X-ray Structure Report

Crystal Data of **2f**·H_2O

August 3, 2002

Experimental

Data Collection

A yellow prism crystal of $C_{16}H_{18}O_4Ru \cdot H_2O$ having approximate dimensions of 0.20 x 0.10 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 ^{o} oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive orthorhombic cell with dimensions:

a = 10.5230(3) Å
b = 13.5805(3) Å
c = 20.7004(5) Å
V = 2958.2(1) Å^3

For Z = 8 and F.W. = 393.40, the calculated density is 1.77 g/cm^3. The systematic absences of:

0kl: k ± 2n
h0l: l ± 2n
hk0: h ± 2n

uniquely determine the space group to be:

Pbca (#61)

The data were collected at a temperature of -50 ± 1^{o}C to a maximum 2θ value of 54.9^{o}. A total of 44 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^{o} in 5.0^{o} step, at χ=45.0^{o} and ϕ = 0.0^{o}. The exposure rate was 180.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 160.0^{o} in 5.0^{o} step, at χ=45.0^{o} and ϕ = 180.0^{o}. The exposure rate was 180.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 28298 reflections that were collected, 3371 were unique (R_{int} = 0.057); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 10.8 cm^{-1}. was applied which resulted in transmission factors ranging from 0.89 to 1.08. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically except for an oxygen atom of H_2O, which was refined isotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F was based on 1948 observed reflections ($I > 3.00\sigma(I)$) and 212 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.026$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.030$$

The standard deviation of an observation of unit weight[4] was 0.43. Unit weights were used. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.64 and -0.37 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package.

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_O|-|F_C|)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$$

where: N_o = number of observations
N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 3.00: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2002).

(10) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{16}H_{18}O_4Ru \cdot H_2O$
Formula Weight	393.40
Crystal Color, Habit	yellow, prism
Crystal Dimensions	0.20 X 0.10 X 0.10 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 180.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 10.5230(3) Å b = 13.5805(3) Å c = 20.7004(5) Å V = 2958.2(1) $Å^3$
Space Group	Pbca (#61)
Z value	8
D_{calc}	1.766 g/cm^3
F_{000}	1600.00
μ(MoKα)	10.82 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	270 mm x 256 mm
Data Images	44 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0°
Exposure Rate	180.0 sec./°
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 160.0°
Exposure Rate	180.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9°
No. of Reflections Measured	Total: 28298 Unique: 3371 (R_{int} = 0.057)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8925 - 1.0806)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	$\Sigma w (\|Fo\| - \|Fc\|)^2$
Least Squares Weights	1
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	1948
No. Variables	212
Reflection/Parameter Ratio	9.19
Residuals: R (I>3.00σ(I))	0.026
Residuals: Rw (I>3.00σ(I))	0.030
Goodness of Fit Indicator	0.43
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.64 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.37 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ru(1)	0.13216(3)	0.08895(2)	0.13956(2)	2.374(6)
O(1)	0.4389(3)	0.0216(3)	0.1579(2)	3.42(8)
O(2)	-0.0330(3)	-0.1197(3)	0.0955(2)	3.51(8)
O(3)	0.2867(3)	-0.0429(3)	0.2523(2)	3.36(8)
O(4)	0.3563(3)	0.0378(3)	0.0359(1)	3.27(7)
O(5)	0.6079(5)	0.1793(4)	0.1204(2)	6.2(1)
C(1)	0.3270(4)	-0.0040(3)	0.1446(3)	2.47(9)
C(2)	0.2353(5)	-0.0370(3)	0.1927(2)	2.6(1)
C(3)	0.1107(4)	-0.0645(3)	0.1775(2)	2.7(1)
C(4)	0.0688(4)	-0.0780(3)	0.1107(2)	2.66(9)
C(5)	0.1473(4)	-0.0252(3)	0.0653(2)	2.49(9)
C(6)	0.2732(4)	0.0031(3)	0.0807(2)	2.48(9)
C(7)	0.2085(5)	-0.0758(5)	0.3050(2)	4.2(1)
C(8)	0.3246(5)	0.0239(4)	-0.0312(2)	3.8(1)
C(9)	0.1545(6)	0.2219(4)	0.0790(4)	5.1(2)
C(10)	0.2359(6)	0.2234(4)	0.1315(6)	7.2(2)
C(11)	0.1886(9)	0.2200(5)	0.1937(6)	7.7(3)
C(12)	0.0697(9)	0.1899(5)	0.2156(3)	6.4(2)
C(13)	-0.0375(7)	0.1485(4)	0.1840(3)	4.9(2)
C(14)	-0.0661(5)	0.1383(4)	0.1203(3)	4.6(1)
C(15)	-0.0732(6)	0.2155(4)	0.0696(3)	5.3(2)
C(16)	0.0368(6)	0.2833(4)	0.0762(3)	4.6(1)
H(1)	0.0527(4)	-0.0766(3)	0.2118(2)	3.3(1)
H(2)	0.1150(4)	-0.0125(3)	0.0233(2)	3.0(1)
H(3)	0.1382(5)	-0.0325(5)	0.3094(2)	5.1(2)
H(4)	0.1787(5)	-0.1403(5)	0.2957(2)	5.1(2)
H(5)	0.2559(5)	-0.0767(5)	0.3440(2)	5.1(2)
H(6)	0.2459(5)	0.0554(4)	-0.0403(2)	4.5(1)
H(7)	0.3892(5)	0.0515(4)	-0.0577(2)	4.5(1)
H(8)	0.3175(5)	-0.0445(4)	-0.0399(2)	4.5(1)
H(9)	0.1921(6)	0.2106(4)	0.0380(4)	6.1(2)
H(10)	0.3246(6)	0.2213(4)	0.1231(6)	8.6(3)
H(11)	0.2553(9)	0.2066(5)	0.2233(6)	9.3(3)
H(12)	0.0804(9)	0.1601(5)	0.2568(3)	7.6(2)
H(13)	-0.0804(7)	0.1017(4)	0.2102(3)	5.9(2)
H(14)	-0.1236(5)	0.0859(4)	0.1121(3)	5.5(2)
H(15)	-0.0742(6)	0.1857(4)	0.0281(3)	6.3(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(16)	-0.1487(6)	0.2527(4)	0.0755(3)	6.3(2)
H(17)	0.0384(6)	0.3263(4)	0.0400(3)	5.5(2)
H(18)	0.0327(6)	0.3210(4)	0.1148(3)	5.5(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0265(1)	0.0246(1)	0.0390(2)	0.0012(2)	-0.0024(2)	-0.0052(2)
O(1)	0.026(2)	0.056(2)	0.047(2)	-0.002(2)	-0.006(1)	-0.001(2)
O(2)	0.035(2)	0.042(2)	0.055(2)	-0.011(2)	-0.001(2)	-0.007(2)
O(3)	0.038(2)	0.054(2)	0.035(2)	0.002(2)	-0.003(2)	0.004(2)
O(4)	0.031(2)	0.054(2)	0.039(2)	-0.007(2)	0.002(2)	0.001(2)
C(1)	0.028(2)	0.028(2)	0.038(3)	0.002(2)	-0.001(2)	-0.004(2)
C(2)	0.036(3)	0.027(2)	0.034(2)	0.005(2)	-0.003(2)	-0.003(2)
C(3)	0.031(3)	0.033(2)	0.039(3)	0.001(2)	0.003(2)	-0.002(2)
C(4)	0.028(2)	0.027(2)	0.047(3)	0.001(2)	0.000(2)	-0.005(2)
C(5)	0.031(3)	0.030(2)	0.034(2)	0.000(2)	-0.003(2)	-0.004(2)
C(6)	0.028(2)	0.027(2)	0.039(3)	-0.000(2)	0.003(2)	-0.001(2)
C(7)	0.052(3)	0.071(4)	0.038(3)	0.007(3)	0.006(2)	0.006(3)
C(8)	0.042(3)	0.060(3)	0.041(3)	-0.008(3)	0.003(2)	0.003(3)
C(9)	0.059(4)	0.035(3)	0.098(5)	0.002(3)	0.032(4)	0.013(3)
C(10)	0.036(3)	0.026(3)	0.21(1)	-0.004(2)	-0.007(6)	-0.011(5)
C(11)	0.095(7)	0.038(4)	0.160(9)	0.022(4)	-0.082(7)	-0.036(5)
C(12)	0.133(7)	0.056(4)	0.054(4)	0.048(5)	-0.020(5)	-0.017(3)
C(13)	0.070(4)	0.044(3)	0.071(4)	0.025(3)	0.036(4)	0.008(3)
C(14)	0.037(3)	0.038(3)	0.101(5)	-0.000(2)	-0.005(3)	-0.000(3)
C(15)	0.070(4)	0.047(3)	0.083(5)	0.010(3)	-0.029(4)	-0.007(3)
C(16)	0.064(4)	0.036(3)	0.074(4)	0.007(3)	0.004(3)	0.009(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ru(1)	C(1)	2.410(4)	Ru(1)	C(2)	2.305(5)
Ru(1)	C(3)	2.238(4)	Ru(1)	C(4)	2.438(4)
Ru(1)	C(5)	2.189(4)	Ru(1)	C(6)	2.246(4)
Ru(1)	C(9)	2.210(6)	Ru(1)	C(10)	2.134(6)
Ru(1)	C(11)	2.185(7)	Ru(1)	C(12)	2.188(6)
Ru(1)	C(13)	2.165(5)	Ru(1)	C(14)	2.227(6)
O(1)	C(1)	1.258(5)	O(2)	C(4)	1.251(5)
O(3)	C(2)	1.349(5)	O(3)	C(7)	1.437(6)
O(4)	C(6)	1.360(5)	O(4)	C(8)	1.441(5)
C(1)	C(2)	1.457(7)	C(1)	C(6)	1.442(7)
C(2)	C(3)	1.400(6)	C(3)	C(4)	1.463(6)
C(4)	C(5)	1.443(6)	C(5)	C(6)	1.416(6)
C(9)	C(10)	1.38(1)	C(9)	C(16)	1.494(8)
C(10)	C(11)	1.38(1)	C(11)	C(12)	1.39(1)
C(12)	C(13)	1.42(1)	C(13)	C(14)	1.360(9)
C(14)	C(15)	1.485(8)	C(15)	C(16)	1.486(8)

Table 4. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
Ru(1)	C(1)	2.410(4)	Ru(1)	C(2)	2.305(5)
Ru(1)	C(3)	2.238(4)	Ru(1)	C(4)	2.438(4)
Ru(1)	C(5)	2.189(4)	Ru(1)	C(6)	2.246(4)
Ru(1)	C(9)	2.210(6)	Ru(1)	C(10)	2.134(6)
Ru(1)	C(11)	2.185(7)	Ru(1)	C(12)	2.188(6)
Ru(1)	C(13)	2.165(5)	Ru(1)	C(14)	2.227(6)
C(3)	H(1)	0.950(6)	C(5)	H(2)	0.950(6)
C(7)	H(3)	0.950(8)	C(7)	H(4)	0.950(8)
C(7)	H(5)	0.950(7)	C(8)	H(6)	0.950(7)
C(8)	H(7)	0.950(7)	C(8)	H(8)	0.950(8)
C(9)	H(9)	0.95(1)	C(10)	H(10)	0.950(9)
C(11)	H(11)	0.95(1)	C(12)	H(12)	0.950(9)
C(13)	H(13)	0.950(9)	C(14)	H(14)	0.950(8)
C(15)	H(15)	0.950(9)	C(15)	H(16)	0.950(8)
C(16)	H(17)	0.950(8)	C(16)	H(18)	0.950(8)

Table 5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Ru(1)	C(2)	35.9(2)	C(1)	Ru(1)	C(3)	65.4(2)
C(2)	Ru(1)	C(3)	35.8(2)	C(1)	Ru(1)	C(4)	75.9(1)
C(2)	Ru(1)	C(4)	63.6(2)	C(3)	Ru(1)	C(4)	36.1(2)
C(1)	Ru(1)	C(5)	66.3(2)	C(2)	Ru(1)	C(5)	77.0(2)
C(3)	Ru(1)	C(5)	66.1(2)	C(4)	Ru(1)	C(5)	35.8(2)
C(1)	Ru(1)	C(6)	35.9(2)	C(2)	Ru(1)	C(6)	64.0(2)
C(3)	Ru(1)	C(6)	76.9(2)	C(4)	Ru(1)	C(6)	64.2(2)
C(5)	Ru(1)	C(6)	37.2(2)	C(1)	Ru(1)	C(9)	111.2(2)
C(2)	Ru(1)	C(9)	145.8(2)	C(3)	Ru(1)	C(9)	166.0(2)
C(4)	Ru(1)	C(9)	130.5(2)	C(5)	Ru(1)	C(9)	99.9(2)
C(1)	Ru(1)	C(10)	91.0(2)	C(2)	Ru(1)	C(10)	115.6(3)
C(3)	Ru(1)	C(10)	151.2(3)	C(4)	Ru(1)	C(10)	156.5(3)
C(5)	Ru(1)	C(10)	120.9(3)	C(1)	Ru(1)	C(11)	100.0(3)
C(2)	Ru(1)	C(11)	103.4(2)	C(3)	Ru(1)	C(11)	127.3(3)
C(4)	Ru(1)	C(11)	163.2(3)	C(5)	Ru(1)	C(11)	156.5(4)
C(1)	Ru(1)	C(12)	123.6(3)	C(2)	Ru(1)	C(12)	105.3(2)
C(3)	Ru(1)	C(12)	107.5(2)	C(4)	Ru(1)	C(12)	132.6(3)
C(5)	Ru(1)	C(12)	166.1(3)	C(1)	Ru(1)	C(13)	151.5(2)
C(2)	Ru(1)	C(13)	117.6(2)	C(3)	Ru(1)	C(13)	96.6(2)
C(4)	Ru(1)	C(13)	103.1(2)	C(5)	Ru(1)	C(13)	128.5(2)
C(1)	Ru(1)	C(14)	164.2(2)	C(2)	Ru(1)	C(14)	138.6(2)
C(3)	Ru(1)	C(14)	104.4(2)	C(4)	Ru(1)	C(14)	88.8(2)
C(5)	Ru(1)	C(14)	99.0(2)	C(6)	Ru(1)	C(9)	92.7(2)
C(6)	Ru(1)	C(10)	93.7(3)	C(9)	Ru(1)	C(10)	37.1(3)
C(6)	Ru(1)	C(11)	121.4(3)	C(9)	Ru(1)	C(11)	66.2(3)
C(10)	Ru(1)	C(11)	37.3(3)	C(6)	Ru(1)	C(12)	156.0(3)
C(9)	Ru(1)	C(12)	85.9(3)	C(10)	Ru(1)	C(12)	71.0(3)
C(11)	Ru(1)	C(12)	37.1(3)	C(6)	Ru(1)	C(13)	165.7(2)
C(9)	Ru(1)	C(13)	91.3(2)	C(10)	Ru(1)	C(13)	97.8(3)
C(11)	Ru(1)	C(13)	72.7(3)	C(12)	Ru(1)	C(13)	38.0(3)
C(6)	Ru(1)	C(14)	132.7(2)	C(9)	Ru(1)	C(14)	75.7(2)
C(10)	Ru(1)	C(14)	102.0(2)	C(11)	Ru(1)	C(14)	95.8(3)
C(12)	Ru(1)	C(14)	70.0(3)	C(13)	Ru(1)	C(14)	36.0(2)
C(2)	O(3)	C(7)	118.9(4)	C(6)	O(4)	C(8)	117.7(4)
Ru(1)	C(1)	O(1)	131.4(3)	Ru(1)	C(1)	C(2)	68.1(2)
O(1)	C(1)	C(2)	123.7(5)	Ru(1)	C(1)	C(6)	65.9(2)
O(1)	C(1)	C(6)	123.3(4)	C(2)	C(1)	C(6)	112.8(4)

Table 5. Bond angles (°) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
Ru(1)	C(2)	O(3)	132.0(3)	Ru(1)	C(2)	C(1)	76.0(3)
O(3)	C(2)	C(1)	112.2(4)	Ru(1)	C(2)	C(3)	69.5(3)
O(3)	C(2)	C(3)	124.4(5)	C(1)	C(2)	C(3)	123.3(4)
Ru(1)	C(3)	C(2)	74.7(3)	Ru(1)	C(3)	C(4)	79.4(3)
C(2)	C(3)	C(4)	121.9(4)	Ru(1)	C(4)	O(2)	135.8(3)
Ru(1)	C(4)	C(3)	64.5(2)	O(2)	C(4)	C(3)	123.6(4)
Ru(1)	C(4)	C(5)	62.6(2)	O(2)	C(4)	C(5)	123.4(5)
C(3)	C(4)	C(5)	112.4(4)	Ru(1)	C(5)	C(4)	81.5(3)
Ru(1)	C(5)	C(6)	73.6(3)	C(4)	C(5)	C(6)	121.6(4)
Ru(1)	C(6)	O(4)	127.9(3)	Ru(1)	C(6)	C(1)	78.3(3)
O(4)	C(6)	C(1)	113.4(4)	Ru(1)	C(6)	C(5)	69.2(3)
O(4)	C(6)	C(5)	122.8(4)	C(1)	C(6)	C(5)	123.8(4)
Ru(1)	C(9)	C(10)	68.5(4)	Ru(1)	C(9)	C(16)	113.0(4)
C(10)	C(9)	C(16)	122.3(6)	Ru(1)	C(10)	C(9)	74.5(4)
Ru(1)	C(10)	C(11)	73.4(4)	C(9)	C(10)	C(11)	120.6(7)
Ru(1)	C(11)	C(10)	69.4(4)	Ru(1)	C(11)	C(12)	71.5(4)
C(10)	C(11)	C(12)	129.6(7)	Ru(1)	C(12)	C(11)	71.3(4)
Ru(1)	C(12)	C(13)	70.1(3)	C(11)	C(12)	C(13)	132.9(7)
Ru(1)	C(13)	C(12)	71.8(4)	Ru(1)	C(13)	C(14)	74.5(4)
C(12)	C(13)	C(14)	131.5(6)	Ru(1)	C(14)	C(13)	69.5(4)
Ru(1)	C(14)	C(15)	112.7(4)	C(13)	C(14)	C(15)	128.7(6)
C(14)	C(15)	C(16)	109.5(5)	C(9)	C(16)	C(15)	107.6(5)

Table 6. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Ru(1)	C(2)	35.9(2)	C(1)	Ru(1)	C(3)	65.4(2)
C(2)	Ru(1)	C(3)	35.8(2)	C(1)	Ru(1)	C(4)	75.9(1)
C(2)	Ru(1)	C(4)	63.6(2)	C(3)	Ru(1)	C(4)	36.1(2)
C(1)	Ru(1)	C(5)	66.3(2)	C(2)	Ru(1)	C(5)	77.0(2)
C(3)	Ru(1)	C(5)	66.1(2)	C(4)	Ru(1)	C(5)	35.8(2)
C(1)	Ru(1)	C(6)	35.9(2)	C(2)	Ru(1)	C(6)	64.0(2)
C(3)	Ru(1)	C(6)	76.9(2)	C(4)	Ru(1)	C(6)	64.2(2)
C(5)	Ru(1)	C(6)	37.2(2)	C(1)	Ru(1)	C(9)	111.2(2)
C(2)	Ru(1)	C(9)	145.8(2)	C(3)	Ru(1)	C(9)	166.0(2)
C(4)	Ru(1)	C(9)	130.5(2)	C(5)	Ru(1)	C(9)	99.9(2)
C(1)	Ru(1)	C(10)	91.0(2)	C(2)	Ru(1)	C(10)	115.6(3)
C(3)	Ru(1)	C(10)	151.2(3)	C(4)	Ru(1)	C(10)	156.5(3)
C(5)	Ru(1)	C(10)	120.9(3)	C(1)	Ru(1)	C(11)	100.0(3)
C(2)	Ru(1)	C(11)	103.4(2)	C(3)	Ru(1)	C(11)	127.3(3)
C(4)	Ru(1)	C(11)	163.2(3)	C(5)	Ru(1)	C(11)	156.5(4)
C(1)	Ru(1)	C(12)	123.6(3)	C(2)	Ru(1)	C(12)	105.3(2)
C(3)	Ru(1)	C(12)	107.5(2)	C(4)	Ru(1)	C(12)	132.6(3)
C(5)	Ru(1)	C(12)	166.1(3)	C(1)	Ru(1)	C(13)	151.5(2)
C(2)	Ru(1)	C(13)	117.6(2)	C(3)	Ru(1)	C(13)	96.6(2)
C(4)	Ru(1)	C(13)	103.1(2)	C(5)	Ru(1)	C(13)	128.5(2)
C(1)	Ru(1)	C(14)	164.2(2)	C(2)	Ru(1)	C(14)	138.6(2)
C(3)	Ru(1)	C(14)	104.4(2)	C(4)	Ru(1)	C(14)	88.8(2)
C(5)	Ru(1)	C(14)	99.0(2)	C(6)	Ru(1)	C(9)	92.7(2)
C(6)	Ru(1)	C(10)	93.7(3)	C(9)	Ru(1)	C(10)	37.1(3)
C(6)	Ru(1)	C(11)	121.4(3)	C(9)	Ru(1)	C(11)	66.2(3)
C(10)	Ru(1)	C(11)	37.3(3)	C(6)	Ru(1)	C(12)	156.0(3)
C(9)	Ru(1)	C(12)	85.9(3)	C(10)	Ru(1)	C(12)	71.0(3)
C(11)	Ru(1)	C(12)	37.1(3)	C(6)	Ru(1)	C(13)	165.7(2)
C(9)	Ru(1)	C(13)	91.3(2)	C(10)	Ru(1)	C(13)	97.8(3)
C(11)	Ru(1)	C(13)	72.7(3)	C(12)	Ru(1)	C(13)	38.0(3)
C(6)	Ru(1)	C(14)	132.7(2)	C(9)	Ru(1)	C(14)	75.7(2)
C(10)	Ru(1)	C(14)	102.0(2)	C(11)	Ru(1)	C(14)	95.8(3)
C(12)	Ru(1)	C(14)	70.0(3)	C(13)	Ru(1)	C(14)	36.0(2)
Ru(1)	C(1)	O(1)	131.4(3)	Ru(1)	C(1)	C(2)	68.1(2)
Ru(1)	C(1)	C(6)	65.9(2)	Ru(1)	C(2)	O(3)	132.0(3)
Ru(1)	C(2)	C(1)	76.0(3)	Ru(1)	C(2)	C(3)	69.5(3)
Ru(1)	C(3)	C(2)	74.7(3)	Ru(1)	C(3)	C(4)	79.4(3)

Table 6. Bond angles involving hydrogens (°) -- continued

atom	atom	atom	angle	atom	atom	atom	angle
Ru(1)	C(3)	H(1)	119.2(4)	C(2)	C(3)	H(1)	118.7(6)
C(4)	C(3)	H(1)	119.4(5)	Ru(1)	C(4)	O(2)	135.8(3)
Ru(1)	C(4)	C(3)	64.5(2)	Ru(1)	C(4)	C(5)	62.6(2)
Ru(1)	C(5)	C(4)	81.5(3)	Ru(1)	C(5)	C(6)	73.6(3)
Ru(1)	C(5)	H(2)	119.3(4)	C(4)	C(5)	H(2)	118.9(5)
C(6)	C(5)	H(2)	119.4(5)	Ru(1)	C(6)	O(4)	127.9(3)
Ru(1)	C(6)	C(1)	78.3(3)	Ru(1)	C(6)	C(5)	69.2(3)
O(3)	C(7)	H(3)	109.1(6)	O(3)	C(7)	H(4)	108.8(6)
H(3)	C(7)	H(4)	109.5(7)	O(3)	C(7)	H(5)	110.5(6)
H(3)	C(7)	H(5)	109.5(7)	H(4)	C(7)	H(5)	109.5(7)
O(4)	C(8)	H(6)	109.5(6)	O(4)	C(8)	H(7)	109.7(6)
H(6)	C(8)	H(7)	109.5(7)	O(4)	C(8)	H(8)	109.2(6)
H(6)	C(8)	H(8)	109.5(7)	H(7)	C(8)	H(8)	109.5(7)
Ru(1)	C(9)	C(10)	68.5(4)	Ru(1)	C(9)	C(16)	113.0(4)
Ru(1)	C(9)	H(9)	114.8(6)	C(10)	C(9)	H(9)	116.5(8)
C(16)	C(9)	H(9)	113.6(8)	Ru(1)	C(10)	C(9)	74.5(4)
Ru(1)	C(10)	C(11)	73.4(4)	Ru(1)	C(10)	H(10)	119.3(8)
C(9)	C(10)	H(10)	117.7(9)	C(11)	C(10)	H(10)	121.5(1)
Ru(1)	C(11)	C(10)	69.4(4)	Ru(1)	C(11)	C(12)	71.5(4)
Ru(1)	C(11)	H(11)	112.1(9)	C(10)	C(11)	H(11)	110.1(1)
C(12)	C(11)	H(11)	113.4(1)	Ru(1)	C(12)	C(11)	71.3(4)
Ru(1)	C(12)	C(13)	70.1(3)	Ru(1)	C(12)	H(12)	110.1(7)
C(11)	C(12)	H(12)	108.1(1)	C(13)	C(12)	H(12)	109.9(9)
Ru(1)	C(13)	C(12)	71.8(4)	Ru(1)	C(13)	C(14)	74.5(4)
Ru(1)	C(13)	H(13)	112.6(6)	C(12)	C(13)	H(13)	112.3(8)
C(14)	C(13)	H(13)	112.4(8)	Ru(1)	C(14)	C(13)	69.5(4)
Ru(1)	C(14)	C(15)	112.7(4)	Ru(1)	C(14)	H(14)	113.8(6)
C(13)	C(14)	H(14)	113.1(7)	C(15)	C(14)	H(14)	111.7(7)
C(14)	C(15)	H(15)	109.9(7)	C(16)	C(15)	H(15)	110.9(7)
C(14)	C(15)	H(16)	109.1(7)	C(16)	C(15)	H(16)	108.1(7)
H(15)	C(15)	H(16)	109.5(8)	C(9)	C(16)	H(17)	111.1(7)
C(15)	C(16)	H(17)	108.8(7)	C(9)	C(16)	H(18)	107.8(7)
C(15)	C(16)	H(18)	112.1(7)	H(17)	C(16)	H(18)	109.5(8)

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(2)	Ru(1)	C(1)	O(1)	-116.3(1)	C(2)	Ru(1)	C(1)	C(2)	0.0(4)
C(2)	Ru(1)	C(1)	C(6)	129.6(8)	C(3)	Ru(1)	C(1)	O(1)	-143.8(1)
C(3)	Ru(1)	C(1)	C(2)	-27.5(5)	C(3)	Ru(1)	C(1)	C(6)	102.1(6)
C(5)	Ru(1)	C(1)	O(1)	142.8(1)	C(5)	Ru(1)	C(1)	C(2)	-100.9(6)
C(5)	Ru(1)	C(1)	C(6)	28.7(5)	C(6)	Ru(1)	C(1)	O(1)	114.1(1)
C(6)	Ru(1)	C(1)	C(2)	-129.6(8)	C(6)	Ru(1)	C(1)	C(6)	0.0(4)
C(9)	Ru(1)	C(1)	O(1)	51.0(1)	C(9)	Ru(1)	C(1)	C(2)	167.3(9)
C(9)	Ru(1)	C(1)	C(6)	-63.1(8)	C(10)	Ru(1)	C(1)	O(1)	19.1(1)
C(10)	Ru(1)	C(1)	C(2)	135.5(9)	C(10)	Ru(1)	C(1)	C(6)	-95.0(9)
C(11)	Ru(1)	C(1)	O(1)	-17.3(2)	C(11)	Ru(1)	C(1)	C(2)	99.1(1)
C(11)	Ru(1)	C(1)	C(6)	-131.3(1)	C(12)	Ru(1)	C(1)	O(1)	-48.5(2)
C(12)	Ru(1)	C(1)	C(2)	67.8(1)	C(12)	Ru(1)	C(1)	C(6)	-162.6(1)
C(13)	Ru(1)	C(1)	O(1)	-89.2(2)	C(13)	Ru(1)	C(1)	C(2)	27.2(2)
C(13)	Ru(1)	C(1)	C(6)	156.8(2)	C(14)	Ru(1)	C(1)	O(1)	164.4(2)
C(14)	Ru(1)	C(1)	C(2)	-79.3(3)	C(14)	Ru(1)	C(1)	C(6)	50.3(3)
C(1)	Ru(1)	C(2)	O(3)	107.4(1)	C(1)	Ru(1)	C(2)	C(1)	0.0(4)
C(1)	Ru(1)	C(2)	C(3)	-134.3(8)	C(3)	Ru(1)	C(2)	O(3)	-118.3(1)
C(3)	Ru(1)	C(2)	C(1)	134.3(8)	C(3)	Ru(1)	C(2)	C(3)	0.0(4)
C(5)	Ru(1)	C(2)	O(3)	174.7(1)	C(5)	Ru(1)	C(2)	C(1)	67.3(5)
C(5)	Ru(1)	C(2)	C(3)	-67.0(5)	C(6)	Ru(1)	C(2)	O(3)	137.5(1)
C(6)	Ru(1)	C(2)	C(1)	30.1(5)	C(6)	Ru(1)	C(2)	C(3)	-104.1(6)
C(9)	Ru(1)	C(2)	O(3)	86.1(2)	C(9)	Ru(1)	C(2)	C(1)	-21.3(2)
C(9)	Ru(1)	C(2)	C(3)	-155.6(2)	C(10)	Ru(1)	C(2)	O(3)	56.4(2)
C(10)	Ru(1)	C(2)	C(1)	-51.0(1)	C(10)	Ru(1)	C(2)	C(3)	174.7(1)
C(11)	Ru(1)	C(2)	O(3)	18.9(2)	C(11)	Ru(1)	C(2)	C(1)	-88.5(1)
C(11)	Ru(1)	C(2)	C(3)	137.2(1)	C(12)	Ru(1)	C(2)	O(3)	-19.5(1)
C(12)	Ru(1)	C(2)	C(1)	-126.9(9)	C(12)	Ru(1)	C(2)	C(3)	98.8(9)
C(13)	Ru(1)	C(2)	O(3)	-58.4(1)	C(13)	Ru(1)	C(2)	C(1)	-165.8(9)
C(13)	Ru(1)	C(2)	C(3)	60.0(9)	C(14)	Ru(1)	C(2)	O(3)	-96.4(1)
C(14)	Ru(1)	C(2)	C(1)	156.2(1)	C(14)	Ru(1)	C(2)	C(3)	21.9(1)
C(1)	Ru(1)	C(3)	C(2)	27.5(5)	C(1)	Ru(1)	C(3)	C(4)	-100.0(6)
C(2)	Ru(1)	C(3)	C(2)	0.0(4)	C(2)	Ru(1)	C(3)	C(4)	-127.5(8)
C(5)	Ru(1)	C(3)	C(2)	101.2(6)	C(5)	Ru(1)	C(3)	C(4)	-26.3(5)
C(6)	Ru(1)	C(3)	C(2)	63.5(5)	C(6)	Ru(1)	C(3)	C(4)	-64.0(5)
C(9)	Ru(1)	C(3)	C(2)	106.4(3)	C(9)	Ru(1)	C(3)	C(4)	-21.1(3)
C(10)	Ru(1)	C(3)	C(2)	-9.9(2)	C(10)	Ru(1)	C(3)	C(4)	-137.4(2)
C(11)	Ru(1)	C(3)	C(2)	-56.2(1)	C(11)	Ru(1)	C(3)	C(4)	176.3(1)

Table 7. Torsion angles (°) -- continued

atom	atom	atom	atom	angle
C(12)	Ru(1)	C(3)	C(2)	-92.0(9)
C(13)	Ru(1)	C(3)	C(2)	-129.4(8)
C(14)	Ru(1)	C(3)	C(2)	-165.3(8)
C(1)	Ru(1)	C(5)	C(4)	98.8(6)
C(2)	Ru(1)	C(5)	C(4)	62.6(5)
C(3)	Ru(1)	C(5)	C(4)	26.5(5)
C(6)	Ru(1)	C(5)	C(4)	126.6(7)
C(9)	Ru(1)	C(5)	C(4)	-152.2(7)
C(10)	Ru(1)	C(5)	C(4)	174.8(1)
C(11)	Ru(1)	C(5)	C(4)	156.4(3)
C(12)	Ru(1)	C(5)	C(4)	-38.5(4)
C(13)	Ru(1)	C(5)	C(4)	-52.4(1)
C(14)	Ru(1)	C(5)	C(4)	-75.3(7)
C(1)	Ru(1)	C(6)	O(4)	-110.6(1)
C(1)	Ru(1)	C(6)	C(5)	133.3(7)
C(2)	Ru(1)	C(6)	C(1)	-30.2(5)
C(3)	Ru(1)	C(6)	O(4)	-176.5(9)
C(3)	Ru(1)	C(6)	C(5)	67.5(5)
C(5)	Ru(1)	C(6)	C(1)	-133.3(7)
C(9)	Ru(1)	C(6)	O(4)	13.1(1)
C(9)	Ru(1)	C(6)	C(5)	-103.0(7)
C(10)	Ru(1)	C(6)	C(1)	86.5(8)
C(11)	Ru(1)	C(6)	O(4)	-50.5(2)
C(11)	Ru(1)	C(6)	C(5)	-166.6(1)
C(12)	Ru(1)	C(6)	C(1)	37.8(2)
C(13)	Ru(1)	C(6)	O(4)	119.2(3)
C(13)	Ru(1)	C(6)	C(5)	3.2(3)
C(14)	Ru(1)	C(6)	C(1)	-163.4(1)
C(1)	Ru(1)	C(9)	C(10)	-61.0(9)
C(2)	Ru(1)	C(9)	C(10)	-47.8(1)
C(3)	Ru(1)	C(9)	C(10)	-134.2(3)
C(5)	Ru(1)	C(9)	C(10)	-129.3(8)
C(6)	Ru(1)	C(9)	C(10)	-92.6(8)
C(10)	Ru(1)	C(9)	C(10)	0.0(7)
C(11)	Ru(1)	C(9)	C(10)	30.8(8)
C(12)	Ru(1)	C(9)	C(10)	63.5(9)
C(13)	Ru(1)	C(9)	C(10)	101.1(9)

atom	atom	atom	atom	angle
C(12)	Ru(1)	C(3)	C(4)	140.5(9)
C(13)	Ru(1)	C(3)	C(4)	103.1(7)
C(14)	Ru(1)	C(3)	C(4)	67.3(7)
C(1)	Ru(1)	C(5)	C(6)	-27.7(4)
C(2)	Ru(1)	C(5)	C(6)	-64.0(5)
C(3)	Ru(1)	C(5)	C(6)	-100.1(6)
C(6)	Ru(1)	C(5)	C(6)	0.0(4)
C(9)	Ru(1)	C(5)	C(6)	81.2(7)
C(10)	Ru(1)	C(5)	C(6)	48.3(1)
C(11)	Ru(1)	C(5)	C(6)	29.8(3)
C(12)	Ru(1)	C(5)	C(6)	-165.0(4)
C(13)	Ru(1)	C(5)	C(6)	-179.0(1)
C(14)	Ru(1)	C(5)	C(6)	158.1(7)
C(1)	Ru(1)	C(6)	C(1)	0.0(4)
C(2)	Ru(1)	C(6)	O(4)	-140.8(9)
C(2)	Ru(1)	C(6)	C(5)	103.2(6)
C(3)	Ru(1)	C(6)	C(1)	-65.8(5)
C(5)	Ru(1)	C(6)	O(4)	116.0(1)
C(5)	Ru(1)	C(6)	C(5)	0.0(4)
C(9)	Ru(1)	C(6)	C(1)	123.7(7)
C(10)	Ru(1)	C(6)	O(4)	-24.1(1)
C(10)	Ru(1)	C(6)	C(5)	-140.1(9)
C(11)	Ru(1)	C(6)	C(1)	60.1(1)
C(12)	Ru(1)	C(6)	O(4)	-72.8(3)
C(12)	Ru(1)	C(6)	C(5)	171.2(2)
C(13)	Ru(1)	C(6)	C(1)	-130.2(3)
C(14)	Ru(1)	C(6)	O(4)	85.9(1)
C(14)	Ru(1)	C(6)	C(5)	-30.1(1)
C(1)	Ru(1)	C(9)	C(16)	-178.3(8)
C(2)	Ru(1)	C(9)	C(16)	-165.1(9)
C(3)	Ru(1)	C(9)	C(16)	108.6(3)
C(5)	Ru(1)	C(9)	C(16)	113.5(9)
C(6)	Ru(1)	C(9)	C(16)	150.2(9)
C(10)	Ru(1)	C(9)	C(16)	-117.2(1)
C(11)	Ru(1)	C(9)	C(16)	-86.5(1)
C(12)	Ru(1)	C(9)	C(16)	-53.8(1)
C(13)	Ru(1)	C(9)	C(16)	-16.1(1)

Table 7. Torsion angles (°) -- continued

atom	atom	atom	atom	angle
C(14)	Ru(1)	C(9)	C(10)	133.9(9)
C(1)	Ru(1)	C(10)	C(9)	125.3(8)
C(2)	Ru(1)	C(10)	C(9)	152.5(8)
C(3)	Ru(1)	C(10)	C(9)	158.9(1)
C(5)	Ru(1)	C(10)	C(9)	62.7(1)
C(6)	Ru(1)	C(10)	C(9)	89.5(8)
C(9)	Ru(1)	C(10)	C(9)	0.0(5)
C(11)	Ru(1)	C(10)	C(9)	-129.4(1)
C(12)	Ru(1)	C(10)	C(9)	-109.3(1)
C(13)	Ru(1)	C(10)	C(9)	-81.9(9)
C(14)	Ru(1)	C(10)	C(9)	-45.5(9)
C(1)	Ru(1)	C(11)	C(10)	78.3(9)
C(2)	Ru(1)	C(11)	C(10)	114.8(9)
C(3)	Ru(1)	C(11)	C(10)	144.8(9)
C(5)	Ru(1)	C(11)	C(10)	26.6(2)
C(6)	Ru(1)	C(11)	C(10)	47.3(1)
C(9)	Ru(1)	C(11)	C(10)	-30.6(8)
C(10)	Ru(1)	C(11)	C(10)	0.0(7)
C(12)	Ru(1)	C(11)	C(10)	-147.5(2)
C(13)	Ru(1)	C(11)	C(10)	-130.1(1)
C(14)	Ru(1)	C(11)	C(10)	-102.1(1)
C(1)	Ru(1)	C(12)	C(11)	57.9(1)
C(2)	Ru(1)	C(12)	C(11)	92.2(9)
C(3)	Ru(1)	C(12)	C(11)	129.5(9)
C(5)	Ru(1)	C(12)	C(11)	-170.2(3)
C(6)	Ru(1)	C(12)	C(11)	32.4(2)
C(9)	Ru(1)	C(12)	C(11)	-54.9(9)
C(10)	Ru(1)	C(12)	C(11)	-20.1(9)
C(11)	Ru(1)	C(12)	C(11)	0.0(8)
C(13)	Ru(1)	C(12)	C(11)	-152.4(1)
C(14)	Ru(1)	C(12)	C(11)	-131.2(1)
C(1)	Ru(1)	C(13)	C(12)	61.7(2)
C(2)	Ru(1)	C(13)	C(12)	79.3(9)
C(3)	Ru(1)	C(13)	C(12)	110.0(8)
C(5)	Ru(1)	C(13)	C(12)	174.6(8)
C(6)	Ru(1)	C(13)	C(12)	172.1(2)
C(9)	Ru(1)	C(13)	C(12)	-81.6(8)

atom	atom	atom	atom	angle
C(14)	Ru(1)	C(9)	C(16)	16.7(9)
C(1)	Ru(1)	C(10)	C(11)	-105.3(9)
C(2)	Ru(1)	C(10)	C(11)	-78.2(1)
C(3)	Ru(1)	C(10)	C(11)	-71.8(2)
C(5)	Ru(1)	C(10)	C(11)	-168.0(9)
C(6)	Ru(1)	C(10)	C(11)	-141.1(9)
C(9)	Ru(1)	C(10)	C(11)	129.4(1)
C(11)	Ru(1)	C(10)	C(11)	0.0(8)
C(12)	Ru(1)	C(10)	C(11)	20.1(9)
C(13)	Ru(1)	C(10)	C(11)	47.5(1)
C(14)	Ru(1)	C(10)	C(11)	83.8(1)
C(1)	Ru(1)	C(11)	C(12)	-134.2(9)
C(2)	Ru(1)	C(11)	C(12)	-97.7(9)
C(3)	Ru(1)	C(11)	C(12)	-67.7(1)
C(5)	Ru(1)	C(11)	C(12)	174.1(2)
C(6)	Ru(1)	C(11)	C(12)	-165.2(8)
C(9)	Ru(1)	C(11)	C(12)	116.9(1)
C(10)	Ru(1)	C(11)	C(12)	147.5(2)
C(12)	Ru(1)	C(11)	C(12)	0.0(6)
C(13)	Ru(1)	C(11)	C(12)	17.4(8)
C(14)	Ru(1)	C(11)	C(12)	45.4(1)
C(1)	Ru(1)	C(12)	C(13)	-149.7(8)
C(2)	Ru(1)	C(12)	C(13)	-115.5(8)
C(3)	Ru(1)	C(12)	C(13)	-78.1(8)
C(5)	Ru(1)	C(12)	C(13)	-17.8(3)
C(6)	Ru(1)	C(12)	C(13)	-175.2(1)
C(9)	Ru(1)	C(12)	C(13)	97.5(9)
C(10)	Ru(1)	C(12)	C(13)	132.3(1)
C(11)	Ru(1)	C(12)	C(13)	152.4(1)
C(13)	Ru(1)	C(12)	C(13)	0.0(5)
C(14)	Ru(1)	C(12)	C(13)	21.3(7)
C(1)	Ru(1)	C(13)	C(14)	-153.7(1)
C(2)	Ru(1)	C(13)	C(14)	-136.1(8)
C(3)	Ru(1)	C(13)	C(14)	-105.4(7)
C(5)	Ru(1)	C(13)	C(14)	-40.8(1)
C(6)	Ru(1)	C(13)	C(14)	-43.3(3)
C(9)	Ru(1)	C(13)	C(14)	63.0(8)

Table 7. Torsion angles (°) -- continued

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(10)	Ru(1)	C(13)	C(12)	-44.9(9)	C(10)	Ru(1)	C(13)	C(14)	99.7(1)
C(11)	Ru(1)	C(13)	C(12)	-17.0(8)	C(11)	Ru(1)	C(13)	C(14)	127.6(1)
C(12)	Ru(1)	C(13)	C(12)	0.0(6)	C(12)	Ru(1)	C(13)	C(14)	144.6(1)
C(14)	Ru(1)	C(13)	C(12)	-144.6(1)	C(14)	Ru(1)	C(13)	C(14)	0.0(5)
C(1)	Ru(1)	C(14)	C(13)	128.9(2)	C(1)	Ru(1)	C(14)	C(15)	-106.6(2)
C(2)	Ru(1)	C(14)	C(13)	68.3(1)	C(2)	Ru(1)	C(14)	C(15)	-167.2(8)
C(3)	Ru(1)	C(14)	C(13)	81.4(8)	C(3)	Ru(1)	C(14)	C(15)	-154.1(8)
C(5)	Ru(1)	C(14)	C(13)	148.8(7)	C(5)	Ru(1)	C(14)	C(15)	-86.7(9)
C(6)	Ru(1)	C(14)	C(13)	166.7(8)	C(6)	Ru(1)	C(14)	C(15)	-68.8(1)
C(9)	Ru(1)	C(14)	C(13)	-113.1(8)	C(9)	Ru(1)	C(14)	C(15)	11.4(9)
C(10)	Ru(1)	C(14)	C(13)	-86.8(1)	C(10)	Ru(1)	C(14)	C(15)	37.8(1)
C(11)	Ru(1)	C(14)	C(13)	-49.5(1)	C(11)	Ru(1)	C(14)	C(15)	75.0(1)
C(12)	Ru(1)	C(14)	C(13)	-22.3(7)	C(12)	Ru(1)	C(14)	C(15)	102.2(1)
C(13)	Ru(1)	C(14)	C(13)	0.0(5)	C(13)	Ru(1)	C(14)	C(15)	124.5(1)
C(7)	O(3)	C(2)	Ru(1)	90.0(8)	C(7)	O(3)	C(2)	C(1)	-179.1(6)
C(7)	O(3)	C(2)	C(3)	-2.6(1)	C(8)	O(4)	C(6)	Ru(1)	-102.6(7)
C(8)	O(4)	C(6)	C(1)	164.2(6)	C(8)	O(4)	C(6)	C(5)	-14.5(1)
Ru(1)	C(1)	C(2)	Ru(1)	0.00(3)	Ru(1)	C(1)	C(2)	O(3)	-130.0(5)
Ru(1)	C(1)	C(2)	C(3)	53.4(5)	O(1)	C(1)	C(2)	Ru(1)	126.0(5)
O(1)	C(1)	C(2)	O(3)	-4.0(8)	O(1)	C(1)	C(2)	C(3)	179.4(5)
C(6)	C(1)	C(2)	Ru(1)	-49.7(5)	C(6)	C(1)	C(2)	O(3)	-179.7(5)
C(6)	C(1)	C(2)	C(3)	3.6(9)	Ru(1)	C(1)	C(6)	Ru(1)	0.00(3)
Ru(1)	C(1)	C(6)	O(4)	126.5(5)	Ru(1)	C(1)	C(6)	C(5)	-54.9(5)
O(1)	C(1)	C(6)	Ru(1)	-124.9(5)	O(1)	C(1)	C(6)	O(4)	1.6(8)
O(1)	C(1)	C(6)	C(5)	-179.8(5)	C(2)	C(1)	C(6)	Ru(1)	50.9(5)
C(2)	C(1)	C(6)	O(4)	177.3(5)	C(2)	C(1)	C(6)	C(5)	-4.0(9)
Ru(1)	C(2)	C(3)	Ru(1)	0.00(3)	Ru(1)	C(2)	C(3)	C(4)	66.7(5)
O(3)	C(2)	C(3)	Ru(1)	127.6(5)	O(3)	C(2)	C(3)	C(4)	-165.7(5)
C(1)	C(2)	C(3)	Ru(1)	-56.2(6)	C(1)	C(2)	C(3)	C(4)	10.5(1)
Ru(1)	C(3)	C(4)	O(2)	-129.5(6)	Ru(1)	C(3)	C(4)	C(5)	41.6(4)
C(2)	C(3)	C(4)	O(2)	166.2(6)	C(2)	C(3)	C(4)	C(5)	-22.7(9)
O(2)	C(4)	C(5)	Ru(1)	128.7(5)	O(2)	C(4)	C(5)	C(6)	-166.6(5)
C(3)	C(4)	C(5)	Ru(1)	-42.4(5)	C(3)	C(4)	C(5)	C(6)	22.3(9)
Ru(1)	C(5)	C(6)	Ru(1)	0.00(3)	Ru(1)	C(5)	C(6)	O(4)	-122.5(6)
Ru(1)	C(5)	C(6)	C(1)	59.0(5)	C(4)	C(5)	C(6)	Ru(1)	-68.8(5)
C(4)	C(5)	C(6)	O(4)	168.7(5)	C(4)	C(5)	C(6)	C(1)	-9.9(1)
Ru(1)	C(9)	C(10)	Ru(1)	0.00(3)	Ru(1)	C(9)	C(10)	C(11)	-59.4(9)

Table 7. Torsion angles (°) -- continued

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(16)	C(9)	C(10)	Ru(1)	104.3(8)	C(16)	C(9)	C(10)	C(11)	44.9(1)
Ru(1)	C(9)	C(16)	C(15)	-41.7(7)	C(10)	C(9)	C(16)	C(15)	-119.9(1)
Ru(1)	C(10)	C(11)	Ru(1)	0.00(3)	Ru(1)	C(10)	C(11)	C(12)	-41.4(1)
C(9)	C(10)	C(11)	Ru(1)	59.9(8)	C(9)	C(10)	C(11)	C(12)	18.5(2)
Ru(1)	C(11)	C(12)	Ru(1)	0.00(3)	Ru(1)	C(11)	C(12)	C(13)	-36.5(1)
C(10)	C(11)	C(12)	Ru(1)	40.7(1)	C(10)	C(11)	C(12)	C(13)	4.3(2)
Ru(1)	C(12)	C(13)	Ru(1)	0.00(3)	Ru(1)	C(12)	C(13)	C(14)	-48.2(8)
C(11)	C(12)	C(13)	Ru(1)	36.8(1)	C(11)	C(12)	C(13)	C(14)	-11.4(2)
Ru(1)	C(13)	C(14)	Ru(1)	0.00(3)	Ru(1)	C(13)	C(14)	C(15)	-103.2(8)
C(12)	C(13)	C(14)	Ru(1)	47.3(1)	C(12)	C(13)	C(14)	C(15)	-55.9(2)
Ru(1)	C(14)	C(15)	C(16)	-37.7(7)	C(13)	C(14)	C(15)	C(16)	43.6(1)
C(14)	C(15)	C(16)	C(9)	51.1(9)					

Table 8. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
RU(1)	O(1)	3.376(3)	(1)	RU(1)	O(2)	3.447(3)	(1)
RU(1)	O(3)	3.361(3)	(1)	RU(1)	O(4)	3.264(3)	(1)
RU(1)	C(1)	2.410(4)	(1)	RU(1)	C(2)	2.305(5)	(1)
RU(1)	C(3)	2.238(4)	(1)	RU(1)	C(4)	2.438(4)	(1)
RU(1)	C(5)	2.189(4)	(1)	RU(1)	C(6)	2.246(4)	(1)
RU(1)	C(9)	2.210(6)	(1)	RU(1)	C(10)	2.134(6)	(1)
RU(1)	C(11)	2.185(7)	(1)	RU(1)	C(12)	2.188(6)	(1)
RU(1)	C(13)	2.165(5)	(1)	RU(1)	C(14)	2.227(6)	(1)
RU(1)	C(15)	3.117(6)	(1)	RU(1)	C(16)	3.114(5)	(1)
O(1)	O(3)	2.674(5)	(1)	O(1)	O(4)	2.681(5)	(1)
O(1)	O(5)	2.890(6)	(1)	O(1)	C(1)	1.258(5)	(1)
O(1)	C(2)	2.396(6)	(1)	O(1)	C(6)	2.378(6)	(1)
O(1)	C(7)	3.223(6)	(-4)	O(1)	C(10)	3.519(7)	(1)
O(2)	O(5)	2.888(6)	(2,1,0,-1)	O(2)	C(3)	2.394(6)	(1)
O(2)	C(4)	1.251(5)	(1)	O(2)	C(5)	2.374(6)	(1)
O(2)	C(7)	3.464(7)	(-4,1,-1)	O(2)	C(8)	3.589(6)	(-1)
O(2)	C(14)	3.558(6)	(1)	O(3)	C(1)	2.330(6)	(1)
O(3)	C(2)	1.349(5)	(1)	O(3)	C(3)	2.432(6)	(1)
O(3)	C(7)	1.437(6)	(1)	O(3)	C(11)	3.451(7)	(2,1,0,-1)
O(3)	C(13)	3.452(7)	(-4)	O(4)	O(4)	3.523(7)	(-1,1,1)
O(4)	C(1)	2.342(6)	(1)	O(4)	C(5)	2.437(6)	(1)
O(4)	C(6)	1.360(5)	(1)	O(4)	C(8)	1.441(5)	(1)
O(4)	C(8)	3.463(6)	(-1,1,1)	O(4)	C(9)	3.399(7)	(1)
O(4)	C(10)	3.446(9)	(1)	O(5)	C(8)	3.396(7)	(-1,1,1)
O(5)	C(12)	3.422(8)	(-4)	O(5)	C(14)	3.476(7)	(1,1,1)
O(5)	C(15)	3.551(8)	(1,1,1)	C(1)	C(2)	1.457(7)	(1)
C(1)	C(3)	2.514(6)	(1)	C(1)	C(4)	2.981(6)	(1)
C(1)	C(5)	2.521(7)	(1)	C(1)	C(6)	1.442(7)	(1)
C(1)	C(10)	3.246(7)	(1)	C(1)	C(11)	3.522(9)	(1)
C(1)	C(16)	3.521(7)	(2,1,0,-1)	C(2)	C(3)	1.400(6)	(1)
C(2)	C(4)	2.502(7)	(1)	C(2)	C(5)	2.800(7)	(1)
C(2)	C(6)	2.414(7)	(1)	C(2)	C(7)	2.399(7)	(1)
C(2)	C(10)	3.505(8)	(2,1,0,-1)	C(2)	C(11)	3.524(8)	(1)
C(2)	C(11)	3.396(9)	(2,1,0,-1)	C(2)	C(12)	3.572(7)	(1)
C(3)	C(4)	1.463(6)	(1)	C(3)	C(5)	2.414(7)	(1)
C(3)	C(6)	2.789(7)	(1)	C(3)	C(7)	2.836(7)	(1)
C(3)	C(10)	3.437(8)	(2,1,0,-1)	C(3)	C(12)	3.569(8)	(1)

Table 8. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(3)	C(13)	3.289(7)	(1)	C(3)	C(14)	3.528(7)	(1)
C(4)	C(5)	1.443(6)	(1)	C(4)	C(6)	2.495(6)	(1)
C(4)	C(10)	3.418(8)	(2,1,0,-1)	C(4)	C(14)	3.269(7)	(1)
C(5)	C(6)	1.416(6)	(1)	C(5)	C(8)	2.814(7)	(1)
C(5)	C(9)	3.368(7)	(1)	C(5)	C(14)	3.357(7)	(1)
C(6)	C(8)	2.397(7)	(1)	C(6)	C(9)	3.224(7)	(1)
C(6)	C(10)	3.196(8)	(1)	C(6)	C(16)	3.593(7)	(2,1,0,-1)
C(7)	C(8)	3.481(7)	(4)	C(8)	C(16)	3.565(8)	(-2)
C(9)	C(10)	1.38(1)	(1)	C(9)	C(11)	2.40(1)	(1)
C(9)	C(12)	3.00(1)	(1)	C(9)	C(13)	3.130(8)	(1)
C(9)	C(14)	2.721(8)	(1)	C(9)	C(15)	2.405(9)	(1)
C(9)	C(16)	1.494(8)	(1)	C(10)	C(11)	1.38(1)	(1)
C(10)	C(12)	2.51(1)	(1)	C(10)	C(13)	3.24(1)	(1)
C(10)	C(14)	3.389(8)	(1)	C(10)	C(15)	3.497(9)	(1)
C(10)	C(16)	2.52(1)	(1)	C(11)	C(12)	1.39(1)	(1)
C(11)	C(13)	2.58(1)	(1)	C(11)	C(14)	3.27(1)	(1)
C(11)	C(16)	3.03(1)	(1)	C(12)	C(13)	1.42(1)	(1)
C(12)	C(14)	2.53(1)	(1)	C(12)	C(15)	3.39(1)	(1)
C(12)	C(16)	3.171(9)	(1)	C(13)	C(14)	1.360(9)	(1)
C(13)	C(15)	2.564(9)	(1)	C(13)	C(16)	2.991(9)	(1)
C(14)	C(15)	1.485(8)	(1)	C(14)	C(16)	2.426(8)	(1)
C(15)	C(16)	1.486(8)	(1)				

*ADC (S, L, TX, TY, TZ) represents:

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z
(2) -X+1/2,Y+1/2,Z
(3) X,-Y+1/2,Z+1/2
(4) -X+1/2,-Y,Z+1/2

L: Lattice translation.
(1) 0, 0, 0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
RU(1)	O(1)	3.376(3)	(1)	RU(1)	O(2)	3.447(3)	(1)
RU(1)	O(3)	3.361(3)	(1)	RU(1)	O(4)	3.264(3)	(1)
RU(1)	C(1)	2.410(4)	(1)	RU(1)	C(2)	2.305(5)	(1)
RU(1)	C(3)	2.238(4)	(1)	RU(1)	C(4)	2.438(4)	(1)
RU(1)	C(5)	2.189(4)	(1)	RU(1)	C(6)	2.246(4)	(1)
RU(1)	C(9)	2.210(6)	(1)	RU(1)	C(10)	2.134(6)	(1)
RU(1)	C(11)	2.185(7)	(1)	RU(1)	C(12)	2.188(6)	(1)
RU(1)	C(13)	2.165(5)	(1)	RU(1)	C(14)	2.227(6)	(1)
RU(1)	C(15)	3.117(6)	(1)	RU(1)	C(16)	3.114(5)	(1)
RU(1)	H(1)	2.83(1)	(1)	RU(1)	H(2)	2.78(1)	(1)
RU(1)	H(9)	2.75(2)	(1)	RU(1)	H(10)	2.73(2)	(1)
RU(1)	H(11)	2.69(3)	(1)	RU(1)	H(12)	2.67(2)	(1)
RU(1)	H(13)	2.68(2)	(1)	RU(1)	H(14)	2.75(2)	(1)
RU(1)	H(15)	3.43(2)	(1)	RU(1)	H(18)	3.36(2)	(1)
O(1)	H(1)	3.24(2)	(-4)	O(1)	H(3)	2.32(3)	(-4)
O(1)	H(4)	3.48(3)	(-4)	O(1)	H(5)	3.59(3)	(-4)
O(1)	H(7)	2.93(3)	(-1,1,1)	O(1)	H(8)	3.55(3)	(-1,1,1)
O(1)	H(10)	3.05(2)	(1)	O(1)	H(11)	3.45(3)	(1)
O(1)	H(12)	2.98(4)	(-4)	O(1)	H(13)	2.95(4)	(-4)
O(1)	H(18)	2.88(4)	(2,1,0,-1)	O(2)	H(1)	2.64(2)	(1)
O(2)	H(2)	2.60(1)	(1)	O(2)	H(2)	3.16(1)	(-1)
O(2)	H(5)	2.62(4)	(-4,1,-1)	O(2)	H(6)	2.66(3)	(-1)
O(2)	H(9)	3.46(4)	(-1)	O(2)	H(10)	3.13(4)	(2,1,0,-1)
O(2)	H(14)	2.97(2)	(1)	O(2)	H(15)	2.94(3)	(-1)
O(3)	H(1)	2.64(1)	(1)	O(3)	H(1)	2.93(1)	(-4)
O(3)	H(3)	1.97(1)	(1)	O(3)	H(4)	1.96(1)	(1)
O(3)	H(5)	1.98(1)	(1)	O(3)	H(11)	3.46(3)	(1)
O(3)	H(11)	3.48(3)	(2,1,0,-1)	O(3)	H(12)	3.51(3)	(1)
O(3)	H(13)	2.53(3)	(-4)	O(3)	H(14)	3.44(4)	(-4)
O(4)	H(2)	2.64(1)	(1)	O(4)	H(6)	1.97(1)	(1)
O(4)	H(7)	1.98(1)	(1)	O(4)	H(7)	2.98(1)	(-1,1,1)
O(4)	H(8)	1.97(1)	(1)	O(4)	H(8)	3.44(1)	(-1,1,1)
O(4)	H(9)	2.91(2)	(1)	O(4)	H(10)	3.10(3)	(1)
O(4)	H(17)	3.08(3)	(2,1,0,-1)	O(4)	H(17)	3.09(3)	(-2)
O(4)	H(18)	3.56(4)	(2,1,0,-1)	O(5)	H(3)	3.24(5)	(-4)
O(5)	H(7)	3.39(3)	(-1,1,1)	O(5)	H(8)	2.60(4)	(-1,1,1)
O(5)	H(10)	3.04(2)	(1)	O(5)	H(12)	2.57(6)	(-4)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(5)	H(14)	3.10(6)	(1,1,1)	O(5)	H(16)	2.90(7)	(1,1,1)
O(5)	H(17)	3.40(5)	(-2)	C(1)	H(1)	3.35(2)	(1)
C(1)	H(2)	3.36(2)	(1)	C(1)	H(3)	3.43(3)	(-4)
C(1)	H(7)	3.55(3)	(-1,1,1)	C(1)	H(10)	3.09(2)	(1)
C(1)	H(11)	3.38(3)	(1)	C(1)	H(13)	3.47(4)	(-4)
C(1)	H(17)	3.46(4)	(2,1,0,-1)	C(1)	H(18)	2.87(4)	(2,1,0,-1)
C(2)	H(1)	2.03(1)	(1)	C(2)	H(3)	2.62(2)	(1)
C(2)	H(4)	2.62(2)	(1)	C(2)	H(5)	3.19(2)	(1)
C(2)	H(11)	3.38(3)	(1)	C(2)	H(11)	3.54(3)	(2,1,0,-1)
C(2)	H(12)	3.40(3)	(1)	C(2)	H(13)	3.37(3)	(-4)
C(2)	H(18)	3.50(4)	(2,1,0,-1)	C(3)	H(1)	0.950(6)	(1)
C(3)	H(2)	3.27(2)	(1)	C(3)	H(3)	2.78(2)	(1)
C(3)	H(4)	2.75(2)	(1)	C(3)	H(10)	3.19(4)	(2,1,0,-1)
C(3)	H(11)	3.54(4)	(2,1,0,-1)	C(3)	H(12)	3.48(3)	(1)
C(3)	H(13)	3.10(2)	(1)	C(3)	H(14)	3.48(3)	(1)
C(4)	H(1)	2.10(1)	(1)	C(4)	H(2)	2.08(1)	(1)
C(4)	H(2)	3.60(1)	(-1)	C(4)	H(5)	3.42(4)	(-4,1,-1)
C(4)	H(10)	2.96(4)	(2,1,0,-1)	C(4)	H(13)	3.56(3)	(1)
C(4)	H(14)	3.01(2)	(1)	C(4)	H(15)	3.22(3)	(-1)
C(5)	H(1)	3.27(2)	(1)	C(5)	H(2)	0.950(6)	(1)
C(5)	H(2)	3.353(6)	(-1)	C(5)	H(6)	2.65(2)	(1)
C(5)	H(8)	2.83(2)	(1)	C(5)	H(9)	3.29(2)	(1)
C(5)	H(14)	3.37(2)	(1)	C(5)	H(15)	3.01(3)	(-1)
C(6)	H(2)	2.06(1)	(1)	C(6)	H(6)	2.62(2)	(1)
C(6)	H(7)	3.18(2)	(1)	C(6)	H(8)	2.62(2)	(1)
C(6)	H(9)	3.07(2)	(1)	C(6)	H(10)	3.14(2)	(1)
C(6)	H(17)	3.23(4)	(2,1,0,-1)	C(6)	H(18)	3.28(4)	(2,1,0,-1)
C(7)	H(1)	2.53(2)	(1)	C(7)	H(3)	0.950(8)	(1)
C(7)	H(4)	0.950(8)	(1)	C(7)	H(5)	0.950(7)	(1)
C(7)	H(6)	3.25(5)	(4)	C(7)	H(7)	3.04(6)	(4)
C(7)	H(11)	3.42(4)	(2,1,0,-1)	C(7)	H(13)	3.29(4)	(-4)
C(7)	H(14)	3.30(5)	(-4)	C(7)	H(16)	3.46(6)	(-3,1,0,-1)
C(7)	H(18)	3.34(6)	(-3,1,0,-1)	C(8)	H(2)	2.53(2)	(1)
C(8)	H(3)	3.32(5)	(4,1,0,0,-1)	C(8)	H(5)	2.81(6)	(4,1,0,0,-1)
C(8)	H(6)	0.950(7)	(1)	C(8)	H(7)	0.950(7)	(1)
C(8)	H(8)	0.950(8)	(1)	C(8)	H(9)	3.23(3)	(1)
C(8)	H(14)	3.08(4)	(-1)	C(8)	H(16)	3.18(5)	(-2)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(8)	H(17)	3.38(4)	(2,1,0,-1)	C(8)	H(17)	3.04(4)	(-2)
C(8)	H(18)	3.50(5)	(-2)	C(9)	H(2)	3.41(2)	(1)
C(9)	H(6)	3.48(3)	(1)	C(9)	H(9)	0.95(1)	(1)
C(9)	H(10)	2.01(2)	(1)	C(9)	H(11)	3.18(4)	(1)
C(9)	H(14)	3.53(3)	(1)	C(9)	H(15)	2.67(3)	(1)
C(9)	H(16)	3.22(3)	(1)	C(9)	H(17)	2.04(2)	(1)
C(9)	H(18)	2.00(2)	(1)	C(10)	H(9)	2.00(3)	(1)
C(10)	H(10)	0.950(9)	(1)	C(10)	H(11)	1.93(3)	(1)
C(10)	H(12)	3.19(4)	(1)	C(10)	H(17)	3.14(3)	(1)
C(10)	H(18)	2.54(2)	(1)	C(11)	H(4)	3.16(5)	(2)
C(11)	H(9)	3.23(4)	(1)	C(11)	H(10)	2.04(3)	(1)
C(11)	H(11)	0.95(1)	(1)	C(11)	H(12)	1.91(2)	(1)
C(11)	H(13)	3.27(4)	(1)	C(11)	H(13)	3.53(4)	(-4)
C(11)	H(18)	2.69(3)	(1)	C(12)	H(4)	3.49(5)	(-3)
C(12)	H(10)	3.32(4)	(1)	C(12)	H(11)	1.97(3)	(1)
C(12)	H(11)	3.55(3)	(-4,1,-1)	C(12)	H(12)	0.950(9)	(1)
C(12)	H(13)	1.99(2)	(1)	C(12)	H(14)	3.27(3)	(1)
C(12)	H(18)	2.77(3)	(1)	C(13)	H(1)	3.25(2)	(1)
C(13)	H(4)	3.26(4)	(-3)	C(13)	H(11)	3.28(4)	(1)
C(13)	H(11)	3.01(4)	(-4,1,-1)	C(13)	H(12)	1.96(2)	(1)
C(13)	H(13)	0.950(9)	(1)	C(13)	H(14)	1.94(2)	(1)
C(13)	H(15)	3.29(3)	(1)	C(13)	H(16)	2.90(3)	(1)
C(13)	H(18)	2.84(2)	(1)	C(14)	H(2)	3.44(3)	(1)
C(14)	H(2)	3.47(3)	(-1)	C(14)	H(5)	3.55(5)	(-4,1,-1)
C(14)	H(8)	3.38(5)	(-1)	C(14)	H(9)	3.35(3)	(1)
C(14)	H(12)	3.23(3)	(1)	C(14)	H(13)	1.93(2)	(1)
C(14)	H(14)	0.950(8)	(1)	C(14)	H(15)	2.02(2)	(1)
C(14)	H(16)	2.01(2)	(1)	C(14)	H(17)	3.24(3)	(1)
C(14)	H(18)	2.69(2)	(1)	C(15)	H(2)	3.39(3)	(-1)
C(15)	H(4)	3.58(6)	(-3)	C(15)	H(7)	3.20(5)	(-2,1,-1)
C(15)	H(8)	3.52(5)	(-1)	C(15)	H(9)	2.87(3)	(1)
C(15)	H(9)	3.47(3)	(-2,1,-1)	C(15)	H(13)	3.30(3)	(1)
C(15)	H(14)	2.04(2)	(1)	C(15)	H(15)	0.950(9)	(1)
C(15)	H(16)	0.950(8)	(1)	C(15)	H(17)	2.00(2)	(1)
C(15)	H(18)	2.04(2)	(1)	C(16)	H(7)	2.75(4)	(-2,1,-1)
C(16)	H(9)	2.07(2)	(1)	C(16)	H(10)	3.29(3)	(1)
C(16)	H(14)	3.25(3)	(1)	C(16)	H(15)	2.03(2)	(1)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(16)	H(16)	2.00(2)	(1)	C(16)	H(17)	0.950(8)	(1)
C(16)	H(18)	0.950(8)	(1)				

*ADC (S, L, TX, TY, TZ) represents:

S: Symmetry operation number. -S is inversion of operation S.
(1) X,Y,Z
(2) -X+1/2,Y+1/2,Z
(3) X,-Y+1/2,Z+1/2
(4) -X+1/2,-Y,Z+1/2

L: Lattice translation.
(1) 0, 0, 0

TX, TY, TZ: Unit cell translation along the x, y, and z directions.

Table 10. Least Squares Planes

Plane number 1

Co-ordinates of the defining atoms projected onto the best plane

Type	Serial	XP	YP	ZP
C	2	1.211	0.697	-0.002
C	3	1.203	-0.702	0.002
C	5	-1.212	-0.705	-0.002
C	6	-1.202	0.710	0.002

Plane number 2

Co-ordinates of the defining atoms projected onto the best plane

Type	Serial	XP	YP	ZP
C	1	-0.007	0.535	0.000
C	2	1.210	-0.265	0.000
C	6	-1.203	-0.270	0.000

Plane number 3

Co-ordinates of the defining atoms projected onto the best plane

Type	Serial	XP	YP	ZP
C	3	1.212	-0.266	0.000
C	4	-0.010	0.539	0.000
C	5	-1.202	-0.273	0.000

Angle between plane 1 and plane 2 is 3.20 Degrees

Angle between plane 1 and plane 3 is 161.00 Degrees

X-ray Structure Report

Crystal Data of **3**·CH_2Cl_2

August 3, 2002

Experimental

Data Collection

A black platelet crystal of $C_{30}H_{30}O_6Ru_2 \cdot CH_2Cl_2$ having approximate dimensions of 0.35 x 0.20 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 stills which were exposed for 1 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 10.7583(5) Å
b = 23.2869(9) Å β = 103.372(2)°
c = 11.4630(7) Å
V = 2793.9(2) Å^3

For Z = 4 and F.W. = 773.64, the calculated density is 1.84 g/cm^3. The systematic absences of:

h0l: h+l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -130 ± 1°C to a maximum 2θ value of 54.9°. A total of 44 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0° in 5.0° step, at χ=45.0° and φ = 0.0°. The exposure rate was 5.0 [sec./°]. The detector at the zero swing position. A second sweep was performed using ω scans from 0.0 to 160.0° in 5.0° step, at χ=45.0° and φ = 180.0°. The exposure rate was 5.0 [sec./°]. The detector at the zero swing position. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 24764 reflections which were collected, 6377 were unique (R_{int} = 0.042); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 13.2 cm^{-1}. was applied which resulted

in transmission factors ranging from 0.87 to 1.16. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F was based on 5076 observed reflections ($I > 3.00\sigma(I)$) and 403 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.056$$

$$R_w = [\Sigma \, w \, (|Fo| - |Fc|)^2 \, / \, \Sigma \, w \, Fo^2]^{1/2} = 0.073$$

The standard deviation of an observation of unit weight[4] was 1.61. Unit weights were used. Plots of $\Sigma \, w \, (|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 4.84 and –2.80 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package.

References

(1) PATTY: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$\Sigma w(|F_o|-|F_c|)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$

where: N_O = number of observations
N_V = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

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(9) CrystalStructure 2.00: Crystal Structure Analysis Package, Rigaku and MSC (2001).

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{30}H_{30}O_6Ru_2 \cdot CH_2Cl_2$
Formula Weight	773.64
Crystal Color, Habit	black, platelet
Crystal Dimensions	0.35 X 0.20 X 0.10 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 stills @ 1.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 10.7583(5) Å b = 23.2869(9) Å c = 11.4630(7) Å β = 103.372(2) ° V = 2793.9(2) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.839 g/cm^3
F_{000}	1552.00
μ(MoKα)	13.18 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Detector Aperture	270 mm x 256 mm
Data Images	44 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0°
Exposure Rate	5.0 sec./°
Detector Swing Angle	0.00°
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 160.0°
Exposure Rate	5.0 sec./°
Detector Swing Angle	0.00°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9°
No. of Reflections Measured	Total: 24764 Unique: 6377 (R_{int} = 0.042)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8651 - 1.1560)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF99 PATTY)
Refinement	Full-matrix least-squares on F
Function Minimized	Σ w (|Fo| - |Fc|)^2
Least Squares Weights	1
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	5076
No. Variables	403
Reflection/Parameter Ratio	12.60
Residuals: R; Rw	0.056 ; 0.073
Goodness of Fit Indicator	1.61
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	4.84 e$^-$/Å^3
Minimum peak in Final Diff. Map	-2.80 e$^-$/Å^3

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ru(1)	-0.14603(6)	-0.25034(3)	-0.20185(5)	1.45(1)
Ru(2)	-0.16084(6)	-0.09613(3)	-0.03015(5)	1.41(1)
Cl(1)	-0.844(1)	0.0901(5)	-0.4551(9)	17.7(4)
Cl(2)	-1.056(2)	0.0523(7)	-0.593(1)	28.5(8)
O(1)	0.0308(5)	-0.1206(3)	-0.0342(5)	1.8(1)
O(2)	0.0713(5)	-0.2368(3)	-0.4301(5)	2.2(1)
O(3)	0.2775(5)	-0.2197(3)	-0.2626(5)	2.0(1)
O(4)	-0.3215(5)	-0.2033(2)	-0.2733(5)	1.8(1)
O(5)	-0.2610(7)	0.0265(3)	-0.2698(7)	3.2(2)
O(6)	-0.4901(6)	-0.0140(3)	-0.3461(6)	2.8(1)
C(1)	0.0372(7)	-0.1505(3)	-0.1261(7)	1.5(1)
C(2)	-0.0754(7)	-0.1645(3)	-0.2124(7)	1.4(1)
C(3)	-0.0687(7)	-0.1965(3)	-0.3197(7)	1.4(1)
C(4)	0.0551(8)	-0.2135(3)	-0.3389(7)	1.6(1)
C(5)	0.1687(7)	-0.1994(4)	-0.2399(7)	1.7(2)
C(6)	0.1604(7)	-0.1689(4)	-0.1427(7)	1.7(2)
C(7)	0.3925(8)	-0.2101(5)	-0.1737(9)	2.9(2)
C(8)	0.024(1)	-0.3017(5)	-0.122(1)	3.7(2)
C(9)	-0.035(1)	-0.2781(4)	-0.033(1)	4.4(3)
C(10)	-0.160(1)	-0.2921(4)	-0.030(1)	3.9(3)
C(11)	-0.253(1)	-0.3158(4)	-0.119(1)	3.8(3)
C(12)	-0.260(1)	-0.3283(5)	-0.242(1)	3.7(2)
C(13)	-0.166(1)	-0.3293(4)	-0.310(1)	4.2(3)
C(14)	-0.048(2)	-0.3653(5)	-0.286(1)	5.4(4)
C(15)	0.008(1)	-0.3643(4)	-0.159(1)	4.0(3)
C(16)	-0.3080(8)	-0.1490(3)	-0.2660(7)	1.7(2)
C(17)	-0.1864(8)	-0.1253(3)	-0.2123(7)	1.5(1)
C(18)	-0.1681(7)	-0.0635(3)	-0.2066(7)	1.6(1)
C(19)	-0.2728(9)	-0.0256(4)	-0.2596(8)	2.1(2)
C(20)	-0.3995(9)	-0.0534(4)	-0.3077(7)	2.1(2)
C(21)	-0.4148(8)	-0.1109(4)	-0.3128(7)	2.0(2)
C(22)	-0.6158(9)	-0.0341(5)	-0.397(1)	3.4(2)
C(23)	-0.3552(8)	-0.0760(4)	-0.0107(7)	1.9(2)
C(24)	-0.3235(8)	-0.1345(4)	0.0152(8)	1.9(2)
C(25)	-0.2202(8)	-0.1502(4)	0.1113(8)	2.1(2)
C(26)	-0.1192(8)	-0.1145(4)	0.1667(7)	2.3(2)
C(27)	-0.0773(8)	-0.0579(4)	0.1441(7)	2.3(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(28)	-0.1386(9)	-0.0134(4)	0.0691(8)	2.3(2)
C(29)	-0.2642(9)	0.0137(4)	0.0726(9)	2.6(2)
C(30)	-0.3543(8)	-0.0331(4)	0.0880(8)	2.1(2)
C(31)	-1.014(2)	0.086(1)	-0.481(2)	8.8(6)
H(1)	-0.1291(7)	-0.1845(3)	-0.3896(7)	1.8(2)
H(2)	0.2357(7)	-0.1601(4)	-0.0837(7)	2.1(2)
H(3)	0.3847(8)	-0.2278(5)	-0.1012(9)	3.5(2)
H(4)	0.4057(8)	-0.1700(5)	-0.1610(9)	3.5(2)
H(5)	0.4630(8)	-0.2262(5)	-0.1991(9)	3.5(2)
H(6)	0.103(1)	-0.2850(5)	-0.125(1)	4.3(3)
H(7)	0.010(1)	-0.2502(4)	0.021(1)	4.7(3)
H(8)	-0.194(1)	-0.2672(4)	0.021(1)	5.2(3)
H(9)	-0.332(1)	-0.2990(4)	-0.115(1)	5.0(3)
H(10)	-0.342(1)	-0.3206(5)	-0.291(1)	4.3(3)
H(11)	-0.199(1)	-0.3223(4)	-0.393(1)	5.0(3)
H(12)	-0.069(2)	-0.4036(5)	-0.312(1)	7.5(5)
H(13)	0.011(2)	-0.3498(5)	-0.328(1)	7.5(5)
H(14)	-0.047(1)	-0.3827(4)	-0.117(1)	5.2(4)
H(15)	0.089(1)	-0.3832(4)	-0.142(1)	5.2(4)
H(16)	-0.0874(7)	-0.0516(3)	-0.2186(7)	2.0(2)
H(17)	-0.4966(8)	-0.1266(4)	-0.3467(7)	2.4(2)
H(18)	-0.6401(9)	-0.0522(5)	-0.352(1)	4.0(2)
H(19)	-0.6722(9)	-0.0003(5)	-0.417(1)	4.0(2)
H(20)	-0.6186(9)	-0.0483(5)	-0.464(1)	4.0(2)
H(21)	-0.4168(8)	-0.0691(4)	-0.0833(7)	2.4(2)
H(22)	-0.3693(8)	-0.1635(4)	-0.0354(8)	2.4(2)
H(23)	-0.1966(8)	-0.1895(4)	0.1091(8)	2.7(2)
H(24)	-0.0446(8)	-0.1378(4)	0.1837(7)	2.8(2)
H(25)	0.0131(8)	-0.0553(4)	0.1585(7)	2.8(2)
H(26)	-0.0804(9)	0.0122(4)	0.0449(8)	2.9(2)
H(27)	-0.2537(9)	0.0403(4)	0.1369(9)	3.2(2)
H(28)	-0.2976(9)	0.0330(4)	-0.0010(9)	3.2(2)
H(29)	-0.3239(8)	-0.0509(4)	0.1638(8)	2.7(2)
H(30)	-0.4378(8)	-0.0186(4)	0.0828(8)	2.7(2)
H(31)	-1.038(2)	0.067(1)	-0.416(2)	10.3(7)
H(32)	-1.049(2)	0.124(1)	-0.488(2)	10.3(7)

$$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0200(3)	0.0187(3)	0.0184(3)	-0.0012(3)	0.0089(2)	-0.0013(2)
Ru(2)	0.0186(3)	0.0188(3)	0.0182(3)	-0.0020(3)	0.0084(2)	-0.0038(2)
Cl(1)	0.29(1)	0.21(1)	0.169(8)	0.05(1)	0.048(8)	0.058(8)
Cl(2)	0.43(2)	0.45(2)	0.30(2)	-0.26(2)	0.27(2)	-0.15(2)
O(1)	0.022(3)	0.027(3)	0.020(3)	-0.001(2)	0.007(2)	-0.005(2)
O(2)	0.022(3)	0.041(4)	0.023(3)	0.002(3)	0.010(2)	-0.009(3)
O(3)	0.021(3)	0.033(3)	0.022(3)	0.003(2)	0.008(2)	-0.005(2)
O(4)	0.024(3)	0.021(3)	0.026(3)	-0.004(2)	0.010(2)	-0.005(2)
O(5)	0.049(4)	0.020(3)	0.050(4)	0.001(3)	0.004(3)	0.005(3)
O(6)	0.035(4)	0.033(4)	0.036(4)	0.013(3)	0.002(3)	-0.000(3)
C(1)	0.021(4)	0.019(4)	0.019(4)	-0.001(3)	0.008(3)	-0.001(3)
C(2)	0.018(3)	0.021(4)	0.017(4)	-0.002(3)	0.007(3)	-0.004(3)
C(3)	0.020(4)	0.019(4)	0.017(4)	-0.003(3)	0.007(3)	-0.000(3)
C(4)	0.022(4)	0.022(4)	0.020(4)	-0.005(3)	0.007(3)	-0.000(3)
C(5)	0.020(4)	0.026(4)	0.020(4)	-0.003(3)	0.008(3)	0.000(3)
C(6)	0.016(4)	0.031(4)	0.021(4)	-0.002(3)	0.006(3)	-0.004(3)
C(7)	0.021(4)	0.054(6)	0.035(5)	0.004(4)	0.009(4)	-0.009(5)
C(8)	0.025(5)	0.038(6)	0.073(8)	-0.004(4)	0.003(5)	0.022(5)
C(9)	0.09(1)	0.025(5)	0.030(5)	-0.004(6)	-0.020(6)	0.006(4)
C(10)	0.10(1)	0.028(5)	0.039(6)	0.014(6)	0.044(6)	0.010(5)
C(11)	0.046(6)	0.025(5)	0.086(9)	0.009(4)	0.045(6)	0.020(5)
C(12)	0.036(6)	0.033(5)	0.068(8)	-0.011(4)	0.002(5)	0.014(5)
C(13)	0.10(1)	0.026(5)	0.029(5)	-0.015(6)	0.011(6)	-0.010(4)
C(14)	0.12(1)	0.023(5)	0.09(1)	0.001(6)	0.09(1)	-0.005(6)
C(15)	0.045(6)	0.029(5)	0.092(9)	0.012(5)	0.044(6)	0.018(6)
C(16)	0.026(4)	0.023(4)	0.017(4)	0.002(3)	0.011(3)	-0.003(3)
C(17)	0.023(4)	0.020(4)	0.017(4)	-0.001(3)	0.009(3)	-0.001(3)
C(18)	0.022(4)	0.022(4)	0.020(4)	-0.002(3)	0.009(3)	-0.002(3)
C(19)	0.035(5)	0.024(4)	0.024(4)	0.004(4)	0.012(4)	0.002(3)
C(20)	0.034(4)	0.028(4)	0.020(4)	0.008(4)	0.007(3)	-0.001(3)
C(21)	0.022(4)	0.032(5)	0.023(4)	0.001(3)	0.005(3)	-0.004(3)
C(22)	0.031(5)	0.048(6)	0.046(6)	0.014(5)	0.001(4)	-0.004(5)
C(23)	0.018(4)	0.032(4)	0.024(4)	0.001(3)	0.009(3)	-0.001(3)
C(24)	0.023(4)	0.027(4)	0.028(4)	-0.006(3)	0.013(3)	-0.006(3)
C(25)	0.032(4)	0.025(4)	0.028(4)	0.001(3)	0.021(4)	0.000(3)
C(26)	0.027(4)	0.041(5)	0.021(4)	0.009(4)	0.011(3)	-0.002(4)
C(27)	0.026(4)	0.041(5)	0.022(4)	-0.002(4)	0.008(3)	-0.011(4)