Appendix A

Crystallographic Data (*Chapter 3*)

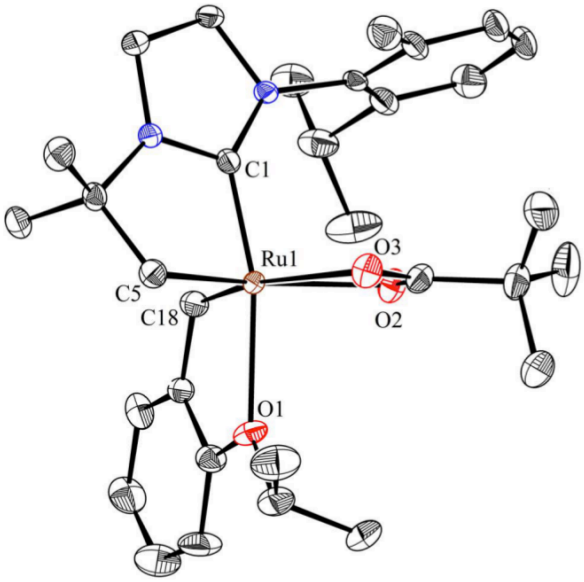

Table A1. Crystal Data and Structure Analysis Details for 3.2

Empirical Formula	$C_{32}H_{46}N_2O_3Ru$
Formula Weight	607.78
Crystallization Solvent	Hexanes
Crystal Shape	Plate
Crystal Color	Purple
Crystal Size	0.11 x 0.32 x 0.37 mm^3
Data Collection	
Preliminary Photograph(s)	Rotation
Type of Diffractometer	Bruker APEX-II CCD
Wavelength	0.71073 Å MoKa

Data Collection Temperature	100 K	
Theta Range for 9786 Reflections Used in Lattice Determination	2.39 to 31.77°	
Unit Cell Dimensions	a = 11.0782(5) Å	a= 90°
	b = 27.9893(11) Å	b= 103.793(2)°
	c = 10.2073(4) Å	g = 90°
Volume	3073.7(2) $Å^3$	
Z	4	
Crystal System	Monoclinic	
Space Group	$P2_1/c$	
Density (Calculated)	1.313 g/cm^3	
F(000)	1280	
Theta Range for Data Collection	2.0 to 39.1°	
Completeness to Theta = 25.000°	99.9%	
Index Ranges	$-19 \leq h \leq 18, -48 \leq k \leq 49, -17 \leq l \leq 17$	
Data Collection Scan Type	φ/ω scans	
Reflections Collected	191072	
Independent Reflections	17585 [$R_{int} = 0.0616$]	
Reflections > 2s(I)	13528	
Average s(I)/(net I)	0.0358	
Absorption Coefficient	0.54 mm^{-1}	
Absorption Correction	Semi-empirical from equivalents	
Max. and Min. Transmission	0.943 and 0.824	

Structure Solution and Refinement

Primary Solution Method	Dual
Hydrogen Placement	Mixed
Refinement method	Full-matrix least-squares on F^2
Data / Restraints / Parameters	17585 / 0 / 434
Treatment of Hydrogen Atoms	Mixed
Goodness-of-Fit on F^2	1.47
Final R Indices [I>2s(I), 13528 reflections]	R1 = 0.0435, *w*R2 = 0.1024
R Indices (All Data)	R1 = 0.0645, *w*R2 = 0.1085
Type of Weighting Scheme Used	Calc
Weighting Scheme Used	$w = 1/[\sigma^2(Fo^2) + (0.0400P)^2]$, where $P = (Fo^2 + 2Fc^2)/3$
Max Shift/Error	0.001
Average Shift/Error	0.000
Extinction Coefficient	N/A
Largest Diff. Peak and Hole	3.79 and -1.14 e/Å^3

Programs Used

Cell Refinement	SAINT V8.27B (Bruker-AXS, 2007)
Data Collection	APEX2 2012.10-0 (Bruker-AXS, 2007)
Data Reduction	SAINT V8.27B (Bruker-AXS, 2007)
Structure Solution	SHELXT (Sheldrick, 2012)
Structure Refinement	SHELXL-2013/2 (Sheldrick, 2013)
Graphics	DIAMOND 3 (Crystal Impact, 1999)

Special Refinement Details: The sample was multiple offset layered plates. In the unit cell determination 108 of 545 reflections were not indexed. Neither cell_now nor TwinRotMat (in Platon) detected any twinning. There are two orientations of the isopropyl group. This disorder is propagated through the molecule, resulting in most atoms being split. The ratio of components is 0.68:0.32; the minor component was modeled isotropically. Although the average bond precision is exemplary given the crystal problems, geometric parameters involving split and non-split atoms have larger errors.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table A2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for 3.2. U(eq) is Defined as One Third of the Trace of the Orthogonalized U^{ij} Tensor

	x	y	z	U_{eq}
Ru(1)	8108(1)	8973(1)	7258(1)	11(1)
O(1)	9330(2)	8344(1)	6798(2)	22(1)
O(2)	6554(1)	8473(1)	7159(1)	23(1)
O(3)	6443(1)	8873(1)	5289(1)	24(1)
N(1)	8148(1)	9953(1)	7887(1)	16(1)
N(2)	6573(3)	9650(1)	8553(3)	14(1)
C(1)	7475(1)	9552(1)	7876(1)	15(1)
C(2)	7620(1)	10372(1)	8402(1)	19(1)
C(3)	6658(6)	10137(2)	9096(6)	18(1)
C(4)	9192(1)	9954(1)	7234(1)	18(1)
C(5)	9058(1)	9486(1)	6437(1)	20(1)
C(6)	10426(1)	9971(1)	8300(1)	23(1)
C(7)	9104(1)	10397(1)	6333(2)	26(1)

C(8)	5452(4)	9391(1)	8475(5)	16(1)
C(9)	5447(3)	9059(1)	9497(3)	21(1)
C(10)	4327(4)	8840(1)	9545(4)	28(1)
C(11)	3249(3)	8941(1)	8603(4)	25(1)
C(12)	3273(3)	9258(1)	7562(4)	23(1)
C(13)	4343(4)	9474(2)	7452(5)	22(1)
C(14)	6704(2)	8955(1)	10627(2)	30(1)
C(15)	7013(2)	8423(1)	10719(2)	48(1)
C(16)	6675(2)	9166(1)	11995(2)	36(1)
C(17)	4419(2)	9783(1)	6349(2)	30(1)
C(18)	9191(1)	8883(1)	8856(1)	19(1)
C(19)	10093(2)	8498(1)	9094(3)	16(1)
C(20)	10913(2)	8392(1)	10324(3)	24(1)
C(21)	11770(2)	8027(1)	10451(4)	33(1)
C(22)	11807(3)	7757(1)	9344(4)	42(1)
C(23)	11012(3)	7842(1)	8087(4)	35(1)
C(24)	10160(2)	8214(1)	7977(3)	21(1)
C(25)	9429(2)	8091(1)	5570(2)	30(1)
C(26)	8701(3)	7630(1)	5448(4)	44(1)
C(27)	8951(3)	8420(1)	4430(3)	43(1)
C(28)	6006(1)	8562(1)	5943(1)	22(1)
C(29)	4837(1)	8282(1)	5278(2)	30(1)
C(30)	4336(2)	8022(1)	6365(2)	50(1)
C(31)	3859(2)	8626(1)	4492(2)	43(1)
C(32)	5184(2)	7928(1)	4288(2)	44(1)
Ru(1A)	7983(1)	8976(1)	7052(1)	17(1)
O(1A)	8954(4)	8328(2)	6550(5)	24(1)
C(19A)	10003(7)	8454(3)	8776(6)	18(1)
C(20A)	10853(7)	8337(3)	9946(7)	27(2)
C(21A)	11665(6)	7944(2)	9956(6)	26(1)
C(22A)	11581(6)	7696(2)	8785(7)	32(1)
C(23A)	10691(6)	7811(2)	7613(6)	29(1)
C(24A)	9906(5)	8193(2)	7612(5)	16(1)
C(25A)	8922(4)	8217(2)	5155(4)	18(1)
C(26A)	8564(7)	7709(3)	4805(7)	38(1)
C(27A)	10089(4)	8372(2)	4738(5)	24(1)
N(2A)	6476(8)	9670(3)	8289(7)	19(2)
C(3A)	6602(14)	10161(5)	8894(13)	19(2)
C(8A)	5532(10)	9325(4)	8629(11)	19(2)
C(9A)	5656(6)	9047(2)	9745(6)	11(1)
C(10A)	4528(7)	8802(3)	9802(7)	17(1)
C(11A)	3453(7)	8880(3)	8896(7)	23(2)
C(12A)	3360(9)	9180(3)	7806(8)	23(2)
C(13A)	4482(10)	9444(4)	7661(10)	17(2)

Table A3. Bond Lengths [Å] and Angles [°] for 3.2

Ru(1)-C(18)	1.7978(15)	C(9)-C(10)	1.396(5)
Ru(1)-C(1)	1.9323(12)	C(9)-C(14)	1.610(4)
Ru(1)-C(5)	2.0709(13)	C(10)-C(11)	1.372(5)
Ru(1)-O(2)	2.2021(10)	C(10)-H(10)	0.9500
Ru(1)-O(1)	2.3336(18)	C(11)-C(12)	1.390(5)
Ru(1)-O(3)	2.3984(12)	C(11)-H(11)	0.9500
O(1)-C(24)	1.378(3)	C(12)-C(13)	1.359(6)
O(1)-C(25)	1.467(3)	C(12)-H(12)	0.9500
O(2)-C(28)	1.2699(17)	C(13)-C(17)	1.437(5)
O(2)-Ru(1A)	2.1402(14)	C(14)-C(9A)	1.315(6)
O(3)-C(28)	1.2624(18)	C(14)-C(15)	1.524(2)
O(3)-Ru(1A)	2.1838(17)	C(14)-C(16)	1.524(2)
N(1)-C(1)	1.3457(16)	C(14)-H(14)	1.0000
N(1)-C(2)	1.4631(16)	C(14)-H(14A)	0.81(7)
N(1)-C(4)	1.4660(16)	C(15)-H(15A)	0.9800
N(2)-C(1)	1.371(3)	C(15)-H(15B)	0.9800
N(2)-C(8)	1.424(5)	C(15)-H(15C)	0.9800
N(2)-C(3)	1.465(7)	C(16)-H(16A)	0.9800
C(1)-N(2A)	1.317(9)	C(16)-H(16B)	0.9800
C(1)-Ru(1A)	1.9640(16)	C(16)-H(16C)	0.9800
C(2)-C(3A)	1.463(15)	C(17)-C(13A)	1.630(10)
C(2)-C(3)	1.558(6)	C(17)-H(17A)	0.9804
C(2)-H(2AA)	0.9900	C(17)-H(17B)	0.9798
C(2)-H(2AB)	0.9900	C(17)-H(17C)	0.9796
C(2)-H(2BC)	0.9900	C(17)-H(17D)	0.8519
C(2)-H(2BD)	0.9900	C(17)-H(17E)	0.9743
C(3)-H(3A)	0.9900	C(17)-H(17F)	1.0594
C(3)-H(3B)	0.9900	C(18)-C(19)	1.449(3)
C(4)-C(6)	1.5310(18)	C(18)-C(19A)	1.513(7)
C(4)-C(5)	1.5318(18)	C(18)-Ru(1A)	2.0186(19)
C(4)-C(7)	1.5336(19)	C(18)-H(18)	0.9500
C(5)-Ru(1A)	2.0508(16)	C(19)-C(20)	1.395(4)
C(5)-H(5A)	0.9900	C(19)-C(24)	1.406(4)
C(5)-H(5B)	0.9900	C(20)-C(21)	1.379(4)
C(5)-H(5C)	0.9900	C(20)-H(20)	0.9500
C(5)-H(5D)	0.9900	C(21)-C(22)	1.368(5)
C(6)-H(6A)	0.9800	C(21)-H(21)	0.9500
C(6)-H(6B)	0.9800	C(22)-C(23)	1.392(4)
C(6)-H(6C)	0.9800	C(22)-H(22)	0.9500
C(7)-H(7A)	0.9800	C(23)-C(24)	1.392(3)
C(7)-H(7B)	0.9800	C(23)-H(23)	0.9500
C(7)-H(7C)	0.9800	C(25)-C(27)	1.479(4)
C(8)-C(9)	1.398(5)	C(25)-C(26)	1.511(4)
C(8)-C(13)	1.429(6)	C(25)-H(25)	1.0000

C(26)-H(26A)	0.9800	C(8A)-C(9A)	1.360(11)
C(26)-H(26B)	0.9800	C(8A)-C(13A)	1.375(14)
C(26)-H(26C)	0.9800	C(9A)-C(10A)	1.439(11)
C(27)-H(27A)	0.9800	C(10A)-C(11A)	1.340(9)
C(27)-H(27B)	0.9800	C(10A)-H(10A)	0.9500
C(27)-H(27C)	0.9800	C(11A)-C(12A)	1.378(10)
C(28)-C(29)	1.528(2)	C(11A)-H(11A)	0.9500
C(28)-Ru(1A)	2.4975(18)	C(12A)-C(13A)	1.483(15)
C(29)-C(31)	1.526(3)	C(12A)-H(12A)	0.9500
C(29)-C(32)	1.528(2)	C(18)-Ru(1)-C(1)	92.11(6)
C(29)-C(30)	1.536(3)	C(18)-Ru(1)-C(5)	99.85(6)
C(30)-H(30A)	0.9800	C(1)-Ru(1)-C(5)	79.03(5)
C(30)-H(30B)	0.9800	C(18)-Ru(1)-O(2)	107.30(5)
C(30)-H(30C)	0.9800	C(1)-Ru(1)-O(2)	101.97(5)
C(31)-H(31A)	0.9800	C(5)-Ru(1)-O(2)	152.74(6)
C(31)-H(31B)	0.9800	C(18)-Ru(1)-O(1)	77.49(7)
C(31)-H(31C)	0.9800	C(1)-Ru(1)-O(1)	166.27(7)
C(32)-H(32A)	0.9800	C(5)-Ru(1)-O(1)	93.79(6)
C(32)-H(32B)	0.9800	O(2)-Ru(1)-O(1)	89.79(6)
C(32)-H(32C)	0.9800	C(18)-Ru(1)-O(3)	163.29(5)
Ru(1A)-O(1A)	2.227(5)	C(1)-Ru(1)-O(3)	96.01(5)
O(1A)-C(24A)	1.373(6)	C(5)-Ru(1)-O(3)	96.03(5)
O(1A)-C(25A)	1.449(7)	O(2)-Ru(1)-O(3)	56.71(4)
C(19A)-C(20A)	1.372(9)	O(1)-Ru(1)-O(3)	96.38(6)
C(19A)-C(24A)	1.377(8)	C(24)-O(1)-C(25)	116.6(2)
C(20A)-C(21A)	1.421(10)	C(24)-O(1)-Ru(1)	108.78(14)
C(20A)-H(20A)	0.9500	C(25)-O(1)-Ru(1)	134.49(16)
C(21A)-C(22A)	1.365(8)	C(28)-O(2)-Ru(1A)	90.47(9)
C(21A)-H(21A)	0.9500	C(28)-O(2)-Ru(1)	96.11(8)
C(22A)-C(23A)	1.394(8)	C(28)-O(3)-Ru(1A)	88.70(9)
C(22A)-H(22A)	0.9500	C(28)-O(3)-Ru(1)	87.26(8)
C(23A)-C(24A)	1.379(9)	C(1)-N(1)-C(2)	113.73(10)
C(23A)-H(23A)	0.9500	C(1)-N(1)-C(4)	119.57(10)
C(25A)-C(26A)	1.496(8)	C(2)-N(1)-C(4)	126.07(10)
C(25A)-C(27A)	1.517(6)	C(1)-N(2)-C(8)	126.9(3)
C(25A)-H(25A)	1.0000	C(1)-N(2)-C(3)	112.9(3)
C(26A)-H(26D)	0.9800	C(8)-N(2)-C(3)	118.1(3)
C(26A)-H(26E)	0.9800	N(2A)-C(1)-N(1)	107.2(4)
C(26A)-H(26F)	0.9800	N(1)-C(1)-N(2)	107.32(16)
C(27A)-H(27D)	0.9800	N(1)-C(1)-Ru(1)	117.30(8)
C(27A)-H(27E)	0.9800	N(2)-C(1)-Ru(1)	134.28(15)
C(27A)-H(27F)	0.9800	N(2A)-C(1)-Ru(1A)	133.8(4)
N(2A)-C(3A)	1.499(18)	N(1)-C(1)-Ru(1A)	118.27(9)
N(2A)-C(8A)	1.522(14)	N(1)-C(2)-C(3A)	101.9(6)
C(3A)-H(3AC)	0.9900	N(1)-C(2)-C(3)	101.6(2)
C(3A)-H(3AD)	0.9900	N(1)-C(2)-H(2AA)	111.5

C(3)-C(2)-H(2AA)	111.5	C(9)-C(8)-C(13)	119.8(4)
N(1)-C(2)-H(2AB)	111.5	N(2)-C(8)-C(13)	123.0(4)
C(3)-C(2)-H(2AB)	111.5	C(10)-C(9)-C(8)	118.7(3)
H(2AA)-C(2)-H(2AB)	109.3	C(10)-C(9)-C(14)	121.3(3)
N(1)-C(2)-H(2BC)	111.4	C(8)-C(9)-C(14)	119.9(3)
C(3A)-C(2)-H(2BC)	111.4	C(11)-C(10)-C(9)	121.1(3)
N(1)-C(2)-H(2BD)	111.4	C(11)-C(10)-H(10)	119.4
C(3A)-C(2)-H(2BD)	111.4	C(9)-C(10)-H(10)	119.4
H(2BC)-C(2)-H(2BD)	109.2	C(10)-C(11)-C(12)	119.7(3)
N(2)-C(3)-C(2)	102.1(4)	C(10)-C(11)-H(11)	120.2
N(2)-C(3)-H(3A)	111.4	C(12)-C(11)-H(11)	120.2
C(2)-C(3)-H(3A)	111.4	C(13)-C(12)-C(11)	121.6(4)
N(2)-C(3)-H(3B)	111.4	C(13)-C(12)-H(12)	119.2
C(2)-C(3)-H(3B)	111.4	C(11)-C(12)-H(12)	119.2
H(3A)-C(3)-H(3B)	109.2	C(12)-C(13)-C(8)	118.8(4)
N(1)-C(4)-C(6)	110.15(10)	C(12)-C(13)-C(17)	123.2(3)
N(1)-C(4)-C(5)	104.65(10)	C(8)-C(13)-C(17)	118.0(4)
C(6)-C(4)-C(5)	111.19(11)	C(9A)-C(14)-C(15)	112.5(3)
N(1)-C(4)-C(7)	109.26(11)	C(9A)-C(14)-C(16)	110.0(3)
C(6)-C(4)-C(7)	108.61(11)	C(15)-C(14)-C(16)	112.16(15)
C(5)-C(4)-C(7)	112.91(11)	C(15)-C(14)-C(9)	111.40(19)
C(4)-C(5)-Ru(1A)	115.02(9)	C(16)-C(14)-C(9)	112.44(16)
C(4)-C(5)-Ru(1)	111.87(8)	C(15)-C(14)-H(14)	106.8
C(4)-C(5)-H(5A)	109.2	C(16)-C(14)-H(14)	106.8
Ru(1)-C(5)-H(5A)	109.2	C(9)-C(14)-H(14)	106.8
C(4)-C(5)-H(5B)	109.2	C(9A)-C(14)-H(14A)	103(5)
Ru(1)-C(5)-H(5B)	109.2	C(15)-C(14)-H(14A)	109(5)
H(5A)-C(5)-H(5B)	107.9	C(16)-C(14)-H(14A)	110(5)
C(4)-C(5)-H(5C)	108.5	C(14)-C(15)-H(15A)	109.5
Ru(1A)-C(5)-H(5C)	108.5	C(14)-C(15)-H(15B)	109.5
C(4)-C(5)-H(5D)	108.5	H(15A)-C(15)-H(15B)	109.5
Ru(1A)-C(5)-H(5D)	108.5	C(14)-C(15)-H(15C)	109.5
H(5C)-C(5)-H(5D)	107.5	H(15A)-C(15)-H(15C)	109.5
C(4)-C(6)-H(6A)	109.5	H(15B)-C(15)-H(15C)	109.5
C(4)-C(6)-H(6B)	109.5	C(14)-C(16)-H(16A)	109.5
H(6A)-C(6)-H(6B)	109.5	C(14)-C(16)-H(16B)	109.5
C(4)-C(6)-H(6C)	109.5	H(16A)-C(16)-H(16B)	109.5
H(6A)-C(6)-H(6C)	109.5	C(14)-C(16)-H(16C)	109.5
H(6B)-C(6)-H(6C)	109.5	H(16A)-C(16)-H(16C)	109.5
C(4)-C(7)-H(7A)	109.5	H(16B)-C(16)-H(16C)	109.5
C(4)-C(7)-H(7B)	109.5	C(13)-C(17)-H(17A)	109.4
H(7A)-C(7)-H(7B)	109.5	C(13)-C(17)-H(17B)	109.5
C(4)-C(7)-H(7C)	109.5	H(17A)-C(17)-H(17B)	109.5
H(7A)-C(7)-H(7C)	109.5	C(13)-C(17)-H(17C)	109.5
H(7B)-C(7)-H(7C)	109.5	H(17A)-C(17)-H(17C)	109.5
C(9)-C(8)-N(2)	117.1(4)	H(17B)-C(17)-H(17C)	109.5

C(13A)-C(17)-H(17D)	106.0	O(3)-C(28)-O(2)	119.89(13)
C(13A)-C(17)-H(17E)	105.0	O(3)-C(28)-C(29)	120.69(13)
H(17D)-C(17)-H(17E)	110.4	O(2)-C(28)-C(29)	119.40(13)
C(13A)-C(17)-H(17F)	110.3	O(3)-C(28)-Ru(1A)	60.95(8)
H(17D)-C(17)-H(17F)	114.7	O(2)-C(28)-Ru(1A)	58.97(7)
H(17E)-C(17)-H(17F)	109.9	C(29)-C(28)-Ru(1A)	176.70(11)
C(19)-C(18)-Ru(1)	122.71(15)	C(31)-C(29)-C(32)	108.65(15)
C(19A)-C(18)-Ru(1A)	109.0(2)	C(31)-C(29)-C(28)	109.30(13)
C(19)-C(18)-H(18)	118.6	C(32)-C(29)-C(28)	107.84(13)
Ru(1)-C(18)-H(18)	118.6	C(31)-C(29)-C(30)	110.17(16)
C(20)-C(19)-C(24)	117.4(2)	C(32)-C(29)-C(30)	111.21(16)
C(20)-C(19)-C(18)	125.8(3)	C(28)-C(29)-C(30)	109.62(14)
C(24)-C(19)-C(18)	116.8(2)	C(29)-C(30)-H(30A)	109.5
C(21)-C(20)-C(19)	121.9(3)	C(29)-C(30)-H(30B)	109.5
C(21)-C(20)-H(20)	119.0	H(30A)-C(30)-H(30B)	109.5
C(19)-C(20)-H(20)	119.0	C(29)-C(30)-H(30C)	109.5
C(22)-C(21)-C(20)	119.1(3)	H(30A)-C(30)-H(30C)	109.5
C(22)-C(21)-H(21)	120.4	H(30B)-C(30)-H(30C)	109.5
C(20)-C(21)-H(21)	120.4	C(29)-C(31)-H(31A)	109.5
C(21)-C(22)-C(23)	121.9(2)	C(29)-C(31)-H(31B)	109.5
C(21)-C(22)-H(22)	119.0	H(31A)-C(31)-H(31B)	109.5
C(23)-C(22)-H(22)	119.0	C(29)-C(31)-H(31C)	109.5
C(22)-C(23)-C(24)	118.1(3)	H(31A)-C(31)-H(31C)	109.5
C(22)-C(23)-H(23)	121.0	H(31B)-C(31)-H(31C)	109.5
C(24)-C(23)-H(23)	121.0	C(29)-C(32)-H(32A)	109.5
O(1)-C(24)-C(23)	124.5(3)	C(29)-C(32)-H(32B)	109.5
O(1)-C(24)-C(19)	113.9(2)	H(32A)-C(32)-H(32B)	109.5
C(23)-C(24)-C(19)	121.6(3)	C(29)-C(32)-H(32C)	109.5
O(1)-C(25)-C(27)	106.6(2)	H(32A)-C(32)-H(32C)	109.5
O(1)-C(25)-C(26)	109.6(2)	H(32B)-C(32)-H(32C)	109.5
C(27)-C(25)-C(26)	112.5(3)	C(1)-Ru(1A)-C(18)	84.86(7)
O(1)-C(25)-H(25)	109.3	C(1)-Ru(1A)-C(5)	78.81(6)
C(27)-C(25)-H(25)	109.3	C(18)-Ru(1A)-C(5)	93.56(7)
C(26)-C(25)-H(25)	109.3	C(1)-Ru(1A)-O(2)	103.14(6)
C(25)-C(26)-H(26A)	109.5	C(18)-Ru(1A)-O(2)	101.89(7)
C(25)-C(26)-H(26B)	109.5	C(5)-Ru(1A)-O(2)	164.52(8)
H(26A)-C(26)-H(26B)	109.5	C(1)-Ru(1A)-O(3)	102.32(6)
C(25)-C(26)-H(26C)	109.5	C(18)-Ru(1A)-O(3)	162.32(7)
H(26A)-C(26)-H(26C)	109.5	C(5)-Ru(1A)-O(3)	103.62(7)
H(26B)-C(26)-H(26C)	109.5	O(2)-Ru(1A)-O(3)	60.90(5)
C(25)-C(27)-H(27A)	109.5	C(1)-Ru(1A)-O(1A)	166.01(12)
C(25)-C(27)-H(27B)	109.5	C(18)-Ru(1A)-O(1A)	81.59(12)
H(27A)-C(27)-H(27B)	109.5	C(5)-Ru(1A)-O(1A)	98.51(14)
C(25)-C(27)-H(27C)	109.5	O(2)-Ru(1A)-O(1A)	83.15(13)
H(27A)-C(27)-H(27C)	109.5	O(3)-Ru(1A)-O(1A)	91.66(11)
H(27B)-C(27)-H(27C)	109.5	C(1)-Ru(1A)-C(28)	105.35(6)

C(18)-Ru(1A)-C(28)	132.28(7)	H(26D)-C(26A)-H(26F)	109.5
C(5)-Ru(1A)-C(28)	133.97(8)	H(26E)-C(26A)-H(26F)	109.5
O(2)-Ru(1A)-C(28)	30.56(4)	C(25A)-C(27A)-H(27D)	109.5
O(3)-Ru(1A)-C(28)	30.35(5)	C(25A)-C(27A)-H(27E)	109.5
O(1A)-Ru(1A)-C(28)	86.48(12)	H(27D)-C(27A)-H(27E)	109.5
C(24A)-O(1A)-C(25A)	123.4(5)	C(25A)-C(27A)-H(27F)	109.5
C(24A)-O(1A)-Ru(1A)	111.4(4)	H(27D)-C(27A)-H(27F)	109.5
C(25A)-O(1A)-Ru(1A)	120.0(3)	H(27E)-C(27A)-H(27F)	109.5
C(20A)-C(19A)-C(24A)	121.4(6)	C(1)-N(2A)-C(3A)	111.0(8)
C(20A)-C(19A)-C(18)	115.8(5)	C(1)-N(2A)-C(8A)	126.1(8)
C(24A)-C(19A)-C(18)	122.8(5)	C(3A)-N(2A)-C(8A)	119.3(9)
C(19A)-C(20A)-C(21A)	119.5(6)	C(2)-C(3A)-N(2A)	103.5(10)
C(19A)-C(20A)-H(20A)	120.2	C(2)-C(3A)-H(3AC)	111.1
C(21A)-C(20A)-H(20A)	120.2	N(2A)-C(3A)-H(3AC)	111.1
C(22A)-C(21A)-C(20A)	118.5(6)	C(2)-C(3A)-H(3AD)	111.1
C(22A)-C(21A)-H(21A)	120.8	N(2A)-C(3A)-H(3AD)	111.1
C(20A)-C(21A)-H(21A)	120.8	H(3AC)-C(3A)-H(3AD)	109.0
C(21A)-C(22A)-C(23A)	121.4(6)	C(9A)-C(8A)-C(13A)	129.7(10)
C(21A)-C(22A)-H(22A)	119.3	C(9A)-C(8A)-N(2A)	128.1(9)
C(23A)-C(22A)-H(22A)	119.3	C(13A)-C(8A)-N(2A)	101.1(8)
C(24A)-C(23A)-C(22A)	119.8(6)	C(14)-C(9A)-C(8A)	125.6(7)
C(24A)-C(23A)-H(23A)	120.1	C(14)-C(9A)-C(10A)	120.9(5)
C(22A)-C(23A)-H(23A)	120.1	C(8A)-C(9A)-C(10A)	113.1(7)
O(1A)-C(24A)-C(19A)	115.0(5)	C(11A)-C(10A)-C(9A)	122.2(7)
O(1A)-C(24A)-C(23A)	125.5(5)	C(11A)-C(10A)-H(10A)	118.9
C(19A)-C(24A)-C(23A)	119.4(5)	C(9A)-C(10A)-H(10A)	118.9
O(1A)-C(25A)-C(26A)	112.5(4)	C(10A)-C(11A)-C(12A)	122.6(8)
O(1A)-C(25A)-C(27A)	113.1(4)	C(10A)-C(11A)-H(11A)	118.7
C(26A)-C(25A)-C(27A)	113.4(4)	C(12A)-C(11A)-H(11A)	118.7
O(1A)-C(25A)-H(25A)	105.7	C(11A)-C(12A)-C(13A)	118.7(8)
C(26A)-C(25A)-H(25A)	105.7	C(11A)-C(12A)-H(12A)	120.6
C(27A)-C(25A)-H(25A)	105.7	C(13A)-C(12A)-H(12A)	120.6
C(25A)-C(26A)-H(26D)	109.5	C(8A)-C(13A)-C(12A)	113.2(9)
C(25A)-C(26A)-H(26E)	109.5	C(8A)-C(13A)-C(17)	126.4(9)
H(26D)-C(26A)-H(26E)	109.5	C(12A)-C(13A)-C(17)	120.0(6)
C(25A)-C(26A)-H(26F)	109.5		

Table A4. Anistropic Displacement Parameters ($Å^2$ x 10^4) for 3.2. The Anistropic Displacement Factor Exponent Takes the Form: $-2p^2[h^2a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	127(1)	119(1)	85(1)	-4(1)	20(1)	-6(1)
O(1)	311(11)	161(7)	216(8)	-35(6)	106(8)	27(7)
O(2)	267(5)	207(5)	224(4)	3(3)	69(4)	-63(4)

O(3)	268(5)	242(5)	214(4)	9(4)	48(4)	-34(4)
N(1)	150(4)	140(4)	219(5)	-7(3)	81(4)	-13(3)
N(2)	143(9)	139(9)	155(11)	-6(8)	77(9)	0(6)
C(1)	131(5)	153(5)	171(5)	14(4)	38(4)	0(4)
C(2)	193(5)	145(5)	232(5)	-5(4)	54(4)	13(4)
C(3)	175(13)	165(13)	204(19)	-17(13)	76(13)	24(8)
C(4)	163(5)	197(6)	183(5)	-4(4)	72(4)	-35(4)
C(5)	204(5)	207(6)	195(5)	3(4)	90(4)	-20(4)
C(6)	160(5)	276(7)	246(6)	-11(5)	45(4)	-24(5)
C(7)	285(7)	237(7)	261(6)	35(5)	104(5)	-39(5)
C(8)	140(10)	121(12)	259(14)	13(11)	129(10)	6(9)
C(9)	150(11)	254(12)	211(13)	-8(9)	32(10)	31(9)
C(10)	303(17)	275(13)	291(17)	62(12)	159(14)	-3(12)
C(11)	170(11)	309(14)	313(15)	-43(12)	122(11)	-68(10)
C(12)	162(10)	281(16)	263(14)	-9(12)	80(10)	-36(9)
C(13)	126(12)	288(15)	229(17)	-30(13)	40(12)	12(10)
C(14)	352(8)	273(8)	335(8)	48(6)	186(6)	85(6)
C(15)	721(14)	323(9)	425(10)	50(8)	197(10)	221(9)
C(16)	401(9)	375(9)	351(8)	-17(7)	154(7)	68(7)
C(17)	277(7)	338(8)	282(7)	-19(6)	54(6)	9(6)
C(18)	189(5)	168(5)	230(6)	18(4)	83(4)	14(4)
C(19)	175(9)	146(9)	190(12)	20(9)	73(9)	3(6)
C(20)	185(10)	243(12)	279(13)	129(11)	13(9)	-11(7)
C(21)	266(11)	293(13)	412(16)	144(12)	21(11)	73(9)
C(22)	386(15)	310(14)	530(20)	101(14)	40(14)	193(11)
C(23)	360(14)	265(12)	429(16)	-7(11)	84(13)	179(10)
C(24)	208(10)	185(9)	252(12)	39(8)	57(9)	31(8)
C(25)	341(12)	277(11)	292(11)	-81(9)	111(9)	31(9)
C(26)	380(14)	183(11)	750(20)	-139(13)	109(15)	-2(10)
C(27)	568(17)	431(15)	290(12)	-42(11)	122(11)	122(13)
C(28)	236(6)	197(6)	241(6)	-54(5)	64(5)	-34(5)
C(29)	256(7)	288(8)	337(8)	-93(6)	46(6)	-91(6)
C(30)	455(11)	527(12)	528(12)	-62(9)	118(9)	-303(9)
C(31)	262(8)	472(11)	500(11)	-155(9)	-21(7)	-6(7)
C(32)	343(9)	408(10)	531(11)	-258(9)	34(8)	-64(7)

Table A5. Hydrogen Coordinates (x 10^3) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for 3.2

	x	y	z	U_{iso}
H(2AA)	721	1059	766	23
H(2AB)	826	1055	906	23
H(2BC)	731	1061	768	23
H(2BD)	824	1053	914	23
H(3A)	696	1014	1009	21

H(3B)	585	1030	885	21
H(5A)	989	936	643	23
H(5B)	861	955	549	23
H(5C)	990	935	650	23
H(5D)	870	956	547	23
H(6A)	1042	1024	891	34
H(6B)	1111	1001	786	34
H(6C)	1054	967	881	34
H(7A)	828	1041	571	38
H(7B)	974	1038	582	38
H(7C)	923	1068	690	38
H(10)	431	862	1024	33
H(11)	249	879	866	30
H(12)	252	933	691	28
H(14)	739	912	1033	36
H(14A)	721(7)	909(2)	1031(7)	36
H(15A)	639	825	1108	72
H(15B)	784	838	1132	72
H(15C)	701	830	982	72
H(16A)	649	951	1190	55
H(16B)	748	912	1263	55
H(16C)	603	901	1234	55
H(17A)	527	990	647	45
H(17B)	386	1006	632	45
H(17C)	418	960	550	45
H(17D)	368	976	587	45
H(17E)	500	964	588	45
H(17F)	471	1013	666	45
H(18)	917	910	958	23
H(20)	1088	858	1110	29
H(21)	1233	796	1130	40
H(22)	1239	750	943	50
H(23)	1105	765	733	42
H(25)	1032	802	562	36
H(26A)	904	743	624	66
H(26B)	877	746	463	66
H(26C)	783	770	540	66
H(27A)	813	854	448	64
H(27B)	887	825	358	64
H(27C)	953	869	447	64
H(30A)	357	785	594	75
H(30B)	416	826	701	75
H(30C)	496	779	684	75
H(31A)	421	880	384	65
H(31B)	361	885	512	65
H(31C)	313	844	401	65

H(32A)	443	776	378	66
H(32B)	577	769	479	66
H(32C)	557	810	366	66
H(20A)	1090	852	1074	33
H(21A)	1225	786	1076	31
H(22A)	1214	744	877	38
H(23A)	1063	763	682	35
H(25A)	823	842	460	22
H(26D)	931	751	500	56
H(26E)	815	769	384	56
H(26F)	800	760	534	56
H(27D)	1020	872	486	37
H(27E)	1001	829	379	37
H(27F)	1081	821	530	37
H(3AC)	583	1035	858	22
H(3AD)	681	1015	989	22
H(10A)	454	858	1051	20
H(11A)	273	872	901	27
H(12A)	259	922	716	27