Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for the manuscript

Synthesis and X-Ray Structure of Ruthenium bis(acetylacetonate)(*N,N,N',N'*-tetramethylethylenediamine)

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X-Ray Structure of [Ru(acac)$_2$(tmed)]

A. Crystal Data

Empirical Formula	$C_{16}H_{30}N_2O_4Ru$
Formula Weight	415.49
Crystal Color, Habit	Red, plate
Crystal Dimensions	0.18 x 0.13 x 0.03 mm
Crystal System	Triclinic
Lattice Type	Primitive
Lattice Parameters	*a* = 7.9351(3) Å *b* = 9.8757(4) Å *c* = 13.0361(6) Å α = 75.5720(10) ° β = 88.3220(10) ° γ = 70.2400(10) ° V = 929.40(7) Å^3
Space Group	P *-1*
Z Value	2
D_{calc}	1.485 g cm^{-3}
F_{000}	432
μ (MoKα)	0.863 mm^{-1}

B. Intensity Measurements

Diffractometer	Bruker APEX CCD[1] graphite monochromated
Radiation	MoKα (λ = 0.71073 Å)
Detector Position	60.00 mm
Exposure Time	15s per frame
Scan Type	ω (0.3° per frame)
$2\theta_{max}$	50.68°
No. of Reflexions measured	Total: 14197 Unique: 3394 (R_{int} = 0.0311)
Corrections	Lorentz polarization Absorption (Tmax = 0.723, Tmin = 0.393)

C. Structure solution and refinement

Structure Solution	Direct Methods (SHELXS)
Refinement	Full-matrix least-squares
Function Minimized	Σ w ($\|F_o\|$ - $\|F_c\|$)^2
Least Squares Weights	w=1/[σ²Fo²+(0.0282P)²+ 0.5443P] where P=(Max(Fo²,0)+2Fc²)/3)
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I > 2.00 σ(I))	3394
No. variables	328

Reflections/parameter Ratio	10.34
Residuals: R, R_w, R_{all}	0.0245; 0.0571; 0.0293
Goodness of Fit Indicator	1.038
Max Shift/Error in final Cycle	0.001
Maximum peak in Final Diff Map	0.537 e.A^{-3}
Minimum peak in Final Diff Map	-0.695 e.A^{-3}

Figure S1. ORTEP of $Ru(acac)_2(tmed)$ (50% probability ellipsoids).

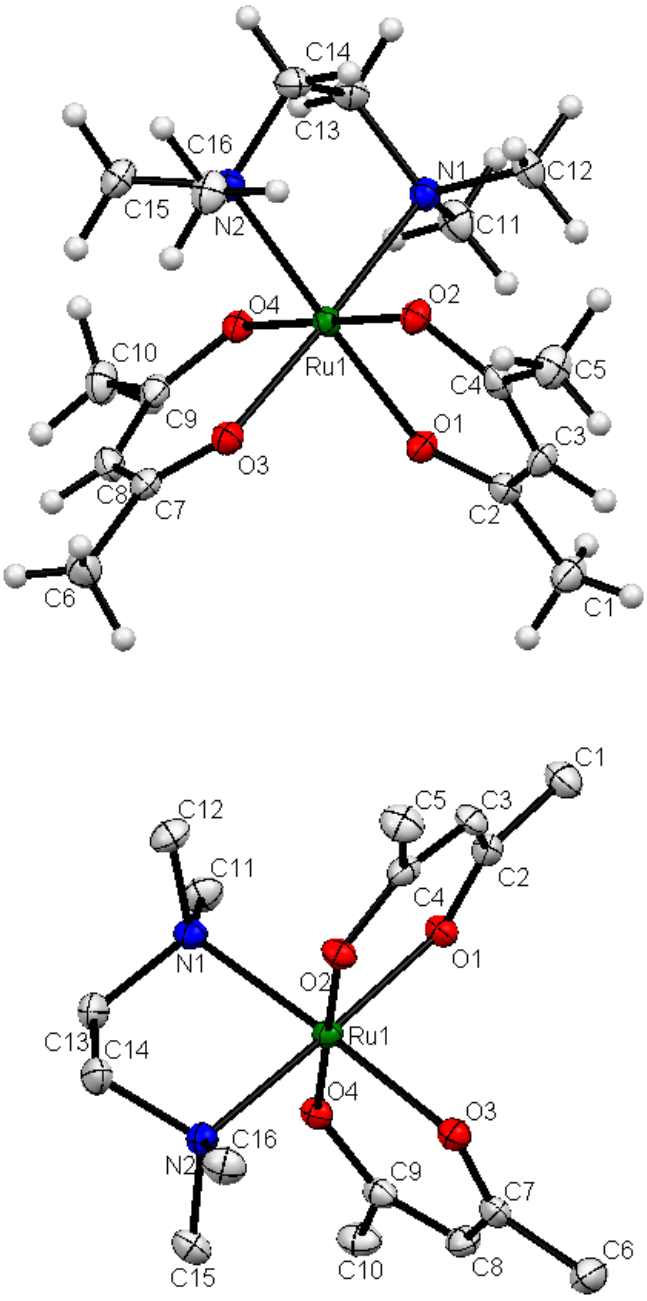

Table S1. Selected bond distances (Å) and angles (deg) for $Ru(acac)_2(tmed)$ compared to $V(acac)_2(tmed)$[2]

$Ru(acac)_2(tmed)$		**$V(acac)_2(tmed)$**	
Ru-O (distance range)	2.0495(16) to 2.0614(16)	V-O (distance range)	2.042(4) to 2.065(4)
Ru-O (mean)	2.0543(32)	V-O (mean)	2.0538(8)
Ru-N (distance range)	2.1416(18) to 2.1470(2)	V-N (distance range)	2.239(4) to 2.243(5)
Ru-N (mean)	2.1443(18)	V-N (mean)	2.241(6)
O(1)-Ru-O(4)	86.68(6)	O(2)-V-O(1)	88.0(2)
O(3)-Ru-O(2)	86.76(6)	O(4)-V-O(3)	88.4(2)
O(1)-Ru-O(3)	89.90(6)	O(4)-V-O(2)	91.4(2)
O(4)-Ru-O(3)	93.26(6)	O(1)-V-O(3)	92.0(2)
O(1)-Ru-O(2)	93.20(6)	O(4)-V-O(1)	94.2(2)
O(4)-Ru-O(2)	179.88(7)	O(2)-V-O(3)	179.8(2)
O(4)-Ru-N(1)	86.91(7)	O(2)-V-N(2)	87.4(2)
O(1)-Ru-N(1)	92.78(7)	O(3)-V-N(2)	92.6(2)
O(2)-Ru-N(1)	93.07(7)	O(4)-V-N(2)	92.6(2)
O(3)-Ru-N(1)	177.32	O(1)-V-N(2)	171.9(2)
O(2)-Ru-N(2)	88.72(7)	O(3)-V-N(1)	89.7(2)
O(4)-Ru-N(2)	91.40(7)	O(2)-V-N(1)	90.6(2)
O(3)-Ru-N(2)	92.75(7)	O(1)-V-N(1)	92.2(2)
O(1)-Ru-N(2)	176.81(7)	O(4)-V-N(1)	173.3(2)
N(1)-Ru-N(2)	84.57(7)	N(2)-V-N(1)	81.1(2)

References

(1) APEX: Area-Detector Software Package; Bruker Analytical X-Ray System, Inc.:Madison, WI (**2001-2003**)

(2) Ma, Y.; Reardon, D.; Gambarotta, S.; Yap, G. *Organometallics*, **1999**, 18, 2773-2781

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $Ru(acac)_2(tmed)$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	6166(1)	6180(1)	7485(1)	13(1)
N(1)	4466(2)	4856(2)	7744(2)	15(1)
N(2)	4438(3)	7420(2)	6084(2)	16(1)
C(2)	9105(3)	3850(2)	8911(2)	17(1)
O(4)	4494(2)	7442(2)	8384(1)	15(1)
O(2)	7849(2)	4908(2)	6584(1)	16(1)
O(1)	7693(2)	4977(2)	8863(1)	16(1)
O(3)	7727(2)	7508(2)	7171(1)	17(1)
C(7)	7424(3)	8645(2)	7543(2)	18(1)
C(9)	4712(3)	8579(2)	8576(2)	17(1)
C(12)	5233(4)	3437(3)	7438(2)	22(1)
C(5)	10349(4)	3027(3)	6204(2)	23(1)
C(8)	6049(3)	9170(3)	8192(2)	19(1)
C(15)	3290(3)	8926(3)	6154(2)	20(1)
C(4)	9273(3)	3820(2)	6983(2)	17(1)
C(3)	9872(3)	3290(3)	8052(2)	18(1)
C(1)	9982(4)	3058(3)	10006(2)	23(1)
C(13)	2805(3)	5821(3)	7060(2)	22(1)
C(14)	3291(4)	6534(3)	5979(2)	23(1)
C(10)	3351(4)	9344(3)	9261(2)	23(1)
C(16)	5457(4)	7615(3)	5124(2)	23(1)
C(11)	3984(4)	4502(3)	8864(2)	23(1)
C(6)	8733(4)	9466(3)	7241(3)	25(1)

Table S3. Anisotropic displacement parameters (A^2 x 10^3) for $Ru(acac)_2(tmed)$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Ru(1)	14(1)	12(1)	13(1)	-4(1)	1(1)	-4(1)
N(1)	16(1)	14(1)	15(1)	-4(1)	1(1)	-4(1)
N(2)	16(1)	17(1)	16(1)	-4(1)	1(1)	-6(1)
C(2)	17(1)	16(1)	19(1)	-3(1)	-2(1)	-7(1)
O(4)	17(1)	15(1)	13(1)	-4(1)	0(1)	-4(1)
O(2)	16(1)	15(1)	15(1)	-4(1)	2(1)	-3(1)
O(1)	16(1)	15(1)	15(1)	-4(1)	-1(1)	-3(1)
O(3)	16(1)	16(1)	19(1)	-4(1)	1(1)	-4(1)
C(7)	18(1)	15(1)	18(1)	0(1)	-5(1)	-4(1)
C(9)	19(1)	15(1)	14(1)	-4(1)	-3(1)	-2(1)
C(12)	26(2)	17(1)	25(2)	-9(1)	3(1)	-9(1)
C(5)	23(2)	23(1)	22(2)	-8(1)	5(1)	-3(1)
C(8)	22(1)	14(1)	21(2)	-6(1)	-2(1)	-5(1)
C(15)	19(1)	19(1)	18(2)	-2(1)	-1(1)	-2(1)
C(4)	18(1)	14(1)	21(1)	-6(1)	4(1)	-8(1)
C(3)	13(1)	14(1)	22(2)	-4(1)	-1(1)	0(1)
C(1)	21(1)	21(1)	23(2)	-5(1)	-3(1)	-2(1)
C(13)	16(1)	20(1)	29(2)	-4(1)	-2(1)	-7(1)
C(14)	25(1)	22(1)	23(2)	-2(1)	-8(1)	-11(1)
C(10)	27(2)	17(1)	23(2)	-7(1)	2(1)	-3(1)
C(16)	27(2)	22(1)	17(2)	-3(1)	3(1)	-7(1)
C(11)	28(2)	21(1)	20(2)	-3(1)	5(1)	-12(1)
C(6)	22(2)	19(1)	34(2)	-6(1)	1(1)	-8(1)

Table S4. Bond lengths [A] for $Ru(acac)_2(tmed)$.

Ru(1)-O(1)	2.0495(16)
Ru(1)-O(4)	2.0509(16)
Ru(1)-O(3)	2.0552(15)
Ru(1)-O(2)	2.0614(16)
Ru(1)-N(1)	2.1416(18)
Ru(1)-N(2)	2.147(2)
N(1)-C(12)	1.476(3)
N(1)-C(11)	1.485(3)
N(1)-C(13)	1.496(3)
N(2)-C(16)	1.478(3)
N(2)-C(15)	1.482(3)
N(2)-C(14)	1.490(3)
C(2)-O(1)	1.274(3)
C(2)-C(3)	1.404(3)
C(2)-C(1)	1.506(3)
O(4)-C(9)	1.276(3)
O(2)-C(4)	1.279(3)
O(3)-C(7)	1.278(3)
C(7)-C(8)	1.399(3)
C(7)-C(6)	1.509(3)
C(9)-C(8)	1.400(3)
C(9)-C(10)	1.504(3)
C(5)-C(4)	1.505(3)
C(4)-C(3)	1.396(3)
C(13)-C(14)	1.512(4)

Table S5. Bond angles [deg] for $Ru(acac)_2(tmed)$

O(1)-Ru(1)-O(4)	86.68(6)
O(1)-Ru(1)-O(3)	89.90(6)
O(4)-Ru(1)-O(3)	93.26(6)
O(1)-Ru(1)-O(2)	93.20(6)
O(4)-Ru(1)-O(2)	179.88(7)
O(3)-Ru(1)-O(2)	86.76(6)
O(1)-Ru(1)-N(1)	92.78(7)
O(4)-Ru(1)-N(1)	86.91(7)
O(3)-Ru(1)-N(1)	177.32(7)
O(2)-Ru(1)-N(1)	93.07(7)
O(1)-Ru(1)-N(2)	176.81(7)
O(4)-Ru(1)-N(2)	91.40(7)
O(3)-Ru(1)-N(2)	92.75(7)
O(2)-Ru(1)-N(2)	88.72(7)
N(1)-Ru(1)-N(2)	84.57(7)
C(12)-N(1)-C(11)	107.50(19)
C(12)-N(1)-C(13)	109.72(19)
C(11)-N(1)-C(13)	108.9(2)
C(12)-N(1)-Ru(1)	113.91(15)
C(11)-N(1)-Ru(1)	112.71(14)
C(13)-N(1)-Ru(1)	103.95(13)
C(16)-N(2)-C(15)	107.1(2)
C(16)-N(2)-C(14)	109.50(19)
C(15)-N(2)-C(14)	109.67(19)
C(16)-N(2)-Ru(1)	112.14(15)
C(15)-N(2)-Ru(1)	112.80(15)
C(14)-N(2)-Ru(1)	105.67(14)
O(1)-C(2)-C(3)	126.2(2)
O(1)-C(2)-C(1)	115.3(2)
C(3)-C(2)-C(1)	118.5(2)
C(9)-O(4)-Ru(1)	123.27(15)
C(4)-O(2)-Ru(1)	122.47(15)
C(2)-O(1)-Ru(1)	123.21(15)
C(7)-O(3)-Ru(1)	122.30(15)
O(3)-C(7)-C(8)	127.0(2)
O(3)-C(7)-C(6)	114.6(2)
C(8)-C(7)-C(6)	118.4(2)
O(4)-C(9)-C(8)	126.1(2)
O(4)-C(9)-C(10)	115.1(2)
C(8)-C(9)-C(10)	118.8(2)
C(7)-C(8)-C(9)	128.1(2)
O(2)-C(4)-C(3)	126.6(2)
O(2)-C(4)-C(5)	115.1(2)
C(3)-C(4)-C(5)	118.2(2)
C(4)-C(3)-C(2)	128.3(2)
N(1)-C(13)-C(14)	110.2(2)
N(2)-C(14)-C(13)	110.4(2)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $Ru(acac)_2(tmed)$.

	x	y	z	U(eq)
H(15C)	2580(30)	8870(30)	6710(20)	15(7)
H(13B)	2160(30)	6540(30)	7425(19)	12(6)
H(11A)	5050(30)	3860(30)	9290(20)	18(7)
H(3)	10950(30)	2460(30)	8220(20)	18(6)
H(15A)	4050(30)	9500(30)	6260(20)	20(7)
H(15B)	2510(30)	9470(30)	5490(20)	20(7)
H(12A)	4390(30)	2870(30)	7549(19)	14(6)
H(12C)	6300(40)	2810(30)	7870(20)	21(7)
H(12B)	5550(40)	3580(30)	6730(20)	26(7)
H(13A)	2050(30)	5270(30)	7010(20)	25(7)
H(11C)	3130(40)	3980(30)	8940(20)	30(7)
H(11B)	3520(40)	5370(30)	9080(20)	27(7)
H(8)	6000(40)	9970(30)	8390(20)	38(8)
H(10B)	3590(30)	10180(30)	9380(20)	25(7)
H(14B)	2240(30)	7120(30)	5530(20)	17(6)
H(16A)	6200(30)	8140(30)	5220(20)	24(7)
H(6A)	9810(40)	8960(30)	7700(30)	41(9)
H(1A)	10900(40)	2210(40)	10010(20)	43(9)
H(16C)	6180(40)	6690(30)	4980(20)	27(7)
H(6B)	9080(40)	9470(30)	6540(30)	36(9)
H(10C)	2200(40)	9630(30)	8920(20)	34(8)
H(5A)	10470(40)	3670(30)	5560(30)	39(9)
H(5B)	9720(40)	2390(40)	6050(30)	48(9)
H(1B)	9140(40)	2850(30)	10430(20)	31(8)
H(14A)	3990(40)	5750(30)	5630(20)	29(7)
H(1C)	10430(40)	3640(40)	10290(30)	46(9)
H(10A)	3410(40)	8710(40)	9910(30)	41(9)
H(16B)	4650(40)	8210(30)	4450(30)	41(9)
H(6C)	8270(40)	10390(40)	7240(30)	54(10)
H(5C)	11480(50)	2420(40)	6450(30)	48(10)