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Table 1. Fractional Positional Parameters and Isotropic Thermal Parameters of Hydrogen Atoms with Their Estimated Standard Deviations in Parentheses

atom	x	y	z	U
H(10A)	0.184(2)	0.081(3)	0.593(4)	0.09(2)
H(10B)	0.146(2)	0.133(3)	0.510(4)	0.08(2)
H(11A)	0.262(3)	0.082(3)	0.535(4)	0.09(2)
H(11B)	0.229(3)	0.137(3)	0.463(4)	0.10(2)
H(12A)	0.307(2)	0.218(2)	0.559(3)	0.06(1)
H(12B)	0.339(2)	0.158(3)	0.641(4)	0.09(2)
H(15)	0.0755(18)	0.3585(19)	0.7257(28)	0.05(1)
H(16)	0.054(2)	0.415(2)	0.846(3)	0.05(1)
H(17)	0.093(2)	0.369(2)	1.016(3)	0.07(1)
H(18)	0.148(2)	0.259(2)	1.039(3)	0.07(1)
H(21)	0.200(2)	0.163(2)	1.057(3)	0.06(1)
H(22)	0.262(2)	0.057(2)	1.074(3)	0.07(1)
H(23)	0.277(2)	0.019(2)	0.934(3)	0.07(1)
H(24)	0.235(2)	0.090(2)	0.783(4)	0.08(2)
H(25)	0.155(2)	0.367(2)	0.623(3)	0.05(1)
H(26)	0.099(2)	0.431(2)	0.475(3)	0.05(1)
H(27)	0.007(2)	0.381(2)	0.353(3)	0.07(1)
H(28)	-0.030(2)	0.272(2)	0.382(3)	0.06(1)
H(31)	-0.052(2)	0.167(2)	0.421(3)	0.07(1)
H(32)	-0.081(3)	0.058(3)	0.470(4)	0.10(2)
H(33)	-0.008(3)	0.023(3)	0.635(4)	0.09(2)
H(34)	0.082(2)	0.092(2)	0.733(3)	0.07(1)

Table 2. Final Anisotropic Temperature Factors (U Values) with Estimated Standard Deviations in Parentheses

atom	U11	U22	U33	U12	U13	U23
Ru(1)	0.0404(1)	0.0501(2)	0.0236(1)	0.0046(1)	0.0127(1)	0.0003(1)
Cl(2)	0.0695(7)	0.0671(7)	0.0596(7)	0.0078(6)	0.0252(6)	-.0006(5)
O(8)	0.050(1)	0.060(2)	0.032(1)	-0.003(1)	0.016(1)	-0.007(1)
O(9)	0.053(2)	0.091(2)	0.064(2)	-0.014(2)	0.025(2)	-0.013(2)
O(35)	0.101(3)	0.085(3)	0.089(3)	0.008(2)	0.041(2)	0.020(2)
O(36)	0.299(8)	0.114(4)	0.151(4)	-0.051(4)	0.172(5)	-0.029(3)
O(37)	0.100(3)	0.139(4)	0.166(5)	0.057(3)	0.058(3)	0.049(4)
O(38)	0.117(4)	0.119(4)	0.171(5)	0.007(3)	-0.018(3)	-0.058(4)
O(39)	0.115(3)	0.102(3)	0.124(4)	0.003(3)	0.043(3)	0.013(3)
O(40)	0.32(1)	0.31(1)	0.28(1)	0.15(1)	0.17(1)	0.09(1)
O(41)	0.152(6)	0.420(13)	0.166(6)	0.012(7)	0.085(5)	0.034(7)
N(3)	0.050(2)	0.048(2)	0.027(1)	0.009(1)	0.016(1)	0.001(1)
N(4)	0.040(1)	0.061(2)	0.031(1)	-0.002(2)	0.016(1)	-0.004(1)
N(5)	0.043(2)	0.058(2)	0.029(1)	-0.001(1)	0.012(1)	0.004(1)
N(6)	0.052(2)	0.056(2)	0.030(1)	0.014(1)	0.021(1)	0.002(1)
N(7)	0.044(2)	0.064(2)	0.034(2)	0.003(2)	0.016(1)	-0.001(1)
C(10)	0.074(3)	0.064(3)	0.045(2)	0.000(2)	0.027(2)	-0.016(2)
C(11)	0.088(4)	0.080(4)	0.062(3)	0.009(3)	0.045(3)	-0.014(3)
C(12)	0.062(3)	0.063(3)	0.050(2)	0.013(2)	0.034(2)	0.006(2)
C(13)	0.049(2)	0.055(2)	0.035(2)	0.009(2)	0.019(2)	0.005(2)

P-148-2

C(14)	0.048(2)	0.059(2)	0.033(2)	0.006(2)	0.012(2)	0.005(2)
C(15)	0.050(2)	0.065(3)	0.042(2)	0.006(2)	0.023(2)	-0.003(2)
C(16)	0.052(2)	0.063(3)	0.067(3)	-0.005(2)	0.033(2)	-0.015(2)
C(17)	0.069(3)	0.078(3)	0.055(3)	-0.020(2)	0.041(2)	-0.024(2)
C(18)	0.068(3)	0.074(3)	0.037(2)	-0.017(2)	0.029(2)	-0.011(2)
C(19)	0.045(2)	0.065(2)	0.030(2)	-0.014(2)	0.018(1)	-0.005(2)
C(20)	0.044(2)	0.062(2)	0.028(2)	-0.010(2)	0.012(1)	-0.001(2)
C(21)	0.067(3)	0.080(3)	0.032(2)	-0.014(2)	0.019(2)	0.003(2)
C(22)	0.070(3)	0.075(3)	0.045(2)	-0.002(2)	0.012(2)	0.020(2)
C(23)	0.068(3)	0.065(3)	0.056(3)	0.008(2)	0.020(2)	0.018(2)
C(24)	0.061(2)	0.058(3)	0.044(2)	0.005(2)	0.021(2)	0.005(2)
C(25)	0.070(3)	0.061(3)	0.042(2)	0.015(2)	0.029(2)	0.003(2)
C(26)	0.089(4)	0.067(3)	0.059(3)	0.030(3)	0.046(3)	0.021(2)
C(27)	0.077(3)	0.106(4)	0.047(3)	0.046(3)	0.034(3)	0.032(3)
C(28)	0.055(3)	0.102(4)	0.041(2)	0.025(3)	0.016(2)	0.011(2)
C(29)	0.046(2)	0.076(3)	0.031(2)	0.018(2)	0.015(2)	0.001(2)
C(30)	0.044(2)	0.073(3)	0.037(2)	0.009(2)	0.013(2)	-0.007(2)
C(31)	0.051(3)	0.097(4)	0.052(3)	0.007(3)	0.007(2)	-0.013(3)
C(32)	0.055(3)	0.093(4)	0.083(4)	-0.013(3)	0.020(3)	-0.024(3)
C(33)	0.070(3)	0.080(4)	0.079(4)	-0.017(3)	0.027(3)	-0.003(3)
C(34)	0.061(3)	0.072(3)	0.054(3)	-0.009(2)	0.020(2)	0.005(2)

a Parameters have the form $\exp[-2\pi^2(a_1^2 U_{11} h^2 + a_2^2 U_{22} k^2 + a_3^2 U_{33} l^2 + 2a_1 a_2 U_{12} hk + 2a_1 a_3 U_{13} hl + 2a_2 a_3 U_{23} kl)]$

P-148-3

**Table 3. Intramolecular Bond Distances (Å) with Their
Estimated Standard Deviations in Parentheses**

atom	atom	distance	atom	atom	distance
Ru(1)	- O(8)	2.113(3)	Ru(1)	- N(3)	2.042(3)
Ru(1)	- N(4)	2.065(3)	Ru(1)	- N(5)	2.057(3)
Ru(1)	- N(6)	2.058(3)	Ru(1)	- N(7)	2.039(4)
Cl(2)	- O(35)	1.420(5)	Cl(2)	- O(36)	1.403(6)
Cl(2)	- O(37)	1.406(5)	Cl(2)	- O(38)	1.393(6)
O(8)	- C(14)	1.282(5)	O(9)	- C(14)	1.241(5)
N(3)	- C(10)	1.475(6)	N(3)	- C(13)	1.294(5)
N(4)	- C(15)	1.349(6)	N(4)	- C(19)	1.363(5)
N(5)	- C(20)	1.364(5)	N(5)	- C(24)	1.343(6)
N(6)	- C(25)	1.344(6)	N(6)	- C(29)	1.362(5)
N(7)	- C(30)	1.372(5)	N(7)	- C(34)	1.342(6)
C(10)	- C(11)	1.532(8)	C(11)	- C(12)	1.515(8)
C(12)	- C(13)	1.487(6)	C(13)	- C(14)	1.495(6)
C(15)	- C(16)	1.382(7)	C(16)	- C(17)	1.377(7)
C(17)	- C(18)	1.375(8)	C(18)	- C(19)	1.382(6)
C(19)	- C(20)	1.469(6)	C(20)	- C(21)	1.388(6)
C(21)	- C(22)	1.373(8)	C(22)	- C(23)	1.372(7)
C(23)	- C(24)	1.381(7)	C(25)	- C(26)	1.380(7)
C(26)	- C(27)	1.378(8)	C(27)	- C(28)	1.363(9)
C(28)	- C(29)	1.395(7)	C(29)	- C(30)	1.462(7)
C(30)	- C(31)	1.401(7)	C(31)	- C(32)	1.360(9)
C(32)	- C(33)	1.380(9)	C(33)	- C(34)	1.375(8)
C(10)	- H(10A)	1.04(6)	C(10)	- H(10B)	0.89(5)
C(11)	- H(11A)	0.97(6)	C(11)	- H(11B)	0.85(6)
C(12)	- H(12A)	0.96(5)	C(12)	- H(12B)	0.99(5)
C(15)	- H(15)	0.98(4)	C(16)	- H(16)	0.95(5)
C(17)	- H(17)	1.00(5)	C(18)	- H(18)	0.90(5)
C(21)	- H(21)	0.89(5)	C(22)	- H(22)	0.95(5)
C(23)	- H(23)	0.98(5)	C(24)	- H(24)	1.02(5)
C(25)	- H(25)	0.89(4)	C(26)	- H(26)	0.96(5)
C(27)	- H(27)	0.88(5)	C(28)	- H(28)	0.88(5)
C(31)	- H(31)	0.87(5)	C(32)	- H(32)	1.00(6)
C(33)	- H(33)	0.94(6)	C(34)	- H(34)	0.92(5)

Table 4. Intramolecular Bond Angles (degrees) with Their Estimated Standard Deviations in Parentheses

atom	atom	atom	angle	atom	atom	atom	angle
O(8)	- Ru(1)	- N(3)	77.9(2)	O(8)	- Ru(1)	- N(4)	90.7(2)
O(8)	- Ru(1)	- N(5)	89.5(2)	O(8)	- Ru(1)	- N(6)	95.5(2)
O(8)	- Ru(1)	- N(7)	171.0(2)	N(3)	- Ru(1)	- N(4)	167.8(2)
N(3)	- Ru(1)	- N(5)	96.7(2)	N(3)	- Ru(1)	- N(6)	87.9(2)
N(3)	- Ru(1)	- N(7)	94.6(2)	N(4)	- Ru(1)	- N(5)	78.9(2)
N(4)	- Ru(1)	- N(6)	97.4(2)	N(4)	- Ru(1)	- N(7)	97.1(2)
N(5)	- Ru(1)	- N(6)	173.8(2)	N(5)	- Ru(1)	- N(7)	96.3(2)
N(6)	- Ru(1)	- N(7)	79.2(2)	O(35)	- Cl(2)	- O(36)	108.0(3)
O(35)	- Cl(2)	- O(37)	111.1(3)	O(35)	- Cl(2)	- O(38)	113.2(3)
O(36)	- Cl(2)	- O(37)	107.6(4)	O(36)	- Cl(2)	- O(38)	107.3(4)
O(37)	- Cl(2)	- O(38)	109.4(4)	Ru(1)	- O(8)	- C(14)	114.9(3)
Ru(1)	- N(3)	- C(10)	133.6(3)	Ru(1)	- N(3)	- C(13)	115.8(3)
C(10)	- N(3)	- C(13)	110.6(4)	Ru(1)	- N(4)	- C(15)	125.4(3)
Ru(1)	- N(4)	- C(19)	115.2(3)	C(15)	- N(4)	- C(19)	118.8(4)
Ru(1)	- N(5)	- C(20)	115.8(3)	Ru(1)	- N(5)	- C(24)	126.1(3)
C(20)	- N(5)	- C(24)	118.1(4)	Ru(1)	- N(6)	- C(25)	126.0(3)
Ru(1)	- N(6)	- C(29)	115.2(3)	C(25)	- N(6)	- C(29)	118.8(4)
Ru(1)	- N(7)	- C(30)	115.0(3)	Ru(1)	- N(7)	- C(34)	126.4(3)
C(30)	- N(7)	- C(34)	118.3(4)	N(3)	- C(10)	- C(11)	105.1(4)
C(10)	- C(11)	- C(12)	106.4(5)	C(11)	- C(12)	- C(13)	102.7(4)

P-148-5

N(3) - C(13) - C(12)	115.0(4)	N(3) - C(13) - C(14)	116.6(4)
C(12) - C(13) - C(14)	128.4(4)	O(8) - C(14) - O(9)	124.2(4)
O(8) - C(14) - C(13)	114.7(4)	O(9) - C(14) - C(13)	121.0(4)
N(4) - C(15) - C(16)	122.4(4)	C(15) - C(16) - C(17)	118.8(5)
C(16) - C(17) - C(18)	119.1(5)	C(17) - C(18) - C(19)	120.5(4)
N(4) - C(19) - C(18)	120.4(4)	N(4) - C(19) - C(20)	115.2(4)
C(18) - C(19) - C(20)	124.4(4)	N(5) - C(20) - C(19)	114.6(4)
N(5) - C(20) - C(21)	120.4(4)	C(19) - C(20) - C(21)	125.0(4)
C(20) - C(21) - C(22)	120.6(4)	C(21) - C(22) - C(23)	118.9(5)
C(22) - C(23) - C(24)	118.7(5)	N(5) - C(24) - C(23)	123.3(4)
N(6) - C(25) - C(26)	122.3(5)	C(25) - C(26) - C(27)	118.9(5)
C(26) - C(27) - C(28)	119.5(5)	C(27) - C(28) - C(29)	120.0(5)
N(6) - C(29) - C(28)	120.4(5)	N(6) - C(29) - C(30)	114.6(4)
C(28) - C(29) - C(30)	125.0(4)	N(7) - C(30) - C(29)	115.1(4)
N(7) - C(30) - C(31)	119.7(5)	C(29) - C(30) - C(31)	125.2(4)
C(30) - C(31) - C(32)	120.9(5)	C(31) - C(32) - C(33)	119.1(6)
C(32) - C(33) - C(34)	118.7(6)	N(7) - C(34) - C(33)	123.4(5)
N(3) - C(10) - H(10A)	107.9(28)	N(3) - C(10) - H(10B)	111.6(32)
C(11) - C(10) - H(10A)	113.5(28)	C(11) - C(10) - H(10B)	115.0(32)
H(10A) - C(10) - H(10B)	103.7(41)	C(10) - C(11) - H(11A)	104.5(31)
C(10) - C(11) - H(11B)	108.6(37)	C(12) - C(11) - H(11A)	114.3(31)
C(12) - C(11) - H(11B)	116.4(38)	H(11A) - C(11) - H(11B)	105.9(49)
C(11) - C(12) - H(12A)	115.4(25)	C(11) - C(12) - H(12B)	111.4(29)
C(13) - C(12) - H(12A)	108.8(25)	C(13) - C(12) - H(12B)	107.2(29)

P-148-6

H(12A)- C(12) - H(12B)	110.7(38) N(4) - C(15) - H(15)	118.7(22)
C(16) - C(15) - H(15)	118.8(22) C(15) - C(16) - H(16)	117.1(24)
C(17) - C(16) - H(16)	124.0(24) C(16) - C(17) - H(17)	120.4(26)
C(18) - C(17) - H(17)	120.2(26) C(17) - C(18) - H(18)	123.9(29)
C(19) - C(18) - H(18)	115.6(29) C(20) - C(21) - H(21)	113.2(28)
C(22) - C(21) - H(21)	126.1(28) C(21) - C(22) - H(22)	122.4(27)
C(23) - C(22) - H(22)	118.7(27) C(22) - C(23) - H(23)	119.7(26)
C(24) - C(23) - H(23)	121.2(26) N(5) - C(24) - H(24)	115.9(27)
C(23) - C(24) - H(24)	120.8(27) N(6) - C(25) - H(25)	114.7(27)
C(26) - C(25) - H(25)	122.6(27) C(25) - C(26) - H(26)	119.6(24)
C(27) - C(26) - H(26)	121.4(24) C(26) - C(27) - H(27)	116.2(29)
C(28) - C(27) - H(27)	124.4(29) C(27) - C(28) - H(28)	123.7(29)
C(29) - C(28) - H(28)	116.2(29) C(30) - C(31) - H(31)	114.1(31)
C(32) - C(31) - H(31)	125.0(31) C(31) - C(32) - H(32)	122.0(31)
C(33) - C(32) - H(32)	118.9(31) C(32) - C(33) - H(33)	121.1(32)
C(34) - C(33) - H(33)	119.8(32) N(7) - C(34) - H(34)	117.1(29)
C(33) - C(34) - H(34)	119.3(29)	

P-1487

Table 5. Intermolecular Torsion Angles (deg.) of Non-hydrogen Atoms with Their Estimated Standard Deviations in Parentheses.

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle						
O(8)	-	Ru(1)	-	N(3)	-	C(10)	-178.1(4)	O(8)	-	Ru(1)	-	N(3)	-	C(13)	-1.0(3)
N(3)	-	Ru(1)	-	O(8)	-	C(14)	-0.4(3)	N(4)	-	Ru(1)	-	O(8)	-	C(14)	175.5(3)
O(8)	-	Ru(1)	-	N(4)	-	C(15)	84.9(4)	O(8)	-	Ru(1)	-	N(4)	-	C(19)	-86.5(3)
N(5)	-	Ru(1)	-	O(8)	-	C(14)	96.6(3)	O(8)	-	Ru(1)	-	N(5)	-	C(20)	90.0(3)
O(8)	-	Ru(1)	-	N(5)	-	C(24)	-91.1(4)	N(6)	-	Ru(1)	-	O(8)	-	C(14)	-87.0(3)
O(8)	-	Ru(1)	-	N(6)	-	C(25)	-13.1(4)	O(8)	-	Ru(1)	-	N(6)	-	C(29)	165.4(3)
N(7)	-	Ru(1)	-	O(8)	-	C(14)	-33.9(7)	O(8)	-	Ru(1)	-	N(7)	-	C(30)	-45.1(7)
O(8)	-	Ru(1)	-	N(7)	-	C(34)	127.3(9)	N(4)	-	Ru(1)	-	N(3)	-	C(10)	162.0(8)
N(4)	-	Ru(1)	-	N(3)	-	C(13)	-20.9(5)	N(3)	-	Ru(1)	-	N(4)	-	C(15)	104.3(7)
N(3)	-	Ru(1)	-	N(4)	-	C(19)	-67.1(6)	N(5)	-	Ru(1)	-	N(3)	-	C(10)	93.8(4)
N(5)	-	Ru(1)	-	N(3)	-	C(13)	-89.1(3)	N(3)	-	Ru(1)	-	N(5)	-	C(20)	167.7(3)
N(3)	-	Ru(1)	-	N(5)	-	C(24)	-13.4(4)	N(6)	-	Ru(1)	-	N(3)	-	C(10)	-82.1(4)
N(6)	-	Ru(1)	-	N(3)	-	C(13)	95.1(3)	N(3)	-	Ru(1)	-	N(6)	-	C(25)	-90.7(4)
N(3)	-	Ru(1)	-	N(6)	-	C(29)	87.8(3)	N(7)	-	Ru(1)	-	N(3)	-	C(10)	-3.1(4)
N(7)	-	Ru(1)	-	N(3)	-	C(13)	174.0(3)	N(3)	-	Ru(1)	-	N(7)	-	C(30)	-77.9(3)
N(3)	-	Ru(1)	-	N(7)	-	C(34)	94.5(4)	N(5)	-	Ru(1)	-	N(4)	-	C(15)	174.3(4)
N(5)	-	Ru(1)	-	N(4)	-	C(19)	2.9(3)	N(4)	-	Ru(1)	-	N(5)	-	C(20)	-0.8(3)
N(4)	-	Ru(1)	-	N(5)	-	C(24)	178.1(4)	N(6)	-	Ru(1)	-	N(4)	-	C(15)	-10.7(4)
N(6)	-	Ru(1)	-	N(4)	-	C(19)	177.9(3)	N(4)	-	Ru(1)	-	N(6)	-	C(25)	78.3(4)
N(4)	-	Ru(1)	-	N(6)	-	C(29)	-103.3(3)	N(7)	-	Ru(1)	-	N(4)	-	C(15)	-90.6(4)

P-148-8

P-148-9

N(7) - Ru(1) - N(4) - C(19)	97.9(3)	N(4) - Ru(1) - N(7) - C(30)	105.2(3)
N(4) - Ru(1) - N(7) - C(34)	-82.4(4)	N(6) - Ru(1) - N(5) - C(20)	-54.2(11)
N(6) - Ru(1) - N(5) - C(24)	124.8(13)	N(5) - Ru(1) - N(6) - C(25)	130.9(13)
N(5) - Ru(1) - N(6) - C(29)	-50.7(11)	N(7) - Ru(1) - N(5) - C(20)	-96.8(3)
N(7) - Ru(1) - N(5) - C(24)	82.1(4)	N(5) - Ru(1) - N(7) - C(30)	-175.2(3)
N(5) - Ru(1) - N(7) - C(34)	-2.8(4)	N(7) - Ru(1) - N(6) - C(25)	174.2(4)
N(7) - Ru(1) - N(6) - C(29)	-7.4(3)	N(6) - Ru(1) - N(7) - C(30)	9.0(3)
N(6) - Ru(1) - N(7) - C(34)	-178.6(4)	Ru(1) - O(8) - C(14) - O(9)	-179.2(5)
Ru(1) - O(8) - C(14) - C(13)	1.5(3)	Ru(1) - N(3) - C(10) - C(11)	173.2(6)
Ru(1) - N(3) - C(13) - C(12)	-176.6(5)	Ru(1) - N(3) - C(13) - C(14)	2.1(3)
C(13) - N(3) - C(10) - C(11)	-4.0(4)	C(10) - N(3) - C(13) - C(12)	1.2(4)
C(10) - N(3) - C(13) - C(14)	179.9(5)	Ru(1) - N(4) - C(15) - C(16)	-172.1(6)
Ru(1) - N(4) - C(19) - C(18)	173.5(5)	Ru(1) - N(4) - C(19) - C(20)	-4.4(3)
C(19) - N(4) - C(15) - C(16)	-1.0(4)	C(15) - N(4) - C(19) - C(18)	1.5(4)
C(15) - N(4) - C(19) - C(20)	-176.4(5)	Ru(1) - N(5) - C(20) - C(19)	-1.3(3)
Ru(1) - N(5) - C(20) - C(21)	179.4(5)	Ru(1) - N(5) - C(24) - C(23)	-178.9(6)
C(24) - N(5) - C(20) - C(19)	179.7(5)	C(24) - N(5) - C(20) - C(21)	0.4(4)
C(20) - N(5) - C(24) - C(23)	0.0(4)	Ru(1) - N(6) - C(25) - C(26)	177.3(7)
Ru(1) - N(6) - C(29) - C(28)	-176.6(5)	Ru(1) - N(6) - C(29) - C(30)	4.6(3)
C(29) - N(6) - C(25) - C(26)	-1.1(5)	C(25) - N(6) - C(29) - C(28)	1.9(5)
C(25) - N(6) - C(29) - C(30)	-176.9(6)	Ru(1) - N(7) - C(30) - C(29)	-9.4(3)
Ru(1) - N(7) - C(30) - C(31)	171.7(5)	Ru(1) - N(7) - C(34) - C(33)	-171.1(7)
C(34) - N(7) - C(30) - C(29)	177.6(6)	C(34) - N(7) - C(30) - C(31)	-1.4(5)
C(30) - N(7) - C(34) - C(33)	1.1(5)	N(3) - C(10) - C(11) - C(12)	5.1(4)
C(10) - C(11) - C(12) - C(13)	-4.4(4)	C(11) - C(12) - C(13) - N(3)	2.2(4)

C(11) - C(12) - C(13) - C(14)	-176.3(6)	N(3) - C(13) - C(14) - O(8)	-2.4(4)
N(3) - C(13) - C(14) - O(9)	178.2(6)	C(12) - C(13) - C(14) - O(8)	176.0(6)
C(12) - C(13) - C(14) - O(9)	-3.3(4)	N(4) - C(15) - C(16) - C(17)	-0.1(5)
C(15) - C(16) - C(17) - C(18)	0.7(5)	C(16) - C(17) - C(18) - C(19)	-0.2(5)
C(17) - C(18) - C(19) - N(4)	-0.9(4)	C(17) - C(18) - C(19) - C(20)	176.8(7)
N(4) - C(19) - C(20) - N(5)	3.7(4)	N(4) - C(19) - C(20) - C(21)	-177.0(6)
C(18) - C(19) - C(20) - N(5)	-174.1(6)	C(18) - C(19) - C(20) - C(21)	5.2(5)
N(5) - C(20) - C(21) - C(22)	-0.7(5)	C(19) - C(20) - C(21) - C(22)	180.0(7)
C(20) - C(21) - C(22) - C(23)	0.7(5)	C(21) - C(22) - C(23) - C(24)	-0.4(5)
C(22) - C(23) - C(24) - N(5)	0.0(5)	N(5) - C(24) - C(23) - C(22)	0.0(5)
N(6) - C(25) - C(26) - C(27)	-0.7(5)	C(25) - C(26) - C(27) - C(28)	1.6(5)
C(26) - C(27) - C(28) - C(29)	-0.7(5)	C(27) - C(28) - C(29) - N(6)	-1.1(5)
C(27) - C(28) - C(29) - C(30)	177.6(8)	N(6) - C(29) - C(30) - N(7)	3.1(4)
N(6) - C(29) - C(30) - C(31)	-178.0(7)	C(28) - C(29) - C(30) - N(7)	-175.6(7)
C(28) - C(29) - C(30) - C(31)	3.3(5)	N(7) - C(30) - C(31) - C(32)	0.4(5)
C(29) - C(30) - C(31) - C(32)	-178.4(8)	C(30) - C(31) - C(32) - C(33)	0.9(6)
C(31) - C(32) - C(33) - C(34)	-1.2(6)	C(32) - C(33) - C(34) - N(7)	0.3(5)

P-148-10

Table 6. Intermolecular Non-bonded Distances (Å) Less Than 3.5 Å with Their Estimated Standard Deviations in Parentheses.

Atom(1)	Atom(2)	dist	e.s.d.	ns	np	Ta	Tb	Tc	x(2)	y(2)	z(2)
O(40)	- O(41)	2.4745	0.0146	2*	1	0	0	1	0.06562	-0.17060	0.81769
O(8)	- C(21)	3.3035	0.0048	1*	2	0	0	2	0.29183	0.35556	0.99230
O(9)	- O(41)	2.7178	0.0077	1*	2	0	0	1	0.43438	0.32940	0.68231
O(9)	- C(31)	3.4819	0.0059	2*	2	0	0	1	0.47070	0.35000	0.98109
O(35)	- C(12)	3.2961	0.0059	2	2	0	0	1	0.20337	0.68116	0.90660
O(35)	- C(13)	3.3085	0.0054	2	2	0	0	1	0.23781	0.71004	0.84595
O(35)	- C(17)	3.3959	0.0059	2*	1	0	1	0	0.09795	0.65717	0.45983
O(35)	- C(24)	3.2757	0.0058	2	2	0	0	1	0.27031	0.60460	0.65381
O(35)	- C(27)	3.3228	0.0067	1*	1	0	1	1	-0.02798	0.64395	0.59111
O(36)	- C(12)	3.4705	0.0072	2	2	0	0	1	0.20337	0.68116	0.90660
O(36)	- C(26)	3.3349	0.0074	2*	1	0	1	1	0.08495	0.61430	0.98273
O(37)	- C(24)	3.4972	0.0066	2	2	0	0	1	0.27031	0.60460	0.65381
O(39)	- O(40)	2.8202	0.0107	2	2	0	0	1	0.40933	0.45399	0.68551
O(39)	- C(32)	3.4755	0.0072	2*	2	0	0	1	0.45686	0.41111	1.01457
O(40)	- C(33)	3.3748	0.0115	2	1	0	0	1	0.00235	0.06734	0.88839
O(41)	- O(41)	2.6995	0.0095	2	1	0	0	0	-0.06562	0.17060	0.18231
C(12)	- C(26)	3.4542	0.0070	1*	2	0	0	1	0.41505	0.11430	0.51727
C(15)	- C(16)	3.4047	0.0059	2	1	0	0	1	-0.07611	0.37163	0.63507
C(17)	- C(23)	3.4120	0.0067	1*	2	0	0	2	0.24475	0.43562	1.06753
C(17)	- C(28)	3.4986	0.0065	2	1	0	0	1	-0.00744	0.29244	1.07483

P-148-11

ns is the symmetry operator number - (* denotes inversion indicator)
np is the lattice point number
Ta, Tb & Tc are unit cell translations

P-148-12

P-148-13

Table 7. Least-squares Planes

Least-squares Plane # 1 (pro-H₂ chelate ring)

plane atoms	xi	yi	zi	w	esd
Ru(1)	-0.0710	0.0010	0.0000	11569723.0	0.0003
O(8)	1.6776	1.1880	-0.0014	158173.9	0.0025
N(3)	1.4056	-1.4093	0.0065	118458.7	0.0029
C(13)	2.6176	-0.9565	-0.0139	73499.6	0.0036
C(14)	2.7773	0.5300	0.0099	70839.4	0.0037
non-plane atoms	xi	yi	zi	w	esd
Cl(2)	0.1635	4.3904	-3.8135	721066.6	0.0012
O(9)	3.9032	1.0519	0.0261	99656.4	0.0032
O(35)	0.6921	5.0970	-4.9256	67855.0	0.0038
O(36)	-0.5915	5.2918	-3.0475	29588.5	0.0052
O(37)	1.1920	3.8922	-2.9943	40585.0	0.0052
O(38)	-0.6834	3.3465	-4.1798	35721.2	0.0055
O(39)	3.7068	3.4159	-1.6408	48586.4	0.0045
O(40)	-2.8690	-2.7858	4.2014	10421.1	0.0097
O(41)	0.5158	-4.3268	-3.0885	14614.4	0.0087
N(4)	-1.2478	1.6916	0.1409	118043.8	0.0029
N(5)	-0.1990	0.2237	2.0412	112956.2	0.0029
N(6)	-0.1637	-0.2147	-2.0449	112956.2	0.0029
N(7)	-1.5882	-1.3497	-0.1731	102334.7	0.0032
C(10)	1.4028	-2.8837	-0.0239	41094.4	0.0048
C(11)	2.8751	-3.2823	-0.1715	28012.8	0.0060
C(12)	3.6758	-1.9984	-0.0895	47648.6	0.0046
C(15)	-1.6567	2.4490	-0.8979	58765.5	0.0042
C(16)	-2.3091	3.6547	-0.7231	47167.7	0.0047
C(17)	-2.5532	4.0976	0.5578	45431.8	0.0047
C(18)	-2.1283	3.3368	1.6216	47164.3	0.0046
C(19)	-1.4690	2.1408	1.4091	74976.2	0.0037
C(20)	-0.9202	1.2954	2.4779	74976.2	0.0037
C(21)	-1.0783	1.5288	3.8374	45808.8	0.0046
C(22)	-0.5252	0.6776	4.7619	41792.3	0.0048
C(23)	0.2001	-0.4006	4.3212	43436.0	0.0048

P-148-14

C(24)	0.3402	-0.5934	2.9610	54159.5	0.0043
C(25)	0.5385	0.4930	-2.9455	48492.0	0.0044
C(26)	0.4574	0.2488	-4.3018	37270.9	0.0050
C(27)	-0.3613	-0.7651	-4.7483	33584.3	0.0054
C(28)	-1.0941	-1.4804	-3.8490	38161.1	0.0052
C(29)	-1.0012	-1.1937	-2.4870	65733.0	0.0039
C(30)	-1.7718	-1.8557	-1.4355	63147.9	0.0040
C(31)	-2.6655	-2.9157	-1.6341	34915.3	0.0056
C(32)	-3.3614	-3.4458	-0.5933	29725.3	0.0061
C(33)	-3.1920	-2.9135	0.6686	30390.4	0.0058
C(34)	-2.3022	-1.8778	0.8335	42670.3	0.0049
H(10A)	0.9669	-3.2222	0.8600	415.4	0.0494
H(10B)	0.8604	-3.1982	-0.6623	429.1	0.0484
H(11A)	3.0343	-3.9013	0.5625	366.5	0.0522
H(11B)	2.9634	-3.7402	-0.8874	328.6	0.0556
H(12A)	4.2345	-1.8148	-0.8421	627.8	0.0404
H(12B)	4.1962	-1.9500	0.7536	418.9	0.0488
H(15)	-1.4358	2.1607	-1.8049	773.9	0.0365
H(16)	-2.5414	4.1421	-1.5106	656.3	0.0391
H(17)	-2.9482	5.0060	0.7138	526.3	0.0440
H(18)	-2.2426	3.5700	2.4807	523.1	0.0442
H(21)	-1.5226	2.2779	4.0153	560.5	0.0426
H(22)	-0.6177	0.8139	5.7003	544.5	0.0434
H(23)	0.5227	-1.0686	4.9671	507.9	0.0445
H(24)	0.8332	-1.4115	2.5968	464.1	0.0466
H(25)	0.9831	1.1830	-2.6095	631.5	0.0400
H(26)	0.9455	0.7998	-4.9108	629.3	0.0402
H(27)	-0.3737	-0.9001	-5.6226	537.6	0.0434
H(28)	-1.6614	-2.1168	-4.0753	544.2	0.0430
H(31)	-2.6991	-3.2028	-2.4565	487.6	0.0455
H(32)	-3.9596	-4.2407	-0.7060	366.1	0.0522
H(33)	-3.5896	-3.3121	1.4205	391.5	0.0504
H(34)	-2.1270	-1.5653	1.6819	506.9	0.0446

Chi squared = 30.4814

Degrees freedom = 2

w is the refinement weight of each atom

xi, yi & zi are the coordinates with respect to the inertial axes

P-148-15

zi represents the atomic displacement from the mean plane

Least-squares Plane # 2 (bpy chelate ring # 1)

plane atoms	xi	yi	zi	w	esd
Ru(1)	-0.0662	0.0000	-0.0001	11569723.0	0.0003
N(4)	1.5381	1.2994	0.0212	118043.8	0.0029
N(5)	1.5113	-1.3207	0.0082	112956.2	0.0030
C(19)	2.7653	0.7075	-0.0318	74976.2	0.0037
C(20)	2.7547	-0.7610	0.0060	74976.2	0.0037

non-plane atoms	xi	yi	zi	w	esd
Cl(2)	-0.0787	5.1446	-2.7198	721066.6	0.0012
O(8)	-0.0510	-0.0237	-2.1133	158173.9	0.0026
O(9)	-1.0167	-0.9921	-3.8746	99656.4	0.0031
O(35)	-0.6188	6.1452	-3.5699	67855.0	0.0039
O(36)	1.2986	5.3816	-2.5936	29588.5	0.0062
O(37)	-0.2416	3.8641	-3.2773	40585.0	0.0048
O(38)	-0.6222	5.1637	-1.4370	35721.2	0.0051
O(39)	-0.6294	1.6218	-5.0674	48586.4	0.0045
O(40)	2.2268	-3.5314	3.9393	10421.1	0.0099
O(41)	-5.0478	-0.3780	1.9116	14614.4	0.0081
N(3)	-1.5205	-1.3689	-0.4248	118458.7	0.0030
N(6)	-1.5525	1.4137	0.1699	112956.2	0.0030
N(7)	-0.3938	-0.0304	2.0119	102334.7	0.0031
C(10)	-2.4399	-2.1664	0.4079	41094.4	0.0050
C(11)	-3.3799	-2.8575	-0.5856	28012.8	0.0060
C(12)	-2.8648	-2.5167	-1.9694	47648.6	0.0046
C(13)	-1.7489	-1.5770	-1.6814	73499.6	0.0038
C(14)	-0.8903	-0.8294	-2.6507	70839.4	0.0038
C(15)	1.4587	2.6422	-0.0822	58765.5	0.0041
C(16)	2.5777	3.4413	-0.2203	47167.7	0.0045
C(17)	3.8189	2.8456	-0.2506	45431.8	0.0047
C(18)	3.9069	1.4763	-0.1583	47164.3	0.0047
C(21)	3.8867	-1.5646	0.0237	45808.8	0.0048
C(22)	3.7726	-2.9325	0.0593	41792.3	0.0050

P-148-16

C(23)	2.5209	-3.4944	0.0617	43436.0	0.0048
C(24)	1.4204	-2.6606	0.0360	54159.5	0.0043
C(25)	-2.0182	2.1920	-0.8213	48492.0	0.0047
C(26)	-3.0578	3.0810	-0.6353	37270.9	0.0054
C(27)	-3.6489	3.1645	0.6061	33584.3	0.0055
C(28)	-3.1763	2.3949	1.6268	38161.1	0.0052
C(29)	-2.1118	1.5207	1.4073	65733.0	0.0039
C(30)	-1.4877	0.6843	2.4313	63147.9	0.0040
C(31)	-1.9079	0.5899	3.7641	34915.3	0.0052
C(32)	-1.2410	-0.1946	4.6520	29725.3	0.0056
C(33)	-0.1256	-0.8888	4.2294	30390.4	0.0057
C(34)	0.2584	-0.7818	2.9131	42670.3	0.0048
H(10A)	-1.8681	-2.8313	0.9708	415.4	0.0490
H(10B)	-2.8468	-1.6615	1.0243	429.1	0.0482
H(11A)	-3.3224	-3.8021	-0.3582	366.5	0.0525
H(11B)	-4.1825	-2.6228	-0.4104	328.6	0.0548
H(12A)	-3.4915	-2.0823	-2.5447	627.8	0.0397
H(12B)	-2.4721	-3.3111	-2.4149	418.9	0.0490
H(15)	0.5758	3.0593	-0.1146	773.9	0.0355
H(16)	2.4331	4.3805	-0.3140	656.3	0.0391
H(17)	4.6395	3.3919	-0.4342	526.3	0.0432
H(18)	4.6803	1.0219	-0.1835	523.1	0.0434
H(21)	4.6450	-1.1036	-0.0290	560.5	0.0419
H(22)	4.5322	-3.5075	0.0718	544.5	0.0424
H(23)	2.4223	-4.4658	0.1806	507.9	0.0444
H(24)	0.4735	-3.0426	0.0848	464.1	0.0463
H(25)	-1.5484	2.1558	-1.5727	631.5	0.0396
H(26)	-3.3338	3.6425	-1.3573	629.3	0.0397
H(27)	-4.3216	3.7345	0.6804	537.6	0.0429
H(28)	-3.4890	2.4287	2.4510	544.2	0.0428
H(31)	-2.6294	1.0455	3.9423	487.6	0.0452
H(32)	-1.5605	-0.3201	5.5925	366.1	0.0523
H(33)	0.3041	-1.5054	4.7927	391.5	0.0507
H(34)	0.9557	-1.2977	2.6039	506.9	0.0443

Chi squared = 140.2439

Degrees freedom = 2

w is the refinement weight of each atom

P-148-17

x_i , y_i & z_i are the coordinates with respect to the inertial axes
 z_i represents the atomic displacement from the mean plane

Least-squares Plane # 3 (bpy chelate ring # 2)

plane atoms	x_i	y_i	z_i	w	esd
Ru(1)	0.0589	0.0003	-0.0005	11569723.0	0.0003
N(6)	-1.5662	1.2621	0.0571	112956.2	0.0030
N(7)	-1.4688	-1.3477	0.0727	102334.7	0.0031
C(29)	-2.7788	0.6505	-0.0462	65733.0	0.0039
C(30)	-2.7228	-0.8102	-0.0754	63147.9	0.0039
non-plane atoms	x_i	y_i	z_i	w	esd
Cl(2)	-0.3168	4.7778	3.3008	721066.6	0.0012
O(8)	1.4849	1.5232	-0.3380	158173.9	0.0025
O(9)	2.4739	2.6863	-1.9633	99656.4	0.0031
O(35)	-0.5065	6.1655	3.5326	67855.0	0.0039
O(36)	0.3453	4.2397	4.4149	29588.5	0.0062
O(37)	0.4964	4.5587	2.1748	40585.0	0.0048
O(38)	-1.5127	4.0788	3.1514	35721.2	0.0052
O(39)	2.3992	4.8115	0.0072	48586.4	0.0045
O(40)	0.3410	-5.7440	-0.4127	10421.1	0.0098
O(41)	-4.1148	0.4781	-3.3119	14614.4	0.0078
N(3)	0.0276	0.1750	-2.0347	118458.7	0.0029
N(4)	0.4804	0.0198	2.0206	118043.8	0.0029
N(5)	1.5819	-1.3793	0.0984	112956.2	0.0030
C(10)	-0.7540	-0.4814	-3.0991	41094.4	0.0050
C(11)	-0.3777	0.2611	-4.3857	28012.8	0.0060
C(12)	0.7156	1.2407	-4.0098	47648.6	0.0046
C(13)	0.8118	1.0744	-2.5352	73499.6	0.0037
C(14)	1.6680	1.8286	-1.5691	70839.4	0.0038
C(15)	-0.0681	0.8560	2.9261	58765.5	0.0041
C(16)	0.3731	0.9231	4.2340	47167.7	0.0045
C(17)	1.4083	0.1048	4.6279	45431.8	0.0046
C(18)	1.9807	-0.7412	3.7072	47164.3	0.0046
C(19)	1.5204	-0.7740	2.4043	74976.2	0.0036

P-148-18

C(20)	2.1106	-1.5929	1.3370	74976.2	0.0036
C(21)	3.1347	-2.5135	1.5144	45808.8	0.0047
C(22)	3.6201	-3.2330	0.4505	41792.3	0.0049
C(23)	3.0872	-3.0173	-0.7953	43436.0	0.0048
C(24)	2.0750	-2.0877	-0.9310	54159.5	0.0043
C(25)	-1.5221	2.6014	0.1552	48492.0	0.0046
C(26)	-2.6612	3.3809	0.1337	37270.9	0.0053
C(27)	-3.8862	2.7669	-0.0074	33584.3	0.0054
C(28)	-3.9493	1.4079	-0.0900	38161.1	0.0050
C(31)	-3.8282	-1.6587	-0.2168	34915.3	0.0052
C(32)	-3.6772	-3.0098	-0.2009	29725.3	0.0056
C(33)	-2.4166	-3.5428	-0.0240	30390.4	0.0057
C(34)	-1.3498	-2.6844	0.1049	42670.3	0.0048
H(10A)	-0.4958	-1.4909	-3.1109	415.4	0.0488
H(10B)	-1.6282	-0.4879	-2.9085	429.1	0.0482
H(11A)	-0.0938	-0.4407	-4.9974	366.5	0.0521
H(11B)	-1.0870	0.5951	-4.7254	328.6	0.0548
H(12A)	0.5295	2.1572	-4.2041	627.8	0.0395
H(12B)	1.5899	0.9715	-4.3933	418.9	0.0489
H(15)	-0.7657	1.4739	2.6326	773.9	0.0356
H(16)	-0.0511	1.5607	4.8044	656.3	0.0389
H(17)	1.8034	0.1926	5.5454	526.3	0.0433
H(18)	2.6651	-1.2916	3.8913	523.1	0.0433
H(21)	3.4405	-2.5414	2.3486	560.5	0.0420
H(22)	4.3220	-3.8705	0.5437	544.5	0.0425
H(23)	3.3588	-3.5892	-1.5480	507.9	0.0442
H(24)	1.6224	-1.9354	-1.8348	464.1	0.0463
H(25)	-0.7179	2.9341	0.3261	631.5	0.0396
H(26)	-2.5880	4.3272	0.2435	629.3	0.0395
H(27)	-4.5903	3.3020	-0.0325	537.6	0.0429
H(28)	-4.7044	0.9553	-0.1460	544.2	0.0427
H(31)	-4.5832	-1.2410	-0.3413	487.6	0.0451
H(32)	-4.4465	-3.6308	-0.3589	366.1	0.0523
H(33)	-2.2664	-4.4672	-0.0958	391.5	0.0506
H(34)	-0.4970	-3.0292	0.1490	506.9	0.0443

Chi squared = 1345.2736

Degrees freedom = 2

P-148-19

w is the refinement weight of each atom

x_i , y_i & z_i are the coordinates with respect to the inertial axes

z_i represents the atomic displacement from the mean plane

Least-squares Plane # 4

plane atoms	x_i	y_i	z_i	w	esd
N(3)	-0.8427	0.0961	-0.0070	118458.7	0.0029
C(10)	-0.3931	-1.3079	0.0291	41094.4	0.0048
C(11)	1.1361	-1.2388	-0.0410	28012.8	0.0060
C(12)	1.5007	0.2310	0.0150	47648.6	0.0046
C(13)	0.1722	0.8988	0.0009	73499.6	0.0037

non-plane atoms	x_i	y_i	z_i	w	esd
Ru(1)	-2.6772	0.9833	-0.1365	11569723.0	0.0003
Cl(2)	-3.5975	5.1129	-4.1318	721066.6	0.0012
O(8)	-1.3776	2.6497	-0.1213	158173.9	0.0025
O(9)	0.7785	3.2054	0.0017	99656.4	0.0033
O(35)	-3.2529	5.9133	-5.2527	67855.0	0.0038
O(36)	-4.6307	5.7616	-3.4383	29588.5	0.0052
O(37)	-2.5100	4.9805	-3.2504	40585.0	0.0051
O(38)	-4.0645	3.8485	-4.4843	35721.2	0.0054
O(39)	-0.0441	5.3421	-1.7769	48586.4	0.0045
O(40)	-4.7043	-2.3985	4.0709	10421.1	0.0098
O(41)	-0.6357	-3.0472	-3.0002	14614.4	0.0088
N(4)	-4.3202	2.2336	-0.1194	118043.8	0.0030
N(5)	-2.9733	1.2183	1.8858	112956.2	0.0030
N(6)	-2.5930	0.6868	-2.1715	112956.2	0.0030
N(7)	-3.6979	-0.7731	-0.3091	102334.7	0.0032
C(14)	-0.1316	2.3624	-0.0362	70839.4	0.0038
C(15)	-4.8863	2.7964	-1.2069	58765.5	0.0042
C(16)	-5.8842	3.7478	-1.1131	47167.7	0.0047
C(17)	-6.3184	4.1333	0.1356	45431.8	0.0048
C(18)	-5.7372	3.5731	1.2490	47164.3	0.0046
C(19)	-4.7338	2.6317	1.1173	74976.2	0.0037
C(20)	-4.0093	2.0293	2.2444	74976.2	0.0037

P-148-20

C(21)	-4.3017	2.2444	3.5845	45808.8	0.0046
C(22)	-3.5638	1.6332	4.5679	41792.3	0.0049
C(23)	-2.5217	0.8173	4.2059	43436.0	0.0048
C(24)	-2.2588	0.6352	2.8625	54159.5	0.0043
C(25)	-2.0948	1.5481	-3.0743	48492.0	0.0044
C(26)	-2.0267	1.2493	-4.4203	37270.9	0.0050
C(27)	-2.4719	0.0197	-4.8531	33584.3	0.0055
C(28)	-2.9968	-0.8583	-3.9525	38161.1	0.0053
C(29)	-3.0669	-0.5153	-2.6022	65733.0	0.0040
C(30)	-3.6520	-1.3495	-1.5537	63147.9	0.0041
C(31)	-4.1673	-2.6386	-1.7399	34915.3	0.0056
C(32)	-4.7211	-3.3248	-0.7050	29725.3	0.0061
C(33)	-4.7884	-2.7277	0.5373	30390.4	0.0058
C(34)	-4.2676	-1.4640	0.6909	42670.3	0.0049
H(10A)	-0.7501	-1.7367	0.9093	415.4	0.0495
H(10B)	-0.7794	-1.7934	-0.6156	429.1	0.0484
H(11A)	1.4384	-1.7561	0.7260	366.5	0.0524
H(11B)	1.3973	-1.6692	-0.7314	328.6	0.0556
H(12A)	2.0149	0.5542	-0.7222	627.8	0.0404
H(12B)	1.9367	0.4628	0.8752	418.9	0.0488
H(15)	-4.5410	2.5623	-2.0904	773.9	0.0364
H(16)	-6.2131	4.1159	-1.9306	656.3	0.0392
H(17)	-6.9796	4.8807	0.2345	526.3	0.0440
H(18)	-5.9619	3.7861	2.0913	523.1	0.0442
H(21)	-4.9623	2.8257	3.7104	560.5	0.0426
H(22)	-3.7423	1.7632	5.4947	544.5	0.0433
H(23)	-2.0445	0.3010	4.8938	507.9	0.0445
H(24)	-1.5211	-0.0024	2.5557	464.1	0.0466
H(25)	-1.9006	2.3514	-2.7522	631.5	0.0400
H(26)	-1.6994	1.9048	-5.0336	629.3	0.0403
H(27)	-2.3969	-0.1394	-5.7202	537.6	0.0434
H(28)	-3.3298	-1.6450	-4.1724	544.2	0.0431
H(31)	-4.0688	-2.9472	-2.5492	487.6	0.0455
H(32)	-5.0410	-4.2682	-0.8056	366.1	0.0523
H(33)	-5.0837	-3.2059	1.2899	391.5	0.0505
H(34)	-4.2408	-1.0869	1.5306	506.9	0.0446

Chi squared = 106.4528

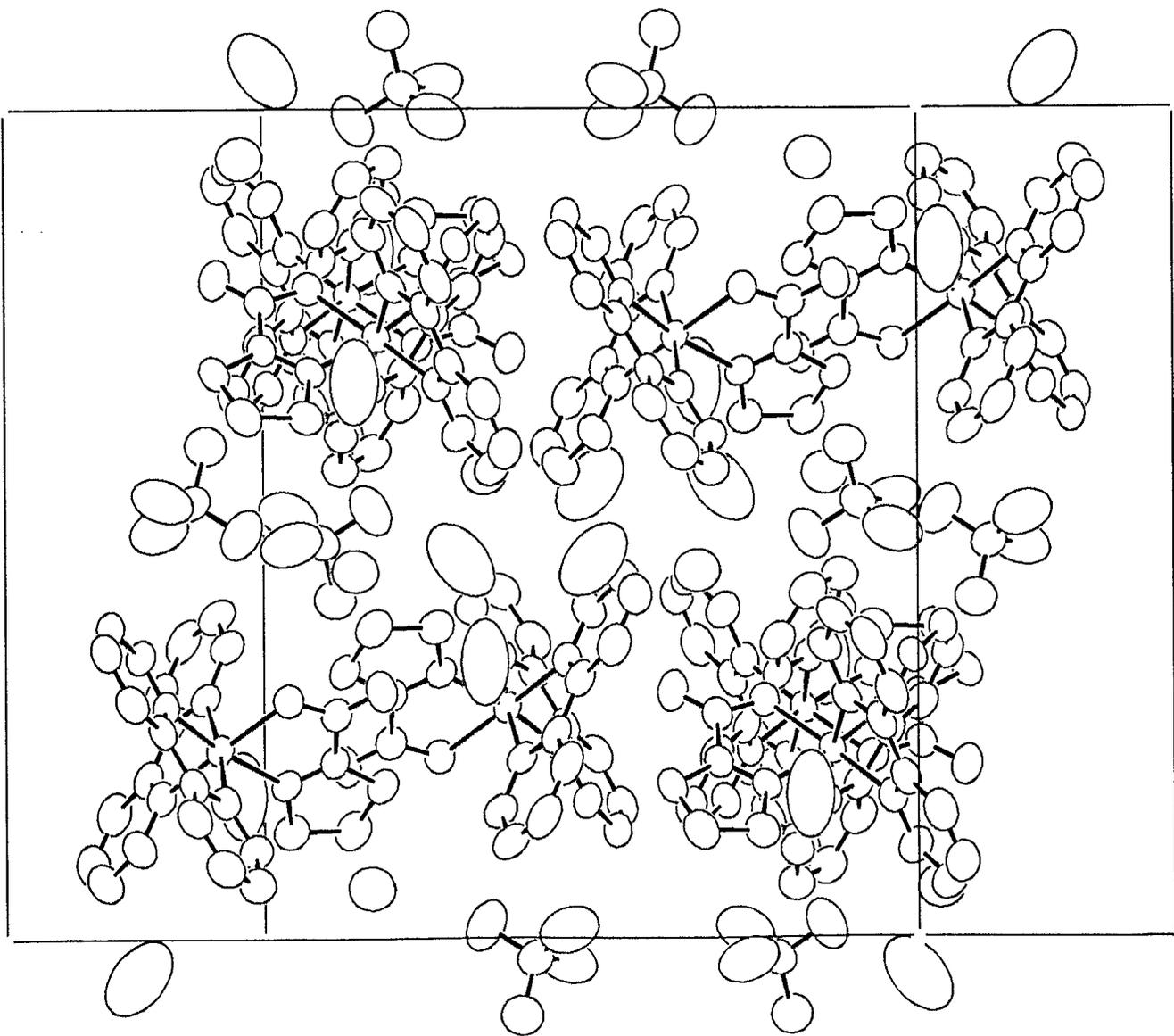
Degrees freedom = 2

w is the refinement weight of each atom
xi, yi & zi are the coordinates with respect to the inertial axes
zi represents the atomic displacement from the mean plane

PLANE/VECTOR ANGLES

Plane/Vector	Plane/Vector	Angle
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1	3	94.22
1	4	3.46
2	3	81.00
2	4	89.65
3	4	97.68

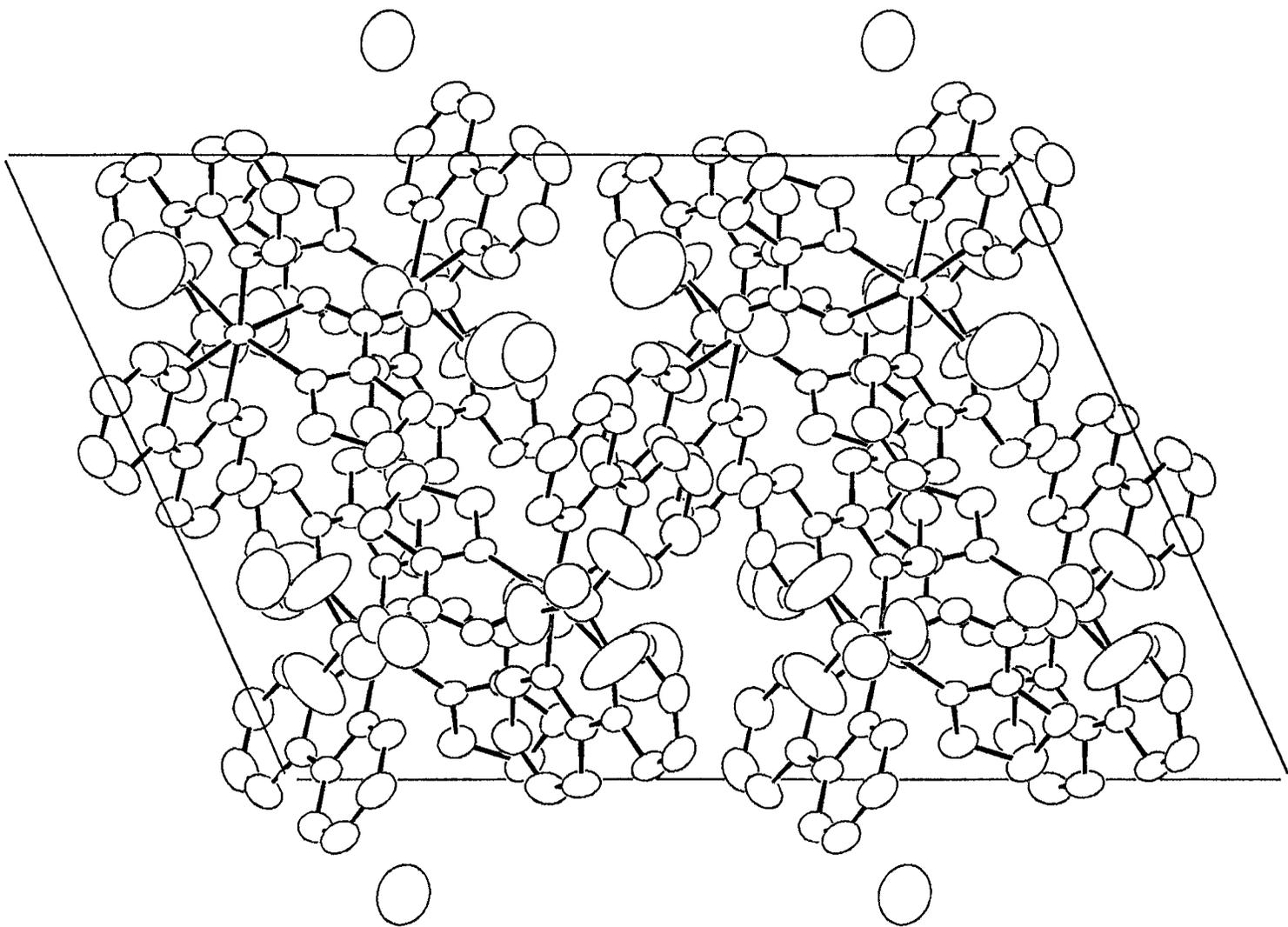
P-148-222



b ↑
a →

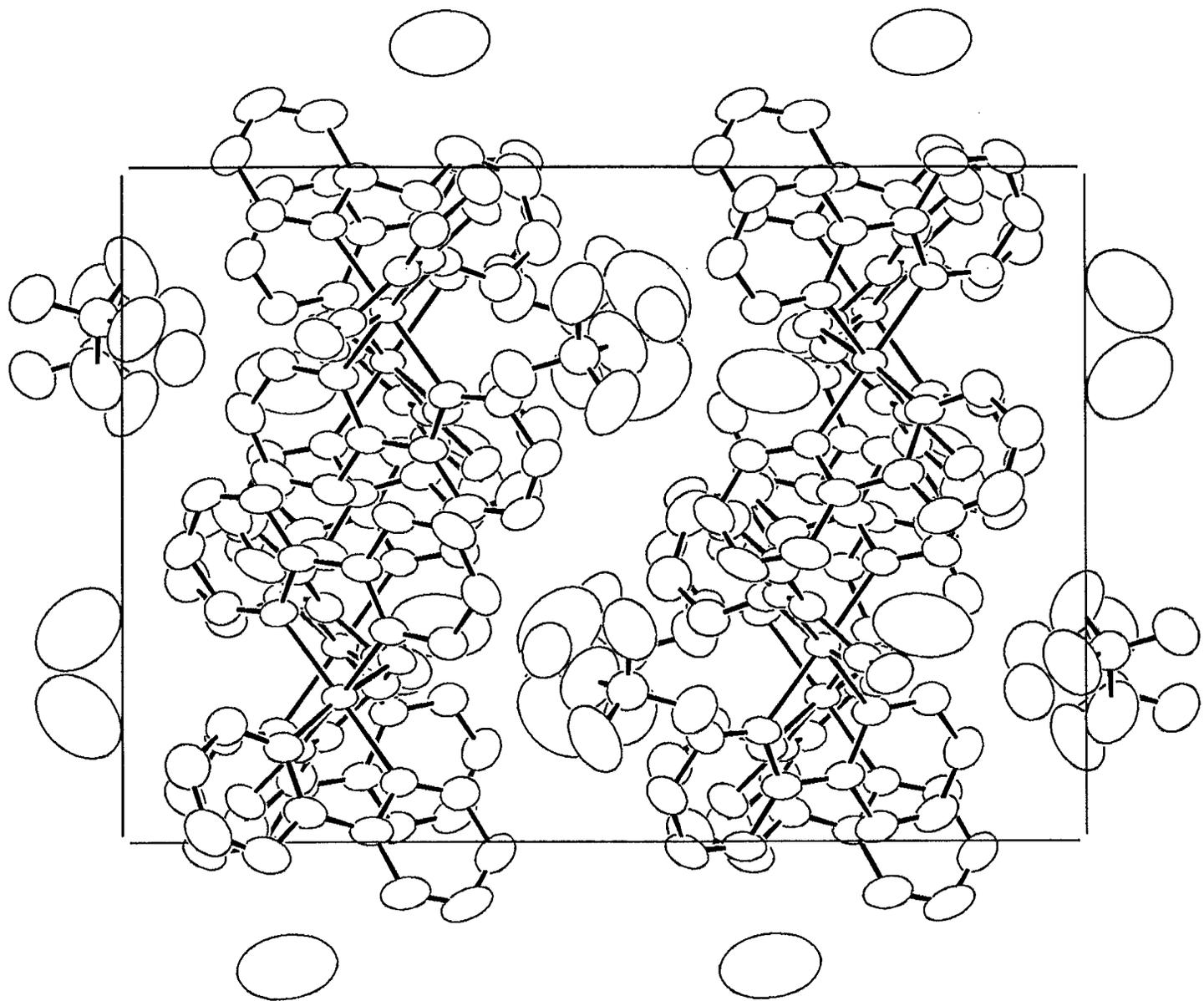
[Ru(Pro-H2)(bpy)2]ClO4·3H2O

P-148-23



$\begin{matrix} c \\ \swarrow \\ a \end{matrix}$

[Ru(Pro-H2)(bpy)2]ClO4·3H2O



P-148-24

[Ru(Pro-H₂)(bpy)₂]C₁₀₄·3H₂O

c ↑
b →