Experimental

Data Collection

A yellow prismatic crystal of $C_{84}H_{86}O_4B_2Ru_2$ having approximate dimensions of 0.10 x 0.10 x 0.20 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7R diffractometer with graphite monochromated Mo-Kα radiation and a rotating anode generator.

Cell constants and an orientation matrix for data collection , obtained from a least-squares refinement using the setting angles of 25 carefully centered reflections in the range $28.68 < 2\theta < 29.85°$ corresponded to a primitive orthorhombic cell with dimensions:

a = 14.82(1) $\AA$

b = 14.96(1) $\AA$

c = 31.85(1) $\AA$

V = 7061(7) $\AA^3$

For Z = 8 and F.W. = 1383.36, the calculated density is 2.60 g/cm^3. The systematic absences of:

h00: h $\neq$ 2n

0k0: k $\neq$ 2n

00l: l $\neq$ 2n

uniquely determine the space group to be:

$P2_12_12_1$ (#19)

The data were collected at a temperature of 23 $\pm$ 1°C using the ω scan technique to a maximum 2θ value of 55.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.26° with a take-off angle of 6.0°. Scans of (1.15 + 0.30 tan θ)° were made at a speed of 8.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 2 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm and the crystal to detector distance was 235 mm, The computer-controlled slits were set to 3.0 mm (horizontal) and 3.0 mm (vertical).

Data Reduction

Of the 8864 reflections which were collected, 8863 were unique (R_{int} = 0.000). The intensities of three representative reflection were measured after every 150 reflections. No decay correction was applied.

The linear absorption coefficient, μ, for Mo-Kα radiation is 9.6 cm^{-1}. Azimuthal scans of several reflections indicated no need for an absorption correction. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient = 2.46500e-08).

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. The final cycle of full-matrix least-squares refinement[3] was based on 4708 observed reflections ($I > 3.00\sigma(I)$) and 831 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

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

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2} = 0.060$$

The standard deviation of an observation of unit weight[4] was 1.04. The weighting scheme was based on counting statistics and included a factor (p = 0.002) to downweight the intense reflections. 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 0.36 and -0.43 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SHELXS-97: Sheldrick, G.M. (1997). Program for the Solution of Crystal Structuers. University of Goettingen, Germany.

(2) DIRDIF94: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M. (1994). The DIRDIF-94 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(|Fo| - |Fc|)^2$

where w = $\frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$

$\sigma_c(Fo)$ = e.s.d. based on counting statistics

p = p-factor

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

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = 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) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{84}H_{86}O_4B_2Ru_2$
Formula Weight	1383.36
Crystal Color, Habit	yellow, prismatic
Crystal Dimensions	0.10 X 0.10 X 0.20 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (28.7 - 29.9°)
Omega Scan Peak Width at Half-height	0.26°
Lattice Parameters	a = 14.82(1)Å b = 14.96(1) Å c = 31.85(1) Å V = 7061(7) Å^3
Space Group	$P2_12_12_1$ (#19)
Z value	8
D_{calc}	2.602 g/cm^3
F_{000}	5760.00
μ(MoKα)	9.57 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factor = 8.53)

Take-off Angle	6.0°
Detector Aperture	3.0 mm horizontal 3.0 mm vertical
Crystal to Detector Distance	235 mm
Voltage, Current	50kV, 200mA
Temperature	23.0°C
Scan Type	ω
Scan Rate	8.0°/min (in ω) (up to 2 scans)
Scan Width	$(1.15 + 0.30 \tan \theta)°$
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 8864 Unique: 8863 (R_{int} = 0.000)
Corrections	Lorentz-polarization Secondary Extinction (coefficient: 2.46500e-08)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS-97)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$w = \frac{1}{\sigma^2(Fo)} = [\sigma_c^2(Fo) + \frac{p^2}{4}Fo^2]^{-1}$
p-factor	0.0020
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4708
No. Variables	831
Reflection/Parameter Ratio	5.67
Residuals: R; Rw	0.056 ; 0.060
Residuals: R1	0.056
No. of Reflections to calc R1	4708

Goodness of Fit Indicator	1.04
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.36 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.43 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
Ru(1)	0.25129(8)	0.56291(6)	0.22595(3)	3.88(2)
Ru(2)	0.64471(6)	0.49532(7)	0.00024(5)	3.76(2)
O(1)	0.164(1)	0.646(1)	0.3400(5)	13.4(6)
O(2)	0.1007(8)	0.520(1)	0.3226(4)	7.9(3)
O(3)	0.5505(10)	0.406(1)	0.1097(4)	9.8(5)
O(4)	0.6630(10)	0.3174(8)	0.0914(3)	7.9(4)
C(1)	0.1461(9)	0.6160(9)	0.2677(5)	4.9(3)
C(2)	0.1036(9)	0.558(1)	0.2370(5)	5.2(3)
C(3)	0.1182(10)	0.573(1)	0.1937(5)	6.4(4)
C(4)	0.174(1)	0.646(1)	0.1804(6)	7.9(5)
C(5)	0.215(1)	0.704(1)	0.2119(7)	7.4(4)
C(6)	0.200(1)	0.689(1)	0.2556(6)	6.5(4)
C(7)	0.137(1)	0.596(1)	0.3126(6)	7.3(4)
C(8)	0.090(1)	0.491(2)	0.3671(5)	10.2(6)
C(9)	0.3341(8)	0.4735(7)	0.2640(4)	3.7(2)
C(10)	0.2990(7)	0.4250(8)	0.2304(4)	3.6(2)
C(11)	0.3294(9)	0.4656(8)	0.1919(4)	3.8(2)
C(12)	0.3870(9)	0.5395(9)	0.2029(5)	4.0(2)
C(13)	0.3908(10)	0.545(1)	0.2486(4)	4.1(2)
C(14)	0.3219(10)	0.4511(10)	0.3112(4)	4.7(3)
C(15)	0.237(1)	0.3431(8)	0.2320(5)	5.3(4)
C(16)	0.312(1)	0.430(1)	0.1474(4)	6.1(4)
C(17)	0.443(1)	0.595(1)	0.1723(5)	5.6(4)
C(18)	0.4483(10)	0.6061(9)	0.2739(5)	5.5(4)

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

atom	x	y	z	B_{eq}
C(19)	0.5806(10)	0.3883(10)	0.0387(5)	4.5(3)
C(20)	0.642(1)	0.3474(7)	0.0084(4)	4.3(2)
C(21)	0.631(1)	0.3666(10)	-0.0346(5)	5.5(3)
C(22)	0.565(1)	0.425(1)	-0.0478(5)	7.0(5)
C(23)	0.502(1)	0.468(1)	-0.0183(6)	6.4(3)
C(24)	0.5125(10)	0.4497(10)	0.0260(6)	5.2(3)
C(25)	0.596(1)	0.373(1)	0.0829(5)	5.9(4)
C(26)	0.687(2)	0.292(2)	0.1358(6)	11.7(8)
C(27)	0.670(1)	0.6336(10)	-0.0166(7)	6.1(3)
C(28)	0.6702(10)	0.6251(9)	0.0299(6)	5.6(3)
C(29)	0.741(1)	0.5639(9)	0.0409(5)	4.7(3)
C(30)	0.7866(8)	0.5378(7)	0.0017(6)	4.6(2)
C(31)	0.745(1)	0.5803(8)	-0.0322(5)	5.3(3)
C(32)	0.609(1)	0.693(1)	-0.0416(7)	8.3(6)
C(33)	0.609(1)	0.674(1)	0.0607(6)	7.3(5)
C(34)	0.767(1)	0.537(1)	0.0848(5)	7.0(5)
C(35)	0.8695(8)	0.4782(9)	-0.0024(7)	6.2(4)
C(36)	0.769(1)	0.572(1)	-0.0782(5)	7.5(5)
C(37)	0.7720(8)	0.5939(8)	0.2189(4)	3.6(2)
C(38)	0.853(1)	0.6227(9)	0.1996(4)	4.4(3)
C(39)	0.851(1)	0.6891(9)	0.1682(4)	4.9(3)
C(40)	0.766(1)	0.7289(9)	0.1566(4)	5.1(3)
C(41)	0.687(1)	0.7020(10)	0.1757(5)	5.1(4)
C(42)	0.6898(9)	0.6355(9)	0.2067(4)	4.0(3)

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

atom	x	y	z	B_{eq}
C(43)	0.8575(9)	0.4489(9)	0.2544(4)	3.9(3)
C(44)	0.9006(10)	0.4133(10)	0.2898(5)	5.4(4)
C(45)	0.968(1)	0.344(1)	0.2856(6)	6.0(4)
C(46)	0.992(1)	0.315(1)	0.2470(7)	6.2(4)
C(47)	0.950(1)	0.346(1)	0.2124(6)	5.9(4)
C(48)	0.881(1)	0.4152(9)	0.2142(5)	5.8(4)
C(49)	0.6817(8)	0.4588(8)	0.2614(4)	3.7(2)
C(50)	0.657(1)	0.4184(9)	0.3009(5)	5.0(3)
C(51)	0.580(1)	0.3628(10)	0.3022(6)	5.5(4)
C(52)	0.530(1)	0.3437(10)	0.2661(6)	5.7(4)
C(53)	0.5557(10)	0.3795(9)	0.2266(6)	5.5(4)
C(54)	0.6302(9)	0.4355(10)	0.2251(5)	4.9(3)
C(55)	0.7851(8)	0.5856(7)	0.3005(4)	3.5(2)
C(56)	0.7121(9)	0.6176(9)	0.3228(4)	4.1(3)
C(57)	0.721(1)	0.6804(9)	0.3559(4)	4.8(3)
C(58)	0.807(1)	0.7119(9)	0.3669(4)	4.9(3)
C(59)	0.881(1)	0.6819(9)	0.3441(5)	5.0(3)
C(60)	0.8707(9)	0.6194(8)	0.3119(4)	4.3(3)
C(61)	1.1239(8)	0.4743(9)	0.0393(4)	3.6(3)
C(62)	1.0879(10)	0.553(1)	0.0564(4)	4.8(3)
C(63)	1.022(1)	0.549(1)	0.0896(5)	5.6(4)
C(64)	0.997(1)	0.466(1)	0.1064(5)	5.7(4)
C(65)	1.031(1)	0.389(1)	0.0889(5)	5.5(4)
C(66)	1.0928(10)	0.3917(10)	0.0548(5)	4.6(3)

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

atom	x	y	z	B_{eq}
C(67)	1.2642(7)	0.3940(7)	-0.0044(4)	3.5(2)
C(68)	1.2973(9)	0.3551(9)	0.0324(4)	4.0(3)
C(69)	1.364(1)	0.2865(9)	0.0295(5)	4.5(3)
C(70)	1.3950(10)	0.2556(9)	-0.0083(6)	5.2(3)
C(71)	1.363(1)	0.294(1)	-0.0451(5)	5.3(4)
C(72)	1.297(1)	0.3622(10)	-0.0432(5)	4.8(3)
C(73)	1.2576(8)	0.5695(7)	0.0010(4)	4.3(2)
C(74)	1.2852(10)	0.616(1)	-0.0365(5)	4.9(3)
C(75)	1.344(1)	0.692(1)	-0.0325(7)	6.6(5)
C(76)	1.373(1)	0.7221(9)	0.0063(8)	6.6(4)
C(77)	1.351(1)	0.677(1)	0.0430(7)	6.6(4)
C(78)	1.292(1)	0.6004(10)	0.0409(6)	5.5(4)
C(79)	1.1227(8)	0.4827(9)	-0.0417(4)	3.7(3)
C(80)	1.0868(10)	0.563(1)	-0.0574(5)	4.9(3)
C(81)	1.024(1)	0.565(1)	-0.0909(5)	6.0(4)
C(82)	0.9950(10)	0.488(1)	-0.1084(5)	5.9(4)
C(83)	1.026(1)	0.404(1)	-0.0930(5)	5.8(4)
C(84)	1.0912(9)	0.4031(10)	-0.0599(5)	4.4(3)
B(1)	0.7749(8)	0.5217(9)	0.2582(4)	3.3(3)
B(2)	1.1927(8)	0.4794(8)	-0.0009(6)	3.6(2)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0415(4)	0.0441(5)	0.0617(6)	0.0005(5)	-0.0088(7)	0.0021(6)
Ru(2)	0.0412(4)	0.0371(4)	0.0647(6)	-0.0021(5)	-0.0068(7)	-0.0049(7)
O(1)	0.26(2)	0.14(1)	0.11(1)	0.04(1)	-0.06(1)	-0.079(10)
O(2)	0.085(8)	0.14(1)	0.072(7)	-0.023(9)	0.012(7)	-0.006(8)
O(3)	0.13(1)	0.16(1)	0.080(9)	0.03(1)	0.039(8)	-0.033(9)
O(4)	0.14(1)	0.090(8)	0.068(7)	0.046(8)	0.001(8)	-0.001(6)
C(1)	0.049(7)	0.054(7)	0.084(8)	0.025(5)	-0.008(5)	-0.022(6)
C(2)	0.040(3)	0.09(1)	0.067(7)	0.014(8)	-0.011(6)	-0.021(8)
C(3)	0.050(7)	0.12(1)	0.069(8)	0.030(8)	-0.019(6)	0.02(1)
C(4)	0.09(1)	0.11(1)	0.11(1)	0.041(8)	-0.030(10)	0.068(9)
C(5)	0.07(1)	0.055(6)	0.15(1)	0.042(8)	0.02(1)	0.028(9)
C(6)	0.045(9)	0.056(7)	0.14(1)	0.019(6)	0.016(10)	-0.031(8)
C(7)	0.09(1)	0.11(1)	0.083(8)	0.043(9)	0.012(10)	-0.020(7)
C(8)	0.12(1)	0.21(2)	0.065(9)	0.00(2)	0.02(1)	-0.01(1)
C(9)	0.050(7)	0.039(6)	0.052(6)	0.010(4)	0.003(4)	-0.002(4)
C(10)	0.040(6)	0.046(3)	0.049(5)	0.006(4)	-0.005(5)	0.012(5)
C(11)	0.052(7)	0.047(6)	0.046(5)	-0.001(4)	-0.002(5)	0.006(4)
C(12)	0.044(4)	0.050(7)	0.060(6)	0.006(4)	-0.005(5)	0.001(6)
C(13)	0.040(4)	0.056(8)	0.060(6)	0.003(5)	-0.001(5)	0.009(6)
C(14)	0.066(9)	0.061(9)	0.050(6)	0.000(8)	-0.007(7)	0.004(7)
C(15)	0.07(1)	0.046(7)	0.08(1)	-0.018(6)	0.01(1)	-0.003(7)
C(16)	0.12(1)	0.071(10)	0.046(7)	0.01(1)	-0.007(8)	-0.011(7)
C(17)	0.066(9)	0.069(10)	0.08(1)	-0.013(8)	0.016(8)	0.020(8)
C(18)	0.063(9)	0.062(9)	0.09(1)	-0.015(7)	-0.023(9)	-0.003(8)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(19)	0.056(8)	0.054(8)	0.062(7)	-0.014(5)	0.005(6)	0.003(5)
C(20)	0.078(8)	0.036(2)	0.051(6)	-0.012(6)	-0.005(7)	-0.009(5)
C(21)	0.11(1)	0.054(7)	0.049(6)	-0.034(7)	-0.012(9)	-0.015(5)
C(22)	0.10(1)	0.08(1)	0.08(1)	-0.031(8)	-0.061(8)	-0.016(8)
C(23)	0.057(5)	0.07(1)	0.113(10)	-0.031(7)	-0.048(8)	0.029(9)
C(24)	0.049(6)	0.048(8)	0.101(9)	-0.016(6)	0.011(7)	-0.002(8)
C(25)	0.10(1)	0.059(9)	0.061(6)	-0.025(6)	0.009(7)	0.003(7)
C(26)	0.22(3)	0.16(2)	0.070(10)	0.08(2)	-0.03(2)	0.00(1)
C(27)	0.054(9)	0.041(5)	0.14(1)	-0.004(6)	0.004(8)	0.019(8)
C(28)	0.046(8)	0.037(6)	0.13(1)	-0.001(5)	-0.023(8)	-0.028(7)
C(29)	0.036(7)	0.043(6)	0.098(7)	-0.004(5)	-0.010(5)	-0.028(6)
C(30)	0.044(3)	0.038(6)	0.093(7)	-0.011(4)	-0.003(7)	-0.008(7)
C(31)	0.056(7)	0.048(8)	0.097(8)	-0.011(6)	0.008(6)	0.020(6)
C(32)	0.08(1)	0.07(1)	0.17(2)	0.023(10)	0.00(1)	0.07(1)
C(33)	0.06(1)	0.09(1)	0.13(2)	0.019(9)	-0.014(10)	-0.05(1)
C(34)	0.07(1)	0.11(1)	0.087(9)	0.000(10)	-0.023(9)	-0.049(9)
C(35)	0.050(7)	0.08(1)	0.11(1)	0.024(6)	-0.01(1)	-0.01(1)
C(36)	0.07(1)	0.12(1)	0.096(9)	0.01(1)	0.015(9)	0.03(1)
C(37)	0.051(6)	0.044(6)	0.043(6)	-0.001(4)	0.000(5)	-0.019(4)
C(38)	0.062(8)	0.053(7)	0.052(8)	-0.013(7)	0.016(7)	-0.018(5)
C(39)	0.084(9)	0.055(8)	0.048(8)	-0.019(7)	0.015(8)	-0.019(5)
C(40)	0.093(9)	0.052(8)	0.050(8)	-0.011(7)	0.005(7)	-0.016(6)
C(41)	0.087(10)	0.051(8)	0.055(9)	0.001(8)	0.000(8)	-0.001(6)
C(42)	0.056(7)	0.057(8)	0.040(7)	0.004(6)	-0.004(6)	-0.008(5)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(43)	0.031(6)	0.039(7)	0.080(7)	-0.009(5)	0.003(6)	-0.005(5)
C(44)	0.058(8)	0.054(9)	0.10(1)	0.009(6)	-0.025(8)	0.007(8)
C(45)	0.055(9)	0.051(9)	0.12(1)	0.003(6)	-0.002(10)	0.017(9)
C(46)	0.053(10)	0.047(9)	0.14(1)	0.002(8)	0.013(8)	-0.001(8)
C(47)	0.066(10)	0.051(8)	0.11(1)	-0.009(6)	0.037(8)	-0.021(8)
C(48)	0.08(1)	0.040(7)	0.10(1)	-0.003(6)	0.055(10)	-0.019(7)
C(49)	0.032(6)	0.037(6)	0.070(7)	0.005(4)	0.008(5)	-0.009(5)
C(50)	0.067(9)	0.051(8)	0.071(8)	-0.004(7)	0.015(8)	-0.003(7)
C(51)	0.065(9)	0.048(8)	0.10(1)	0.003(6)	0.042(8)	-0.009(8)
C(52)	0.058(10)	0.047(8)	0.11(1)	-0.004(7)	0.027(9)	-0.020(9)
C(53)	0.059(8)	0.045(8)	0.10(1)	-0.001(6)	-0.004(10)	-0.018(8)
C(54)	0.051(7)	0.058(8)	0.076(9)	-0.001(6)	-0.007(7)	-0.026(9)
C(55)	0.059(6)	0.031(6)	0.045(6)	-0.006(5)	-0.004(5)	0.003(4)
C(56)	0.065(8)	0.044(7)	0.045(7)	0.007(6)	0.002(6)	0.005(5)
C(57)	0.090(10)	0.045(7)	0.048(8)	-0.002(7)	0.012(7)	0.003(5)
C(58)	0.101(9)	0.043(8)	0.041(9)	-0.019(7)	-0.006(7)	0.007(7)
C(59)	0.082(10)	0.046(7)	0.064(9)	-0.003(7)	-0.027(7)	0.010(5)
C(60)	0.055(7)	0.039(6)	0.068(9)	0.001(6)	-0.012(7)	0.007(5)
C(61)	0.042(7)	0.055(6)	0.040(7)	-0.002(5)	-0.016(5)	0.003(5)
C(62)	0.060(9)	0.060(8)	0.061(9)	0.001(8)	0.000(6)	-0.014(8)
C(63)	0.061(9)	0.093(9)	0.057(9)	0.008(9)	-0.003(6)	-0.033(8)
C(64)	0.055(9)	0.11(1)	0.054(10)	0.010(8)	-0.013(8)	-0.003(8)
C(65)	0.055(9)	0.09(1)	0.062(10)	0.011(8)	-0.015(6)	0.023(8)
C(66)	0.050(8)	0.058(8)	0.067(10)	-0.008(7)	-0.011(6)	0.016(7)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(67)	0.035(6)	0.042(5)	0.057(5)	-0.009(4)	-0.017(6)	-0.003(6)
C(68)	0.041(7)	0.052(8)	0.058(8)	-0.001(5)	-0.011(6)	0.005(6)
C(69)	0.040(8)	0.048(8)	0.083(9)	-0.003(5)	-0.018(7)	0.018(7)
C(70)	0.052(8)	0.046(7)	0.10(1)	-0.002(6)	0.015(8)	0.001(7)
C(71)	0.056(9)	0.058(8)	0.09(1)	-0.007(6)	0.010(9)	-0.024(8)
C(72)	0.059(9)	0.053(8)	0.071(9)	-0.009(6)	0.019(8)	-0.016(8)
C(73)	0.043(6)	0.043(5)	0.078(6)	0.007(5)	0.003(9)	0.005(7)
C(74)	0.046(8)	0.063(8)	0.077(9)	-0.003(6)	-0.003(8)	0.016(8)
C(75)	0.05(1)	0.064(9)	0.14(1)	-0.010(7)	0.02(1)	0.01(1)
C(76)	0.049(9)	0.049(8)	0.15(1)	-0.002(7)	-0.02(1)	0.011(10)
C(77)	0.061(10)	0.061(9)	0.13(1)	-0.006(7)	0.00(1)	-0.030(9)
C(78)	0.066(9)	0.051(8)	0.09(1)	0.000(6)	-0.020(9)	-0.015(8)
C(79)	0.039(7)	0.059(6)	0.043(7)	-0.001(6)	0.002(5)	0.007(6)
C(80)	0.052(8)	0.062(8)	0.071(9)	0.013(8)	-0.003(6)	0.016(8)
C(81)	0.046(8)	0.10(1)	0.08(1)	-0.007(10)	-0.005(7)	0.038(10)
C(82)	0.049(8)	0.11(1)	0.059(10)	0.012(9)	-0.012(7)	0.010(9)
C(83)	0.07(1)	0.10(1)	0.053(9)	-0.015(9)	-0.019(7)	0.001(8)
C(84)	0.040(8)	0.066(8)	0.064(9)	-0.001(7)	-0.009(6)	-0.012(7)
B(1)	0.034(6)	0.044(7)	0.048(6)	-0.001(4)	0.007(5)	-0.011(4)
B(2)	0.038(6)	0.049(6)	0.051(6)	0.002(4)	-0.005(5)	-0.011(9)

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)	2.20(1)	Ru(1)	C(2)	2.22(1)
Ru(1)	C(3)	2.23(1)	Ru(1)	C(4)	2.22(1)
Ru(1)	C(5)	2.23(1)	Ru(1)	C(6)	2.25(1)
Ru(1)	C(9)	2.18(1)	Ru(1)	C(10)	2.19(1)
Ru(1)	C(11)	2.15(1)	Ru(1)	C(12)	2.17(1)
Ru(1)	C(13)	2.21(1)	Ru(2)	C(19)	2.23(1)
Ru(2)	C(20)	2.23(1)	Ru(2)	C(21)	2.23(1)
Ru(2)	C(22)	2.19(1)	Ru(2)	C(23)	2.23(1)
Ru(2)	C(24)	2.23(1)	Ru(2)	C(27)	2.17(1)
Ru(2)	C(28)	2.19(1)	Ru(2)	C(29)	2.18(1)
Ru(2)	C(30)	2.20(1)	Ru(2)	C(31)	2.21(2)
O(1)	C(7)	1.21(2)	O(2)	C(7)	1.30(2)
O(2)	C(8)	1.49(2)	O(3)	C(25)	1.19(2)
O(4)	C(25)	1.33(2)	O(4)	C(26)	1.51(2)
C(1)	C(2)	1.45(2)	C(1)	C(6)	1.41(2)
C(1)	C(7)	1.47(2)	C(2)	C(3)	1.41(2)
C(3)	C(4)	1.43(3)	C(4)	C(5)	1.46(3)
C(5)	C(6)	1.43(2)	C(9)	C(10)	1.39(2)
C(9)	C(13)	1.44(2)	C(9)	C(14)	1.55(2)
C(10)	C(11)	1.44(2)	C(10)	C(15)	1.54(2)
C(11)	C(12)	1.44(2)	C(11)	C(16)	1.54(2)
C(12)	C(13)	1.46(2)	C(12)	C(17)	1.52(2)
C(13)	C(18)	1.49(2)	C(19)	C(20)	1.46(2)
C(19)	C(24)	1.42(2)	C(19)	C(25)	1.44(2)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(20)	C(21)	1.41(2)	C(21)	C(22)	1.38(2)
C(22)	C(23)	1.47(2)	C(23)	C(24)	1.44(2)
C(27)	C(28)	1.48(2)	C(27)	C(31)	1.46(2)
C(27)	C(32)	1.50(2)	C(28)	C(29)	1.43(2)
C(28)	C(33)	1.52(2)	C(29)	C(30)	1.47(2)
C(29)	C(34)	1.51(2)	C(30)	C(31)	1.40(2)
C(30)	C(35)	1.52(2)	C(31)	C(36)	1.51(2)
C(37)	C(38)	1.41(2)	C(37)	C(42)	1.42(2)
C(37)	B(1)	1.65(2)	C(38)	C(39)	1.41(2)
C(39)	C(40)	1.43(2)	C(40)	C(41)	1.39(2)
C(41)	C(42)	1.40(2)	C(43)	C(44)	1.40(2)
C(43)	C(48)	1.42(2)	C(43)	B(1)	1.64(2)
C(44)	C(45)	1.44(2)	C(45)	C(46)	1.35(3)
C(46)	C(47)	1.34(3)	C(47)	C(48)	1.46(2)
C(49)	C(50)	1.44(2)	C(49)	C(54)	1.43(2)
C(49)	B(1)	1.67(2)	C(50)	C(51)	1.41(2)
C(51)	C(52)	1.40(2)	C(52)	C(53)	1.42(2)
C(53)	C(54)	1.39(2)	C(55)	C(56)	1.38(2)
C(55)	C(60)	1.41(2)	C(55)	B(1)	1.66(2)
C(56)	C(57)	1.42(2)	C(57)	C(58)	1.41(2)
C(58)	C(59)	1.39(2)	C(59)	C(60)	1.40(2)
C(61)	C(62)	1.40(2)	C(61)	C(66)	1.41(2)
C(61)	B(2)	1.64(2)	C(62)	C(63)	1.44(2)
C(63)	C(64)	1.41(2)	C(64)	C(65)	1.37(2)

Table 3. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(65)	C(66)	1.42(2)	C(67)	C(68)	1.40(2)
C(67)	C(72)	1.41(2)	C(67)	B(2)	1.66(2)
C(68)	C(69)	1.42(2)	C(69)	C(70)	1.37(2)
C(70)	C(71)	1.39(2)	C(71)	C(72)	1.41(2)
C(73)	C(74)	1.44(2)	C(73)	C(78)	1.44(2)
C(73)	B(2)	1.66(2)	C(74)	C(75)	1.44(2)
C(75)	C(76)	1.38(3)	C(76)	C(77)	1.39(3)
C(77)	C(78)	1.44(2)	C(79)	C(80)	1.41(2)
C(79)	C(84)	1.40(2)	C(79)	B(2)	1.66(2)
C(80)	C(81)	1.41(2)	C(81)	C(82)	1.36(2)
C(82)	C(83)	1.41(2)	C(83)	C(84)	1.43(2)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Ru(1)	C(2)	38.2(5)	C(1)	Ru(1)	C(3)	68.0(6)
C(1)	Ru(1)	C(4)	80.2(7)	C(1)	Ru(1)	C(5)	66.9(6)
C(1)	Ru(1)	C(6)	37.0(5)	C(1)	Ru(1)	C(9)	106.6(5)
C(1)	Ru(1)	C(10)	122.1(5)	C(1)	Ru(1)	C(11)	158.5(5)
C(1)	Ru(1)	C(12)	157.1(5)	C(1)	Ru(1)	C(13)	120.8(5)
C(2)	Ru(1)	C(3)	37.0(6)	C(2)	Ru(1)	C(4)	67.3(7)
C(2)	Ru(1)	C(5)	79.8(7)	C(2)	Ru(1)	C(6)	68.0(6)
C(2)	Ru(1)	C(9)	116.6(6)	C(2)	Ru(1)	C(10)	106.3(6)
C(2)	Ru(1)	C(11)	126.2(6)	C(2)	Ru(1)	C(12)	164.5(6)
C(2)	Ru(1)	C(13)	150.4(5)	C(3)	Ru(1)	C(4)	37.6(7)
C(3)	Ru(1)	C(5)	68.3(7)	C(3)	Ru(1)	C(6)	80.6(7)
C(3)	Ru(1)	C(9)	142.7(6)	C(3)	Ru(1)	C(10)	112.4(6)
C(3)	Ru(1)	C(11)	106.9(6)	C(3)	Ru(1)	C(12)	132.5(5)
C(3)	Ru(1)	C(13)	171.2(6)	C(4)	Ru(1)	C(5)	38.4(7)
C(4)	Ru(1)	C(6)	68.3(8)	C(4)	Ru(1)	C(9)	172.9(7)
C(4)	Ru(1)	C(10)	137.3(7)	C(4)	Ru(1)	C(11)	108.9(7)
C(4)	Ru(1)	C(12)	110.1(7)	C(4)	Ru(1)	C(13)	139.7(7)
C(5)	Ru(1)	C(6)	37.2(6)	C(5)	Ru(1)	C(9)	146.0(7)
C(5)	Ru(1)	C(10)	170.8(6)	C(5)	Ru(1)	C(11)	132.1(6)
C(5)	Ru(1)	C(12)	107.9(6)	C(5)	Ru(1)	C(13)	114.1(7)
C(6)	Ru(1)	C(9)	118.3(6)	C(6)	Ru(1)	C(10)	151.3(6)
C(6)	Ru(1)	C(11)	164.3(6)	C(6)	Ru(1)	C(12)	126.3(6)
C(6)	Ru(1)	C(13)	106.5(6)	C(9)	Ru(1)	C(10)	37.2(4)
C(9)	Ru(1)	C(11)	64.1(4)	C(9)	Ru(1)	C(12)	64.4(5)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(9)	Ru(1)	C(13)	38.4(5)	C(10)	Ru(1)	C(11)	38.8(4)
C(10)	Ru(1)	C(12)	64.5(5)	C(10)	Ru(1)	C(13)	63.8(5)
C(11)	Ru(1)	C(12)	38.9(5)	C(11)	Ru(1)	C(13)	65.0(5)
C(12)	Ru(1)	C(13)	38.9(4)	C(19)	Ru(2)	C(20)	38.2(5)
C(19)	Ru(2)	C(21)	67.3(5)	C(19)	Ru(2)	C(22)	79.1(6)
C(19)	Ru(2)	C(23)	67.0(6)	C(19)	Ru(2)	C(24)	37.2(5)
C(19)	Ru(2)	C(27)	153.4(7)	C(19)	Ru(2)	C(28)	118.3(7)
C(19)	Ru(2)	C(29)	106.9(6)	C(19)	Ru(2)	C(30)	127.2(6)
C(19)	Ru(2)	C(31)	163.0(6)	C(20)	Ru(2)	C(21)	36.7(5)
C(20)	Ru(2)	C(22)	66.2(6)	C(20)	Ru(2)	C(23)	80.1(6)
C(20)	Ru(2)	C(24)	68.7(6)	C(20)	Ru(2)	C(27)	168.3(7)
C(20)	Ru(2)	C(28)	146.5(6)	C(20)	Ru(2)	C(29)	114.3(5)
C(20)	Ru(2)	C(30)	107.7(5)	C(20)	Ru(2)	C(31)	129.7(6)
C(21)	Ru(2)	C(22)	36.3(6)	C(21)	Ru(2)	C(23)	68.0(7)
C(21)	Ru(2)	C(24)	80.8(6)	C(21)	Ru(2)	C(27)	135.7(7)
C(21)	Ru(2)	C(28)	173.8(7)	C(21)	Ru(2)	C(29)	139.4(6)
C(21)	Ru(2)	C(30)	110.2(6)	C(21)	Ru(2)	C(31)	108.9(6)
C(22)	Ru(2)	C(23)	38.8(6)	C(22)	Ru(2)	C(24)	68.9(7)
C(22)	Ru(2)	C(27)	112.0(8)	C(22)	Ru(2)	C(28)	144.6(7)
C(22)	Ru(2)	C(29)	171.0(7)	C(22)	Ru(2)	C(30)	131.7(7)
C(22)	Ru(2)	C(31)	108.0(7)	C(23)	Ru(2)	C(24)	37.8(5)
C(23)	Ru(2)	C(27)	105.9(6)	C(23)	Ru(2)	C(28)	116.1(6)
C(23)	Ru(2)	C(29)	149.5(7)	C(23)	Ru(2)	C(30)	164.8(7)
C(23)	Ru(2)	C(31)	128.2(7)	C(24)	Ru(2)	C(27)	122.2(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(24)	Ru(2)	C(28)	105.3(6)	C(24)	Ru(2)	C(29)	119.9(6)
C(24)	Ru(2)	C(30)	157.1(7)	C(24)	Ru(2)	C(31)	159.6(6)
C(27)	Ru(2)	C(28)	39.8(6)	C(27)	Ru(2)	C(29)	65.5(6)
C(27)	Ru(2)	C(30)	64.2(5)	C(27)	Ru(2)	C(31)	38.8(6)
C(28)	Ru(2)	C(29)	38.3(5)	C(28)	Ru(2)	C(30)	64.5(5)
C(28)	Ru(2)	C(31)	64.9(6)	C(29)	Ru(2)	C(30)	39.4(5)
C(29)	Ru(2)	C(31)	64.4(6)	C(30)	Ru(2)	C(31)	37.0(6)
C(7)	O(2)	C(8)	122(1)	C(25)	O(4)	C(26)	121(1)
Ru(1)	C(1)	C(2)	71.7(8)	Ru(1)	C(1)	C(6)	73.5(9)
Ru(1)	C(1)	C(7)	125(1)	C(2)	C(1)	C(6)	121(1)
C(2)	C(1)	C(7)	119(1)	C(6)	C(1)	C(7)	118(1)
Ru(1)	C(2)	C(1)	70.1(8)	Ru(1)	C(2)	C(3)	71.9(9)
C(1)	C(2)	C(3)	119(1)	Ru(1)	C(3)	C(2)	71.1(8)
Ru(1)	C(3)	C(4)	71.0(8)	C(2)	C(3)	C(4)	119(1)
Ru(1)	C(4)	C(3)	71.4(8)	Ru(1)	C(4)	C(5)	71.0(9)
C(3)	C(4)	C(5)	119(1)	Ru(1)	C(5)	C(4)	70.7(8)
Ru(1)	C(5)	C(6)	72.2(10)	C(4)	C(5)	C(6)	120(1)
Ru(1)	C(6)	C(1)	69.5(8)	Ru(1)	C(6)	C(5)	70.7(9)
C(1)	C(6)	C(5)	118(1)	O(1)	C(7)	O(2)	119(2)
O(1)	C(7)	C(1)	123(2)	O(2)	C(7)	C(1)	116(1)
Ru(1)	C(9)	C(10)	71.5(7)	Ru(1)	C(9)	C(13)	71.7(8)
Ru(1)	C(9)	C(14)	127.2(9)	C(10)	C(9)	C(13)	109(1)
C(10)	C(9)	C(14)	126(1)	C(13)	C(9)	C(14)	123(1)
Ru(1)	C(10)	C(9)	71.3(7)	Ru(1)	C(10)	C(11)	69.4(7)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Ru(1)	C(10)	C(15)	124.0(9)	C(9)	C(10)	C(11)	108(1)
C(9)	C(10)	C(15)	127(1)	C(11)	C(10)	C(15)	123(1)
Ru(1)	C(11)	C(10)	71.8(7)	Ru(1)	C(11)	C(12)	71.2(7)
Ru(1)	C(11)	C(16)	127.4(10)	C(10)	C(11)	C(12)	107(1)
C(10)	C(11)	C(16)	125(1)	C(12)	C(11)	C(16)	126(1)
Ru(1)	C(12)	C(11)	69.9(7)	Ru(1)	C(12)	C(13)	71.9(9)
Ru(1)	C(12)	C(17)	129.1(10)	C(11)	C(12)	C(13)	107(1)
C(11)	C(12)	C(17)	125(1)	C(13)	C(12)	C(17)	126(1)
Ru(1)	C(13)	C(9)	69.9(8)	Ru(1)	C(13)	C(12)	69.2(8)
Ru(1)	C(13)	C(18)	129(1)	C(9)	C(13)	C(12)	106(1)
C(9)	C(13)	C(18)	127(1)	C(12)	C(13)	C(18)	126(1)
Ru(2)	C(19)	C(20)	70.9(7)	Ru(2)	C(19)	C(24)	71.5(8)
Ru(2)	C(19)	C(25)	125(1)	C(20)	C(19)	C(24)	121(1)
C(20)	C(19)	C(25)	118(1)	C(24)	C(19)	C(25)	119(1)
Ru(2)	C(20)	C(19)	70.9(7)	Ru(2)	C(20)	C(21)	71.7(8)
C(19)	C(20)	C(21)	119(1)	Ru(2)	C(21)	C(20)	71.6(7)
Ru(2)	C(21)	C(22)	70.4(9)	C(20)	C(21)	C(22)	120(1)
Ru(2)	C(22)	C(21)	73.3(8)	Ru(2)	C(22)	C(23)	71.9(8)
C(21)	C(22)	C(23)	122(1)	Ru(2)	C(23)	C(22)	69.3(8)
Ru(2)	C(23)	C(24)	71.2(9)	C(22)	C(23)	C(24)	118(1)
Ru(2)	C(24)	C(19)	71.3(8)	Ru(2)	C(24)	C(23)	71.1(9)
C(19)	C(24)	C(23)	118(1)	O(3)	C(25)	O(4)	122(1)
O(3)	C(25)	C(19)	123(1)	O(4)	C(25)	C(19)	114(1)
Ru(2)	C(27)	C(28)	70.9(9)	Ru(2)	C(27)	C(31)	72.2(8)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Ru(2)	C(27)	C(32)	126(1)	C(28)	C(27)	C(31)	106(1)
C(28)	C(27)	C(32)	125(1)	C(31)	C(27)	C(32)	127(1)
Ru(2)	C(28)	C(27)	69.3(9)	Ru(2)	C(28)	C(29)	70.4(7)
Ru(2)	C(28)	C(33)	126(1)	C(27)	C(28)	C(29)	107(1)
C(27)	C(28)	C(33)	127(1)	C(29)	C(28)	C(33)	125(1)
Ru(2)	C(29)	C(28)	71.3(8)	Ru(2)	C(29)	C(30)	71.0(7)
Ru(2)	C(29)	C(34)	126(1)	C(28)	C(29)	C(30)	107(1)
C(28)	C(29)	C(34)	126(1)	C(30)	C(29)	C(34)	126(1)
Ru(2)	C(30)	C(29)	69.7(7)	Ru(2)	C(30)	C(31)	72.0(9)
Ru(2)	C(30)	C(35)	126.9(8)	C(29)	C(30)	C(31)	109(1)
C(29)	C(30)	C(35)	126(1)	C(31)	C(30)	C(35)	123(1)
Ru(2)	C(31)	C(27)	69.0(9)	Ru(2)	C(31)	C(30)	71.0(8)
Ru(2)	C(31)	C(36)	124(1)	C(27)	C(31)	C(30)	108(1)
C(27)	C(31)	C(36)	123(1)	C(30)	C(31)	C(36)	127(1)
C(38)	C(37)	C(42)	118(1)	C(38)	C(37)	B(1)	120(1)
C(42)	C(37)	B(1)	121(1)	C(37)	C(38)	C(39)	120(1)
C(38)	C(39)	C(40)	119(1)	C(39)	C(40)	C(41)	120(1)
C(40)	C(41)	C(42)	118(1)	C(37)	C(42)	C(41)	122(1)
C(44)	C(43)	C(48)	118(1)	C(44)	C(43)	B(1)	122(1)
C(48)	C(43)	B(1)	119(1)	C(43)	C(44)	C(45)	120(1)
C(44)	C(45)	C(46)	119(1)	C(45)	C(46)	C(47)	121(1)
C(46)	C(47)	C(48)	122(1)	C(43)	C(48)	C(47)	117(1)
C(50)	C(49)	C(54)	117(1)	C(50)	C(49)	B(1)	119(1)
C(54)	C(49)	B(1)	121(1)	C(49)	C(50)	C(51)	118(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(50)	C(51)	C(52)	121(1)	C(51)	C(52)	C(53)	120(1)
C(52)	C(53)	C(54)	118(1)	C(49)	C(54)	C(53)	123(1)
C(56)	C(55)	C(60)	116(1)	C(56)	C(55)	B(1)	123(1)
C(60)	C(55)	B(1)	119(1)	C(55)	C(56)	C(57)	122(1)
C(56)	C(57)	C(58)	119(1)	C(57)	C(58)	C(59)	118(1)
C(58)	C(59)	C(60)	120(1)	C(55)	C(60)	C(59)	121(1)
C(62)	C(61)	C(66)	118(1)	C(62)	C(61)	B(2)	120(1)
C(66)	C(61)	B(2)	121(1)	C(61)	C(62)	C(63)	121(1)
C(62)	C(63)	C(64)	119(1)	C(63)	C(64)	C(65)	119(1)
C(64)	C(65)	C(66)	121(1)	C(61)	C(66)	C(65)	120(1)
C(68)	C(67)	C(72)	118(1)	C(68)	C(67)	B(2)	119(1)
C(72)	C(67)	B(2)	122(1)	C(67)	C(68)	C(69)	119(1)
C(68)	C(69)	C(70)	122(1)	C(69)	C(70)	C(71)	119(1)
C(70)	C(71)	C(72)	119(1)	C(67)	C(72)	C(71)	121(1)
C(74)	C(73)	C(78)	118(1)	C(74)	C(73)	B(2)	121(1)
C(78)	C(73)	B(2)	119(1)	C(73)	C(74)	C(75)	118(1)
C(74)	C(75)	C(76)	121(1)	C(75)	C(76)	C(77)	121(1)
C(76)	C(77)	C(78)	119(1)	C(73)	C(78)	C(77)	120(1)
C(80)	C(79)	C(84)	116(1)	C(80)	C(79)	B(2)	122(1)
C(84)	C(79)	B(2)	120(1)	C(79)	C(80)	C(81)	122(1)
C(80)	C(81)	C(82)	119(1)	C(81)	C(82)	C(83)	120(1)
C(82)	C(83)	C(84)	118(1)	C(79)	C(84)	C(83)	121(1)
C(37)	B(1)	C(43)	113.4(10)	C(37)	B(1)	C(49)	113.1(10)
C(37)	B(1)	C(55)	103.9(9)	C(43)	B(1)	C(49)	104.3(9)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(43)	B(1)	C(55)	111(1)	C(49)	B(1)	C(55)	110(1)
C(61)	B(2)	C(67)	114(1)	C(61)	B(2)	C(73)	111(1)
C(61)	B(2)	C(79)	102.9(8)	C(67)	B(2)	C(73)	105.0(8)
C(67)	B(2)	C(79)	111(1)	C(73)	B(2)	C(79)	111(1)

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru(1)	C(1)	C(2)	C(3)	-53(1)	Ru(1)	C(1)	C(6)	C(5)	52(1)
Ru(1)	C(1)	C(7)	O(1)	99(2)	Ru(1)	C(1)	C(7)	O(2)	-79(2)
Ru(1)	C(2)	C(1)	C(6)	56(1)	Ru(1)	C(2)	C(1)	C(7)	-120(1)
Ru(1)	C(2)	C(3)	C(4)	-53(1)	Ru(1)	C(3)	C(2)	C(1)	52(1)
Ru(1)	C(3)	C(4)	C(5)	-54(1)	Ru(1)	C(4)	C(3)	C(2)	53(1)
Ru(1)	C(4)	C(5)	C(6)	-54(1)	Ru(1)	C(5)	C(4)	C(3)	54(1)
Ru(1)	C(5)	C(6)	C(1)	-52(1)	Ru(1)	C(6)	C(1)	C(2)	-55(1)
Ru(1)	C(6)	C(1)	C(7)	121(1)	Ru(1)	C(6)	C(5)	C(4)	53(1)
Ru(1)	C(9)	C(10)	C(11)	59.7(8)	Ru(1)	C(9)	C(10)	C(15)	-119(1)
Ru(1)	C(9)	C(13)	C(12)	-60.0(10)	Ru(1)	C(9)	C(13)	C(18)	124(1)
Ru(1)	C(10)	C(9)	C(13)	-61.7(9)	Ru(1)	C(10)	C(9)	C(14)	122(1)
Ru(1)	C(10)	C(11)	C(12)	62.6(8)	Ru(1)	C(10)	C(11)	C(16)	-123(1)
Ru(1)	C(11)	C(10)	C(9)	-60.8(8)	Ru(1)	C(11)	C(10)	C(15)	117(1)
Ru(1)	C(11)	C(12)	C(13)	62.3(10)	Ru(1)	C(11)	C(12)	C(17)	-124(1)
Ru(1)	C(12)	C(11)	C(10)	-63.0(8)	Ru(1)	C(12)	C(11)	C(16)	123(1)
Ru(1)	C(12)	C(13)	C(9)	60.5(9)	Ru(1)	C(12)	C(13)	C(18)	-124(1)
Ru(1)	C(13)	C(9)	C(10)	61.6(9)	Ru(1)	C(13)	C(9)	C(14)	-122(1)
Ru(1)	C(13)	C(12)	C(11)	-61.0(9)	Ru(1)	C(13)	C(12)	C(17)	125(1)
Ru(2)	C(19)	C(20)	C(21)	-54(1)	Ru(2)	C(19)	C(24)	C(23)	55(1)
Ru(2)	C(19)	C(25)	O(3)	91(2)	Ru(2)	C(19)	C(25)	O(4)	-90(1)
Ru(2)	C(20)	C(19)	C(24)	52(1)	Ru(2)	C(20)	C(19)	C(25)	-120(1)
Ru(2)	C(20)	C(21)	C(22)	-52(1)	Ru(2)	C(21)	C(20)	C(19)	54(1)
Ru(2)	C(21)	C(22)	C(23)	-55(1)	Ru(2)	C(22)	C(21)	C(20)	53(1)
Ru(2)	C(22)	C(23)	C(24)	-53(1)	Ru(2)	C(23)	C(22)	C(21)	55(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru(2)	C(23)	C(24)	C(19)	-55(1)	Ru(2)	C(24)	C(19)	C(20)	-52(1)
Ru(2)	C(24)	C(19)	C(25)	121(1)	Ru(2)	C(24)	C(23)	C(22)	52(1)
Ru(2)	C(27)	C(28)	C(29)	60(1)	Ru(2)	C(27)	C(28)	C(33)	-121(1)
Ru(2)	C(27)	C(31)	C(30)	-60(1)	Ru(2)	C(27)	C(31)	C(36)	118(1)
Ru(2)	C(28)	C(27)	C(31)	-63(1)	Ru(2)	C(28)	C(27)	C(32)	121(1)
Ru(2)	C(28)	C(29)	C(30)	62.2(9)	Ru(2)	C(28)	C(29)	C(34)	-121(1)
Ru(2)	C(29)	C(28)	C(27)	-59(1)	Ru(2)	C(29)	C(28)	C(33)	121(1)
Ru(2)	C(29)	C(30)	C(31)	61.5(9)	Ru(2)	C(29)	C(30)	C(35)	-121(1)
Ru(2)	C(30)	C(29)	C(28)	-62.4(9)	Ru(2)	C(30)	C(29)	C(34)	121(1)
Ru(2)	C(30)	C(31)	C(27)	58(1)	Ru(2)	C(30)	C(31)	C(36)	-119(1)
Ru(2)	C(31)	C(27)	C(28)	62(1)	Ru(2)	C(31)	C(27)	C(32)	-122(1)
Ru(2)	C(31)	C(30)	C(29)	-60.0(8)	Ru(2)	C(31)	C(30)	C(35)	122(1)
O(1)	C(7)	O(2)	C(8)	0(3)	O(1)	C(7)	C(1)	C(2)	-172(1)
O(1)	C(7)	C(1)	C(6)	10(2)	O(2)	C(7)	C(1)	C(2)	8(2)
O(2)	C(7)	C(1)	C(6)	-168(1)	O(3)	C(25)	O(4)	C(26)	0(2)
O(3)	C(25)	C(19)	C(20)	178(1)	O(3)	C(25)	C(19)	C(24)	4(2)
O(4)	C(25)	C(19)	C(20)	-3(2)	O(4)	C(25)	C(19)	C(24)	-177(1)
C(1)	Ru(1)	C(2)	C(3)	132(1)	C(1)	Ru(1)	C(3)	C(2)	-29(1)
C(1)	Ru(1)	C(3)	C(4)	102(1)	C(1)	Ru(1)	C(4)	C(3)	-66(1)
C(1)	Ru(1)	C(4)	C(5)	65(1)	C(1)	Ru(1)	C(5)	C(4)	-103(1)
C(1)	Ru(1)	C(5)	C(6)	29.1(10)	C(1)	Ru(1)	C(6)	C(5)	-132(1)
C(1)	Ru(1)	C(9)	C(10)	121.7(8)	C(1)	Ru(1)	C(9)	C(13)	-119.0(8)
C(1)	Ru(1)	C(9)	C(14)	0(1)	C(1)	Ru(1)	C(10)	C(9)	-74.3(9)
C(1)	Ru(1)	C(10)	C(11)	166.6(7)	C(1)	Ru(1)	C(10)	C(15)	49(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	Ru(1)	C(11)	C(10)	-32(1)	C(1)	Ru(1)	C(11)	C(12)	-148(1)
C(1)	Ru(1)	C(11)	C(16)	89(1)	C(1)	Ru(1)	C(12)	C(11)	150(1)
C(1)	Ru(1)	C(12)	C(13)	33(1)	C(1)	Ru(1)	C(12)	C(17)	-88(1)
C(1)	Ru(1)	C(13)	C(9)	77.4(10)	C(1)	Ru(1)	C(13)	C(12)	-165.5(8)
C(1)	Ru(1)	C(13)	C(18)	-44(1)	C(1)	C(2)	Ru(1)	C(3)	-132(1)
C(1)	C(2)	Ru(1)	C(4)	-103(1)	C(1)	C(2)	Ru(1)	C(5)	-65(1)
C(1)	C(2)	Ru(1)	C(6)	-28.6(10)	C(1)	C(2)	Ru(1)	C(9)	83(1)
C(1)	C(2)	Ru(1)	C(10)	121.6(9)	C(1)	C(2)	Ru(1)	C(11)	159.2(8)
C(1)	C(2)	Ru(1)	C(12)	172(1)	C(1)	C(2)	Ru(1)	C(13)	56(1)
C(1)	C(2)	C(3)	C(4)	0(2)	C(1)	C(6)	Ru(1)	C(2)	29.5(10)
C(1)	C(6)	Ru(1)	C(3)	65(1)	C(1)	C(6)	Ru(1)	C(4)	102(1)
C(1)	C(6)	Ru(1)	C(5)	132(1)	C(1)	C(6)	Ru(1)	C(9)	-79(1)
C(1)	C(6)	Ru(1)	C(10)	-54(1)	C(1)	C(6)	Ru(1)	C(11)	-174(1)
C(1)	C(6)	Ru(1)	C(12)	-157.5(9)	C(1)	C(6)	Ru(1)	C(13)	-119.6(10)
C(1)	C(6)	C(5)	C(4)	1(2)	C(1)	C(7)	O(2)	C(8)	178(1)
C(2)	Ru(1)	C(1)	C(6)	-132(1)	C(2)	Ru(1)	C(1)	C(7)	114(1)
C(2)	Ru(1)	C(3)	C(4)	132(1)	C(2)	Ru(1)	C(4)	C(3)	-28(1)
C(2)	Ru(1)	C(4)	C(5)	102(1)	C(2)	Ru(1)	C(5)	C(4)	-66(1)
C(2)	Ru(1)	C(5)	C(6)	66(1)	C(2)	Ru(1)	C(6)	C(5)	-102(1)
C(2)	Ru(1)	C(9)	C(10)	81.9(9)	C(2)	Ru(1)	C(9)	C(13)	-158.8(7)
C(2)	Ru(1)	C(9)	C(14)	-39(1)	C(2)	Ru(1)	C(10)	C(9)	-112.8(8)
C(2)	Ru(1)	C(10)	C(11)	128.2(8)	C(2)	Ru(1)	C(10)	C(15)	10(1)
C(2)	Ru(1)	C(11)	C(10)	-69.2(9)	C(2)	Ru(1)	C(11)	C(12)	174.2(8)
C(2)	Ru(1)	C(11)	C(16)	52(1)	C(2)	Ru(1)	C(12)	C(11)	-17(2)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(2)	Ru(1)	C(12)	C(13)	-135(2)	C(2)	Ru(1)	C(12)	C(17)	102(2)
C(2)	Ru(1)	C(13)	C(9)	40(1)	C(2)	Ru(1)	C(13)	C(12)	157(1)
C(2)	Ru(1)	C(13)	C(18)	-81(1)	C(2)	C(1)	Ru(1)	C(3)	28(1)
C(2)	C(1)	Ru(1)	C(4)	65(1)	C(2)	C(1)	Ru(1)	C(5)	103(1)
C(2)	C(1)	Ru(1)	C(6)	132(1)	C(2)	C(1)	Ru(1)	C(9)	-112.2(10)
C(2)	C(1)	Ru(1)	C(10)	-74(1)	C(2)	C(1)	Ru(1)	C(11)	-51(1)
C(2)	C(1)	Ru(1)	C(12)	-175(1)	C(2)	C(1)	Ru(1)	C(13)	-151.5(9)
C(2)	C(1)	C(6)	C(5)	-2(2)	C(2)	C(3)	Ru(1)	C(4)	-132(1)
C(2)	C(3)	Ru(1)	C(5)	-102(1)	C(2)	C(3)	Ru(1)	C(6)	-65(1)
C(2)	C(3)	Ru(1)	C(9)	59(1)	C(2)	C(3)	Ru(1)	C(10)	87(1)
C(2)	C(3)	Ru(1)	C(11)	128(1)	C(2)	C(3)	Ru(1)	C(12)	162(1)
C(2)	C(3)	Ru(1)	C(13)	150(3)	C(2)	C(3)	C(4)	C(5)	0(2)
C(3)	Ru(1)	C(1)	C(6)	-104(1)	C(3)	Ru(1)	C(1)	C(7)	142(1)
C(3)	Ru(1)	C(4)	C(5)	131(1)	C(3)	Ru(1)	C(5)	C(4)	-29(1)
C(3)	Ru(1)	C(5)	C(6)	103(1)	C(3)	Ru(1)	C(6)	C(5)	-66(1)
C(3)	Ru(1)	C(9)	C(10)	46(1)	C(3)	Ru(1)	C(9)	C(13)	165.7(10)
C(3)	Ru(1)	C(9)	C(14)	-75(1)	C(3)	Ru(1)	C(10)	C(9)	-151.6(8)
C(3)	Ru(1)	C(10)	C(11)	89.3(8)	C(3)	Ru(1)	C(10)	C(15)	-27(1)
C(3)	Ru(1)	C(11)	C(10)	-105.0(8)	C(3)	Ru(1)	C(11)	C(12)	138.5(9)
C(3)	Ru(1)	C(11)	C(16)	16(1)	C(3)	Ru(1)	C(12)	C(11)	-59(1)
C(3)	Ru(1)	C(12)	C(13)	-177(1)	C(3)	Ru(1)	C(12)	C(17)	60(1)
C(3)	Ru(1)	C(13)	C(9)	-102(4)	C(3)	Ru(1)	C(13)	C(12)	14(5)
C(3)	Ru(1)	C(13)	C(18)	135(4)	C(3)	C(2)	Ru(1)	C(4)	29(1)
C(3)	C(2)	Ru(1)	C(5)	67(1)	C(3)	C(2)	Ru(1)	C(6)	104(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(3)	C(2)	Ru(1)	C(9)	-144(1)	C(3)	C(2)	Ru(1)	C(10)	-105(1)
C(3)	C(2)	Ru(1)	C(11)	-68(1)	C(3)	C(2)	Ru(1)	C(12)	-54(2)
C(3)	C(2)	Ru(1)	C(13)	-171(1)	C(3)	C(2)	C(1)	C(6)	2(2)
C(3)	C(2)	C(1)	C(7)	-174(1)	C(3)	C(4)	Ru(1)	C(5)	-131(1)
C(3)	C(4)	Ru(1)	C(6)	-103(1)	C(3)	C(4)	Ru(1)	C(9)	96(5)
C(3)	C(4)	Ru(1)	C(10)	60(1)	C(3)	C(4)	Ru(1)	C(11)	93(1)
C(3)	C(4)	Ru(1)	C(12)	134(1)	C(3)	C(4)	Ru(1)	C(13)	166(1)
C(3)	C(4)	C(5)	C(6)	0(2)	C(4)	Ru(1)	C(1)	C(6)	-66(1)
C(4)	Ru(1)	C(1)	C(7)	179(1)	C(4)	Ru(1)	C(5)	C(6)	132(1)
C(4)	Ru(1)	C(6)	C(5)	-29(1)	C(4)	Ru(1)	C(9)	C(10)	-40(5)
C(4)	Ru(1)	C(9)	C(13)	78(5)	C(4)	Ru(1)	C(9)	C(14)	-162(5)
C(4)	Ru(1)	C(10)	C(9)	173.2(10)	C(4)	Ru(1)	C(10)	C(11)	54(1)
C(4)	Ru(1)	C(10)	C(15)	-63(1)	C(4)	Ru(1)	C(11)	C(10)	-144.5(8)
C(4)	Ru(1)	C(11)	C(12)	98.9(9)	C(4)	Ru(1)	C(11)	C(16)	-22(1)
C(4)	Ru(1)	C(12)	C(11)	-95.4(10)	C(4)	Ru(1)	C(12)	C(13)	146(1)
C(4)	Ru(1)	C(12)	C(17)	24(1)	C(4)	Ru(1)	C(13)	C(9)	-169(1)
C(4)	Ru(1)	C(13)	C(12)	-52(1)	C(4)	Ru(1)	C(13)	C(18)	68(1)
C(4)	C(3)	Ru(1)	C(5)	29(1)	C(4)	C(3)	Ru(1)	C(6)	66(1)
C(4)	C(3)	Ru(1)	C(9)	-168(1)	C(4)	C(3)	Ru(1)	C(10)	-140(1)
C(4)	C(3)	Ru(1)	C(11)	-99(1)	C(4)	C(3)	Ru(1)	C(12)	-64(1)
C(4)	C(3)	Ru(1)	C(13)	-77(4)	C(4)	C(5)	Ru(1)	C(6)	-132(1)
C(4)	C(5)	Ru(1)	C(9)	170(1)	C(4)	C(5)	Ru(1)	C(10)	66(4)
C(4)	C(5)	Ru(1)	C(11)	64(1)	C(4)	C(5)	Ru(1)	C(12)	100(1)
C(4)	C(5)	Ru(1)	C(13)	141(1)	C(5)	Ru(1)	C(1)	C(6)	-29(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(5)	Ru(1)	C(1)	C(7)	-142(1)	C(5)	Ru(1)	C(9)	C(10)	-165(1)
C(5)	Ru(1)	C(9)	C(13)	-45(1)	C(5)	Ru(1)	C(9)	C(14)	73(1)
C(5)	Ru(1)	C(10)	C(9)	116(4)	C(5)	Ru(1)	C(10)	C(11)	-2(4)
C(5)	Ru(1)	C(10)	C(15)	-120(4)	C(5)	Ru(1)	C(11)	C(10)	179.4(9)
C(5)	Ru(1)	C(11)	C(12)	62(1)	C(5)	Ru(1)	C(11)	C(16)	-58(1)
C(5)	Ru(1)	C(12)	C(11)	-136.0(9)	C(5)	Ru(1)	C(12)	C(13)	106(1)
C(5)	Ru(1)	C(12)	C(17)	-15(1)	C(5)	Ru(1)	C(13)	C(9)	153.9(9)
C(5)	Ru(1)	C(13)	C(12)	-89(1)	C(5)	Ru(1)	C(13)	C(18)	31(1)
C(5)	C(4)	Ru(1)	C(6)	28(1)	C(5)	C(4)	Ru(1)	C(9)	-131(5)
C(5)	C(4)	Ru(1)	C(10)	-167.6(9)	C(5)	C(4)	Ru(1)	C(11)	-135(1)
C(5)	C(4)	Ru(1)	C(12)	-93(1)	C(5)	C(4)	Ru(1)	C(13)	-61(1)
C(5)	C(6)	Ru(1)	C(9)	148(1)	C(5)	C(6)	Ru(1)	C(10)	173(1)
C(5)	C(6)	Ru(1)	C(11)	53(2)	C(5)	C(6)	Ru(1)	C(12)	70(1)
C(5)	C(6)	Ru(1)	C(13)	108(1)	C(5)	C(6)	C(1)	C(7)	174(1)
C(6)	Ru(1)	C(1)	C(7)	-113(1)	C(6)	Ru(1)	C(9)	C(10)	159.9(8)
C(6)	Ru(1)	C(9)	C(13)	-80.8(9)	C(6)	Ru(1)	C(9)	C(14)	38(1)
C(6)	Ru(1)	C(10)	C(9)	-39(1)	C(6)	Ru(1)	C(10)	C(11)	-158(1)
C(6)	Ru(1)	C(10)	C(15)	84(1)	C(6)	Ru(1)	C(11)	C(10)	138(2)
C(6)	Ru(1)	C(11)	C(12)	21(2)	C(6)	Ru(1)	C(11)	C(16)	-99(2)
C(6)	Ru(1)	C(12)	C(11)	-172.8(9)	C(6)	Ru(1)	C(12)	C(13)	69(1)
C(6)	Ru(1)	C(12)	C(17)	-52(1)	C(6)	Ru(1)	C(13)	C(9)	115.0(9)
C(6)	Ru(1)	C(13)	C(12)	-128.0(10)	C(6)	Ru(1)	C(13)	C(18)	-7(1)
C(6)	C(1)	Ru(1)	C(9)	115(1)	C(6)	C(1)	Ru(1)	C(10)	152(1)
C(6)	C(1)	Ru(1)	C(11)	175(1)	C(6)	C(1)	Ru(1)	C(12)	52(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(6)	C(1)	Ru(1)	C(13)	75(1)	C(6)	C(5)	Ru(1)	C(9)	-56(1)
C(6)	C(5)	Ru(1)	C(10)	-160(3)	C(6)	C(5)	Ru(1)	C(11)	-163.0(9)
C(6)	C(5)	Ru(1)	C(12)	-127(1)	C(6)	C(5)	Ru(1)	C(13)	-85(1)
C(7)	C(1)	Ru(1)	C(9)	1(1)	C(7)	C(1)	Ru(1)	C(10)	39(1)
C(7)	C(1)	Ru(1)	C(11)	62(2)	C(7)	C(1)	Ru(1)	C(12)	-61(2)
C(7)	C(1)	Ru(1)	C(13)	-37(1)	C(9)	Ru(1)	C(10)	C(11)	-119(1)
C(9)	Ru(1)	C(10)	C(15)	123(1)	C(9)	Ru(1)	C(11)	C(10)	36.0(7)
C(9)	Ru(1)	C(11)	C(12)	-80.6(8)	C(9)	Ru(1)	C(11)	C(16)	157(1)
C(9)	Ru(1)	C(12)	C(11)	79.7(8)	C(9)	Ru(1)	C(12)	C(13)	-37.9(9)
C(9)	Ru(1)	C(12)	C(17)	-160(1)	C(9)	Ru(1)	C(13)	C(12)	117(1)
C(9)	Ru(1)	C(13)	C(18)	-122(1)	C(9)	C(10)	Ru(1)	C(11)	119(1)
C(9)	C(10)	Ru(1)	C(12)	80.6(8)	C(9)	C(10)	Ru(1)	C(13)	37.1(7)
C(9)	C(10)	C(11)	C(12)	1(1)	C(9)	C(10)	C(11)	C(16)	175(1)
C(9)	C(13)	Ru(1)	C(10)	-36.0(7)	C(9)	C(13)	Ru(1)	C(11)	-79.1(8)
C(9)	C(13)	Ru(1)	C(12)	-117(1)	C(9)	C(13)	C(12)	C(11)	0(1)
C(9)	C(13)	C(12)	C(17)	-173(1)	C(10)	Ru(1)	C(9)	C(13)	119(1)
C(10)	Ru(1)	C(9)	C(14)	-121(1)	C(10)	Ru(1)	C(11)	C(12)	-116(1)
C(10)	Ru(1)	C(11)	C(16)	121(1)	C(10)	Ru(1)	C(12)	C(11)	38.3(7)
C(10)	Ru(1)	C(12)	C(13)	-79.3(10)	C(10)	Ru(1)	C(12)	C(17)	158(1)
C(10)	Ru(1)	C(13)	C(12)	81.1(9)	C(10)	Ru(1)	C(13)	C(18)	-158(1)
C(10)	C(9)	Ru(1)	C(11)	-37.5(7)	C(10)	C(9)	Ru(1)	C(12)	-80.9(8)
C(10)	C(9)	Ru(1)	C(13)	-119(1)	C(10)	C(9)	C(13)	C(12)	1(1)
C(10)	C(9)	C(13)	C(18)	-173(1)	C(10)	C(11)	Ru(1)	C(12)	116(1)
C(10)	C(11)	Ru(1)	C(13)	78.7(8)	C(10)	C(11)	C(12)	C(13)	0(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(10)	C(11)	C(12)	C(17)	172(1)	C(11)	Ru(1)	C(9)	C(13)	81.8(9)
C(11)	Ru(1)	C(9)	C(14)	-159(1)	C(11)	Ru(1)	C(10)	C(15)	-117(1)
C(11)	Ru(1)	C(12)	C(13)	-117(1)	C(11)	Ru(1)	C(12)	C(17)	120(1)
C(11)	Ru(1)	C(13)	C(12)	37.9(8)	C(11)	Ru(1)	C(13)	C(18)	158(1)
C(11)	C(10)	Ru(1)	C(12)	-38.5(7)	C(11)	C(10)	Ru(1)	C(13)	-81.9(8)
C(11)	C(10)	C(9)	C(13)	-2(1)	C(11)	C(10)	C(9)	C(14)	-177(1)
C(11)	C(12)	Ru(1)	C(13)	117(1)	C(11)	C(12)	C(13)	C(18)	174(1)
C(12)	Ru(1)	C(9)	C(13)	38.4(8)	C(12)	Ru(1)	C(9)	C(14)	157(1)
C(12)	Ru(1)	C(10)	C(15)	-155(1)	C(12)	Ru(1)	C(11)	C(16)	-121(1)
C(12)	Ru(1)	C(13)	C(18)	120(1)	C(12)	C(11)	Ru(1)	C(13)	-37.9(8)
C(12)	C(11)	C(10)	C(15)	-179(1)	C(12)	C(13)	C(9)	C(14)	176(1)
C(13)	Ru(1)	C(9)	C(14)	119(1)	C(13)	Ru(1)	C(10)	C(15)	160(1)
C(13)	Ru(1)	C(11)	C(16)	-159(1)	C(13)	Ru(1)	C(12)	C(17)	-122(1)
C(13)	C(9)	C(10)	C(15)	179(1)	C(13)	C(12)	C(11)	C(16)	-174(1)
C(14)	C(9)	C(10)	C(15)	3(2)	C(14)	C(9)	C(13)	C(18)	2(2)
C(15)	C(10)	C(11)	C(16)	-5(2)	C(16)	C(11)	C(12)	C(17)	-1(2)
C(17)	C(12)	C(13)	C(18)	1(2)	C(19)	Ru(2)	C(20)	C(21)	131(1)
C(19)	Ru(2)	C(21)	C(20)	-30(1)	C(19)	Ru(2)	C(21)	C(22)	102(1)
C(19)	Ru(2)	C(22)	C(21)	-66(1)	C(19)	Ru(2)	C(22)	C(23)	66(1)
C(19)	Ru(2)	C(23)	C(22)	-101(1)	C(19)	Ru(2)	C(23)	C(24)	30.2(9)
C(19)	Ru(2)	C(24)	C(23)	-130(1)	C(19)	Ru(2)	C(27)	C(28)	41(1)
C(19)	Ru(2)	C(27)	C(31)	157(1)	C(19)	Ru(2)	C(27)	C(32)	-78(2)
C(19)	Ru(2)	C(28)	C(27)	-160.2(10)	C(19)	Ru(2)	C(28)	C(29)	81(1)
C(19)	Ru(2)	C(28)	C(33)	-38(1)	C(19)	Ru(2)	C(29)	C(28)	-114(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(19)	Ru(2)	C(29)	C(30)	128.8(8)	C(19)	Ru(2)	C(29)	C(34)	7(1)
C(19)	Ru(2)	C(30)	C(29)	-69.5(9)	C(19)	Ru(2)	C(30)	C(31)	171.2(9)
C(19)	Ru(2)	C(30)	C(35)	51(1)	C(19)	Ru(2)	C(31)	C(27)	-144(1)
C(19)	Ru(2)	C(31)	C(30)	-24(2)	C(19)	Ru(2)	C(31)	C(36)	98(2)
C(19)	C(20)	Ru(2)	C(21)	-131(1)	C(19)	C(20)	Ru(2)	C(22)	-103(1)
C(19)	C(20)	Ru(2)	C(23)	-65.1(10)	C(19)	C(20)	Ru(2)	C(24)	-27.6(9)
C(19)	C(20)	Ru(2)	C(27)	173(2)	C(19)	C(20)	Ru(2)	C(28)	57(1)
C(19)	C(20)	Ru(2)	C(29)	86.6(10)	C(19)	C(20)	Ru(2)	C(30)	128.4(9)
C(19)	C(20)	Ru(2)	C(31)	162.8(9)	C(19)	C(20)	C(21)	C(22)	1(2)
C(19)	C(24)	Ru(2)	C(20)	28.3(9)	C(19)	C(24)	Ru(2)	C(21)	64.4(10)
C(19)	C(24)	Ru(2)	C(22)	100(1)	C(19)	C(24)	Ru(2)	C(23)	130(1)
C(19)	C(24)	Ru(2)	C(27)	-156.6(10)	C(19)	C(24)	Ru(2)	C(28)	-116.8(10)
C(19)	C(24)	Ru(2)	C(29)	-78(1)	C(19)	C(24)	Ru(2)	C(30)	-56(1)
C(19)	C(24)	Ru(2)	C(31)	-175(1)	C(19)	C(24)	C(23)	C(22)	-2(2)
C(19)	C(25)	O(4)	C(26)	-178(1)	C(20)	Ru(2)	C(19)	C(24)	-134(1)
C(20)	Ru(2)	C(19)	C(25)	112(1)	C(20)	Ru(2)	C(21)	C(22)	133(1)
C(20)	Ru(2)	C(22)	C(21)	-28(1)	C(20)	Ru(2)	C(22)	C(23)	104(1)
C(20)	Ru(2)	C(23)	C(22)	-64(1)	C(20)	Ru(2)	C(23)	C(24)	67.8(10)
C(20)	Ru(2)	C(24)	C(23)	-101(1)	C(20)	Ru(2)	C(27)	C(28)	-128(2)
C(20)	Ru(2)	C(27)	C(31)	-12(3)	C(20)	Ru(2)	C(27)	C(32)	110(2)
C(20)	Ru(2)	C(28)	C(27)	163(1)	C(20)	Ru(2)	C(28)	C(29)	44(1)
C(20)	Ru(2)	C(28)	C(33)	-75(1)	C(20)	Ru(2)	C(29)	C(28)	-154(1)
C(20)	Ru(2)	C(29)	C(30)	88.6(9)	C(20)	Ru(2)	C(29)	C(34)	-33(1)
C(20)	Ru(2)	C(30)	C(29)	-107.0(8)	C(20)	Ru(2)	C(30)	C(31)	133.7(9)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(20)	Ru(2)	C(30)	C(35)	14(1)	C(20)	Ru(2)	C(31)	C(27)	176(1)
C(20)	Ru(2)	C(31)	C(30)	-63(1)	C(20)	Ru(2)	C(31)	C(36)	59(1)
C(20)	C(19)	Ru(2)	C(21)	29.1(9)	C(20)	C(19)	Ru(2)	C(22)	65.1(9)
C(20)	C(19)	Ru(2)	C(23)	103(1)	C(20)	C(19)	Ru(2)	C(24)	134(1)
C(20)	C(19)	Ru(2)	C(27)	-176(1)	C(20)	C(19)	Ru(2)	C(28)	-147.9(9)
C(20)	C(19)	Ru(2)	C(29)	-108.1(9)	C(20)	C(19)	Ru(2)	C(30)	-69(1)
C(20)	C(19)	Ru(2)	C(31)	-51(2)	C(20)	C(19)	C(24)	C(23)	2(2)
C(20)	C(21)	Ru(2)	C(22)	-133(1)	C(20)	C(21)	Ru(2)	C(23)	-103(1)
C(20)	C(21)	Ru(2)	C(24)	-66(1)	C(20)	C(21)	Ru(2)	C(27)	166.1(10)
C(20)	C(21)	Ru(2)	C(28)	124(5)	C(20)	C(21)	Ru(2)	C(29)	59(1)
C(20)	C(21)	Ru(2)	C(30)	92(1)	C(20)	C(21)	Ru(2)	C(31)	132(1)
C(20)	C(21)	C(22)	C(23)	-1(2)	C(21)	Ru(2)	C(19)	C(24)	-105(1)
C(21)	Ru(2)	C(19)	C(25)	141(1)	C(21)	Ru(2)	C(22)	C(23)	132(1)
C(21)	Ru(2)	C(23)	C(22)	-27.9(10)	C(21)	Ru(2)	C(23)	C(24)	103(1)
C(21)	Ru(2)	C(24)	C(23)	-65(1)	C(21)	Ru(2)	C(27)	C(28)	-173(1)
C(21)	Ru(2)	C(27)	C(31)	-57(1)	C(21)	Ru(2)	C(27)	C(32)	65(2)
C(21)	Ru(2)	C(28)	C(27)	46(6)	C(21)	Ru(2)	C(28)	C(29)	-71(6)
C(21)	Ru(2)	C(28)	C(33)	167(5)	C(21)	Ru(2)	C(29)	C(28)	170(1)
C(21)	Ru(2)	C(29)	C(30)	54(1)	C(21)	Ru(2)	C(29)	C(34)	-67(1)
C(21)	Ru(2)	C(30)	C(29)	-145.8(8)	C(21)	Ru(2)	C(30)	C(31)	94.9(9)
C(21)	Ru(2)	C(30)	C(35)	-24(1)	C(21)	Ru(2)	C(31)	C(27)	141(1)
C(21)	Ru(2)	C(31)	C(30)	-98.7(10)	C(21)	Ru(2)	C(31)	C(36)	23(1)
C(21)	C(20)	Ru(2)	C(22)	28(1)	C(21)	C(20)	Ru(2)	C(23)	66(1)
C(21)	C(20)	Ru(2)	C(24)	103(1)	C(21)	C(20)	Ru(2)	C(27)	-55(3)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(21)	C(20)	Ru(2)	C(28)	-170(1)	C(21)	C(20)	Ru(2)	C(29)	-141(1)
C(21)	C(20)	Ru(2)	C(30)	-100(1)	C(21)	C(20)	Ru(2)	C(31)	-65(1)
C(21)	C(20)	C(19)	C(24)	-2(2)	C(21)	C(20)	C(19)	C(25)	-175(1)
C(21)	C(22)	Ru(2)	C(23)	-132(1)	C(21)	C(22)	Ru(2)	C(24)	-103(1)
C(21)	C(22)	Ru(2)	C(27)	138(1)	C(21)	C(22)	Ru(2)	C(28)	169(1)
C(21)	C(22)	Ru(2)	C(29)	66(4)	C(21)	C(22)	Ru(2)	C(30)	64(1)
C(21)	C(22)	Ru(2)	C(31)	97(1)	C(21)	C(22)	C(23)	C(24)	2(2)
C(22)	Ru(2)	C(19)	C(24)	-69(1)	C(22)	Ru(2)	C(19)	C(25)	177(1)
C(22)	Ru(2)	C(23)	C(24)	131(1)	C(22)	Ru(2)	C(24)	C(23)	-29(1)
C(22)	Ru(2)	C(27)	C(28)	152(1)	C(22)	Ru(2)	C(27)	C(31)	-91(1)
C(22)	Ru(2)	C(27)	C(32)	32(2)	C(22)	Ru(2)	C(28)	C(27)	-47(1)
C(22)	Ru(2)	C(28)	C(29)	-165(1)	C(22)	Ru(2)	C(28)	C(33)	73(2)
C(22)	Ru(2)	C(29)	C(28)	114(4)	C(22)	Ru(2)	C(29)	C(30)	-2(4)
C(22)	Ru(2)	C(29)	C(34)	-124(4)	C(22)	Ru(2)	C(30)	C(29)	179.4(10)
C(22)	Ru(2)	C(30)	C(31)	60(1)	C(22)	Ru(2)	C(30)	C(35)	-59(2)
C(22)	Ru(2)	C(31)	C(27)	103(1)	C(22)	Ru(2)	C(31)	C(30)	-137.1(10)
C(22)	Ru(2)	C(31)	C(36)	-14(1)	C(22)	C(21)	Ru(2)	C(23)	29(1)
C(22)	C(21)	Ru(2)	C(24)	66(1)	C(22)	C(21)	Ru(2)	C(27)	-60(1)
C(22)	C(21)	Ru(2)	C(28)	-102(6)	C(22)	C(21)	Ru(2)	C(29)	-167(1)
C(22)	C(21)	Ru(2)	C(30)	-134(1)	C(22)	C(21)	Ru(2)	C(31)	-94(1)
C(22)	C(23)	Ru(2)	C(24)	-131(1)	C(22)	C(23)	Ru(2)	C(27)	105(1)
C(22)	C(23)	Ru(2)	C(28)	146(1)	C(22)	C(23)	Ru(2)	C(29)	174(1)
C(22)	C(23)	Ru(2)	C(30)	58(2)	C(22)	C(23)	Ru(2)	C(31)	69(1)
C(23)	Ru(2)	C(19)	C(24)	-30.6(9)	C(23)	Ru(2)	C(19)	C(25)	-143(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(23)	Ru(2)	C(27)	C(28)	111(1)	C(23)	Ru(2)	C(27)	C(31)	-132(1)
C(23)	Ru(2)	C(27)	C(32)	-8(2)	C(23)	Ru(2)	C(28)	C(27)	-83(1)
C(23)	Ru(2)	C(28)	C(29)	158.1(10)	C(23)	Ru(2)	C(28)	C(33)	37(1)
C(23)	Ru(2)	C(29)	C(28)	-41(1)	C(23)	Ru(2)	C(29)	C(30)	-158(1)
C(23)	Ru(2)	C(29)	C(34)	80(1)	C(23)	Ru(2)	C(30)	C(29)	134(2)
C(23)	Ru(2)	C(30)	C(31)	14(2)	C(23)	Ru(2)	C(30)	C(35)	-104(2)
C(23)	Ru(2)	C(31)	C(27)	65(1)	C(23)	Ru(2)	C(31)	C(30)	-175.1(10)
C(23)	Ru(2)	C(31)	C(36)	-52(1)	C(23)	C(22)	Ru(2)	C(24)	29.3(10)
C(23)	C(22)	Ru(2)	C(27)	-88(1)	C(23)	C(22)	Ru(2)	C(28)	-57(1)
C(23)	C(22)	Ru(2)	C(29)	-160(3)	C(23)	C(22)	Ru(2)	C(30)	-162.6(9)
C(23)	C(22)	Ru(2)	C(31)	-129(1)	C(23)	C(24)	Ru(2)	C(27)	73(1)
C(23)	C(24)	Ru(2)	C(28)	113(1)	C(23)	C(24)	Ru(2)	C(29)	151.7(10)
C(23)	C(24)	Ru(2)	C(30)	173(1)	C(23)	C(24)	Ru(2)	C(31)	54(2)
C(23)	C(24)	C(19)	C(25)	176(1)	C(24)	Ru(2)	C(19)	C(25)	-113(1)
C(24)	Ru(2)	C(27)	C(28)	74(1)	C(24)	Ru(2)	C(27)	C(31)	-169.8(10)
C(24)	Ru(2)	C(27)	C(32)	-46(2)	C(24)	Ru(2)	C(28)	C(27)	-122(1)
C(24)	Ru(2)	C(28)	C(29)	119(1)	C(24)	Ru(2)	C(28)	C(33)	0(1)
C(24)	Ru(2)	C(29)	C(28)	-76(1)	C(24)	Ru(2)	C(29)	C(30)	167.0(8)
C(24)	Ru(2)	C(29)	C(34)	45(1)	C(24)	Ru(2)	C(30)	C(29)	-30(1)
C(24)	Ru(2)	C(30)	C(31)	-149(1)	C(24)	Ru(2)	C(30)	C(35)	91(2)
C(24)	Ru(2)	C(31)	C(27)	25(2)	C(24)	Ru(2)	C(31)	C(30)	145(1)
C(24)	Ru(2)	C(31)	C(36)	-92(2)	C(24)	C(19)	Ru(2)	C(27)	48(1)
C(24)	C(19)	Ru(2)	C(28)	77(1)	C(24)	C(19)	Ru(2)	C(29)	117.5(10)
C(24)	C(19)	Ru(2)	C(30)	155.9(9)	C(24)	C(19)	Ru(2)	C(31)	174(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(24)	C(23)	Ru(2)	C(27)	-122(1)	C(24)	C(23)	Ru(2)	C(28)	-81(1)
C(24)	C(23)	Ru(2)	C(29)	-54(1)	C(24)	C(23)	Ru(2)	C(30)	-169(1)
C(24)	C(23)	Ru(2)	C(31)	-158.8(9)	C(25)	C(19)	Ru(2)	C(27)	-64(2)
C(25)	C(19)	Ru(2)	C(28)	-35(1)	C(25)	C(19)	Ru(2)	C(29)	4(1)
C(25)	C(19)	Ru(2)	C(30)	42(1)	C(25)	C(19)	Ru(2)	C(31)	60(2)
C(27)	Ru(2)	C(28)	C(29)	-118(1)	C(27)	Ru(2)	C(28)	C(33)	121(1)
C(27)	Ru(2)	C(29)	C(28)	38(1)	C(27)	Ru(2)	C(29)	C(30)	-78.5(9)
C(27)	Ru(2)	C(29)	C(34)	159(1)	C(27)	Ru(2)	C(30)	C(29)	82.1(9)
C(27)	Ru(2)	C(30)	C(31)	-37.1(9)	C(27)	Ru(2)	C(30)	C(35)	-156(2)
C(27)	Ru(2)	C(31)	C(30)	119(1)	C(27)	Ru(2)	C(31)	C(36)	-117(2)
C(27)	C(28)	Ru(2)	C(29)	118(1)	C(27)	C(28)	Ru(2)	C(30)	79(1)
C(27)	C(28)	Ru(2)	C(31)	38.5(10)	C(27)	C(28)	C(29)	C(30)	2(1)
C(27)	C(28)	C(29)	C(34)	178(1)	C(27)	C(31)	Ru(2)	C(28)	-39.5(10)
C(27)	C(31)	Ru(2)	C(29)	-82(1)	C(27)	C(31)	Ru(2)	C(30)	-119(1)
C(27)	C(31)	C(30)	C(29)	-1(1)	C(27)	C(31)	C(30)	C(35)	-178(1)
C(28)	Ru(2)	C(27)	C(31)	115(1)	C(28)	Ru(2)	C(27)	C(32)	-120(2)
C(28)	Ru(2)	C(29)	C(30)	-116(1)	C(28)	Ru(2)	C(29)	C(34)	121(1)
C(28)	Ru(2)	C(30)	C(29)	37.8(9)	C(28)	Ru(2)	C(30)	C(31)	-81.5(10)
C(28)	Ru(2)	C(30)	C(35)	159(2)	C(28)	Ru(2)	C(31)	C(30)	80.3(9)
C(28)	Ru(2)	C(31)	C(36)	-156(1)	C(28)	C(27)	Ru(2)	C(29)	-36.8(9)
C(28)	C(27)	Ru(2)	C(30)	-80(1)	C(28)	C(27)	Ru(2)	C(31)	-115(1)
C(28)	C(27)	C(31)	C(30)	2(1)	C(28)	C(27)	C(31)	C(36)	-178(1)
C(28)	C(29)	Ru(2)	C(30)	116(1)	C(28)	C(29)	Ru(2)	C(31)	81(1)
C(28)	C(29)	C(30)	C(31)	0(1)	C(28)	C(29)	C(30)	C(35)	176(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(29)	Ru(2)	C(27)	C(31)	79.0(10)	C(29)	Ru(2)	C(27)	C(32)	-157(2)
C(29)	Ru(2)	C(28)	C(33)	-120(2)	C(29)	Ru(2)	C(30)	C(31)	-119(1)
C(29)	Ru(2)	C(30)	C(35)	121(2)	C(29)	Ru(2)	C(31)	C(30)	37.8(8)
C(29)	Ru(2)	C(31)	C(36)	160(1)	C(29)	C(28)	Ru(2)	C(30)	-38.8(9)
C(29)	C(28)	Ru(2)	C(31)	-79.9(10)	C(29)	C(28)	C(27)	C(31)	-3(1)
C(29)	C(28)	C(27)	C(32)	-177(1)	C(29)	C(30)	Ru(2)	C(31)	119(1)
C(29)	C(30)	C(31)	C(36)	-179(1)	C(30)	Ru(2)	C(27)	C(31)	35.4(10)
C(30)	Ru(2)	C(27)	C(32)	159(2)	C(30)	Ru(2)	C(28)	C(33)	-159(1)
C(30)	Ru(2)	C(29)	C(34)	-121(1)	C(30)	Ru(2)	C(31)	C(36)	122(1)
C(30)	C(29)	Ru(2)	C(31)	-35.5(8)	C(30)	C(29)	C(28)	C(33)	-175(1)
C(30)	C(31)	C(27)	C(32)	177(1)	C(31)	Ru(2)	C(27)	C(32)	123(2)
C(31)	Ru(2)	C(28)	C(33)	159(1)	C(31)	Ru(2)	C(29)	C(34)	-157(1)
C(31)	Ru(2)	C(30)	C(35)	-119(2)	C(31)	C(27)	C(28)	C(33)	175(1)
C(31)	C(30)	C(29)	C(34)	-176(1)	C(32)	C(27)	C(28)	C(33)	0(2)
C(32)	C(27)	C(31)	C(36)	-4(2)	C(33)	C(28)	C(29)	C(34)	0(2)
C(34)	C(29)	C(30)	C(35)	0(2)	C(35)	C(30)	C(31)	C(36)	3(2)
C(37)	C(38)	C(39)	C(40)	1(1)	C(37)	C(42)	C(41)	C(40)	0(2)
C(37)	B(1)	C(43)	C(44)	147(1)	C(37)	B(1)	C(43)	C(48)	-37(1)
C(37)	B(1)	C(49)	C(50)	-156(1)	C(37)	B(1)	C(49)	C(54)	30(1)
C(37)	B(1)	C(55)	C(56)	90(1)	C(37)	B(1)	C(55)	C(60)	-80(1)
C(38)	C(37)	C(42)	C(41)	1(1)	C(38)	C(37)	B(1)	C(43)	-33(1)
C(38)	C(37)	B(1)	C(49)	-151(1)	C(38)	C(37)	B(1)	C(55)	88(1)
C(38)	C(39)	C(40)	C(41)	0(2)	C(39)	C(38)	C(37)	C(42)	-1(1)
C(39)	C(38)	C(37)	B(1)	-175(1)	C(39)	C(40)	C(41)	C(42)	0(2)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(41)	C(42)	C(37)	B(1)	174(1)	C(42)	C(37)	B(1)	C(43)	153(1)
C(42)	C(37)	B(1)	C(49)	34(1)	C(42)	C(37)	B(1)	C(55)	-84(1)
C(43)	C(44)	C(45)	C(46)	1(2)	C(43)	C(48)	C(47)	C(46)	-1(2)
C(43)	B(1)	C(49)	C(50)	79(1)	C(43)	B(1)	C(49)	C(54)	-93(1)
C(43)	B(1)	C(55)	C(56)	-146(1)	C(43)	B(1)	C(55)	C(60)	42(1)
C(44)	C(43)	C(48)	C(47)	0(2)	C(44)	C(43)	B(1)	C(49)	-88(1)
C(44)	C(43)	B(1)	C(55)	30(1)	C(44)	C(45)	C(46)	C(47)	-3(2)
C(45)	C(44)	C(43)	C(48)	0(2)	C(45)	C(44)	C(43)	B(1)	175(1)
C(45)	C(46)	C(47)	C(48)	3(2)	C(47)	C(48)	C(43)	B(1)	-175(1)
C(48)	C(43)	B(1)	C(49)	85(1)	C(48)	C(43)	B(1)	C(55)	-154(1)
C(49)	C(50)	C(51)	C(52)	2(2)	C(49)	C(54)	C(53)	C(52)	0(2)
C(49)	B(1)	C(55)	C(56)	-30(1)	C(49)	B(1)	C(55)	C(60)	157(1)
C(50)	C(49)	C(54)	C(53)	3(1)	C(50)	C(49)	B(1)	C(55)	-40(1)
C(50)	C(51)	C(52)	C(53)	0(2)	C(51)	C(50)	C(49)	C(54)	-4(1)
C(51)	C(50)	C(49)	B(1)	-177(1)	C(51)	C(52)	C(53)	C(54)	-1(2)
C(53)	C(54)	C(49)	B(1)	176(1)	C(54)	C(49)	B(1)	C(55)	146(1)
C(55)	C(56)	C(57)	C(58)	0(2)	C(55)	C(60)	C(59)	C(58)	1(2)
C(56)	C(55)	C(60)	C(59)	0(1)	C(56)	C(57)	C(58)	C(59)	1(2)
C(57)	C(56)	C(55)	C(60)	0(1)	C(57)	C(56)	C(55)	B(1)	-172(1)
C(57)	C(58)	C(59)	C(60)	-2(2)	C(59)	C(60)	C(55)	B(1)	172(1)
C(61)	C(62)	C(63)	C(64)	2(2)	C(61)	C(66)	C(65)	C(64)	2(2)
C(61)	B(2)	C(67)	C(68)	-34(1)	C(61)	B(2)	C(67)	C(72)	149(1)
C(61)	B(2)	C(73)	C(74)	-145(1)	C(61)	B(2)	C(73)	C(78)	37(1)
C(61)	B(2)	C(79)	C(80)	87(1)	C(61)	B(2)	C(79)	C(84)	-87(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(62)	C(61)	C(66)	C(65)	-3(2)	C(62)	C(61)	B(2)	C(67)	153(1)
C(62)	C(61)	B(2)	C(73)	34(1)	C(62)	C(61)	B(2)	C(79)	-85(1)
C(62)	C(63)	C(64)	C(65)	-4(2)	C(63)	C(62)	C(61)	C(66)	1(2)
C(63)	C(62)	C(61)	B(2)	175(1)	C(63)	C(64)	C(65)	C(66)	1(2)
C(65)	C(66)	C(61)	B(2)	-177(1)	C(66)	C(61)	B(2)	C(67)	-32(1)
C(66)	C(61)	B(2)	C(73)	-151(1)	C(66)	C(61)	B(2)	C(79)	88(1)
C(67)	C(68)	C(69)	C(70)	-1(2)	C(67)	C(72)	C(71)	C(70)	1(2)
C(67)	B(2)	C(73)	C(74)	89(1)	C(67)	B(2)	C(73)	C(78)	-86(1)
C(67)	B(2)	C(79)	C(80)	-149(1)	C(67)	B(2)	C(79)	C(84)	35(1)
C(68)	C(67)	C(72)	C(71)	-1(1)	C(68)	C(67)	B(2)	C(73)	88(1)
C(68)	C(67)	B(2)	C(79)	-150(1)	C(68)	C(69)	C(70)	C(71)	1(2)
C(69)	C(68)	C(67)	C(72)	1(1)	C(69)	C(68)	C(67)	B(2)	-175(1)
C(69)	C(70)	C(71)	C(72)	-2(2)	C(71)	C(72)	C(67)	B(2)	174(1)
C(72)	C(67)	B(2)	C(73)	-87(1)	C(72)	C(67)	B(2)	C(79)	33(1)
C(73)	C(74)	C(75)	C(76)	-1(2)	C(73)	C(78)	C(77)	C(76)	1(2)
C(73)	B(2)	C(79)	C(80)	-32(1)	C(73)	B(2)	C(79)	C(84)	152(1)
C(74)	C(73)	C(78)	C(77)	1(2)	C(74)	C(73)	B(2)	C(79)	-31(1)
C(74)	C(75)	C(76)	C(77)	4(2)	C(75)	C(74)	C(73)	C(78)	-1(1)
C(75)	C(74)	C(73)	B(2)	-178(1)	C(75)	C(76)	C(77)	C(78)	-4(2)
C(77)	C(78)	C(73)	B(2)	177(1)	C(78)	C(73)	B(2)	C(79)	152(1)
C(79)	C(80)	C(81)	C(82)	1(2)	C(79)	C(84)	C(83)	C(82)	2(2)
C(80)	C(79)	C(84)	C(83)	0(2)	C(80)	C(81)	C(82)	C(83)	0(2)
C(81)	C(80)	C(79)	C(84)	-2(2)	C(81)	C(80)	C(79)	B(2)	-177(1)
C(81)	C(82)	C(83)	C(84)	-2(2)	C(83)	C(84)	C(79)	B(2)	175(1)