71.45(14)
C(1')-C(5')-C(4')	107.4(2)
C(1')-C(5')-Ru	73.24(12)
C(4')-C(5')-Ru	70.70(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	27(1)	29(1)	18(1)	1(1)	9(1)	0(1)
Cl	50(1)	37(1)	52(1)	13(1)	17(1)	14(1)
O(1)	48(1)	63(1)	32(1)	2(1)	23(1)	-8(1)
O(2)	92(2)	89(2)	31(1)	-26(1)	26(1)	-56(1)
N	30(1)	35(1)	27(1)	-1(1)	13(1)	-4(1)
C(1)	31(1)	28(1)	21(1)	3(1)	9(1)	5(1)
C(2)	29(1)	39(1)	20(1)	0(1)	7(1)	-5(1)
C(3)	49(1)	31(1)	22(1)	-1(1)	12(1)	-8(1)
C(4)	50(1)	30(1)	21(1)	1(1)	13(1)	8(1)
C(5)	28(1)	43(1)	19(1)	1(1)	9(1)	6(1)
C(6)	32(1)	30(1)	20(1)	-1(1)	11(1)	-3(1)
C(7)	40(1)	41(1)	33(1)	-9(1)	22(1)	-14(1)
C(8)	32(1)	32(1)	25(1)	5(1)	11(1)	5(1)
C(9)	36(1)	31(1)	22(1)	3(1)	14(1)	3(1)
C(10)	50(1)	34(1)	25(1)	1(1)	14(1)	-1(1)
C(11)	70(2)	42(1)	27(1)	-1(1)	21(1)	1(1)
C(12)	80(2)	72(2)	41(2)	-21(1)	8(1)	-22(2)
C(13)	31(1)	44(1)	39(1)	1(1)	13(1)	-8(1)
C(1')	59(2)	54(1)	31(1)	-2(1)	30(1)	-8(1)
C(2')	85(2)	73(2)	25(1)	16(1)	26(1)	31(2)
C(3')	34(1)	137(3)	19(1)	-13(1)	6(1)	12(2)
C(4')	83(2)	60(2)	29(1)	-24(1)	29(1)	-32(2)
C(5')	46(1)	53(1)	25(1)	-5(1)	15(1)	13(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(2)	4664	15206	-2762	35
H(3)	3794	17059	-3183	40
H(4)	1797	17131	-3905	40
H(5)	775	15403	-4188	35
H(7A)	918	13490	-4474	43
H(7B)	1817	12635	-3694	43
H(11A)	1282	14251	282	67
H(11B)	1698	15527	553	67
H(11C)	2532	14498	985	67
H(12A)	4316	16484	-106	99
H(12B)	4110	15484	727	99
H(12C)	3300	16552	468	99
H(13A)	-694	11965	-2822	56
H(13B)	148	11348	-3425	56
H(13C)	-723	12241	-4159	56
H(1')	4256	16120	-6158	54
H(2')	2261	16784	-6807	71
H(3')	994	15083	-6855	76
H(4')	2241	13283	-6216	65
H(5')	4285	13966	-5762	48