

Inorganic Chemistry

including bioinorganic chemistry

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TITLE : RuA4bd

Supporting information P-2694-111
cis-[RuA4(1,3-bd)](ClO4)2
P 1
of 108

CRYSTAL :

Chemical Formula

Ru1 N4 C4 H18 Cl2 O8

Formula Weight

422.20

Crystal Size

0.30 * 0.30 * 0.30 mm**3

Unit-cell Dimensions :

a = 16.887 (4) A

b = 16.934 (5) A

c = 10.805 (3) A

alpha = 90.000000 (0) degrees

beta = 90.000000 (0) degrees

gamma = 90.000000 (0) degrees

Volume of unit cell

3090 (1) A**3

Crystal System

Orthorhombic

Space Group

P b 21 a(# 29)

Z value

8

Densities: Dobs ;Dcalc

1.80; 1.82 g/cm**3

DATA COLLECTION :

Diffractometer used

Mac Science MXC18

Radiation

Mo K-alpha (lambda= 0.71073)

Total Reflections Measured

3189

Reflection (hkl) limits

0 < h < 20

0 < k < 20

0 < l < 12

Unique Reflections

2824

Internal Consistency : Rint

0.00

REFINEMENT :

Least squares refinement method

Full matrix

Absorption correction

refdiff psi-scan

Function minimized

Sum[w(|Fo|-|Fc|)**2]

Weight method

Count statistics

w=exp(0.00 sin(theta)**2/lambda**2)/(sig**2(Fo) + 0.008 * Fo**2)

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F(000)	1695
Linear absorption coefficient	13.781/cm
Reflections used in L.S.	2419
Data reduction cut-off	3.00
Maximum sin(theta)/lambda	0.595
L.S. parameters	337
L.S. matrix elements	56953
Extinction coefficient	0.0000
Eta coefficient	1.0000
Residuals, R	0.0501
Residuals, Rw	0.0759
Max shift/e. s. d.	0.3473
Average shift/e. s. d.	0.0427
Sum w(Fobs-Fcal)**2	0.50521E+04
Sum (Fobs-Fcal)	0.64805E+04
Goodness of fit	$\sqrt{0.24266E+01}$

FOURIER :

Fourier map type	Fo-Fc
Sim weighting	OFF
Fourier map grid	0.200 A
Maximum peak in final Fourier map	1.74 e/A**3 @ (0.284 0.012 0.685)
Minimum peak in final Fourier map	-0.70 e/A**3 @ (0.308 0.024 0.019)

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FRACTIONAL ATOMIC COORDINATES & U(iso)

Atom	x/a	y/b	z/c	U(iso)
Ru(1)	0.22446(5)	-0.22000	0.00815(7)	0.023
Ru(2)	0.02130(5)	0.00939(8)	0.47141(9)	0.024
Cl(1)	0.44175(17)	-0.26464(21)	-0.25029(29)	0.027
Cl(2)	0.01950(18)	0.26943(22)	0.25835(30)	0.032
Cl(3)	-0.23275(17)	0.02355(23)	0.26175(32)	0.035
Cl(4)	0.1910(2)	-0.4533(3)	0.2338(4)	0.043
N(1)	0.1313(7)	-0.3054(7)	-0.0061(9)	0.019(2)
N(2)	0.3090(9)	-0.3177(9)	0.0025(11)	0.031
N(5)	-0.0778(7)	-0.0677(9)	0.4839(11)	0.029
N(4)	0.3271(10)	-0.1427(9)	0.0011(10)	0.036
N(7)	0.0207(6)	0.0166(10)	0.6711(11)	0.037
N(3)	0.2279(6)	-0.2190(11)	-0.1908(9)	0.040
N(8)	0.1093(8)	0.1002(10)	0.4778(11)	0.038
O(1)	0.4081(9)	-0.1904(9)	-0.2606(19)	0.089
O(9)	-0.1845(8)	-0.0439(8)	0.2445(14)	0.068
O(13)	0.1280(7)	-0.3980(8)	0.2462(12)	0.065
O(2)	0.3813(7)	-0.3229(7)	-0.2633(11)	0.059
O(3)	0.5016(9)	-0.2713(9)	-0.3385(13)	0.069
C(8)	0.1117(17)	-0.0898(18)	0.4924(24)	0.078
N(6)	-0.0616(8)	0.1055(9)	0.4838(11)	0.030
C(1)	0.2350(12)	-0.2202(17)	0.2171(13)	0.069
O(5)	-0.0575(8)	0.2424(13)	0.2657(15)	0.095
O(10)	-0.2321(8)	0.0355(14)	0.3934(13)	0.100
O(4)	0.4711(7)	-0.2681(15)	-0.1249(13)	0.105
O(11)	-0.3096(8)	0.0153(12)	0.2259(18)	0.105
O(14)	0.2019(12)	-0.4658(9)	0.0950(15)	0.116
O(12)	-0.1994(11)	0.0918(10)	0.2184(19)	0.106
O(15)	0.2650(9)	-0.4207(13)	0.2509(23)	0.132
O(6)	0.0575(12)	0.2612(12)	0.3724(18)	0.125
O(7)	0.0560(15)	0.2284(16)	0.1687(26)	0.193
C(4)	0.1412(18)	-0.1190(19)	-0.0173(25)	0.091
C(2)	0.1745(15)	-0.1847(16)	0.1824(18)	0.106
C(3)	0.1585(17)	-0.1314(15)	0.0971(20)	0.107
C(7)	0.0925(18)	-0.0703(17)	0.3745(24)	0.116
C(6)	0.0510(17)	-0.0405(19)	0.3011(16)	0.114
O(8)	0.0283(16)	0.3494(11)	0.2288(23)	0.139
C(5)	0.0153(12)	0.0235(13)	0.2630(16)	0.062
O(16)	0.1761(12)	-0.5260(10)	0.2822(21)	0.137

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ANISOTROPIC THERMAL PARAMETERS

Atom	U11	U22	U33	U12	U13	U23
Ru(1)	0.0228(5)	0.0192(5)	0.0263(5)	-0.0023(5)	0.0043(3)	-0.0027(4)
Ru(2)	0.0219(5)	0.0212(6)	0.0299(5)	-0.0022(4)	0.0039(3)	-0.0077(4)
Cl(1)	0.024(1)	0.023(2)	0.035(2)	0.003(1)	0.007(1)	-0.003(1)
Cl(2)	0.033(2)	0.027(2)	0.035(2)	-0.004(1)	0.002(1)	0.000(1)
Cl(3)	0.030(2)	0.025(2)	0.051(2)	0.005(1)	0.000(1)	0.000(1)
Cl(4)	0.038(2)	0.035(2)	0.055(2)	0.002(2)	0.004(1)	-0.001(2)
N(2)	0.032(7)	0.027(8)	0.035(6)	0.008(6)	0.008(4)	0.004(5)
N(5)	0.018(6)	0.032(8)	0.038(6)	0.014(5)	0.000(4)	-0.003(5)
N(4)	0.05(1)	0.03(1)	0.03(1)	-0.03(1)	0.00(0)	0.00(0)
N(7)	0.038(5)	0.036(7)	0.037(6)	0.001(5)	0.002(4)	-0.001(7)
N(3)	0.039(7)	0.054(8)	0.025(5)	0.011(6)	0.006(4)	-0.001(7)
N(8)	0.024(6)	0.048(8)	0.041(7)	-0.018(6)	0.005(5)	-0.009(5)
O(1)	0.068(9)	0.049(8)	0.151(15)	0.024(7)	0.043(9)	0.034(9)
O(9)	0.070(9)	0.045(7)	0.088(9)	0.024(6)	-0.013(7)	-0.011(7)
O(13)	0.061(7)	0.049(7)	0.086(9)	0.015(6)	0.051(7)	0.011(6)
O(2)	0.059(7)	0.058(8)	0.061(7)	-0.043(6)	0.021(6)	-0.036(6)
O(3)	0.082(8)	0.060(9)	0.065(8)	-0.002(7)	0.044(8)	-0.011(7)
C(8)	0.07(2)	0.07(2)	0.09(1)	0.05(1)	-0.01(1)	-0.03(1)
N(6)	0.030(7)	0.025(7)	0.036(6)	0.007(5)	0.002(4)	-0.001(4)
C(1)	0.09(1)	0.08(2)	0.04(1)	0.03(1)	0.01(1)	-0.03(1)
O(5)	0.035(6)	0.165(19)	0.086(10)	-0.017(9)	-0.012(6)	0.040(12)
O(10)	0.07(1)	0.16(2)	0.07(1)	0.01(1)	0.00(1)	-0.05(1)
O(4)	0.058(8)	0.205(23)	0.052(8)	-0.021(11)	-0.011(6)	-0.005(11)
O(11)	0.037(7)	0.120(15)	0.159(17)	0.002(9)	-0.003(8)	-0.062(15)
O(14)	0.21(2)	0.06(1)	0.08(1)	0.06(1)	0.05(1)	-0.01(1)
O(12)	0.11(1)	0.05(1)	0.16(2)	0.00(1)	0.06(1)	0.03(1)
O(15)	0.05(1)	0.10(2)	0.24(2)	-0.01(1)	-0.05(1)	0.08(2)
O(6)	0.15(1)	0.10(1)	0.12(1)	-0.04(1)	-0.10(1)	0.05(1)
O(7)	0.19(2)	0.17(2)	0.22(3)	-0.09(2)	0.17(2)	-0.14(2)
C(4)	0.08(2)	0.07(2)	0.12(2)	0.06(2)	0.00(1)	-0.01(2)
C(2)	0.14(2)	0.13(2)	0.04(1)	0.11(2)	0.00(1)	-0.04(1)
C(3)	0.17(2)	0.09(2)	0.06(1)	0.11(2)	0.05(1)	0.02(1)
C(7)	0.16(2)	0.11(2)	0.08(2)	0.10(2)	0.04(2)	-0.02(1)
C(6)	0.15(2)	0.16(3)	0.03(1)	0.12(2)	0.00(1)	-0.02(1)
O(8)	0.23(3)	0.03(1)	0.16(2)	-0.03(1)	0.03(2)	0.02(1)
C(5)	0.10(1)	0.04(1)	0.05(1)	-0.01(1)	0.02(1)	-0.02(1)
O(16)	0.16(2)	0.06(1)	0.19(2)	0.05(1)	0.13(2)	0.07(1)

$$T=\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+U_{12}hka^{*}b^{*}+U_{23}klb^{*}c^{*}+U_{13}hla^{*}c^{*})]$$

INTRAMOLECULAR BOND LENGTHS (H omitted)

Minimum bond length= 1.10Å : Maximum bond length= 2.30Å

Ru(1)-N(1)	2.142(13)	Ru(1)-N(2)	2.186(15)
Ru(1)-N(4)	2.174(17)	Ru(1)-N(3)	2.151(10)
Ru(1)-C(1)	2.265(15)	Ru(1)-C(4)	2.23(4)
Ru(1)-C(2)	2.15(3)	Ru(1)-C(3)	2.10(3)
Ru(2)-N(5)	2.128(14)	Ru(2)-N(7)	2.162(12)
Ru(2)-N(8)	2.140(15)	Ru(2)-C(8)	2.28(3)
Ru(2)-N(6)	2.151(15)	Ru(2)-C(7)	2.09(3)
Ru(2)-C(6)	2.09(3)	Ru(2)-C(5)	2.266(18)
Cl(1)-O(1)	1.384(16)	Cl(1)-O(2)	1.426(13)
Cl(1)-O(3)	1.394(15)	Cl(1)-O(4)	1.444(15)
Cl(2)-O(5)	1.381(15)	Cl(2)-O(6)	1.40(2)
Cl(2)-O(7)	1.34(3)	Cl(2)-O(8)	1.399(19)
Cl(3)-O(9)	1.415(15)	Cl(3)-O(10)	1.437(15)
Cl(3)-O(11)	1.361(15)	Cl(3)-O(12)	1.369(18)
Cl(4)-O(13)	1.424(14)	Cl(4)-O(14)	1.525(17)
Cl(4)-O(15)	1.379(18)	Cl(4)-O(16)	1.362(19)
O(1)-O(2)	2.29(2)	O(1)-O(3)	2.25(3)
O(1)-O(4)	2.24(3)	O(9)-O(10)	2.25(3)
C(8)-C(7)	1.36(4)	C(1)-C(2)	1.24(4)
O(5)-O(6)	2.28(3)	O(5)-O(7)	2.20(3)
O(10)-O(11)	2.26(3)	O(10)-O(12)	2.19(3)
O(11)-O(12)	2.27(3)	O(14)-O(15)	2.13(3)
O(6)-O(7)	2.27(4)	O(6)-O(8)	2.21(3)
O(7)-O(8)	2.20(4)	C(4)-C(3)	1.29(4)
C(2)-C(3)	1.32(4)	C(7)-C(6)	1.17(4)
C(6)-C(5)	1.31(4)		

INTRAMOLECULAR BOND ANGLES (H omitted)

Minimum bond length= 1.10Å : Maximum bond length= 2.30Å			
N(1)-Ru(1)-N(2)	88.1(6)	N(1)-Ru(1)-N(4)	171.7(5)
N(1)-Ru(1)-N(3)	87.3(5)	N(1)-Ru(1)-C(1)	97.4(7)
N(1)-Ru(1)-C(4)	92.6(9)	N(1)-Ru(1)-C(2)	87.9(8)
N(1)-Ru(1)-C(3)	97.2(9)	N(2)-Ru(1)-N(4)	86.2(6)
N(2)-Ru(1)-N(3)	87.7(6)	N(2)-Ru(1)-C(1)	88.6(7)
N(2)-Ru(1)-C(4)	171.2(8)	N(2)-Ru(1)-C(2)	119.5(8)
N(2)-Ru(1)-C(3)	154.1(7)	N(4)-Ru(1)-N(3)	86.5(5)
N(4)-Ru(1)-C(1)	88.4(7)	N(4)-Ru(1)-C(4)	92.1(10)
N(4)-Ru(1)-C(2)	100.1(8)	N(4)-Ru(1)-C(3)	90.5(9)
N(3)-Ru(1)-C(1)	173.9(6)	N(3)-Ru(1)-C(4)	83.6(9)
N(3)-Ru(1)-C(2)	152.2(8)	N(3)-Ru(1)-C(3)	117.8(8)
C(1)-Ru(1)-C(4)	100.0(10)	C(1)-Ru(1)-C(2)	32.6(9)
C(1)-Ru(1)-C(3)	65.6(9)	C(4)-Ru(1)-C(2)	69.3(10)
C(4)-Ru(1)-C(3)	34.4(10)	C(2)-Ru(1)-C(3)	36.1(10)
N(5)-Ru(2)-N(7)	88.2(5)	N(5)-Ru(2)-N(8)	170.3(6)
N(5)-Ru(2)-C(8)	93.9(9)	N(5)-Ru(2)-N(6)	87.1(6)
N(5)-Ru(2)-C(7)	95.0(10)	N(5)-Ru(2)-C(6)	89.8(9)
N(5)-Ru(2)-C(5)	95.3(7)	N(7)-Ru(2)-N(8)	86.0(5)
N(7)-Ru(2)-C(8)	86.8(8)	N(7)-Ru(2)-N(6)	83.8(5)
N(7)-Ru(2)-C(7)	122.6(9)	N(7)-Ru(2)-C(6)	154.8(9)
N(7)-Ru(2)-C(5)	170.3(7)	N(8)-Ru(2)-C(8)	93.5(9)
N(8)-Ru(2)-N(6)	84.6(6)	N(8)-Ru(2)-C(7)	94.6(10)
N(8)-Ru(2)-C(6)	98.8(9)	N(8)-Ru(2)-C(5)	89.3(7)
C(8)-Ru(2)-N(6)	170.6(8)	C(8)-Ru(2)-C(7)	35.8(10)
C(8)-Ru(2)-C(6)	68.2(11)	C(8)-Ru(2)-C(5)	101.9(9)
N(6)-Ru(2)-C(7)	153.5(9)	N(6)-Ru(2)-C(6)	121.2(9)
N(6)-Ru(2)-C(5)	87.3(7)	C(7)-Ru(2)-C(6)	32.6(11)
C(7)-Ru(2)-C(5)	66.1(10)	C(6)-Ru(2)-C(5)	34.6(10)
O(1)-Cl(1)-O(2)	109.1(9)	O(1)-Cl(1)-O(3)	108.4(10)
O(1)-Cl(1)-O(4)	104.7(13)	O(2)-Cl(1)-O(3)	113.3(8)
O(2)-Cl(1)-O(4)	108.1(10)	O(3)-Cl(1)-O(4)	112.9(8)
O(5)-Cl(2)-O(6)	110.5(11)	O(5)-Cl(2)-O(7)	107.6(14)
O(5)-Cl(2)-O(8)	115.8(14)	O(6)-Cl(2)-O(7)	111.9(14)
O(6)-Cl(2)-O(8)	104.4(14)	O(7)-Cl(2)-O(8)	106.7(16)
O(9)-Cl(3)-O(10)	103.9(11)	O(9)-Cl(3)-O(11)	115.4(11)
O(9)-Cl(3)-O(12)	113.6(10)	O(10)-Cl(3)-O(11)	107.7(10)
O(10)-Cl(3)-O(12)	102.5(13)	O(11)-Cl(3)-O(12)	112.4(12)
O(13)-Cl(4)-O(14)	105.9(9)	O(13)-Cl(4)-O(15)	113.6(11)
O(13)-Cl(4)-O(16)	114.9(11)	O(14)-Cl(4)-O(15)	94.5(13)
O(14)-Cl(4)-O(16)	105.9(12)	O(15)-Cl(4)-O(16)	118.6(14)
Cl(1)-O(1)-O(2)	36.1(6)	Cl(1)-O(1)-O(3)	35.9(6)
Cl(1)-O(1)-O(4)	38.6(8)	O(2)-O(1)-O(3)	62.5(7)
O(2)-O(1)-O(4)	61.7(8)	O(3)-O(1)-O(4)	63.6(7)
Cl(3)-O(9)-O(10)	38.4(6)	Cl(1)-O(2)-O(1)	34.9(6)
Cl(1)-O(3)-O(1)	35.7(6)	Ru(2)-C(8)-C(7)	64.4(17)
Ru(1)-C(1)-C(2)	68.6(12)	Cl(2)-O(5)-O(6)	35.0(7)
Cl(2)-O(5)-O(7)	35.6(9)	O(6)-O(5)-O(7)	60.9(10)
Cl(3)-O(10)-O(9)	37.7(7)	Cl(3)-O(10)-O(11)	35.0(6)

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<cont

Cl(3)-O(10)-O(12)	37.6(7)	O(9)-O(10)-O(11)	62.8(8)
O(9)-O(10)-O(12)	63.4(7)	O(11)-O(10)-O(12)	61.3(8)
Cl(1)-O(4)-O(1)	36.7(8)	Cl(3)-O(11)-O(10)	37.3(7)
Cl(3)-O(11)-O(12)	33.9(7)	O(10)-O(11)-O(12)	57.8(8)
Cl(4)-O(14)-O(15)	40.1(7)	Cl(3)-O(12)-O(10)	39.9(8)
Cl(3)-O(12)-O(11)	33.7(7)	O(10)-O(12)-O(11)	60.9(8)
Cl(4)-O(15)-O(14)	45.4(9)	Cl(2)-O(6)-O(5)	34.5(7)
Cl(2)-O(6)-O(7)	33.3(9)	Cl(2)-O(6)-O(8)	37.8(8)
O(5)-O(6)-O(7)	57.7(9)	O(5)-O(6)-O(8)	63.2(10)
O(7)-O(6)-O(8)	58.8(11)	Cl(2)-O(7)-O(5)	36.8(9)
Cl(2)-O(7)-O(6)	34.8(9)	Cl(2)-O(7)-O(8)	37.5(10)
O(5)-O(7)-O(6)	61.4(10)	O(5)-O(7)-O(8)	64.7(12)
O(6)-O(7)-O(8)	59.2(11)	Ru(1)-C(4)-C(3)	67.2(18)
Ru(1)-C(2)-C(1)	78.8(14)	Ru(1)-C(2)-C(3)	70.0(14)
C(1)-C(2)-C(3)	135.2(26)	Ru(1)-C(3)-C(4)	78.4(18)
Ru(1)-C(3)-C(2)	73.9(16)	C(4)-C(3)-C(2)	146.2(28)
Ru(2)-C(7)-C(8)	79.8(18)	Ru(2)-C(7)-C(6)	73.6(19)
C(8)-C(7)-C(6)	152.1(31)	Ru(2)-C(6)-C(7)	73.8(17)
Ru(2)-C(6)-C(5)	80.3(16)	C(7)-C(6)-C(5)	147.8(29)
Cl(2)-O(8)-O(6)	37.8(9)	Cl(2)-O(8)-O(7)	35.8(9)
O(6)-O(8)-O(7)	62.0(11)	Ru(2)-C(5)-C(6)	65.1(12)

INTRAMOLECULAR TORSION ANGLES (H omitted)

Minimum bond length= 1.10Å : Maximum bond length= 2.30Å			
N(1)-Ru(1)-C(1)-C(2)	-74.2(15)	N(1)-Ru(1)-C(4)-C(3)	99.0(17)
N(1)-Ru(1)-C(2)-C(1)	107.3(15)	N(1)-Ru(1)-C(2)-C(3)	-105.3(16)
N(1)-Ru(1)-C(3)-C(4)	-84.1(18)	N(1)-Ru(1)-C(3)-C(2)	76.3(15)
N(2)-Ru(1)-C(1)-C(2)	-162.1(16)	N(2)-Ru(1)-C(4)-C(3)	-166.5(67)
N(2)-Ru(1)-C(2)-C(1)	20.7(13)	N(2)-Ru(1)-C(2)-C(3)	168.1(18)
N(2)-Ru(1)-C(3)-C(4)	175.3(30)	N(2)-Ru(1)-C(3)-C(2)	-24.3(16)
N(4)-Ru(1)-C(1)-C(2)	111.7(16)	N(4)-Ru(1)-C(4)-C(3)	-87.8(18)
N(4)-Ru(1)-C(2)-C(1)	-70.7(15)	N(4)-Ru(1)-C(2)-C(3)	76.7(16)
N(4)-Ru(1)-C(3)-C(4)	93.0(18)	N(4)-Ru(1)-C(3)-C(2)	-106.6(15)
N(3)-Ru(1)-C(1)-C(2)	145.3(69)	N(3)-Ru(1)-C(4)-C(3)	-174.0(18)
N(3)-Ru(1)-C(2)-C(1)	-172.6(26)	N(3)-Ru(1)-C(2)-C(3)	-25.2(16)
N(3)-Ru(1)-C(3)-C(4)	6.7(16)	N(3)-Ru(1)-C(3)-C(2)	167.0(18)
C(4)-Ru(1)-C(1)-C(2)	19.8(17)	C(1)-Ru(1)-C(4)-C(3)	1.0(17)
C(1)-Ru(1)-C(2)-C(1)	0.0(15)	C(2)-Ru(1)-C(1)-C(2)	0.0(17)
C(1)-Ru(1)-C(2)-C(3)	147.4(24)	C(1)-Ru(1)-C(3)-C(4)	-178.9(20)
C(3)-Ru(1)-C(1)-C(2)	20.4(16)	C(1)-Ru(1)-C(3)-C(2)	-18.6(15)
C(4)-Ru(1)-C(2)-C(1)	-159.1(18)	C(2)-Ru(1)-C(4)-C(3)	12.2(17)
C(4)-Ru(1)-C(2)-C(3)	-11.7(16)	C(4)-Ru(1)-C(3)-C(4)	0.0(20)
C(4)-Ru(1)-C(3)-C(2)	160.3(27)	C(3)-Ru(1)-C(4)-C(3)	0.0(18)
C(3)-Ru(1)-C(2)-C(1)	-147.4(24)	C(2)-Ru(1)-C(3)-C(4)	-160.3(27)
C(2)-Ru(1)-C(3)-C(2)	0.0(16)	C(3)-Ru(1)-C(2)-C(3)	0.0(17)
N(5)-Ru(2)-C(8)-C(7)	93.2(18)	N(5)-Ru(2)-C(7)-C(8)	-89.7(17)
N(5)-Ru(2)-C(7)-C(6)	81.7(19)	N(5)-Ru(2)-C(6)-C(7)	-99.7(19)
N(5)-Ru(2)-C(6)-C(5)	99.7(15)	N(5)-Ru(2)-C(5)-C(6)	-81.9(16)
N(7)-Ru(2)-C(8)-C(7)	-178.9(18)	N(7)-Ru(2)-C(7)-C(8)	1.3(15)
N(7)-Ru(2)-C(7)-C(6)	172.7(23)	N(7)-Ru(2)-C(6)-C(7)	-14.4(18)
N(7)-Ru(2)-C(6)-C(5)	-175.1(29)	N(7)-Ru(2)-C(5)-C(6)	167.4(45)
N(8)-Ru(2)-C(8)-C(7)	-93.1(18)	N(8)-Ru(2)-C(7)-C(8)	89.5(17)
N(8)-Ru(2)-C(7)-C(6)	-99.0(19)	N(8)-Ru(2)-C(6)-C(7)	84.9(19)
N(8)-Ru(2)-C(6)-C(5)	-75.8(15)	N(8)-Ru(2)-C(5)-C(6)	106.7(16)
N(6)-Ru(2)-C(8)-C(7)	-171.1(59)	C(8)-Ru(2)-C(7)-C(8)	0.0(18)
C(7)-Ru(2)-C(8)-C(7)	0.0(20)	C(8)-Ru(2)-C(7)-C(6)	171.4(30)
C(6)-Ru(2)-C(8)-C(7)	5.0(18)	C(8)-Ru(2)-C(6)-C(7)	-5.4(19)
C(8)-Ru(2)-C(6)-C(5)	-166.0(18)	C(5)-Ru(2)-C(8)-C(7)	-3.1(17)
C(8)-Ru(2)-C(5)-C(6)	13.2(17)	N(6)-Ru(2)-C(7)-C(8)	176.8(31)
N(6)-Ru(2)-C(7)-C(6)	-11.8(17)	N(6)-Ru(2)-C(6)-C(7)	173.9(23)
N(6)-Ru(2)-C(6)-C(5)	13.2(12)	N(6)-Ru(2)-C(5)-C(6)	-168.7(16)
C(6)-Ru(2)-C(7)-C(8)	-171.4(30)	C(7)-Ru(2)-C(6)-C(7)	0.0(21)
C(6)-Ru(2)-C(7)-C(6)	0.0(20)	C(7)-Ru(2)-C(6)-C(5)	-160.6(28)
C(5)-Ru(2)-C(7)-C(8)	176.7(20)	C(5)-Ru(2)-C(7)-C(6)	-11.9(18)
C(7)-Ru(2)-C(5)-C(6)	11.3(17)	C(5)-Ru(2)-C(6)-C(7)	160.6(28)
C(6)-Ru(2)-C(5)-C(6)	0.0(19)	C(5)-Ru(2)-C(6)-C(5)	0.0(13)
O(1)-Cl(1)-O(2)-O(1)	0.0(12)	O(2)-Cl(1)-O(1)-O(2)	0.0(9)
O(2)-Cl(1)-O(1)-O(3)	-123.8(9)	O(2)-Cl(1)-O(1)-O(4)	115.4(10)
O(1)-Cl(1)-O(3)-O(1)	0.0(12)	O(3)-Cl(1)-O(1)-O(2)	123.8(9)
O(3)-Cl(1)-O(1)-O(3)	0.0(10)	O(3)-Cl(1)-O(1)-O(4)	-120.8(11)
O(1)-Cl(1)-O(4)-O(1)	0.0(12)	O(4)-Cl(1)-O(1)-O(2)	-115.4(10)
O(4)-Cl(1)-O(1)-O(3)	120.8(11)	O(4)-Cl(1)-O(1)-O(4)	0.0(12)

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O(3)-Cl(1)-O(2)-O(1)	-120.9(11)	O(2)-Cl(1)-O(3)-O(1)	121.2(10)
O(4)-Cl(1)-O(2)-O(1)	113.2(12)	O(2)-Cl(1)-O(4)-O(1)	-116.1(10)
O(4)-Cl(1)-O(3)-O(1)	-115.5(12)	O(3)-Cl(1)-O(4)-O(1)	117.7(11)
O(5)-Cl(2)-O(6)-O(5)	0.0(13)	O(6)-Cl(2)-O(5)-O(6)	0.0(14)
O(6)-Cl(2)-O(5)-O(7)	-122.5(16)	O(5)-Cl(2)-O(6)-O(7)	119.9(16)
O(5)-Cl(2)-O(6)-O(8)	-125.1(14)	O(5)-Cl(2)-O(7)-O(5)	0.0(13)
O(7)-Cl(2)-O(5)-O(6)	122.5(16)	O(5)-Cl(2)-O(7)-O(6)	-121.5(13)
O(7)-Cl(2)-O(5)-O(7)	0.0(18)	O(5)-Cl(2)-O(7)-O(8)	124.8(14)
O(8)-Cl(2)-O(5)-O(6)	-118.4(15)	O(5)-Cl(2)-O(8)-O(6)	121.7(13)
O(8)-Cl(2)-O(5)-O(7)	119.2(17)	O(5)-Cl(2)-O(8)-O(7)	-119.7(16)
O(7)-Cl(2)-O(6)-O(5)	-119.9(16)	O(6)-Cl(2)-O(7)-O(5)	121.5(13)
O(6)-Cl(2)-O(7)-O(6)	0.0(16)	O(7)-Cl(2)-O(6)-O(7)	0.0(19)
O(7)-Cl(2)-O(6)-O(8)	115.0(17)	O(6)-Cl(2)-O(7)-O(8)	-113.6(15)
O(8)-Cl(2)-O(6)-O(5)	125.1(14)	O(6)-Cl(2)-O(8)-O(6)	0.0(13)
O(8)-Cl(2)-O(6)-O(7)	-115.0(17)	O(6)-Cl(2)-O(8)-O(7)	118.7(15)
O(8)-Cl(2)-O(6)-O(8)	0.0(15)	O(8)-Cl(2)-O(7)-O(5)	-124.8(14)
O(8)-Cl(2)-O(7)-O(6)	113.6(15)	O(7)-Cl(2)-O(8)-O(6)	-118.7(15)
O(7)-Cl(2)-O(8)-O(7)	0.0(18)	O(8)-Cl(2)-O(7)-O(8)	0.0(16)
O(9)-Cl(3)-O(10)-O(9)	0.0(10)	O(10)-Cl(3)-O(9)-O(10)	0.0(11)
O(9)-Cl(3)-O(10)-O(11)	-122.8(11)	O(9)-Cl(3)-O(10)-O(12)	118.5(11)
O(11)-Cl(3)-O(9)-O(10)	-117.6(12)	O(9)-Cl(3)-O(11)-O(10)	115.4(11)
O(9)-Cl(3)-O(11)-O(12)	-132.5(12)	O(12)-Cl(3)-O(9)-O(10)	110.6(12)
O(9)-Cl(3)-O(12)-O(10)	-111.4(11)	O(9)-Cl(3)-O(12)-O(11)	133.3(12)
O(11)-Cl(3)-O(10)-O(9)	122.8(11)	O(10)-Cl(3)-O(11)-O(10)	0.0(12)
O(11)-Cl(3)-O(10)-O(11)	0.0(13)	O(11)-Cl(3)-O(10)-O(12)	-118.7(12)
O(10)-Cl(3)-O(11)-O(12)	112.1(13)	O(12)-Cl(3)-O(10)-O(9)	-118.5(11)
O(10)-Cl(3)-O(12)-O(10)	0.0(11)	O(12)-Cl(3)-O(10)-O(11)	118.7(12)
O(10)-Cl(3)-O(12)-O(11)	-115.3(12)	O(12)-Cl(3)-O(10)-O(12)	0.0(12)
O(12)-Cl(3)-O(11)-O(10)	-112.1(13)	O(11)-Cl(3)-O(12)-O(10)	115.3(12)
O(11)-Cl(3)-O(12)-O(11)	0.0(14)	O(12)-Cl(3)-O(11)-O(12)	0.0(14)
O(13)-Cl(4)-O(14)-O(15)	116.2(12)	O(13)-Cl(4)-O(15)-O(14)	-109.6(11)
O(14)-Cl(4)-O(15)-O(14)	0.0(10)	O(15)-Cl(4)-O(14)-O(15)	0.0(13)
O(16)-Cl(4)-O(14)-O(15)	-121.4(14)	O(16)-Cl(4)-O(15)-O(14)	110.9(14)
Cl(1)-O(1)-O(2)-Cl(1)	0.0(4)	Cl(1)-O(1)-O(3)-Cl(1)	0.0(4)
Cl(1)-O(1)-O(4)-Cl(1)	0.0(4)	O(3)-O(1)-O(2)-Cl(1)	33.4(7)
O(2)-O(1)-O(3)-Cl(1)	-33.5(7)	O(4)-O(1)-O(2)-Cl(1)	-39.8(8)
O(2)-O(1)-O(4)-Cl(1)	37.1(8)	O(4)-O(1)-O(3)-Cl(1)	36.8(9)
O(3)-O(1)-O(4)-Cl(1)	-34.3(8)	Cl(3)-O(9)-O(10)-Cl(3)	0.0(4)
Cl(3)-O(9)-O(10)-O(11)	32.9(8)	Cl(3)-O(9)-O(10)-O(12)	-36.9(8)
Ru(2)-C(8)-C(7)-Ru(2)	0.0(1)	Ru(2)-C(8)-C(7)-C(6)	-17.8(59)
Ru(1)-C(1)-C(2)-Ru(1)	0.0(1)	Ru(1)-C(1)-C(2)-C(3)	-46.0(30)
Cl(2)-O(5)-O(6)-Cl(2)	0.0(4)	Cl(2)-O(5)-O(6)-O(7)	-34.2(11)
Cl(2)-O(5)-O(6)-O(8)	34.2(10)	Cl(2)-O(5)-O(7)-Cl(2)	0.0(4)
Cl(2)-O(5)-O(7)-O(6)	33.6(11)	Cl(2)-O(5)-O(7)-O(8)	-33.6(11)
O(7)-O(5)-O(6)-Cl(2)	34.2(11)	O(6)-O(5)-O(7)-Cl(2)	-33.6(11)
O(6)-O(5)-O(7)-O(6)	0.0(8)	O(7)-O(5)-O(6)-O(7)	0.0(12)
O(7)-O(5)-O(6)-O(8)	68.4(12)	O(6)-O(5)-O(7)-O(8)	-67.2(11)
Cl(3)-O(10)-O(11)-Cl(3)	0.0(4)	Cl(3)-O(10)-O(11)-O(12)	-37.6(9)
Cl(3)-O(10)-O(12)-Cl(3)	0.0(4)	Cl(3)-O(10)-O(12)-O(11)	35.0(9)
O(9)-O(10)-O(11)-Cl(3)	-35.3(8)	O(9)-O(10)-O(11)-O(12)	-73.0(9)

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O(9)-O(10)-O(12)-Cl(3)	37.0(8)	O(9)-O(10)-O(12)-O(11)	72.0(8)
O(12)-O(10)-O(11)-Cl(3)	37.6(9)	O(11)-O(10)-O(12)-Cl(3)	-35.0(9)
O(11)-O(10)-O(12)-O(11)	0.0(8)	O(12)-O(10)-O(11)-O(12)	0.0(8)
Cl(3)-O(11)-O(12)-Cl(3)	0.0(4)	Cl(3)-O(11)-O(12)-O(10)	-41.6(10)
O(10)-O(11)-O(12)-Cl(3)	41.6(10)	O(10)-O(11)-O(12)-O(10)	0.0(8)
Cl(4)-O(14)-O(15)-Cl(4)	0.0(4)	Cl(2)-O(6)-O(7)-Cl(2)	0.0(4)
Cl(2)-O(6)-O(7)-O(5)	-35.6(11)	Cl(2)-O(6)-O(7)-O(8)	40.5(12)
Cl(2)-O(6)-O(8)-Cl(2)	0.0(4)	Cl(2)-O(6)-O(8)-O(7)	-35.5(11)
O(5)-O(6)-O(7)-Cl(2)	35.6(11)	O(5)-O(6)-O(7)-O(5)	0.0(8)
O(5)-O(6)-O(7)-O(8)	76.1(11)	O(5)-O(6)-O(8)-Cl(2)	-31.3(9)
O(5)-O(6)-O(8)-O(7)	-66.9(11)	O(8)-O(6)-O(7)-Cl(2)	-40.5(12)
O(7)-O(6)-O(8)-Cl(2)	35.5(11)	O(8)-O(6)-O(7)-O(5)	-76.1(11)
O(7)-O(6)-O(8)-O(7)	0.0(12)	O(8)-O(6)-O(7)-O(8)	0.0(11)
Cl(2)-O(7)-O(8)-Cl(2)	0.0(4)	Cl(2)-O(7)-O(8)-O(6)	37.5(11)
O(5)-O(7)-O(8)-Cl(2)	32.9(11)	O(5)-O(7)-O(8)-O(6)	70.4(10)
O(6)-O(7)-O(8)-Cl(2)	-37.5(11)	O(6)-O(7)-O(8)-O(6)	0.0(9)
Ru(1)-C(4)-C(3)-Ru(1)	0.0(1)	Ru(1)-C(4)-C(3)-C(2)	-35.5(42)
Ru(1)-C(2)-C(3)-Ru(1)	0.0(1)	Ru(1)-C(2)-C(3)-C(4)	36.3(44)
C(1)-C(2)-C(3)-Ru(1)	48.7(30)	C(1)-C(2)-C(3)-C(4)	84.9(56)
Ru(2)-C(7)-C(6)-Ru(2)	0.0(1)	Ru(2)-C(7)-C(6)-C(5)	37.8(48)
C(8)-C(7)-C(6)-Ru(2)	18.3(60)	C(8)-C(7)-C(6)-C(5)	56.1(65)
Ru(2)-C(6)-C(5)-Ru(2)	0.0(1)	C(7)-C(6)-C(5)-Ru(2)	-36.7(49)