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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{20}H_{26}O_8Ru$
Formula Weight	495.49
Crystal Color, Habit	yellow, prismatic
Crystal Dimensions	0.10 X 0.10 X 0.05 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	25 (29.4 - 30.0°)
Omega Scan Peak Width at Half-height	0.22°
Lattice Parameters	a = 7.816(5)Å b = 25.190(5) Å c = 11.050(6) Å β = 109.01(4)°
	V = 2056(1) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.600 g/cm^3
F_{000}	1016.00
μ(MoKα)	8.06 cm^{-1}

B. Intensity Measurements

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

Attenuator	Zr foil (factor = 8.40)
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	16.0°/min (in ω)
Scan Width	$(0.52 + 0.30 \tan\theta)°$
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 5088 Unique: 4852 (R_{int} = 0.026)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS-86)
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))	2892
No. Variables	288
Reflection/Parameter Ratio	10.04
Residuals: R; Rw	0.040 ; 0.041
Residuals: R1	0.000
No. of Reflections to calc R1	0

Goodness of Fit Indicator	0.66
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.40 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.40 $e^-/Å^3$

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

atom	x	y	z	B_{eq}
Ru	0.34750(5)	0.36829(2)	0.83668(4)	2.609(7)
O(1)	0.7587(6)	0.3916(2)	1.1207(4)	4.8(1)
O(2)	0.8349(6)	0.3207(2)	1.0277(4)	4.5(1)
O(3)	0.6345(6)	0.4519(2)	0.6810(4)	4.6(1)
O(4)	0.4501(6)	0.5056(2)	0.7431(4)	4.4(1)
O(5)	0.2238(6)	0.4158(2)	0.4933(4)	5.4(1)
O(6)	0.0709(7)	0.3411(2)	0.4932(5)	7.1(1)
O(7)	0.6714(6)	0.2760(2)	0.7349(5)	5.1(1)
O(8)	0.5055(7)	0.2322(2)	0.8350(5)	5.6(1)
C(1)	0.6379(7)	0.3800(2)	0.8927(5)	2.8(1)
C(2)	0.5471(7)	0.4301(2)	0.8636(5)	2.8(1)
C(3)	0.7441(6)	0.3661(3)	1.0244(5)	3.5(1)
C(4)	0.5507(8)	0.4618(2)	0.7529(6)	3.4(1)
C(5)	0.9553(10)	0.3033(3)	1.1510(7)	6.0(2)
C(6)	0.439(1)	0.5408(3)	0.6381(8)	5.8(2)
C(7)	0.3667(7)	0.3526(2)	0.6453(5)	3.3(1)
C(8)	0.3690(8)	0.3040(2)	0.7090(6)	3.7(1)
C(9)	0.2051(8)	0.3677(3)	0.5376(6)	4.4(1)
C(10)	0.5335(9)	0.2706(2)	0.7593(6)	4.1(1)
C(11)	0.074(1)	0.4373(4)	0.3887(8)	7.9(3)
C(12)	0.657(1)	0.1977(3)	0.8947(9)	7.1(2)
C(13)	0.3417(8)	0.3955(3)	1.0326(5)	3.7(1)
C(14)	0.3524(9)	0.3400(3)	1.0289(7)	4.6(2)
C(15)	0.214(1)	0.3115(3)	0.9362(8)	5.5(2)

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

atom	x	y	z	B_{eq}
C(16)	0.0776(9)	0.3313(3)	0.8262(8)	5.3(2)
C(17)	0.0454(7)	0.3808(3)	0.7591(7)	5.3(2)
C(18)	0.1279(8)	0.4308(3)	0.7906(6)	4.1(1)
C(19)	0.1356(9)	0.4626(3)	0.9069(7)	4.6(2)
C(20)	0.1702(9)	0.4261(3)	1.0200(6)	4.3(2)
H(1)	0.6983	0.3639	0.8345	2.3(4)
H(2)	0.5527	0.4539	0.9401	2.7(4)
H(3)	0.8851	0.2975	1.2065	8.6(2)
H(4)	1.0092	0.2705	1.1401	10.1(2)
H(5)	1.0439	0.3290	1.1855	8.7(2)
H(6)	0.3929	0.5225	0.5605	8.3(2)
H(7)	0.3669	0.5703	0.6413	5.5(3)
H(8)	0.5601	0.5530	0.6477	6.1(2)
H(9)	0.4710	0.3657	0.6153	4.0(3)
H(10)	0.2575	0.2804	0.6938	5.0(3)
H(11)	-0.0324	0.4402	0.4132	10.2(1)
H(12)	0.1030	0.4718	0.3649	17.54(8)
H(13)	0.0470	0.4147	0.3152	13.6(1)
H(14)	0.7017	0.1814	0.8337	6.6(2)
H(15)	0.6322	0.1727	0.9487	7.5(2)
H(16)	0.7594	0.2201	0.9493	12.0(1)
H(17)	0.4530	0.4124	1.0835	4.8(3)
H(18)	0.4624	0.3195	1.0806	5.9(3)
H(19)	0.2389	0.2749	0.9536	6.0(2)

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

atom	x	y	z	B_{eq}
H(20)	-0.0418	0.3012	0.7547	9.2(2)
H(21)	-0.0714	0.3755	0.6521	9.1(2)
H(22)	0.1287	0.4517	0.7108	3.8(3)
H(23)	0.2408	0.4884	0.9386	5.5(3)
H(24)	-0.0031	0.4891	0.8655	7.8(2)
H(25)	0.1959	0.4400	1.1193	3.0(4)
H(26)	0.0711	0.3942	1.0303	8.7(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	0.0288(2)	0.0321(2)	0.0407(2)	-0.0030(2)	0.0147(1)	-0.0062(2)
O(1)	0.053(2)	0.078(3)	0.044(2)	0.010(2)	0.005(2)	-0.004(2)
O(2)	0.057(3)	0.053(3)	0.063(3)	0.019(2)	0.024(2)	0.019(2)
O(3)	0.061(3)	0.061(3)	0.061(3)	0.007(2)	0.034(2)	0.011(2)
O(4)	0.066(3)	0.040(2)	0.065(3)	0.008(2)	0.027(2)	0.009(2)
O(5)	0.056(3)	0.084(4)	0.051(3)	0.003(3)	0.000(2)	0.008(3)
O(6)	0.060(3)	0.124(5)	0.068(3)	-0.033(3)	-0.004(3)	-0.018(3)
O(7)	0.059(3)	0.059(3)	0.088(3)	0.009(2)	0.042(3)	-0.005(3)
O(8)	0.082(3)	0.048(3)	0.099(4)	0.006(2)	0.051(3)	0.007(3)
C(1)	0.031(2)	0.036(3)	0.040(3)	-0.002(2)	0.014(2)	-0.001(2)
C(2)	0.031(3)	0.036(3)	0.040(3)	-0.008(2)	0.011(2)	-0.004(2)
C(3)	0.027(2)	0.054(3)	0.055(3)	-0.007(3)	0.016(2)	0.005(3)
C(4)	0.040(3)	0.034(3)	0.054(4)	-0.008(2)	0.014(3)	0.000(3)
C(5)	0.065(4)	0.089(6)	0.075(5)	0.029(4)	0.026(4)	0.048(4)
C(6)	0.086(5)	0.059(4)	0.080(5)	0.015(4)	0.032(4)	0.027(4)
C(7)	0.039(3)	0.048(3)	0.041(3)	-0.010(2)	0.016(2)	-0.018(2)
C(8)	0.047(3)	0.038(3)	0.062(4)	-0.007(3)	0.026(3)	-0.019(3)
C(9)	0.049(3)	0.072(4)	0.043(3)	-0.005(4)	0.012(3)	-0.013(4)
C(10)	0.061(4)	0.041(3)	0.061(4)	-0.005(3)	0.031(3)	-0.019(3)
C(11)	0.064(5)	0.153(9)	0.065(5)	0.024(5)	-0.003(4)	0.030(6)
C(12)	0.124(7)	0.054(4)	0.099(7)	0.033(5)	0.048(6)	0.012(4)
C(13)	0.046(3)	0.058(4)	0.040(3)	-0.004(3)	0.019(3)	-0.003(3)
C(14)	0.057(4)	0.057(4)	0.077(5)	0.009(3)	0.046(4)	0.020(4)
C(15)	0.086(5)	0.042(4)	0.110(6)	-0.008(4)	0.074(5)	0.001(4)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(16)	0.052(4)	0.062(4)	0.104(6)	-0.025(3)	0.051(4)	-0.036(4)
C(17)	0.022(3)	0.087(6)	0.089(5)	-0.002(3)	0.014(3)	-0.030(4)
C(18)	0.037(3)	0.070(4)	0.049(4)	0.012(3)	0.013(3)	0.001(3)
C(19)	0.053(4)	0.056(4)	0.066(4)	0.010(3)	0.018(3)	-0.014(3)
C(20)	0.054(4)	0.059(4)	0.061(4)	0.005(3)	0.030(3)	-0.012(3)

The general temperature factor expression:

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

Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ru	C(1)	2.169(5)	Ru	C(2)	2.155(5)
Ru	C(7)	2.204(5)	Ru	C(8)	2.190(5)
Ru	C(13)	2.285(6)	Ru	C(14)	2.229(6)
Ru	C(15)	2.256(6)	Ru	C(16)	2.274(6)
Ru	C(17)	2.256(6)	Ru	C(18)	2.261(6)
O(1)	C(3)	1.216(7)	O(2)	C(3)	1.341(7)
O(2)	C(5)	1.449(8)	O(3)	C(4)	1.209(7)
O(4)	C(4)	1.337(7)	O(4)	C(6)	1.441(8)
O(5)	C(9)	1.334(8)	O(5)	C(11)	1.454(8)
O(6)	C(9)	1.207(7)	O(7)	C(10)	1.201(7)
O(8)	C(10)	1.343(8)	O(8)	C(12)	1.440(9)
C(1)	C(2)	1.431(7)	C(1)	C(3)	1.464(7)
C(1)	H(1)	1.000(5)	C(2)	C(4)	1.469(8)
C(2)	H(2)	1.026(5)	C(5)	H(3)	0.957(7)
C(5)	H(4)	0.953(8)	C(5)	H(5)	0.934(9)
C(6)	H(6)	0.936(8)	C(6)	H(7)	0.942(7)
C(6)	H(8)	0.966(8)	C(7)	C(8)	1.408(8)
C(7)	C(9)	1.475(8)	C(7)	H(9)	1.030(5)
C(8)	C(10)	1.486(8)	C(8)	H(10)	1.023(6)
C(11)	H(11)	0.958(9)	C(11)	H(12)	0.96(1)
C(11)	H(13)	0.96(1)	C(12)	H(14)	0.950(8)
C(12)	H(15)	0.929(9)	C(12)	H(16)	1.005(10)
C(13)	C(14)	1.401(8)	C(13)	C(20)	1.513(8)
C(13)	H(17)	0.968(6)	C(14)	C(15)	1.42(1)

Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(14)	H(18)	1.006(7)	C(15)	C(16)	1.42(1)
C(15)	H(19)	0.949(7)	C(16)	C(17)	1.43(1)
C(16)	H(20)	1.261(7)	C(17)	C(18)	1.407(9)
C(17)	H(21)	1.243(7)	C(18)	C(19)	1.498(9)
C(18)	H(22)	1.029(6)	C(19)	C(20)	1.503(9)
C(19)	H(23)	1.016(7)	C(19)	H(24)	1.227(6)
C(20)	H(25)	1.106(6)	C(20)	H(26)	1.149(7)

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Ru	C(2)	38.7(2)	C(1)	Ru	C(7)	84.6(2)
C(1)	Ru	C(8)	89.5(2)	C(1)	Ru	C(13)	91.8(2)
C(1)	Ru	C(14)	94.6(2)	C(1)	Ru	C(15)	123.7(3)
C(1)	Ru	C(16)	159.6(3)	C(1)	Ru	C(17)	163.2(2)
C(1)	Ru	C(18)	128.0(2)	C(2)	Ru	C(7)	89.4(2)
C(2)	Ru	C(8)	114.8(2)	C(2)	Ru	C(13)	83.7(2)
C(2)	Ru	C(14)	108.2(2)	C(2)	Ru	C(15)	145.1(3)
C(2)	Ru	C(16)	157.1(2)	C(2)	Ru	C(17)	124.9(2)
C(2)	Ru	C(18)	89.4(2)	C(7)	Ru	C(8)	37.4(2)
C(7)	Ru	C(13)	172.5(2)	C(7)	Ru	C(14)	150.6(2)
C(7)	Ru	C(15)	122.7(2)	C(7)	Ru	C(16)	103.3(2)
C(7)	Ru	C(17)	92.9(2)	C(7)	Ru	C(18)	101.1(2)
C(8)	Ru	C(13)	149.5(2)	C(8)	Ru	C(14)	113.4(3)
C(8)	Ru	C(15)	89.4(2)	C(8)	Ru	C(16)	85.9(2)
C(8)	Ru	C(17)	98.5(2)	C(8)	Ru	C(18)	125.6(2)
C(13)	Ru	C(14)	36.1(2)	C(13)	Ru	C(15)	64.7(2)
C(13)	Ru	C(16)	82.3(2)	C(13)	Ru	C(17)	88.7(2)
C(13)	Ru	C(18)	75.9(2)	C(14)	Ru	C(15)	36.9(3)
C(14)	Ru	C(16)	69.2(3)	C(14)	Ru	C(17)	95.6(3)
C(14)	Ru	C(18)	102.3(2)	C(15)	Ru	C(16)	36.5(3)
C(15)	Ru	C(17)	71.4(3)	C(15)	Ru	C(18)	96.5(3)
C(16)	Ru	C(17)	36.8(3)	C(16)	Ru	C(18)	69.6(3)
C(17)	Ru	C(18)	36.3(2)	C(3)	O(2)	C(5)	117.4(5)
C(4)	O(4)	C(6)	116.8(5)	C(9)	O(5)	C(11)	118.3(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(10)	O(8)	C(12)	116.4(6)	Ru	C(1)	C(2)	70.1(3)
Ru	C(1)	C(3)	116.9(3)	Ru	C(1)	H(1)	115.5(4)
C(2)	C(1)	C(3)	120.9(5)	C(2)	C(1)	H(1)	121.1(5)
C(3)	C(1)	H(1)	108.0(5)	Ru	C(2)	C(1)	71.2(3)
Ru	C(2)	C(4)	119.2(4)	Ru	C(2)	H(2)	111.8(3)
C(1)	C(2)	C(4)	121.6(5)	C(1)	C(2)	H(2)	116.4(5)
C(4)	C(2)	H(2)	111.1(5)	O(1)	C(3)	O(2)	121.9(5)
O(1)	C(3)	C(1)	127.2(6)	O(2)	C(3)	C(1)	110.8(5)
O(3)	C(4)	O(4)	123.2(6)	O(3)	C(4)	C(2)	126.5(5)
O(4)	C(4)	C(2)	110.3(5)	O(2)	C(5)	H(3)	108.4(6)
O(2)	C(5)	H(4)	108.8(7)	O(2)	C(5)	H(5)	110.0(6)
H(3)	C(5)	H(4)	108.6(7)	H(3)	C(5)	H(5)	110.3(9)
H(4)	C(5)	H(5)	110.7(7)	O(4)	C(6)	H(6)	109.8(6)
O(4)	C(6)	H(7)	109.5(7)	O(4)	C(6)	H(8)	108.0(6)
H(6)	C(6)	H(7)	111.4(8)	H(6)	C(6)	H(8)	109.3(8)
H(7)	C(6)	H(8)	108.8(7)	Ru	C(7)	C(8)	70.8(3)
Ru	C(7)	C(9)	114.8(4)	Ru	C(7)	H(9)	124.0(4)
C(8)	C(7)	C(9)	119.7(5)	C(8)	C(7)	H(9)	123.9(5)
C(9)	C(7)	H(9)	102.5(5)	Ru	C(8)	C(7)	71.9(3)
Ru	C(8)	C(10)	114.6(4)	Ru	C(8)	H(10)	107.2(4)
C(7)	C(8)	C(10)	123.2(5)	C(7)	C(8)	H(10)	123.5(6)
C(10)	C(8)	H(10)	108.6(5)	O(5)	C(9)	O(6)	122.7(6)
O(5)	C(9)	C(7)	111.3(5)	O(6)	C(9)	C(7)	125.9(7)
O(7)	C(10)	O(8)	124.2(6)	O(7)	C(10)	C(8)	125.6(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
O(8)	C(10)	C(8)	110.2(6)	O(5)	C(11)	H(11)	110.6(7)
O(5)	C(11)	H(12)	110.9(8)	O(5)	C(11)	H(13)	110.6(8)
H(11)	C(11)	H(12)	108.2(9)	H(11)	C(11)	H(13)	108.1(9)
H(12)	C(11)	H(13)	108.3(8)	O(8)	C(12)	H(14)	111.9(8)
O(8)	C(12)	H(15)	113.2(8)	O(8)	C(12)	H(16)	108.3(6)
H(14)	C(12)	H(15)	111.3(7)	H(14)	C(12)	H(16)	105.0(9)
H(15)	C(12)	H(16)	106.6(9)	Ru	C(13)	C(14)	69.7(4)
Ru	C(13)	C(20)	110.8(4)	Ru	C(13)	H(17)	113.0(4)
C(14)	C(13)	C(20)	124.5(6)	C(14)	C(13)	H(17)	114.0(6)
C(20)	C(13)	H(17)	115.4(6)	Ru	C(14)	C(13)	74.1(4)
Ru	C(14)	C(15)	72.6(4)	Ru	C(14)	H(18)	116.9(4)
C(13)	C(14)	C(15)	119.1(6)	C(13)	C(14)	H(18)	123.0(7)
C(15)	C(14)	H(18)	117.3(7)	Ru	C(15)	C(14)	70.5(3)
Ru	C(15)	C(16)	72.4(4)	Ru	C(15)	H(19)	128.2(5)
C(14)	C(15)	C(16)	128.6(6)	C(14)	C(15)	H(19)	106.7(8)
C(16)	C(15)	H(19)	124.1(8)	Ru	C(16)	C(15)	71.0(3)
Ru	C(16)	C(17)	70.9(3)	Ru	C(16)	H(20)	139.7(4)
C(15)	C(16)	C(17)	134.9(6)	C(15)	C(16)	H(20)	121.5(7)
C(17)	C(16)	H(20)	103.3(7)	Ru	C(17)	C(16)	72.3(4)
Ru	C(17)	C(18)	72.1(3)	Ru	C(17)	H(21)	134.4(4)
C(16)	C(17)	C(18)	131.5(6)	C(16)	C(17)	H(21)	110.6(6)
C(18)	C(17)	H(21)	117.8(7)	Ru	C(18)	C(17)	71.6(4)
Ru	C(18)	C(19)	111.4(4)	Ru	C(18)	H(22)	109.4(4)
C(17)	C(18)	C(19)	125.4(6)	C(17)	C(18)	H(22)	112.0(6)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(19)	C(18)	H(22)	116.9(6)	C(18)	C(19)	C(20)	109.4(5)
C(18)	C(19)	H(23)	116.0(6)	C(18)	C(19)	H(24)	100.8(5)
C(20)	C(19)	H(23)	101.4(6)	C(20)	C(19)	H(24)	122.7(6)
H(23)	C(19)	H(24)	107.4(5)	C(13)	C(20)	C(19)	107.6(5)
C(13)	C(20)	H(25)	101.6(5)	C(13)	C(20)	H(26)	103.8(5)
C(19)	C(20)	H(25)	123.9(6)	C(19)	C(20)	H(26)	124.5(6)
H(25)	C(20)	H(26)	91.9(5)				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru	C(1)	C(2)	C(4)	-113.3(5)	Ru	C(1)	C(3)	O(1)	-76.9(7)
Ru	C(1)	C(3)	O(2)	105.7(4)	Ru	C(2)	C(1)	C(3)	-110.2(4)
Ru	C(2)	C(4)	O(3)	-89.3(7)	Ru	C(2)	C(4)	O(4)	92.5(5)
Ru	C(7)	C(8)	C(10)	-108.1(5)	Ru	C(7)	C(9)	O(5)	95.8(5)
Ru	C(7)	C(9)	O(6)	-83.9(7)	Ru	C(8)	C(7)	C(9)	-108.2(5)
Ru	C(8)	C(10)	O(7)	-96.3(7)	Ru	C(8)	C(10)	O(8)	85.0(5)
Ru	C(13)	C(14)	C(15)	-59.1(5)	Ru	C(13)	C(20)	C(19)	-42.3(6)
Ru	C(14)	C(13)	C(20)	101.9(6)	Ru	C(14)	C(15)	C(16)	-46.2(6)
Ru	C(15)	C(14)	C(13)	59.8(5)	Ru	C(15)	C(16)	C(17)	-33.9(8)
Ru	C(16)	C(15)	C(14)	45.5(6)	Ru	C(16)	C(17)	C(18)	-44.4(7)
Ru	C(17)	C(16)	C(15)	33.9(8)	Ru	C(17)	C(18)	C(19)	-103.6(6)
Ru	C(18)	C(17)	C(16)	44.5(7)	Ru	C(18)	C(19)	C(20)	-42.1(6)
O(1)	C(3)	O(2)	C(5)	-1.2(8)	O(1)	C(3)	C(1)	C(2)	5.1(8)
O(2)	C(3)	C(1)	C(2)	-172.4(4)	O(3)	C(4)	O(4)	C(6)	2.1(9)
O(3)	C(4)	C(2)	C(1)	-4.4(9)	O(4)	C(4)	C(2)	C(1)	177.4(5)
O(5)	C(9)	C(7)	C(8)	177.0(5)	O(6)	C(9)	O(5)	C(11)	1(1)
O(6)	C(9)	C(7)	C(8)	-2.8(10)	O(7)	C(10)	O(8)	C(12)	3.5(9)
O(7)	C(10)	C(8)	C(7)	-12.5(10)	O(8)	C(10)	C(8)	C(7)	168.7(5)
C(1)	Ru	C(2)	C(4)	116.4(5)	C(1)	Ru	C(7)	C(8)	96.3(3)
C(1)	Ru	C(7)	C(9)	-149.1(5)	C(1)	Ru	C(8)	C(7)	-81.7(3)
C(1)	Ru	C(8)	C(10)	37.2(5)	C(1)	Ru	C(13)	C(14)	-95.4(4)
C(1)	Ru	C(13)	C(20)	144.3(4)	C(1)	Ru	C(14)	C(13)	86.7(4)
C(1)	Ru	C(14)	C(15)	-145.1(4)	C(1)	Ru	C(15)	C(14)	43.3(5)
C(1)	Ru	C(15)	C(16)	-173.0(3)	C(1)	Ru	C(16)	C(15)	17.0(8)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(1)	Ru	C(16)	C(17)	172.3(5)	C(1)	Ru	C(17)	C(16)	-170.6(7)
C(1)	Ru	C(17)	C(18)	-24(1)	C(1)	Ru	C(18)	C(17)	171.4(4)
C(1)	Ru	C(18)	C(19)	-66.9(5)	C(1)	C(2)	Ru	C(7)	-82.1(3)
C(1)	C(2)	Ru	C(8)	-53.8(4)	C(1)	C(2)	Ru	C(13)	100.8(3)
C(1)	C(2)	Ru	C(14)	73.9(3)	C(1)	C(2)	Ru	C(15)	76.1(5)
C(1)	C(2)	Ru	C(16)	153.5(6)	C(1)	C(2)	Ru	C(17)	-175.2(3)
C(1)	C(2)	Ru	C(18)	176.7(3)	C(1)	C(3)	O(2)	C(5)	176.4(5)
C(2)	Ru	C(1)	C(3)	115.4(5)	C(2)	Ru	C(7)	C(8)	134.7(3)
C(2)	Ru	C(7)	C(9)	-110.6(5)	C(2)	Ru	C(8)	C(7)	-51.5(4)
C(2)	Ru	C(8)	C(10)	67.5(5)	C(2)	Ru	C(13)	C(14)	-133.2(4)
C(2)	Ru	C(13)	C(20)	106.4(4)	C(2)	Ru	C(14)	C(13)	49.7(4)
C(2)	Ru	C(14)	C(15)	177.9(4)	C(2)	Ru	C(15)	C(14)	-3.5(6)
C(2)	Ru	C(15)	C(16)	140.3(4)	C(2)	Ru	C(16)	C(15)	-110.1(7)
C(2)	Ru	C(16)	C(17)	45.2(9)	C(2)	Ru	C(17)	C(16)	-160.3(4)
C(2)	Ru	C(17)	C(18)	-13.7(5)	C(2)	Ru	C(18)	C(17)	168.8(4)
C(2)	Ru	C(18)	C(19)	-69.5(5)	C(2)	C(1)	Ru	C(7)	95.8(3)
C(2)	C(1)	Ru	C(8)	132.9(3)	C(2)	C(1)	Ru	C(13)	-77.6(3)
C(2)	C(1)	Ru	C(14)	-113.7(3)	C(2)	C(1)	Ru	C(15)	-138.1(3)
C(2)	C(1)	Ru	C(16)	-150.1(6)	C(2)	C(1)	Ru	C(17)	13.6(9)
C(2)	C(1)	Ru	C(18)	-4.2(4)	C(2)	C(4)	O(4)	C(6)	-179.6(5)
C(3)	C(1)	Ru	C(7)	-148.8(4)	C(3)	C(1)	Ru	C(8)	-111.7(4)
C(3)	C(1)	Ru	C(13)	37.8(4)	C(3)	C(1)	Ru	C(14)	1.7(5)
C(3)	C(1)	Ru	C(15)	-22.7(5)	C(3)	C(1)	Ru	C(16)	-34.8(8)
C(3)	C(1)	Ru	C(17)	129.0(8)	C(3)	C(1)	Ru	C(18)	111.2(4)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(3)	C(1)	C(2)	C(4)	136.5(5)	C(4)	C(2)	Ru	C(7)	34.3(4)
C(4)	C(2)	Ru	C(8)	62.6(5)	C(4)	C(2)	Ru	C(13)	-142.8(4)
C(4)	C(2)	Ru	C(14)	-169.7(4)	C(4)	C(2)	Ru	C(15)	-167.5(4)
C(4)	C(2)	Ru	C(16)	-90.1(8)	C(4)	C(2)	Ru	C(17)	-58.8(5)
C(4)	C(2)	Ru	C(18)	-66.9(4)	C(7)	Ru	C(8)	C(10)	119.0(6)
C(7)	Ru	C(13)	C(14)	-156(1)	C(7)	Ru	C(13)	C(20)	83(1)
C(7)	Ru	C(14)	C(13)	173.9(4)	C(7)	Ru	C(14)	C(15)	-57.9(6)
C(7)	Ru	C(15)	C(14)	150.4(4)	C(7)	Ru	C(15)	C(16)	-65.8(4)
C(7)	Ru	C(16)	C(15)	127.9(4)	C(7)	Ru	C(16)	C(17)	-76.8(4)
C(7)	Ru	C(17)	C(16)	108.4(4)	C(7)	Ru	C(17)	C(18)	-105.0(4)
C(7)	Ru	C(18)	C(17)	79.5(4)	C(7)	Ru	C(18)	C(19)	-158.8(4)
C(7)	C(8)	Ru	C(13)	-174.4(4)	C(7)	C(8)	Ru	C(14)	-176.5(3)
C(7)	C(8)	Ru	C(15)	154.6(4)	C(7)	C(8)	Ru	C(16)	118.2(4)
C(7)	C(8)	Ru	C(17)	83.5(4)	C(7)	C(8)	Ru	C(18)	57.0(4)
C(7)	C(9)	O(5)	C(11)	-178.5(6)	C(8)	Ru	C(7)	C(9)	114.6(6)
C(8)	Ru	C(13)	C(14)	-3.3(6)	C(8)	Ru	C(13)	C(20)	-123.6(5)
C(8)	Ru	C(14)	C(13)	178.2(4)	C(8)	Ru	C(14)	C(15)	-53.6(4)
C(8)	Ru	C(15)	C(14)	132.4(4)	C(8)	Ru	C(15)	C(16)	-83.9(4)
C(8)	Ru	C(16)	C(15)	94.6(4)	C(8)	Ru	C(16)	C(17)	-110.1(4)
C(8)	Ru	C(17)	C(16)	71.3(4)	C(8)	Ru	C(17)	C(18)	-142.1(4)
C(8)	Ru	C(18)	C(17)	48.3(5)	C(8)	Ru	C(18)	C(19)	170.0(4)
C(8)	C(7)	Ru	C(13)	157(1)	C(8)	C(7)	Ru	C(14)	6.5(6)
C(8)	C(7)	Ru	C(15)	-30.7(5)	C(8)	C(7)	Ru	C(16)	-64.6(4)
C(8)	C(7)	Ru	C(17)	-100.3(4)	C(8)	C(7)	Ru	C(18)	-136.0(3)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(8)	C(10)	O(8)	C(12)	-177.7(6)	C(9)	C(7)	Ru	C(13)	-87(1)
C(9)	C(7)	Ru	C(14)	121.1(6)	C(9)	C(7)	Ru	C(15)	84.0(5)
C(9)	C(7)	Ru	C(16)	50.1(5)	C(9)	C(7)	Ru	C(17)	14.3(5)
C(9)	C(7)	Ru	C(18)	-21.3(5)	C(9)	C(7)	C(8)	C(10)	143.7(6)
C(10)	C(8)	Ru	C(13)	-55.5(6)	C(10)	C(8)	Ru	C(14)	-57.6(5)
C(10)	C(8)	Ru	C(15)	-86.4(5)	C(10)	C(8)	Ru	C(16)	-122.8(5)
C(10)	C(8)	Ru	C(17)	-157.5(5)	C(10)	C(8)	Ru	C(18)	175.9(4)
C(13)	Ru	C(14)	C(15)	128.2(6)	C(13)	Ru	C(15)	C(14)	-30.8(4)
C(13)	Ru	C(15)	C(16)	112.9(4)	C(13)	Ru	C(16)	C(15)	-57.2(4)
C(13)	Ru	C(16)	C(17)	98.1(4)	C(13)	Ru	C(17)	C(16)	-78.9(4)
C(13)	Ru	C(17)	C(18)	67.7(4)	C(13)	Ru	C(18)	C(17)	-107.5(4)
C(13)	Ru	C(18)	C(19)	14.1(4)	C(13)	C(14)	Ru	C(15)	-128.2(6)
C(13)	C(14)	Ru	C(16)	-106.1(4)	C(13)	C(14)	Ru	C(17)	-80.0(4)
C(13)	C(14)	Ru	C(18)	-43.8(4)	C(13)	C(14)	C(15)	C(16)	13(1)
C(13)	C(20)	C(19)	C(18)	55.6(7)	C(14)	Ru	C(13)	C(20)	-120.3(6)
C(14)	Ru	C(15)	C(16)	143.7(6)	C(14)	Ru	C(16)	C(15)	-22.3(4)
C(14)	Ru	C(16)	C(17)	133.0(4)	C(14)	Ru	C(17)	C(16)	-43.4(4)
C(14)	Ru	C(17)	C(18)	103.2(4)	C(14)	Ru	C(18)	C(17)	-82.6(5)
C(14)	Ru	C(18)	C(19)	39.0(5)	C(14)	C(13)	Ru	C(15)	31.4(4)
C(14)	C(13)	Ru	C(16)	65.0(4)	C(14)	C(13)	Ru	C(17)	101.4(4)
C(14)	C(13)	Ru	C(18)	135.8(4)	C(14)	C(13)	C(20)	C(19)	-121.5(7)
C(14)	C(15)	Ru	C(16)	-143.7(6)	C(14)	C(15)	Ru	C(17)	-128.4(4)
C(14)	C(15)	Ru	C(18)	-101.9(4)	C(14)	C(15)	C(16)	C(17)	11(1)
C(15)	Ru	C(13)	C(20)	-88.9(5)	C(15)	Ru	C(16)	C(17)	155.3(6)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(15)	Ru	C(17)	C(16)	-15.2(4)	C(15)	Ru	C(17)	C(18)	131.4(5)
C(15)	Ru	C(18)	C(17)	-45.7(5)	C(15)	Ru	C(18)	C(19)	76.0(5)
C(15)	C(14)	Ru	C(16)	22.1(4)	C(15)	C(14)	Ru	C(17)	48.2(4)
C(15)	C(14)	Ru	C(18)	84.4(4)	C(15)	C(14)	C(13)	C(20)	42.9(9)
C(15)	C(16)	Ru	C(17)	-155.3(6)	C(15)	C(16)	Ru	C(18)	-134.9(4)
C(15)	C(16)	C(17)	C(18)	-10(1)	C(16)	Ru	C(13)	C(20)	-55.3(5)
C(16)	Ru	C(17)	C(18)	146.6(6)	C(16)	Ru	C(18)	C(17)	-20.6(4)
C(16)	Ru	C(18)	C(19)	101.1(5)	C(16)	C(15)	Ru	C(17)	15.3(4)
C(16)	C(15)	Ru	C(18)	41.9(4)	C(16)	C(17)	Ru	C(18)	-146.6(6)
C(16)	C(17)	C(18)	C(19)	-59.1(10)	C(17)	Ru	C(13)	C(20)	-18.9(5)
C(17)	Ru	C(18)	C(19)	121.7(7)	C(17)	C(16)	Ru	C(18)	20.3(4)
C(17)	C(18)	C(19)	C(20)	40.0(8)	C(18)	Ru	C(13)	C(20)	15.4(4)

Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
O(1)	H(13)	2.623(4)	65601	O(1)	H(26)	2.924(5)	65501
O(1)	H(23)	3.094(5)	66703	O(1)	H(14)	3.132(5)	4
O(1)	H(7)	3.238(4)	66703	O(1)	H(11)	3.342(4)	65601
O(1)	C(11)	3.379(10)	65601	O(1)	H(24)	3.537(5)	66703
O(2)	H(26)	2.607(4)	65501	O(2)	C(16)	3.373(8)	65501
O(2)	C(15)	3.436(8)	65501	O(2)	H(20)	3.488(4)	65501
O(3)	H(6)	2.685(4)	66603	O(3)	H(12)	2.973(4)	66603
O(3)	H(24)	3.049(5)	65501	O(3)	H(21)	3.093(4)	65501
O(3)	C(6)	3.387(9)	66603	O(3)	H(8)	3.453(4)	66603
O(3)	H(25)	3.485(5)	66703	O(3)	C(17)	3.530(8)	65501
O(4)	H(17)	2.751(4)	66703	O(4)	H(25)	3.018(5)	66703
O(4)	H(11)	3.440(5)	56603	O(4)	C(13)	3.518(7)	66703
O(4)	H(23)	3.563(5)	66703	O(5)	H(8)	2.758(5)	66603
O(5)	C(6)	3.567(9)	66603	O(5)	H(6)	3.591(5)	66603
O(6)	H(16)	2.786(5)	45404	O(6)	H(14)	2.905(5)	45404
O(6)	C(12)	3.21(1)	45404	O(6)	H(3)	3.217(5)	45401
O(6)	H(19)	3.290(6)	55404	O(6)	H(15)	3.319(6)	45404
O(6)	H(5)	3.351(5)	45401	O(6)	H(4)	3.357(6)	45404
O(7)	H(20)	2.271(5)	65501	O(7)	H(3)	2.580(4)	55404
O(7)	H(18)	3.088(5)	55404	O(7)	C(16)	3.309(8)	65501
O(7)	C(5)	3.332(9)	55404	O(7)	H(15)	3.337(5)	55404
O(7)	H(4)	3.352(4)	55404	O(7)	H(16)	3.443(5)	55404
O(7)	H(21)	3.516(5)	65501	O(8)	H(18)	3.015(5)	55404
C(1)	H(26)	3.248(5)	65501	C(2)	H(23)	3.064(5)	66703

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(3)	H(26)	2.631(5)	65501	C(3)	H(13)	3.531(6)	65601
C(4)	H(25)	3.196(5)	66703	C(4)	H(24)	3.370(6)	65501
C(4)	H(23)	3.497(6)	66703	C(5)	H(20)	2.867(7)	65504
C(5)	H(26)	2.937(7)	65501	C(5)	H(10)	3.085(7)	65504
C(5)	H(14)	3.280(8)	4	C(5)	H(13)	3.292(9)	65601
C(5)	C(15)	3.591(10)	65501	C(6)	H(11)	3.081(8)	56603
C(6)	H(17)	3.143(8)	66703	C(6)	H(25)	3.252(8)	66703
C(6)	H(6)	3.308(8)	66603	C(6)	H(15)	3.453(7)	65602
C(7)	H(15)	3.518(5)	55404	C(8)	H(4)	3.258(6)	45404
C(8)	H(19)	3.329(6)	55404	C(8)	H(18)	3.591(5)	55404
C(10)	H(18)	2.938(6)	55404	C(10)	H(20)	3.424(7)	65501
C(10)	H(3)	3.447(6)	55404	C(10)	H(19)	3.600(6)	55404
C(11)	H(8)	3.023(9)	66603	C(11)	H(22)	3.227(9)	56603
C(11)	H(24)	3.260(9)	56603	C(11)	H(7)	3.359(9)	56603
C(11)	H(25)	3.409(9)	55401	C(11)	H(5)	3.49(1)	45401
C(12)	H(3)	3.155(9)	55404	C(12)	H(7)	3.233(8)	64602
C(12)	H(18)	3.332(9)	55404	C(12)	H(21)	3.475(8)	65504
C(12)	H(9)	3.592(9)	4	C(14)	H(5)	3.407(6)	45501
C(15)	H(4)	3.326(6)	45501	C(15)	H(5)	3.455(7)	45501
C(15)	H(10)	3.599(7)	4	C(16)	H(1)	3.106(7)	45501
C(16)	H(4)	3.220(6)	45404	C(17)	H(1)	3.116(6)	45501
C(18)	H(12)	3.195(6)	56603	C(19)	H(2)	3.245(7)	66703
C(19)	H(24)	3.252(7)	56703	C(19)	H(12)	3.402(7)	56603
C(19)	H(25)	3.512(6)	56703	C(20)	H(24)	2.991(6)	56703

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
C(20)	H(5)	3.389(7)	45501	H(1)	H(20)	2.926(1)	65501
H(1)	H(26)	3.106(1)	65501	H(1)	H(21)	3.1226(9)	65501
H(2)	H(23)	2.2598(5)	66703	H(2)	H(2)	2.9208(2)	66703
H(2)	H(17)	3.38	66703	H(2)	H(25)	3.5036(8)	66703
H(3)	H(14)	2.3716(7)	4	H(3)	H(20)	2.5685(1)	65504
H(3)	H(16)	3.1752(4)	4	H(3)	H(13)	3.2802(2)	65601
H(3)	H(10)	3.551(2)	65504	H(4)	H(10)	2.239(1)	65504
H(4)	H(20)	2.3128(1)	65504	H(4)	H(19)	3.1455(9)	65501
H(4)	H(26)	3.4343(1)	65501	H(4)	H(19)	3.5323(2)	65504
H(5)	H(26)	2.43	65501	H(5)	H(13)	2.59	65601
H(5)	H(10)	3.2071(6)	65504	H(5)	H(25)	3.2145(3)	65501
H(5)	H(20)	3.4805(1)	65504	H(5)	H(14)	3.572(2)	4
H(6)	H(6)	2.7073(9)	66603	H(6)	H(11)	3.073(2)	56603
H(6)	H(8)	3.0967(1)	66603	H(7)	H(11)	2.498(2)	56603
H(7)	H(15)	2.77	65602	H(7)	H(14)	2.8813(1)	65602
H(7)	H(17)	2.9380(1)	66703	H(7)	H(13)	3.442(2)	56603
H(7)	H(21)	3.5822(5)	56603	H(7)	H(25)	3.585(2)	66703
H(8)	H(25)	2.6645(5)	66703	H(8)	H(12)	2.753(2)	66603
H(8)	H(13)	3.073(2)	66603	H(8)	H(17)	3.13	66703
H(8)	H(15)	3.3825(3)	65602	H(8)	H(9)	3.50	66603
H(9)	H(15)	2.7254(6)	55404	H(9)	H(21)	3.474(2)	65501
H(10)	H(19)	2.96	55404	H(10)	H(18)	3.4299(6)	55404
H(11)	H(22)	3.03	56603	H(11)	H(12)	3.4811(1)	56603
H(11)	H(11)	3.52	56603	H(12)	H(22)	2.5904(7)	56603

Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distance	ADC
H(12)	H(24)	2.60	56603	H(12)	H(25)	3.1332(2)	55401
H(13)	H(25)	2.8444(5)	55401	H(13)	H(24)	3.09	56603
H(13)	H(26)	3.26	55401	H(14)	H(18)	2.8131(4)	55404
H(15)	H(21)	2.9158(8)	65504	H(15)	H(20)	3.5704(7)	65504
H(16)	H(21)	3.2616(2)	65504	H(16)	H(20)	3.2670(1)	65504
H(17)	H(23)	3.523(1)	66703	H(23)	H(24)	3.3290(9)	56703
H(24)	H(25)	2.3791(6)	56703	H(24)	H(24)	3.01	56703
H(24)	H(26)	3.2644(1)	56703				

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ± 4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

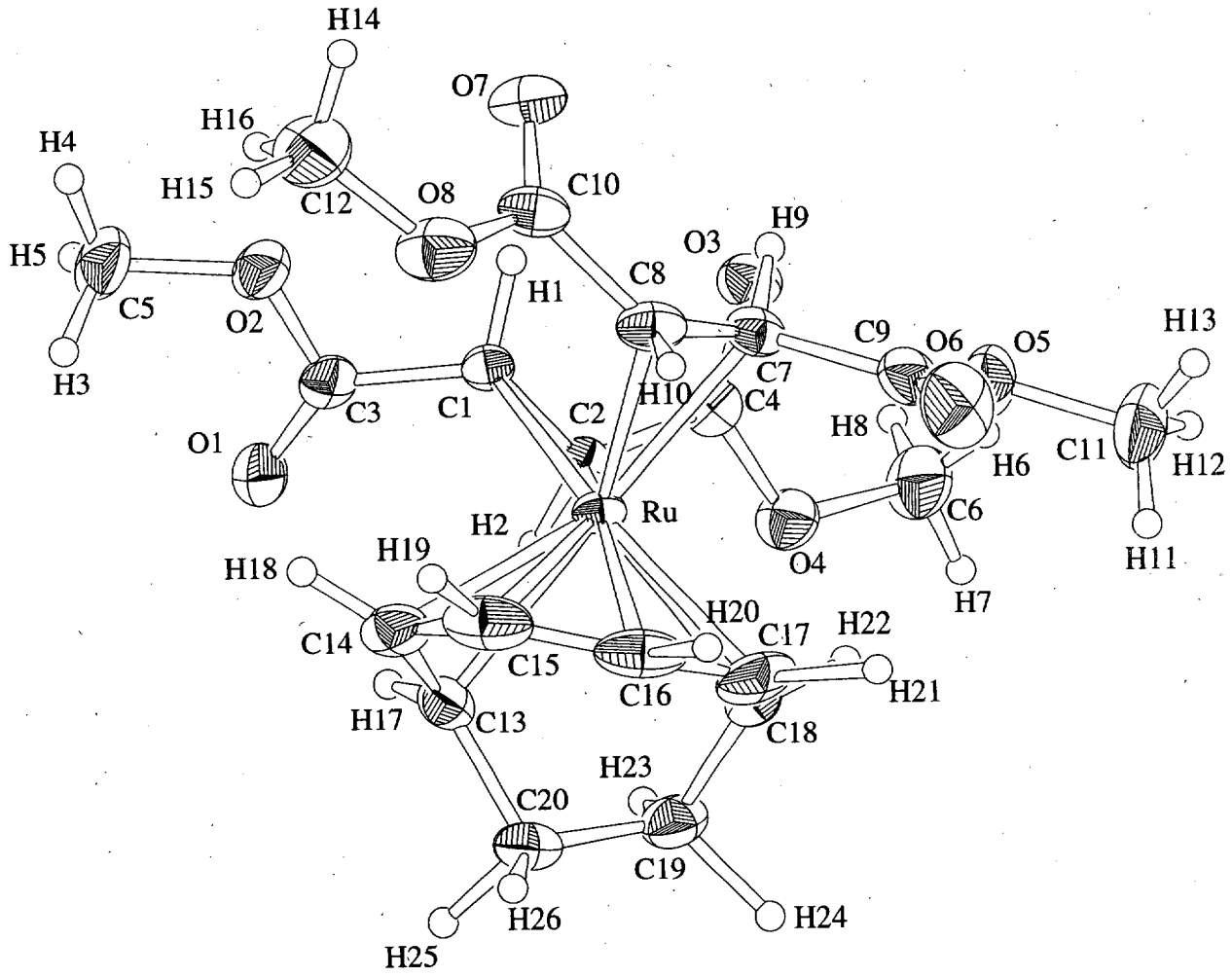
The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	X,	Y,	Z	(2)	-X,	1/2+Y,	1/2-Z
(3)	-X,	-Y,	-Z	(4)	X,	1/2-Y,	1/2+Z



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"Novel Ruthenium Complex-Catalyzed Dimerization of 2,5-Norbornadiene to Pentacyclo[6.6.0.0^{2,6}.0^{3,13}.0^{10,14}]tetradeca-4,11-diene Involving Carbon-Carbon Bond Cleavage"

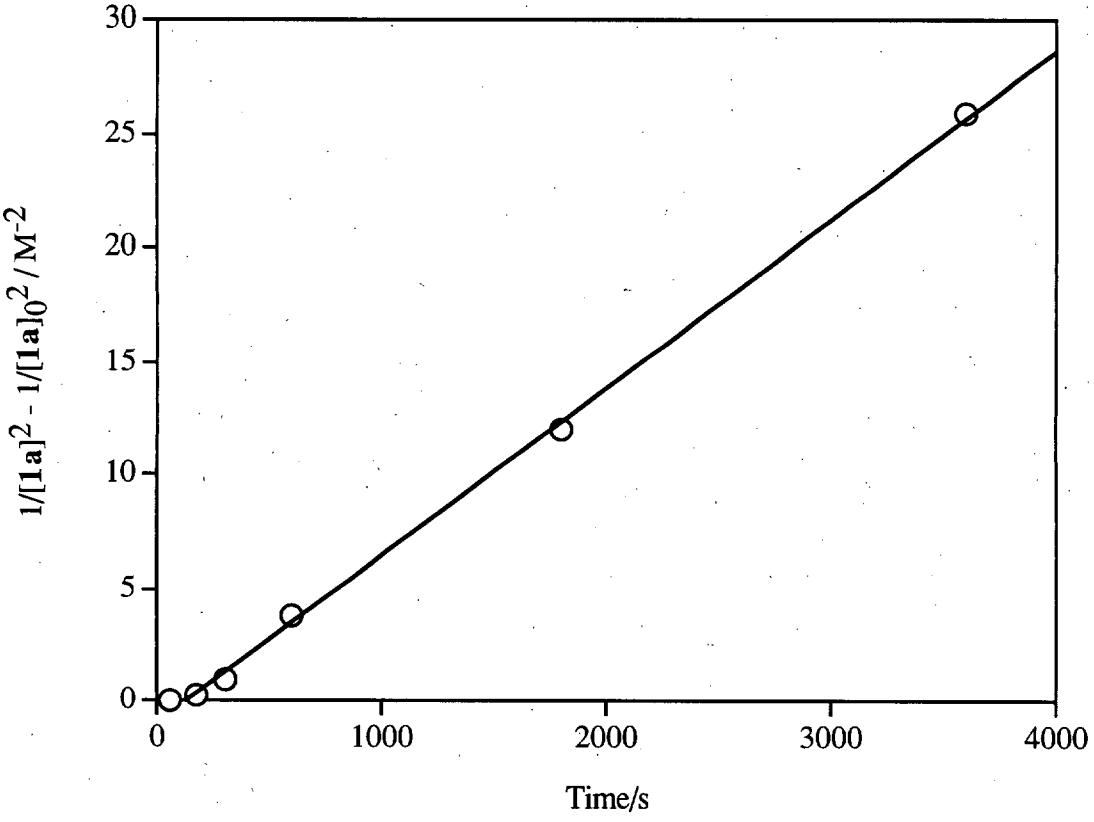

Figure 7. The kinetic analysis of Ru(cod)(cot)-catalyzed dimerization of **1a**. The reaction was carried out at 120 °C in sealed tubes, where the amounts of **1a**, Ru(cod)(cot), *N*,*N*-dimethylacrylamide and toluene were 5.0 mmol, 0.10 mmol, 1.0 mmol and 3.0 mL, respectively. The line is the linear fit. Slope = 7.38 x 10^{-3} $M^{-2}s^{-1}$; linear correlation coefficient = 0.999.

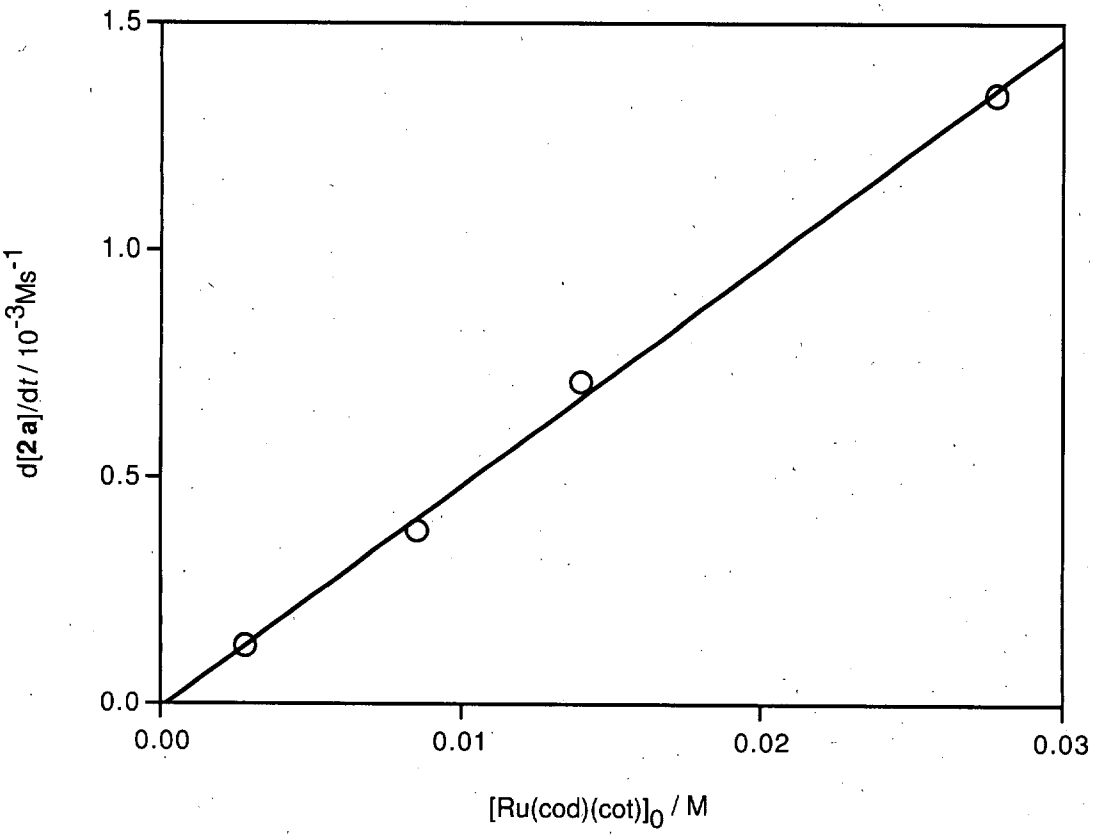

Figure 8. Plot of d[**2a**]/dt vs Ru(cod)(cot) concentration for the dimerization of **1a**. The reaction was carried out at 120 °C in sealed tubes, where the amounts of **1a**, Ru(cod)(cot), *N*,*N*-dimethylacrylamide and toluene were 5.0 mmol, 0.010 - 0.10 mmol, 1.0 mmol and 3.0 mL, respectively. The line is the linear fit. Intercept = -7.64 x 10^{-6} Ms^{-1}; slope = 4.88 x 10^{-2} s^{-1}; linear correlation coefficient = 0.999.