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Supporting Information

Ruthenium-catalyzed Asymmetric Hydrosilylation of Ketones and Imine

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Experimental Section

General. ^{1}H (270 MHz) and ^{31}P-NMR spectra (109 MHz) were recorded on a JEOL JNM-EX-270 spectrometer as solutions in $CDCl_3$. The coupling constants (J) were in hertz (Hz). GLC analyses were performed on a Shimadzu GC-14A instrument (25 m HiCap-CBP-10-S25 capillary column) with a flame-ionization detector and nitrogen as carrier gas. Elemental analyses were performed on a Perkin-Elmer 2400 series II CHN analyzer. All reactions were carried out under a dry nitrogen atmosphere. Solvents were dried by the usual methods and distilled before use.

Preparation of [$RuCl_2(PPh_3)$(1)]. In a 20-mL round-bottomed flask were placed $RuCl_2(PPh_3)_3$ (480 mg, 0.50 mmol) and (*S*)-[2-(4'-phenyloxazolin-2'-yl)ferrocenyl]diphenylphosphine (**1**) (257 mg, 0.50 mmol) under nitrogen. Anhydrous toluene (15 ml) was added, and then the resulting solution was magnetically stirred at room temperature for 20 h. The original purple solution turned to a red suspension. After addition of hexane (20 mL), the reaction mixture was filtered. Recrystallization of the resultant solid from dichloromethane/n-hexane gave [$RuCl_2(PPh_3)$(**1**)] (409 mg, 0.43

mmol; 86%) as a red solid. ^{1}H-NMR δ 2.68 (dd, 1H, J = 8 and 9 Hz), 3.92 (dd, 1H, J = 1 and 9 Hz), 4.12 (s, 5H), 4.23 (dd, 1H, J = 1 and 8 Hz), 4.71 (m, 1H), 4.80 (m, 1H), 5.04 (m, 1H), 6.6-8.2 (m, 30H). ^{31}P-NMR δ 40.8 (d, J = 45 Hz) and 75.7 (d, J = 45 Hz). Anal Calcd for $C_{49}H_{41}Cl_2FeNOP_2Ru \cdot CH_2Cl_2$: C, 58.05; H, 4.19; N, 1.35. Found: C, 57.58; H, 4.26; N, 1.42.

Similarly, complexes [$RuCl_2(PPh_3)$(**L**)] (L=**2** or **3**) were prepared from $RuCl_2(PPh_3)_3$ and **2** or **3**, respectively.

[$RuCl_2(PPh_3)$(**2**)]. A red solid. ^{1}H-NMR δ 0.57 (d, 3H, J = 7 Hz), 0.97 (d, 3H, J = 7 Hz), 2.12 (dd, 1H, J = 8 and 8 Hz), 3.21 (m, 1H), 3.28 (m, 1H), 3.80 (dd, 1H, J = 3 and 8 Hz), 4.02 (s, 5H), 4.59 (m, 1H), 4.68 (m, 1H), 4.84 (m, 1H), 6.5-8.4 (m, 25H). ^{31}P-NMR δ 40.1 (d, J = 45 Hz) and 77.0 (d, J = 45 Hz). Anal Calcd for $C_{46}H_{43}Cl_2FeNOP_2Ru$: C, 60.34; H, 4.73; N, 1.53. Found: C, 60.30; H, 4.89; N, 1.52. Yield, 81%.

[$RuCl_2(PPh_3)$(**3**)]. A black solid. ^{1}H-NMR δ 0.82 (s, 9H), 3.99 (m, 1H), 4.42 (m, 1H), 4.44 (s, 5H), 4.48 (m, 1H), 4.60 (m, 1H), 4.87 (m, 1H), 5.06 (m, 1H), 6.9-7.8 (m, 25H). ^{31}P-NMR δ 41.8 (d, J = 41 Hz) and 68.9 (d, J = 41 Hz). Anal Calcd for $C_{47}H_{45}Cl_2FeNOP_2Ru$: C, 60.72; H, 4.88; N, 1.51. Found: C, 60.80; H, 4.91; N, 1.44. Yield, 87%.

X-ray Structural Determination of [$RuCl_2(PPh_3)$(1)]·CH_2Cl_2 (Figure 1). Data for [$RuCl_2(PPh_3)$(**1**)]·CH_2Cl_2 (a red crystal, grown by slow diffusion of n-hexane into a dichloromethane solution of [$RuCl_2(PPh_3)$(**1**)] at room temperature) of $C_{50}H_{43}Cl_4FeNOP_2Ru$ was collected on a Rigaku AFC7R diffractometer with graphite monochromated Mo-Kα radiation (λ=0.71069 Å) and a 12kW rotating anode generator. Crystal data for [$RuCl_2(PPh_3)$(**1**)]·CH_2Cl_2 are as follows: monoclinic, space group $P2_1$(#4); a = 11.370(8), b = 17.914(8), c = 12.210(4) Å, β = 114.63(3)°; V = 2260(1) Å^3; Z = 2; D_{calcd} = 1.520 g cm^{-3}; μ(MoKα) = 10.01 cm^{-1}; The final R value was 0.040 (Rw = 0.043) for 4264 unique reflections with I >3σ(I). The structure was solved by the Patterson method (DIRDIF92 PATTY). All non-hydrogen atoms were refined anisotropically. Hydrogen atom position was geometrically calculated or taken from a difference Fourier map.

General Procedure for Ruthenium-Catalyzed Asymmetric Hydrosilylation of Ketones. In a 20-ml flask were placed [$RuCl_2(PPh_3)$(**1**)] (0.01 mmol; 1.0 mol%) and AgOTf or $Cu(OTf)_2$ (0.01 mmol; 1.0 mol%) under N_2. Anhydrous diethyl ether (10 mL) was added, and then the mixture was magnetically stirred at room temperature for 1 h. After addition of a ketone (1.0 mmol), the reaction flask was dipped in a thermoregulated bath at 0 °C. Diphenylsilane (2.0 mmol) was slowly added by a syringe. The reaction was run by keeping the temperature at 0 °C. For the work-up, methanol (1 mL) was slowly added at 0 °C to the reaction mixture, which was stirred for 0.5 h. After gas evolution ceased, 1 N HCl aq. (5 mL) was added to the reaction mixture which was stirred for 1 h at room temperature. The reaction mixture was extracted with brine (50 mL) and diethyl ether (50 mL x 3) and then dried over anhydrous $MgSO_4$. For the GLC analyses, naphthalene was added as an internal standard. For isolation, the extract was concentrated under reduced pressure by an aspirator, and then distilled in vacuum by Kugelrohr to give the corresponding alcohol together with the unreacted starting ketone. Dimethoxydiphenylsilane was left in the residue. The ee value and the configuration of the alcohol were determined by GLC on a cyclodextrin phase (Chiraldex GT-A, 30 m).

General Procedure for Ruthenium-Catalyzed Asymmetric Hydrosilylation of an Imine (13). The reaction was carried out by a similar method as described in the previous section. The ee value of **14** was determined by GC analysis of the corresponding trifluoroacetamide on a cyclodextrin phase (Chiraldex GT-A, 30 m).

Experimental

Data Collection

A red prismatic crystal of $C_{50}H_{43}Cl_4FeNOP_2Ru$ having approximate dimensions of 0.20 x 0.20 x 0.20 mm was mounted in a glass capillary. 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 $29.66 < 2\theta < 29.96°$ corresponded to a primitive monoclinic cell with dimensions:

$$\begin{aligned} a &= 11.370(8)\ \AA \\ b &= 17.914(8)\ \AA \qquad \beta = 114.63(3)° \\ c &= 12.210(4)\ \AA \\ V &= 2260(1)\ \AA^3 \end{aligned}$$

For Z = 2 and F.W. = 1034.57, the calculated density is 1.52 g/cm^3. Based on the systematic absences of:

$$0k0:\ k \neq 2n$$

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$$P2_1\ (\#4)$$

The data were collected at a temperature of 23 $\pm$ 1°C using the ω-2θ 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 0.41° with a take-off angle of 6.0°. Scans of (1.78 + 0.30 tan θ)° were made at a speed of 16.0°/min (in omega). The weak reflections ($I < 10.0\sigma(I)$) were rescanned (maximum of 1 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 9.0 mm (horizontal) and 13.0 mm (vertical).

Data Reduction

Of the 5626 reflections which were collected, 5367 were unique ($R_{int} = 0.045$). The intensities of three representative reflection were measured after every 150 reflections. Over the course of data collection, the standards decreased by 0.7%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 10.0 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.75 to 1.00. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient = 1.65930e-07).

Structure Solution and Refinement

The structure was solved by heavy-atom Patterson methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included, but their positions were not refined; isotropic B values were refined The final cycle of full-matrix least-squares refinement[3] was based on 4262 observed reflections ($I > 3.00\sigma(I)$) and 580 variable parameters and converged (largest parameter shift was 4.72 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.040$$

$$R_w = \sqrt{\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2} = 0.043$$

The standard deviation of an observation of unit weight[4] was 1.66. The weighting scheme was based on counting statistics and included a factor (p = 0.001) 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 0.97 and -0.91 $e^-/\AA^3$, 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) 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) 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	$C_{50}H_{43}Cl_4FeNOP_2Ru$
Formula Weight	1034.57
Crystal Color, Habit	red, prismatic
Crystal Dimensions	0.20 X 0.20 X 0.20 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (29.7 - 30.0°)
Omega Scan Peak Width at Half-height	0.41°
Lattice Parameters	a = 11.370(8)Å b = 17.914(8) Å c = 12.210(4) Å β = 114.63(3)°
	V = 2260(1) Å^3
Space Group	$P2_1$ (#4)
Z value	2
D_{calc}	1.520 g/cm^3
F_{000}	1052.00
μ(MoKα)	10.01 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Attenuator	Zr foil (factor = 8.44)
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	235 mm
Temperature	23.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω)
Scan Width	$(1.78 + 0.30 \tan \theta)°$
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 5626 Unique: 5367 ($R_{int} = 0.045$)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.7545 - 0.9999) Decay (0.66% decline) Secondary Extinction (coefficient: 1.65930e-07)

C. Structure Solution and Refinement

Structure Solution	Patterson Methods (DIRDIF92 PATTY)
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	0.0010
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>3.00σ(I))	4262
No. Variables	580
Reflection/Parameter Ratio	7.35
Residuals: R; Rw	0.040 ; 0.043

Goodness of Fit Indicator	1.66
Max Shift/Error in Final Cycle	4.72
Maximum peak in Final Diff. Map	0.97 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.91 $e^-/\AA^3$

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

atom	x	y	z	B_{eq}
Ru(1)	-0.29597(4)	-0.3457(7)	0.24512(3)	1.987(7)
Fe(1)	-0.09641(8)	-0.4939(7)	0.57798(8)	2.99(2)
Cl(1)	-0.0710(1)	-0.3361(7)	0.2871(2)	4.28(4)
Cl(2)	-0.3060(2)	-0.2123(7)	0.2359(2)	3.57(4)
Cl(3)	0.3556(3)	0.4317(7)	0.4967(3)	7.87(8)
Cl(4)	0.4962(5)	0.5012(8)	0.7272(4)	16.0(2)
P(1)	-0.3093(1)	-0.3492(7)	0.4196(1)	2.03(2)
P(2)	-0.5114(1)	-0.3523(7)	0.1212(1)	2.17(2)
O(1)	-0.2717(4)	-0.5857(7)	0.2691(4)	3.25(9)
N(1)	-0.2774(5)	-0.4622(8)	0.2322(4)	2.35(8)
C(1)	-0.2687(5)	-0.4399(8)	0.4894(5)	2.29(9)
C(2)	-0.2630(5)	-0.5080(8)	0.4278(5)	2.22(9)
C(3)	-0.2440(6)	-0.5696(8)	0.5078(6)	3.1(1)
C(4)	-0.2391(7)	-0.5408(8)	0.6170(6)	3.4(1)
C(5)	-0.2543(6)	-0.4627(8)	0.6078(5)	3.0(1)
C(6)	0.0591(9)	-0.437(1)	0.688(1)	8.2(3)
C(7)	0.0540(8)	-0.435(1)	0.576(1)	8.1(3)
C(8)	0.0587(7)	-0.508(1)	0.5395(8)	7.0(2)
C(9)	0.0713(8)	-0.5524(9)	0.635(1)	6.3(2)
C(10)	0.0710(9)	-0.509(1)	0.7257(9)	7.2(2)
C(11)	-0.2699(5)	-0.5147(8)	0.3074(5)	2.33(9)
C(12)	-0.2832(5)	-0.4980(8)	0.1196(5)	2.44(9)
C(13)	-0.3088(6)	-0.5809(8)	0.1401(6)	3.0(1)
C(14)	-0.1638(5)	-0.4891(8)	0.0969(5)	2.56(10)

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

atom	x	y	z	B_{eq}
C(15)	-0.1748(6)	-0.4663(8)	-0.0161(6)	3.7(1)
C(16)	-0.0671(7)	-0.4672(9)	-0.0415(7)	4.4(2)
C(17)	0.0510(7)	-0.4904(9)	0.0423(7)	4.4(2)
C(18)	0.0615(7)	-0.5104(9)	0.1535(7)	5.0(2)
C(19)	-0.0450(6)	-0.5107(9)	0.1803(6)	4.0(2)
C(20)	-0.1993(5)	-0.2874(8)	0.5387(5)	2.8(1)
C(21)	-0.2158(7)	-0.2781(9)	0.6440(6)	4.1(1)
C(22)	-0.1287(8)	-0.2384(9)	0.7407(7)	5.7(2)
C(23)	-0.0230(9)	-0.2063(9)	0.7328(8)	6.0(2)
C(24)	-0.0042(7)	-0.2130(9)	0.6284(8)	4.9(2)
C(25)	-0.0930(6)	-0.2521(8)	0.5307(6)	3.4(1)
C(26)	-0.4626(5)	-0.3283(8)	0.4276(5)	2.39(10)
C(27)	-0.5053(7)	-0.2544(8)	0.4086(6)	3.3(1)
C(28)	-0.6219(7)	-0.2340(8)	0.4105(7)	4.1(2)
C(29)	-0.6990(6)	-0.2872(8)	0.4288(6)	3.9(1)
C(30)	-0.6594(6)	-0.3616(8)	0.4471(6)	3.6(1)
C(31)	-0.5400(6)	-0.3814(8)	0.4487(5)	2.8(1)
C(32)	-0.6452(6)	-0.2958(8)	0.1228(5)	2.7(1)
C(33)	-0.6428(7)	-0.2189(8)	0.1097(6)	3.5(1)
C(34)	-0.7488(8)	-0.1757(8)	0.1019(6)	4.6(2)
C(35)	-0.8550(8)	-0.2090(9)	0.1075(7)	5.3(2)
C(36)	-0.8587(7)	-0.2844(9)	0.1224(8)	5.0(2)
C(37)	-0.7539(6)	-0.3284(8)	0.1309(6)	3.6(2)
C(38)	-0.5786(5)	-0.4484(8)	0.0931(5)	2.40(9)

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

atom	x	y	z	B_{eq}
C(39)	-0.6241(5)	-0.4814(8)	-0.0187(5)	3.0(1)
C(40)	-0.6628(6)	-0.5564(8)	-0.0325(7)	4.0(1)
C(41)	-0.6568(7)	-0.5962(8)	0.0648(7)	4.2(1)
C(42)	-0.6128(6)	-0.5646(8)	0.1761(7)	3.7(1)
C(43)	-0.5725(6)	-0.4895(8)	0.1918(5)	3.0(1)
C(44)	-0.5151(6)	-0.3244(8)	-0.0252(5)	2.8(1)
C(45)	-0.6279(8)	-0.3051(8)	-0.1237(6)	4.4(2)
C(46)	-0.6246(9)	-0.2854(9)	-0.2326(6)	5.2(2)
C(47)	-0.5077(9)	-0.2832(9)	-0.2422(7)	5.2(2)
C(48)	-0.3985(9)	-0.3014(8)	-0.1466(7)	4.3(2)
C(49)	-0.4018(6)	-0.3214(8)	-0.0383(6)	3.3(1)
C(50)	0.385(1)	0.448(1)	0.644(1)	8.8(3)
H(1)	-0.2360	-0.6200	0.4910	3(1)
H(2)	-0.2241	-0.5688	0.6871	4(1)
H(3)	-0.2525	-0.4289	0.6720	3(1)
H(4)	0.0553	-0.3907	0.7343	10(3)
H(5)	0.0478	-0.3882	0.5295	8(3)
H(6)	0.0572	-0.5237	0.4638	9(2)
H(7)	0.0764	-0.6056	0.6346	10(2)
H(8)	0.0772	-0.5256	0.8042	6(3)
H(9)	-0.3565	-0.4774	0.0516	3(1)
H(10)	-0.2580	-0.6125	0.1139	5(1)
H(11)	-0.3984	-0.5929	0.0935	3(1)
H(12)	-0.2581	-0.4488	-0.0759	7(1)

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

atom	x	y	z	B_{eq}
H(13)	-0.0756	-0.4496	-0.1205	6(1)
H(14)	0.1259	-0.4918	0.0249	5(1)
H(15)	0.1453	-0.5228	0.2135	7(2)
H(16)	-0.0353	-0.5251	0.2601	7(1)
H(17)	-0.2925	-0.2987	0.6490	1(1)
H(18)	-0.1434	-0.2321	0.8129	4(2)
H(19)	0.0402	-0.1794	0.8016	4(2)
H(20)	0.0721	-0.1895	0.6233	7(2)
H(21)	-0.0816	-0.2541	0.4553	3(1)
H(22)	-0.4505	-0.2150	0.3972	0(1)
H(23)	-0.6507	-0.1821	0.3977	5(1)
H(24)	-0.7805	-0.2726	0.4294	6(1)
H(25)	-0.7138	-0.3976	0.4586	6(1)
H(26)	-0.5103	-0.4312	0.4657	1(1)
H(27)	-0.5679	-0.1948	0.1060	6(1)
H(28)	-0.7457	-0.1209	0.0956	5(1)
H(29)	-0.9287	-0.1785	0.0985	5(2)
H(30)	-0.9328	-0.3058	0.1282	6(2)
H(31)	-0.7554	-0.3801	0.1425	7(1)
H(32)	-0.6305	-0.4510	-0.0887	2(1)
H(33)	-0.6921	-0.5788	-0.1120	1(1)
H(34)	-0.6843	-0.6465	0.0554	5(1)
H(35)	-0.6096	-0.5922	0.2437	6(1)
H(36)	-0.5410	-0.4659	0.2701	0(1)

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

atom	x	y	z	B_{eq}
H(37)	-0.7097	-0.3026	-0.1136	8(2)
H(38)	-0.7041	-0.2740	-0.3033	4(2)
H(39)	-0.5048	-0.2676	-0.3169	5(2)
H(40)	-0.3155	-0.3000	-0.1529	4(2)
H(41)	-0.3214	-0.3322	0.0309	6(1)
H(42)	0.3032	0.4694	0.6407	10(3)
H(43)	0.3957	0.4012	0.6809	20(3)

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

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0286(2)	0.0236(2)	0.0276(2)	-0.0038(2)	0.0160(2)	-0.0010(2)
Fe(1)	0.0340(4)	0.0409(5)	0.0346(4)	0.0080(4)	0.0104(4)	0.0063(4)
Cl(1)	0.0358(7)	0.060(1)	0.076(1)	-0.0160(9)	0.0333(7)	-0.019(1)
Cl(2)	0.061(1)	0.0243(7)	0.052(1)	-0.0080(8)	0.0257(9)	0.0008(7)
Cl(3)	0.140(3)	0.058(1)	0.096(2)	-0.004(2)	0.044(2)	0.003(1)
Cl(4)	0.219(5)	0.291(7)	0.120(3)	-0.163(5)	0.094(3)	-0.063(4)
P(1)	0.0279(5)	0.0253(6)	0.0260(5)	-0.0021(7)	0.0132(5)	-0.0013(7)
P(2)	0.0324(6)	0.0235(7)	0.0272(5)	0.0011(7)	0.0132(5)	0.0006(7)
O(1)	0.055(3)	0.024(2)	0.047(2)	0.002(2)	0.023(2)	-0.002(2)
N(1)	0.036(2)	0.025(2)	0.033(2)	-0.004(2)	0.018(2)	-0.007(2)
C(1)	0.032(2)	0.022(2)	0.031(2)	-0.001(2)	0.011(2)	-0.001(2)
C(2)	0.027(2)	0.025(2)	0.033(2)	-0.004(2)	0.014(1)	-0.002(2)
C(3)	0.043(3)	0.032(3)	0.045(3)	0.006(2)	0.020(3)	0.013(2)
C(4)	0.050(3)	0.043(3)	0.041(3)	0.002(3)	0.023(3)	0.016(3)
C(5)	0.036(3)	0.044(3)	0.034(3)	-0.001(2)	0.014(2)	0.009(3)
C(6)	0.035(4)	0.112(7)	0.130(8)	-0.007(4)	0.000(6)	-0.065(6)
C(7)	0.036(4)	0.111(7)	0.152(8)	0.002(4)	0.029(6)	0.076(7)
C(8)	0.038(4)	0.175(9)	0.051(4)	0.020(6)	0.018(3)	-0.013(5)
C(9)	0.048(4)	0.063(7)	0.110(6)	0.032(4)	0.015(5)	0.010(4)
C(10)	0.049(4)	0.163(9)	0.046(5)	0.033(6)	0.003(3)	0.026(5)
C(11)	0.030(3)	0.027(2)	0.033(2)	-0.002(2)	0.015(2)	-0.004(2)
C(12)	0.032(2)	0.031(2)	0.030(2)	0.003(2)	0.013(2)	-0.009(2)
C(13)	0.040(3)	0.032(2)	0.043(2)	0.002(3)	0.019(3)	-0.015(3)
C(14)	0.034(2)	0.031(3)	0.037(2)	0.000(2)	0.020(2)	-0.006(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(15)	0.046(3)	0.063(4)	0.035(3)	0.007(3)	0.019(3)	0.000(3)
C(16)	0.058(3)	0.073(5)	0.053(4)	0.005(4)	0.040(3)	0.000(4)
C(17)	0.047(3)	0.070(5)	0.064(4)	-0.003(3)	0.036(3)	-0.010(4)
C(18)	0.036(3)	0.095(7)	0.060(4)	0.009(4)	0.023(3)	-0.002(4)
C(19)	0.038(3)	0.071(5)	0.044(4)	0.010(3)	0.019(2)	0.006(3)
C(20)	0.036(3)	0.035(3)	0.030(2)	-0.006(2)	0.008(2)	-0.005(2)
C(21)	0.053(4)	0.068(4)	0.042(3)	-0.020(4)	0.027(3)	-0.018(3)
C(22)	0.078(5)	0.096(6)	0.045(5)	-0.037(4)	0.030(4)	-0.036(4)
C(23)	0.070(5)	0.081(6)	0.068(5)	-0.040(5)	0.023(4)	-0.041(5)
C(24)	0.045(4)	0.061(5)	0.071(4)	-0.021(4)	0.016(3)	-0.019(4)
C(25)	0.042(3)	0.040(3)	0.047(4)	-0.009(2)	0.020(3)	-0.003(3)
C(26)	0.032(2)	0.035(3)	0.027(2)	0.006(2)	0.016(2)	-0.002(2)
C(27)	0.053(3)	0.031(3)	0.051(4)	0.007(3)	0.031(3)	0.005(3)
C(28)	0.060(4)	0.043(4)	0.064(4)	0.023(3)	0.039(4)	0.008(3)
C(29)	0.041(4)	0.057(4)	0.053(4)	0.016(3)	0.024(3)	-0.002(3)
C(30)	0.038(3)	0.053(4)	0.055(4)	0.005(3)	0.029(3)	0.006(3)
C(31)	0.037(3)	0.037(3)	0.039(3)	0.000(2)	0.021(3)	-0.001(3)
C(32)	0.037(3)	0.032(3)	0.034(3)	0.011(2)	0.015(2)	0.007(2)
C(33)	0.064(4)	0.032(3)	0.043(4)	0.011(3)	0.026(3)	0.008(3)
C(34)	0.086(5)	0.043(4)	0.052(4)	0.036(3)	0.036(4)	0.015(3)
C(35)	0.069(5)	0.074(4)	0.062(5)	0.041(4)	0.029(4)	0.011(4)
C(36)	0.048(4)	0.073(4)	0.082(5)	0.022(4)	0.039(4)	-0.002(5)
C(37)	0.039(3)	0.049(5)	0.053(3)	0.005(2)	0.025(3)	0.000(3)
C(38)	0.024(2)	0.029(2)	0.039(2)	-0.003(2)	0.014(2)	-0.004(2)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(39)	0.032(3)	0.043(3)	0.037(3)	0.004(2)	0.012(2)	-0.007(3)
C(40)	0.037(3)	0.046(3)	0.058(4)	-0.001(3)	0.009(3)	-0.022(3)
C(41)	0.048(4)	0.030(4)	0.076(4)	-0.012(3)	0.018(4)	-0.014(3)
C(42)	0.041(3)	0.038(3)	0.061(4)	-0.001(3)	0.019(3)	0.008(3)
C(43)	0.043(3)	0.037(3)	0.036(3)	-0.004(3)	0.020(3)	-0.005(2)
C(44)	0.048(3)	0.034(3)	0.027(2)	0.001(2)	0.018(2)	0.000(2)
C(45)	0.055(4)	0.068(5)	0.038(3)	0.015(4)	0.013(3)	0.009(3)
C(46)	0.085(5)	0.071(5)	0.034(3)	0.016(5)	0.016(4)	0.016(4)
C(47)	0.100(4)	0.068(5)	0.038(3)	0.001(5)	0.038(3)	0.016(4)
C(48)	0.082(5)	0.049(4)	0.046(3)	-0.012(4)	0.040(3)	0.000(3)
C(49)	0.047(3)	0.044(3)	0.037(3)	-0.006(3)	0.021(3)	-0.006(2)

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($\AA$)

atom	atom	distance	atom	atom	distance
Ru(1)	Cl(1)	2.396(3)	Ru(1)	Cl(2)	2.392(2)
Ru(1)	P(1)	2.199(2)	Ru(1)	P(2)	2.283(2)
Ru(1)	N(1)	2.110(7)	Fe(1)	C(1)	2.044(7)
Fe(1)	C(2)	2.030(7)	Fe(1)	C(3)	2.047(9)
Fe(1)	C(4)	2.052(9)	Fe(1)	C(5)	2.052(8)
Fe(1)	C(6)	2.00(1)	Fe(1)	C(7)	2.02(1)
Fe(1)	C(8)	2.02(1)	Fe(1)	C(9)	2.03(1)
Fe(1)	C(10)	2.02(1)	Cl(3)	C(50)	1.71(2)
Cl(4)	C(50)	1.58(2)	P(1)	C(1)	1.802(7)
P(1)	C(20)	1.841(7)	P(1)	C(26)	1.824(7)
P(2)	C(32)	1.835(8)	P(2)	C(38)	1.858(7)
P(2)	C(44)	1.839(7)	O(1)	C(11)	1.353(9)
O(1)	C(13)	1.454(10)	N(1)	C(11)	1.292(10)
N(1)	C(12)	1.494(9)	C(1)	C(2)	1.449(10)
C(1)	C(5)	1.44(1)	C(2)	C(3)	1.43(1)
C(2)	C(11)	1.444(10)	C(3)	C(4)	1.41(1)
C(3)	H(1)	0.94(2)	C(4)	C(5)	1.41(1)
C(4)	H(2)	0.94(1)	C(5)	H(3)	0.98(1)
C(6)	C(7)	1.34(2)	C(6)	C(10)	1.35(2)
C(6)	H(4)	1.01(2)	C(7)	C(8)	1.39(2)
C(7)	H(5)	0.99(2)	C(8)	C(9)	1.37(2)
C(8)	H(6)	0.96(1)	C(9)	C(10)	1.36(2)
C(9)	H(7)	0.96(2)	C(10)	H(8)	0.98(2)
C(12)	C(13)	1.55(1)	C(12)	C(14)	1.503(9)

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

atom	atom	distance	atom	atom	distance
C(12)	H(9)	0.972(9)	C(13)	H(10)	0.95(1)
C(13)	H(11)	0.962(9)	C(14)	C(15)	1.39(1)
C(14)	C(19)	1.37(1)	C(15)	C(16)	1.38(1)
C(15)	H(12)	0.98(1)	C(16)	C(17)	1.37(1)
C(16)	H(13)	0.98(1)	C(17)	C(18)	1.36(1)
C(17)	H(14)	0.959(8)	C(18)	C(19)	1.38(1)
C(18)	H(15)	0.95(1)	C(19)	H(16)	0.969(10)
C(20)	C(21)	1.39(1)	C(20)	C(25)	1.40(1)
C(21)	C(22)	1.38(1)	C(21)	H(17)	0.97(1)
C(22)	C(23)	1.37(2)	C(22)	H(18)	0.97(1)
C(23)	C(24)	1.38(2)	C(23)	H(19)	0.98(1)
C(24)	C(25)	1.39(1)	C(24)	H(20)	0.99(1)
C(25)	H(21)	0.982(9)	C(26)	C(27)	1.40(1)
C(26)	C(31)	1.39(1)	C(27)	C(28)	1.39(1)
C(27)	H(22)	0.99(1)	C(28)	C(29)	1.37(1)
C(28)	H(23)	0.98(2)	C(29)	C(30)	1.39(1)
C(29)	H(24)	0.966(9)	C(30)	C(31)	1.40(1)
C(30)	H(25)	0.94(1)	C(31)	H(26)	0.95(2)
C(32)	C(33)	1.39(1)	C(32)	C(37)	1.41(1)
C(33)	C(34)	1.40(1)	C(33)	H(27)	0.97(1)
C(34)	C(35)	1.37(2)	C(34)	H(28)	0.99(2)
C(35)	C(36)	1.37(2)	C(35)	H(29)	0.97(1)
C(36)	C(37)	1.40(1)	C(36)	H(30)	0.95(1)
C(37)	H(31)	0.94(2)	C(38)	C(39)	1.38(1)

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

atom	atom	distance	atom	atom	distance
C(38)	C(43)	1.39(1)	C(39)	C(40)	1.40(1)
C(39)	H(32)	0.99(1)	C(40)	C(41)	1.36(1)
C(40)	H(33)	0.97(1)	C(41)	C(42)	1.36(1)
C(41)	H(34)	0.94(2)	C(42)	C(43)	1.41(1)
C(42)	H(35)	0.95(1)	C(43)	H(36)	0.97(1)
C(44)	C(45)	1.39(1)	C(44)	C(49)	1.36(1)
C(45)	C(46)	1.39(1)	C(45)	H(37)	0.99(1)
C(46)	C(47)	1.38(2)	C(46)	H(38)	0.98(1)
C(47)	C(48)	1.34(2)	C(47)	H(39)	0.97(1)
C(48)	C(49)	1.39(1)	C(48)	H(40)	0.98(1)
C(49)	H(41)	0.971(9)	C(50)	H(42)	0.99(2)
C(50)	H(43)	0.93(2)			

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ru(1)	Cl(2)	87.97(9)	Cl(1)	Ru(1)	P(1)	107.07(7)
Cl(1)	Ru(1)	P(2)	154.16(7)	Cl(1)	Ru(1)	N(1)	87.5(2)
Cl(2)	Ru(1)	P(1)	93.06(9)	Cl(2)	Ru(1)	P(2)	90.19(9)
Cl(2)	Ru(1)	N(1)	171.3(2)	P(1)	Ru(1)	P(2)	98.77(7)
P(1)	Ru(1)	N(1)	95.3(2)	P(2)	Ru(1)	N(1)	90.7(2)
C(1)	Fe(1)	C(2)	41.7(3)	C(1)	Fe(1)	C(3)	69.8(3)
C(1)	Fe(1)	C(4)	68.9(3)	C(1)	Fe(1)	C(5)	41.3(3)
C(1)	Fe(1)	C(6)	119.9(5)	C(1)	Fe(1)	C(7)	112.0(4)
C(1)	Fe(1)	C(8)	132.2(5)	C(1)	Fe(1)	C(9)	169.5(5)
C(1)	Fe(1)	C(10)	150.7(5)	C(2)	Fe(1)	C(3)	41.0(3)
C(2)	Fe(1)	C(4)	68.2(3)	C(2)	Fe(1)	C(5)	68.8(3)
C(2)	Fe(1)	C(6)	154.4(6)	C(2)	Fe(1)	C(7)	122.2(5)
C(2)	Fe(1)	C(8)	110.6(4)	C(2)	Fe(1)	C(9)	129.5(5)
C(2)	Fe(1)	C(10)	165.4(6)	C(3)	Fe(1)	C(4)	40.2(3)
C(3)	Fe(1)	C(5)	68.2(4)	C(3)	Fe(1)	C(6)	164.0(7)
C(3)	Fe(1)	C(7)	153.4(7)	C(3)	Fe(1)	C(8)	117.7(5)
C(3)	Fe(1)	C(9)	106.9(5)	C(3)	Fe(1)	C(10)	126.2(6)
C(4)	Fe(1)	C(5)	40.1(3)	C(4)	Fe(1)	C(6)	128.1(6)
C(4)	Fe(1)	C(7)	166.4(7)	C(4)	Fe(1)	C(8)	148.8(6)
C(4)	Fe(1)	C(9)	115.4(5)	C(4)	Fe(1)	C(10)	106.3(5)
C(5)	Fe(1)	C(6)	109.7(5)	C(5)	Fe(1)	C(7)	131.7(6)
C(5)	Fe(1)	C(8)	170.9(6)	C(5)	Fe(1)	C(9)	147.8(5)
C(5)	Fe(1)	C(10)	116.4(5)	C(6)	Fe(1)	C(7)	38.9(7)
C(6)	Fe(1)	C(8)	66.7(6)	C(6)	Fe(1)	C(9)	65.9(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(6)	Fe(1)	C(10)	39.3(7)	C(7)	Fe(1)	C(8)	40.3(6)
C(7)	Fe(1)	C(9)	66.2(6)	C(7)	Fe(1)	C(10)	65.8(6)
C(8)	Fe(1)	C(9)	39.7(5)	C(8)	Fe(1)	C(10)	66.6(5)
C(9)	Fe(1)	C(10)	39.2(6)	Ru(1)	P(1)	C(1)	112.1(3)
Ru(1)	P(1)	C(20)	116.7(3)	Ru(1)	P(1)	C(26)	120.0(2)
C(1)	P(1)	C(20)	102.2(4)	C(1)	P(1)	C(26)	102.8(3)
C(20)	P(1)	C(26)	100.6(3)	Ru(1)	P(2)	C(32)	129.0(3)
Ru(1)	P(2)	C(38)	114.6(2)	Ru(1)	P(2)	C(44)	102.4(3)
C(32)	P(2)	C(38)	103.5(3)	C(32)	P(2)	C(44)	100.3(3)
C(38)	P(2)	C(44)	103.3(3)	C(11)	O(1)	C(13)	105.9(6)
Ru(1)	N(1)	C(11)	130.3(5)	Ru(1)	N(1)	C(12)	121.8(5)
C(11)	N(1)	C(12)	107.8(6)	Fe(1)	C(1)	P(1)	132.6(4)
Fe(1)	C(1)	C(2)	68.6(4)	Fe(1)	C(1)	C(5)	69.7(4)
P(1)	C(1)	C(2)	124.9(5)	P(1)	C(1)	C(5)	128.9(6)
C(2)	C(1)	C(5)	105.6(7)	Fe(1)	C(2)	C(1)	69.7(4)
Fe(1)	C(2)	C(3)	70.1(4)	Fe(1)	C(2)	C(11)	124.4(5)
C(1)	C(2)	C(3)	108.8(6)	C(1)	C(2)	C(11)	127.1(6)
C(3)	C(2)	C(11)	124.1(7)	Fe(1)	C(3)	C(2)	68.8(4)
Fe(1)	C(3)	C(4)	70.1(5)	Fe(1)	C(3)	H(1)	126.2(7)
C(2)	C(3)	C(4)	107.4(7)	C(2)	C(3)	H(1)	126.4(9)
C(4)	C(3)	H(1)	126.2(8)	Fe(1)	C(4)	C(3)	69.7(5)
Fe(1)	C(4)	C(5)	70.0(5)	Fe(1)	C(4)	H(2)	124.5(7)
C(3)	C(4)	C(5)	109.5(8)	C(3)	C(4)	H(2)	125(1)
C(5)	C(4)	H(2)	124(1)	Fe(1)	C(5)	C(1)	69.0(4)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Fe(1)	C(5)	C(4)	69.9(5)	Fe(1)	C(5)	H(3)	125.4(6)
C(1)	C(5)	C(4)	108.7(8)	C(1)	C(5)	H(3)	125(1)
C(4)	C(5)	H(3)	125(1)	Fe(1)	C(6)	C(7)	71.5(8)
Fe(1)	C(6)	C(10)	71.3(8)	Fe(1)	C(6)	H(4)	124.1(10)
C(7)	C(6)	C(10)	109(1)	C(7)	C(6)	H(4)	123(2)
C(10)	C(6)	H(4)	127(2)	Fe(1)	C(7)	C(6)	69.7(8)
Fe(1)	C(7)	C(8)	69.9(8)	Fe(1)	C(7)	H(5)	125.9(9)
C(6)	C(7)	C(8)	108(1)	C(6)	C(7)	H(5)	125(2)
C(8)	C(7)	H(5)	126(2)	Fe(1)	C(8)	C(7)	69.8(7)
Fe(1)	C(8)	C(9)	70.4(6)	Fe(1)	C(8)	H(6)	126.3(8)
C(7)	C(8)	C(9)	106(1)	C(7)	C(8)	H(6)	127(2)
C(9)	C(8)	H(6)	126(2)	Fe(1)	C(9)	C(8)	69.9(6)
Fe(1)	C(9)	C(10)	70.1(7)	Fe(1)	C(9)	H(7)	124.4(10)
C(8)	C(9)	C(10)	108(1)	C(8)	C(9)	H(7)	124(1)
C(10)	C(9)	H(7)	127(1)	Fe(1)	C(10)	C(6)	69.4(7)
Fe(1)	C(10)	C(9)	70.7(7)	Fe(1)	C(10)	H(8)	124(1)
C(6)	C(10)	C(9)	107(1)	C(6)	C(10)	H(8)	125(2)
C(9)	C(10)	H(8)	126(2)	O(1)	C(11)	N(1)	116.9(6)
O(1)	C(11)	C(2)	114.6(6)	N(1)	C(11)	C(2)	128.5(7)
N(1)	C(12)	C(13)	101.6(6)	N(1)	C(12)	C(14)	115.3(6)
N(1)	C(12)	H(9)	108.4(8)	C(13)	C(12)	C(14)	112.1(6)
C(13)	C(12)	H(9)	110(1)	C(14)	C(12)	H(9)	108.8(7)
O(1)	C(13)	C(12)	104.0(6)	O(1)	C(13)	H(10)	112.7(8)
O(1)	C(13)	H(11)	112.6(7)	C(12)	C(13)	H(10)	109(1)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(12)	C(13)	H(11)	109(1)	H(10)	C(13)	H(11)	108(1)
C(12)	C(14)	C(15)	119.9(7)	C(12)	C(14)	C(19)	121.4(7)
C(15)	C(14)	C(19)	118.4(7)	C(14)	C(15)	C(16)	119.7(8)
C(14)	C(15)	H(12)	119.7(8)	C(16)	C(15)	H(12)	120.6(8)
C(15)	C(16)	C(17)	121.4(8)	C(15)	C(16)	H(13)	118.9(10)
C(17)	C(16)	H(13)	119.7(9)	C(16)	C(17)	C(18)	118.4(8)
C(16)	C(17)	H(14)	121(1)	C(18)	C(17)	H(14)	119(1)
C(17)	C(18)	C(19)	121.1(9)	C(17)	C(18)	H(15)	118.1(9)
C(19)	C(18)	H(15)	120(1)	C(14)	C(19)	C(18)	121.0(8)
C(14)	C(19)	H(16)	119.2(8)	C(18)	C(19)	H(16)	119.7(9)
P(1)	C(20)	C(21)	119.7(6)	P(1)	C(20)	C(25)	122.5(6)
C(21)	C(20)	C(25)	117.6(7)	C(20)	C(21)	C(22)	122.0(9)
C(20)	C(21)	H(17)	119.0(9)	C(22)	C(21)	H(17)	119.0(9)
C(21)	C(22)	C(23)	119.5(10)	C(21)	C(22)	H(18)	120(1)
C(23)	C(22)	H(18)	120(1)	C(22)	C(23)	C(24)	120.4(9)
C(22)	C(23)	H(19)	119(1)	C(24)	C(23)	H(19)	119(1)
C(23)	C(24)	C(25)	119.9(10)	C(23)	C(24)	H(20)	119(1)
C(25)	C(24)	H(20)	120(1)	C(20)	C(25)	C(24)	120.5(9)
C(20)	C(25)	H(21)	120.2(9)	C(24)	C(25)	H(21)	119(1)
P(1)	C(26)	C(27)	117.3(6)	P(1)	C(26)	C(31)	124.2(6)
C(27)	C(26)	C(31)	118.5(7)	C(26)	C(27)	C(28)	121.1(8)
C(26)	C(27)	H(22)	120(1)	C(28)	C(27)	H(22)	118(1)
C(27)	C(28)	C(29)	120.0(8)	C(27)	C(28)	H(23)	120.5(10)
C(29)	C(28)	H(23)	119.5(9)	C(28)	C(29)	C(30)	120.2(8)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(28)	C(29)	H(24)	119(1)	C(30)	C(29)	H(24)	120(1)
C(29)	C(30)	C(31)	119.5(8)	C(29)	C(30)	H(25)	119(1)
C(31)	C(30)	H(25)	121(1)	C(26)	C(31)	C(30)	120.7(8)
C(26)	C(31)	H(26)	119.4(8)	C(30)	C(31)	H(26)	120.0(8)
P(2)	C(32)	C(33)	119.3(7)	P(2)	C(32)	C(37)	121.9(6)
C(33)	C(32)	C(37)	118.7(8)	C(32)	C(33)	C(34)	119.9(9)
C(32)	C(33)	H(27)	120(1)	C(34)	C(33)	H(27)	119(1)
C(33)	C(34)	C(35)	120.3(9)	C(33)	C(34)	H(28)	119(1)
C(35)	C(34)	H(28)	119.8(9)	C(34)	C(35)	C(36)	120.9(9)
C(34)	C(35)	H(29)	119(1)	C(36)	C(35)	H(29)	119(1)
C(35)	C(36)	C(37)	119(1)	C(35)	C(36)	H(30)	118(1)
C(37)	C(36)	H(30)	121(1)	C(32)	C(37)	C(36)	120.5(9)
C(32)	C(37)	H(31)	119.5(8)	C(36)	C(37)	H(31)	120.0(9)
P(2)	C(38)	C(39)	122.5(6)	P(2)	C(38)	C(43)	117.6(6)
C(39)	C(38)	C(43)	119.7(7)	C(38)	C(39)	C(40)	120.0(8)
C(38)	C(39)	H(32)	118(1)	C(40)	C(39)	H(32)	121(1)
C(39)	C(40)	C(41)	119.8(9)	C(39)	C(40)	H(33)	118(1)
C(41)	C(40)	H(33)	121(1)	C(40)	C(41)	C(42)	121.2(9)
C(40)	C(41)	H(34)	119(1)	C(42)	C(41)	H(34)	118(1)
C(41)	C(42)	C(43)	119.8(9)	C(41)	C(42)	H(35)	121(1)
C(43)	C(42)	H(35)	119(1)	C(38)	C(43)	C(42)	119.5(8)
C(38)	C(43)	H(36)	119(1)	C(42)	C(43)	H(36)	121(1)
P(2)	C(44)	C(45)	123.3(7)	P(2)	C(44)	C(49)	119.0(6)
C(45)	C(44)	C(49)	117.7(7)	C(44)	C(45)	C(46)	120.6(10)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(44)	C(45)	H(37)	118.7(9)	C(46)	C(45)	H(37)	120.6(10)
C(45)	C(46)	C(47)	119.9(10)	C(45)	C(46)	H(38)	120(1)
C(47)	C(46)	H(38)	119.2(10)	C(46)	C(47)	C(48)	119.5(9)
C(46)	C(47)	H(39)	119(1)	C(48)	C(47)	H(39)	120(1)
C(47)	C(48)	C(49)	120.6(10)	C(47)	C(48)	H(40)	119.9(9)
C(49)	C(48)	H(40)	119(1)	C(44)	C(49)	C(48)	121.7(8)
C(44)	C(49)	H(41)	118.8(8)	C(48)	C(49)	H(41)	119.5(9)
Cl(3)	C(50)	Cl(4)	122(1)	Cl(3)	C(50)	H(42)	104(1)
Cl(3)	C(50)	H(43)	107(1)	Cl(4)	C(50)	H(42)	105(1)
Cl(4)	C(50)	H(43)	108(1)	H(42)	C(50)	H(43)	107(1)