Synthesis of Ruthenium Boryl Analogues of the Shvo Metal–Ligand Bifunctional Hydrogenation Catalyst

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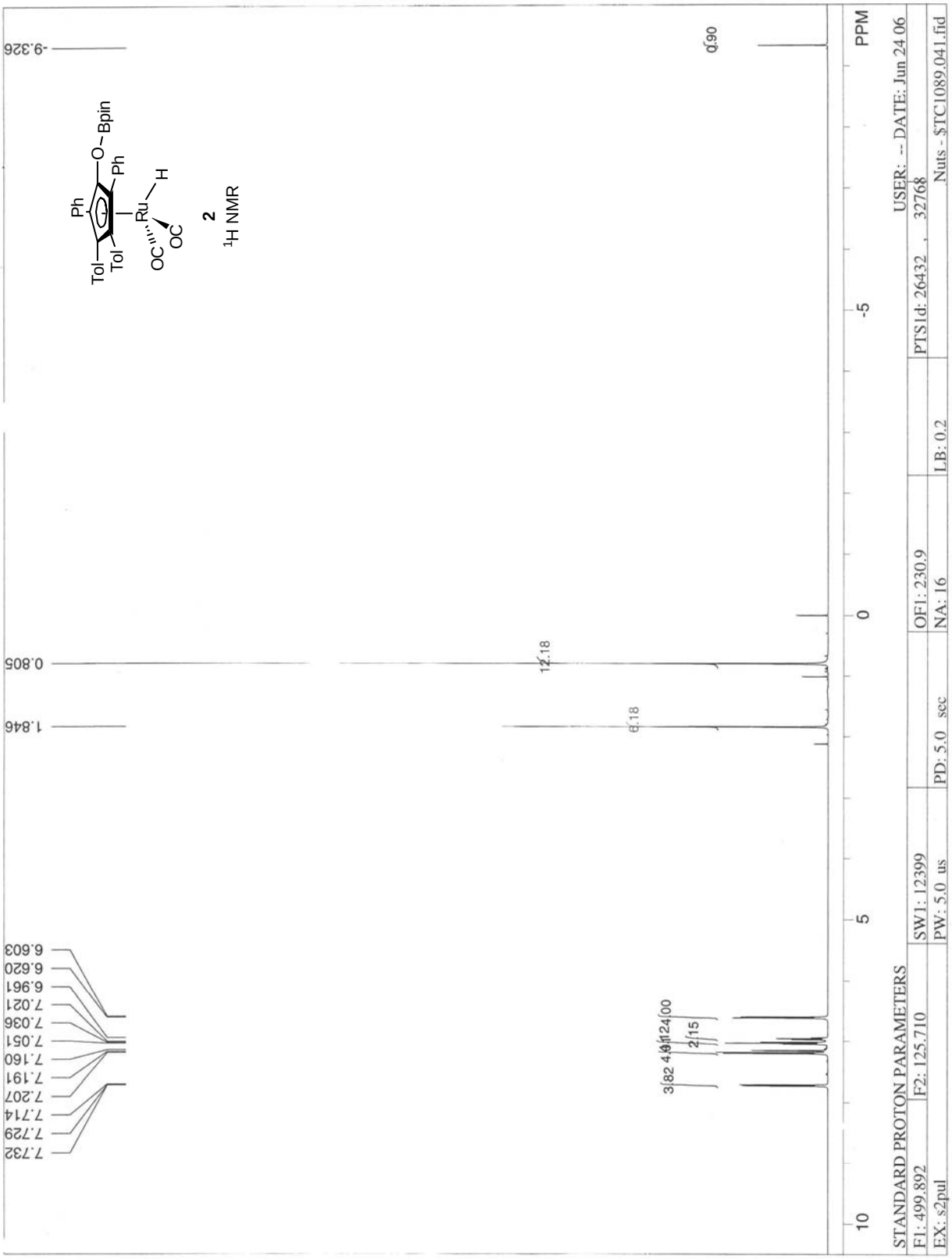
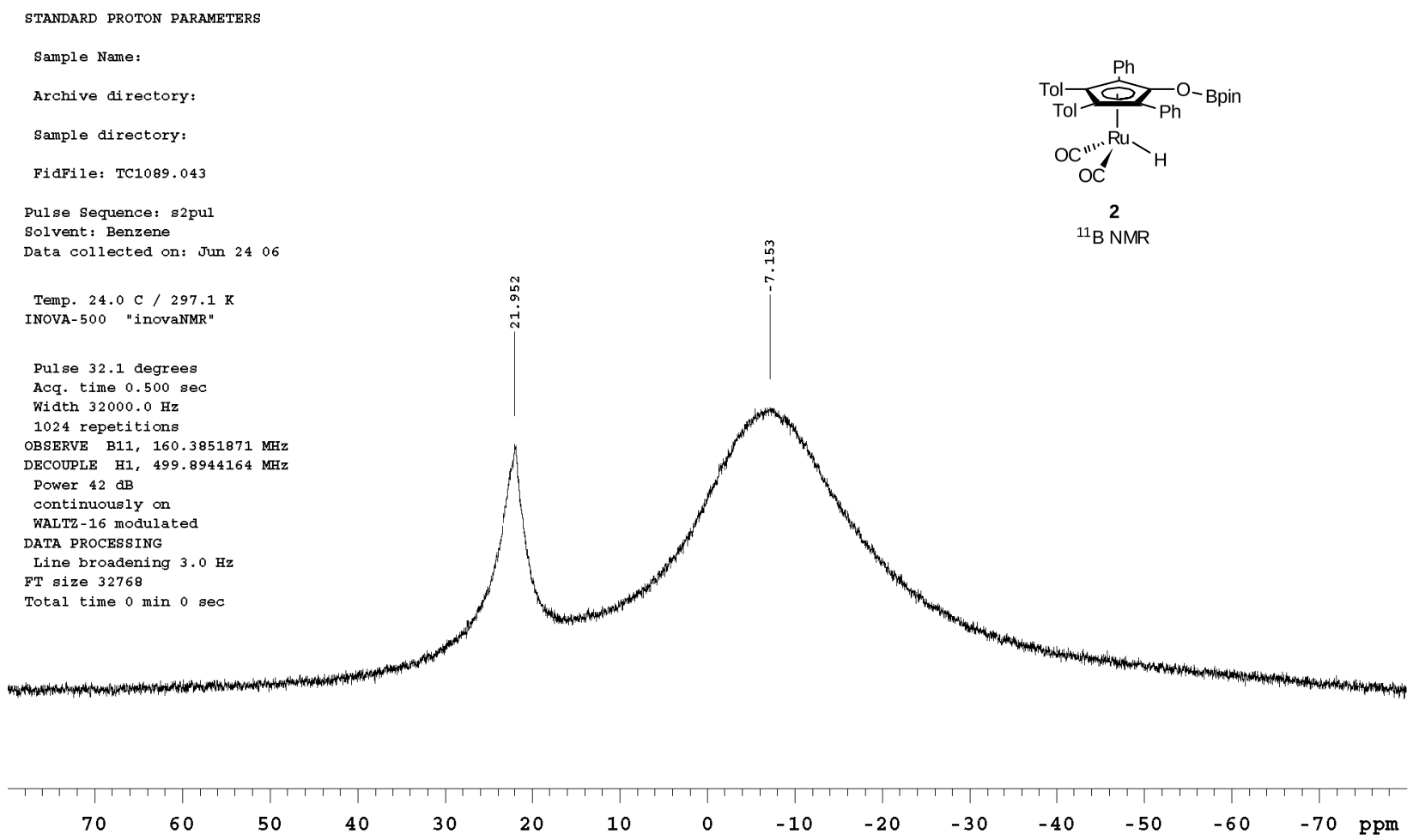
Madison, Wisconsin 53706

Supporting Information

Contents:

I. NMR Spectra of Complexes 2, 3, 5, 7, 8

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DECOUPLE H1, 499.8944164 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 32768
Total time 0 min 0 sec
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-7.153
Ph
Tol
O
Bpin
Tol
Ph
Ru
OC
H
OC
2
11B NMR
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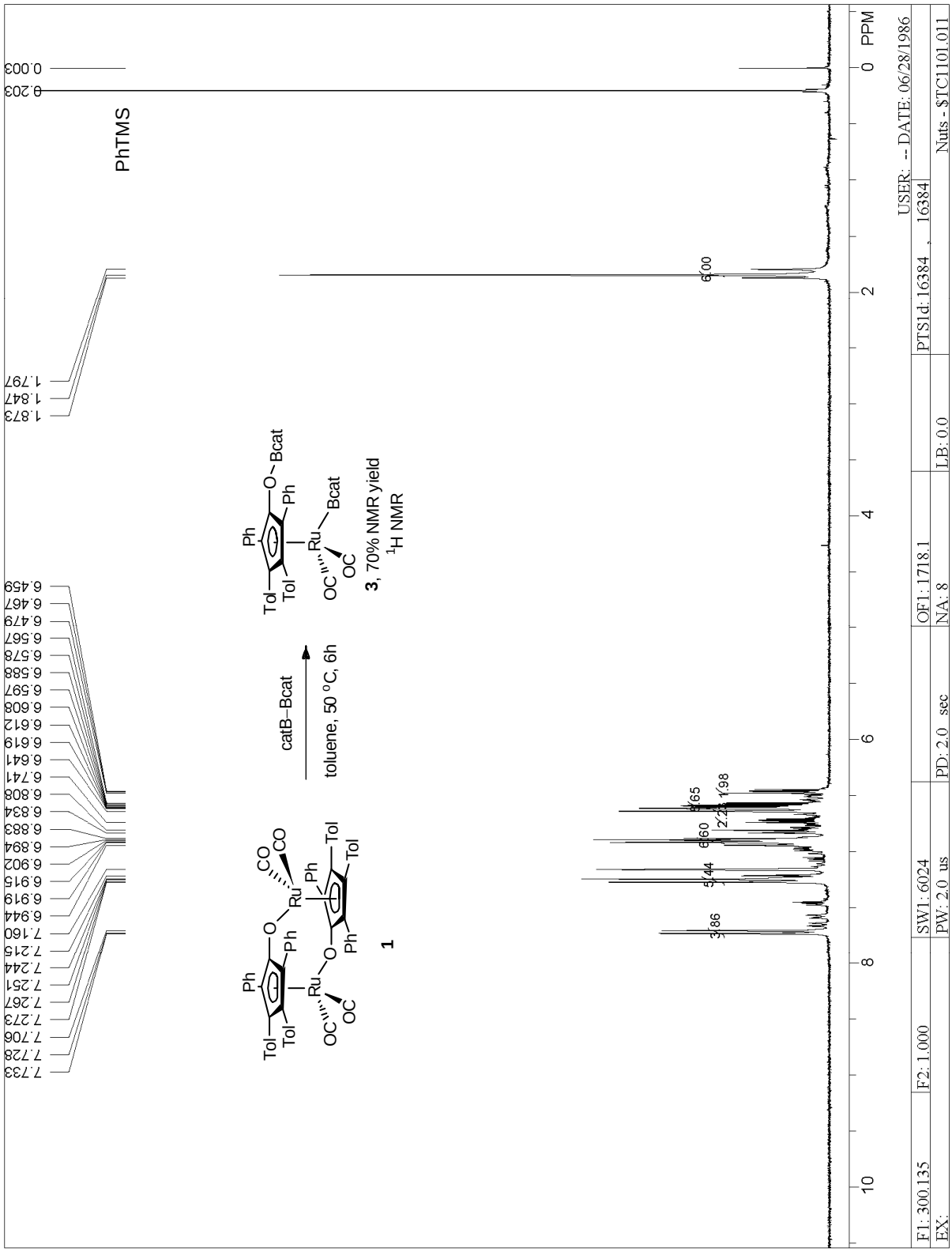
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6.467
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6.588
6.597
6.608
6.612
6.619
6.641
6.741
6.808
6.834
6.883
6.894
6.902
6.915
6.919
6.944
7.160
7.215
7.244
7.251
7.267
7.273
7.706
7.728
7.733
catB–Bcat
toluene, 50 °C, 6h
1
3, 70% NMR yield
1H NMR
6.00
3.86
5.44
6.60
2.22
1.98
3.65
0 PPM
2
4
6
8
10
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F2: 1.000
SW1: 6024
OF1: 1718.1
PTS1d: 16384 , 16384
EX:
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PD: 2.0 sec
NA: 8
LB: 0.0
USER: -- DATE: 06/28/1986
Nuts - $TC1101.011

STANDARD PROTON PARAMETERS

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Archive directory:

Sample directory:

FidFile: TC.1051.053

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Solvent: Benzene
Data collected on: May 21 06

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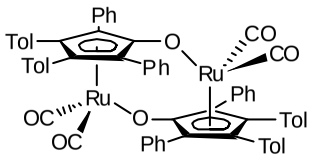

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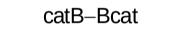
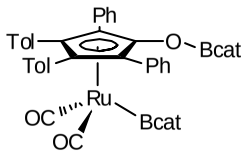
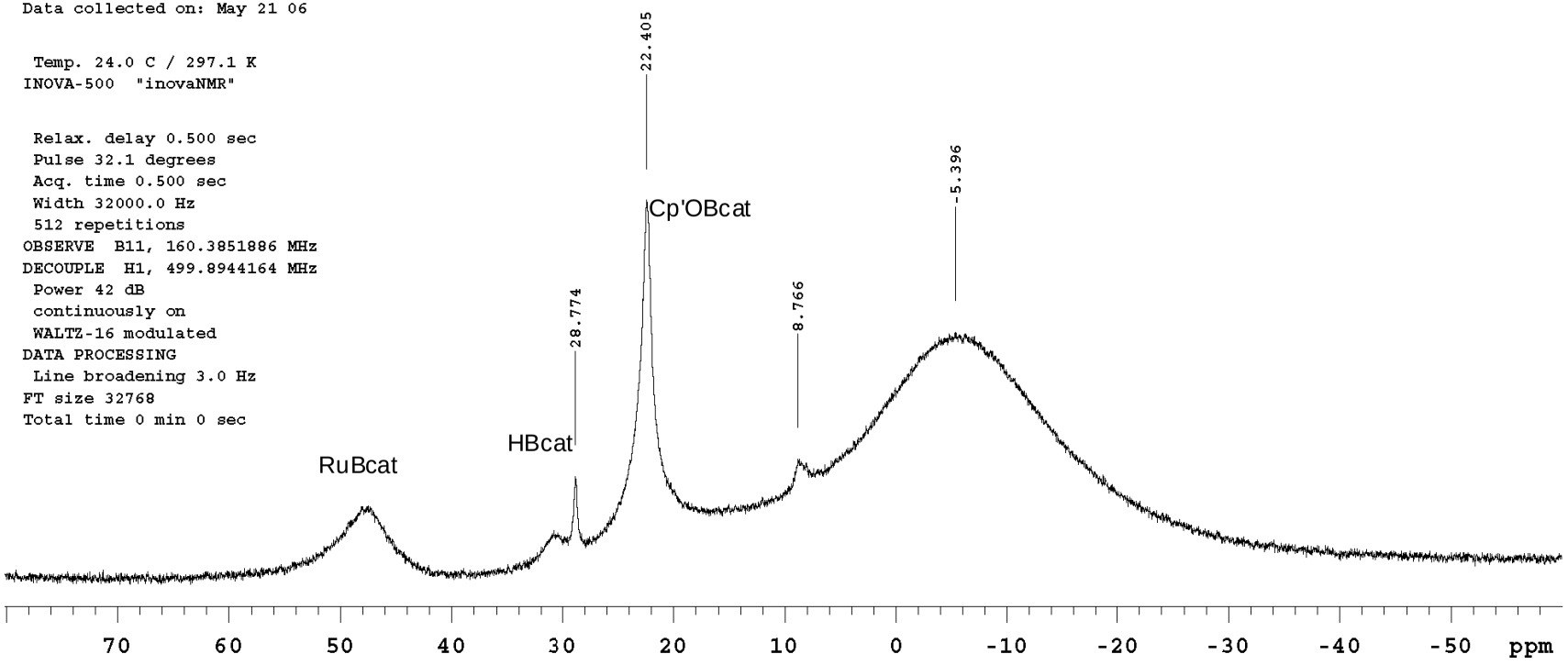
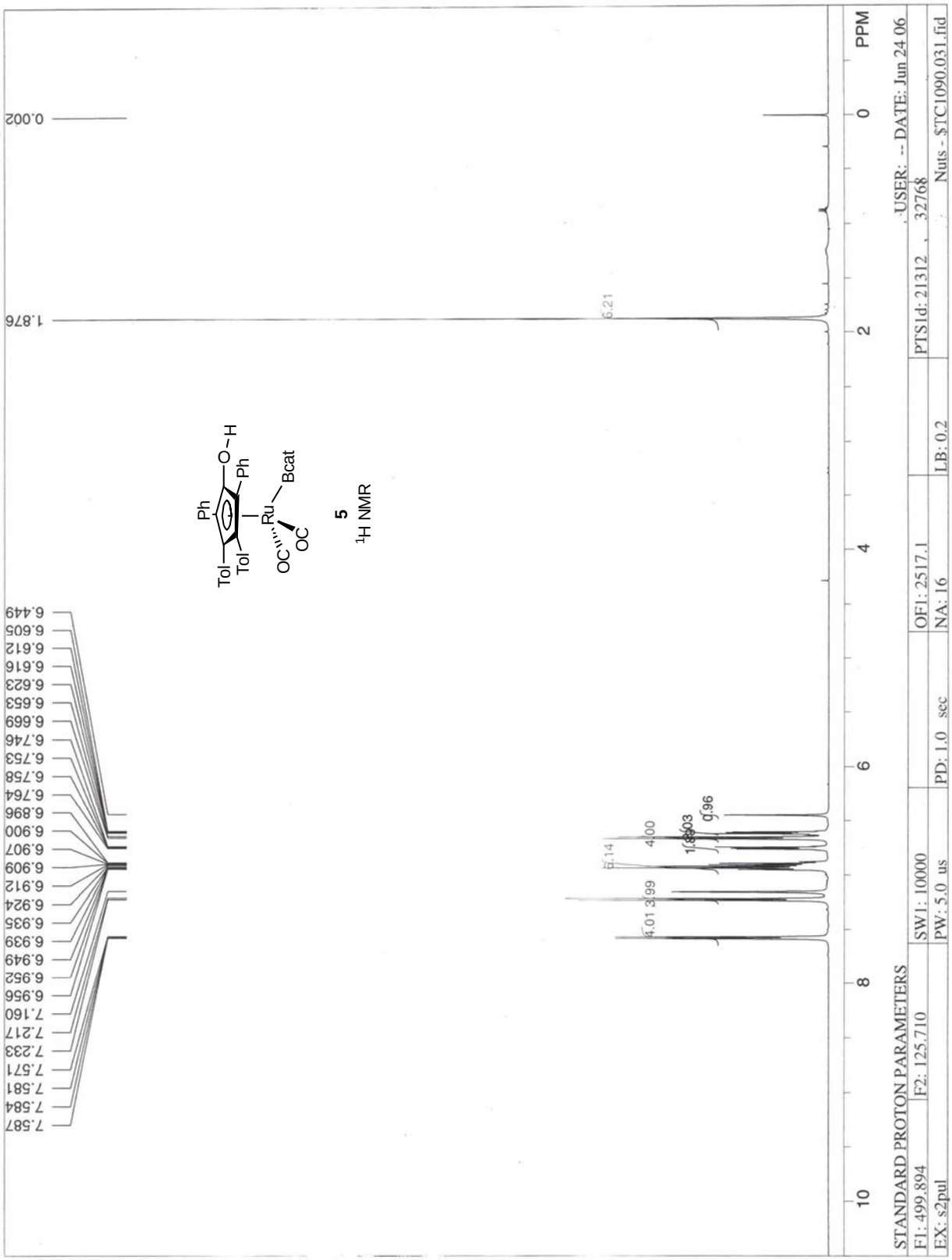




3, 70% NMR yield
^{11}B NMR

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O
H
Ph
Tol
Tol
Ru
Bcat
OC
OC
5
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6.449
6.605
6.612
6.616
6.623
6.653
6.669
6.746
6.753
6.758
6.764
6.896
6.900
6.907
6.909
6.912
6.924
6.935
6.939
6.949
6.952
6.956
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7.233
7.571
7.581
7.584
7.587
8.14
4.00
4.01
3.99
1.89
3.03
9.96
PPM
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F2: 125.710
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32768
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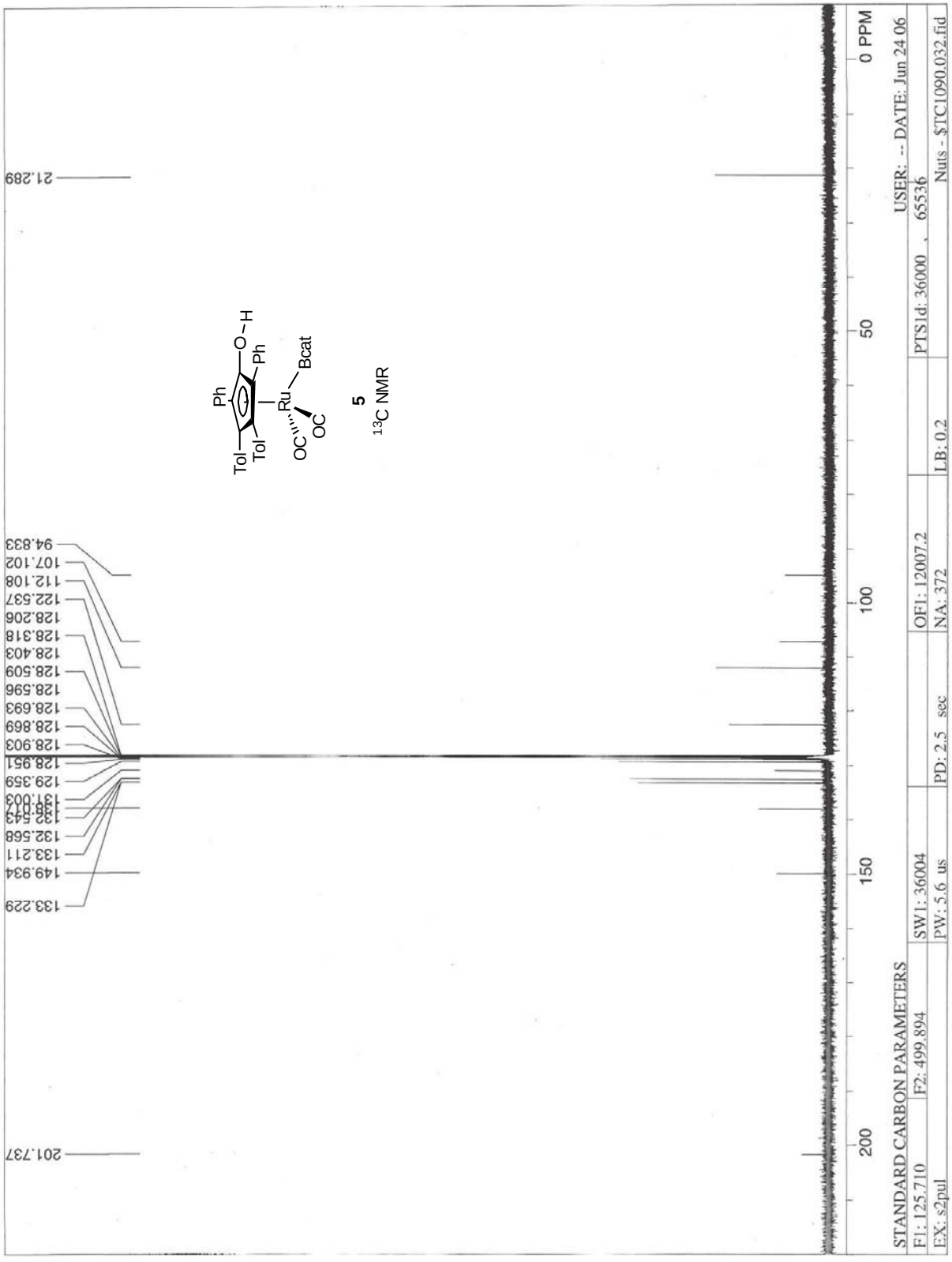
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O
H
Ph
Tol
Tol
Ru
Bcat
OC
OC
5
^{13}C NMR
21.289
94.833
107.102
112.108
122.537
128.206
128.318
128.403
128.509
128.596
128.693
128.869
128.903
128.951
129.359
131.003
132.543
132.568
133.211
149.934
133.229
201.737
200
150
100
50
0 PPM
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F2: 499.894
EX: s2pul
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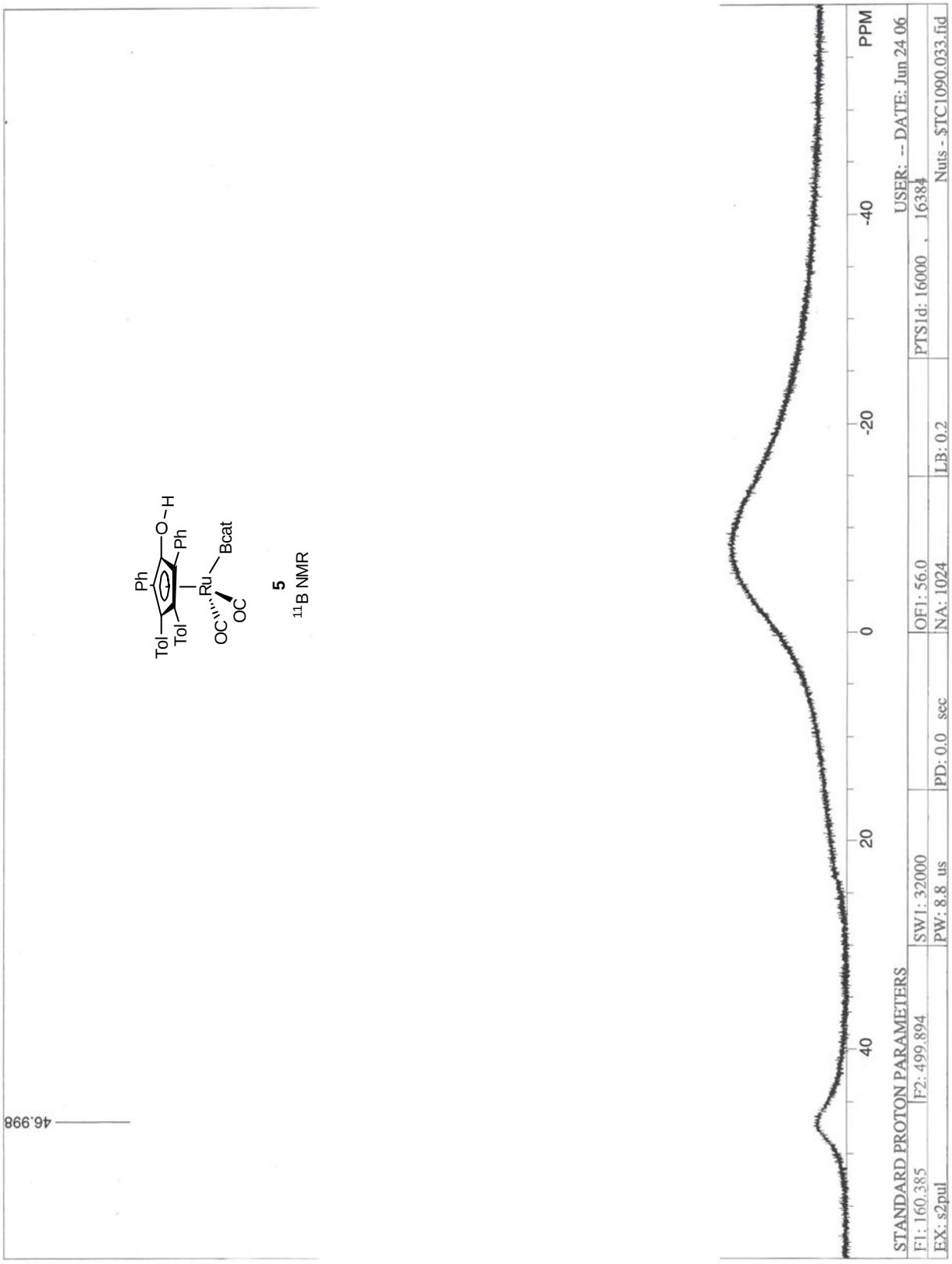
Ph
O–H
Ph
Tol
Tol
Ru
Bcat
OC
OC
46.998
PPM
40
20
0
-20
-40
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F1: 160.385
F2: 499.894
SW1: 32000
PW: 8.8 us
PD: 0.0 sec
OF1: 56.0
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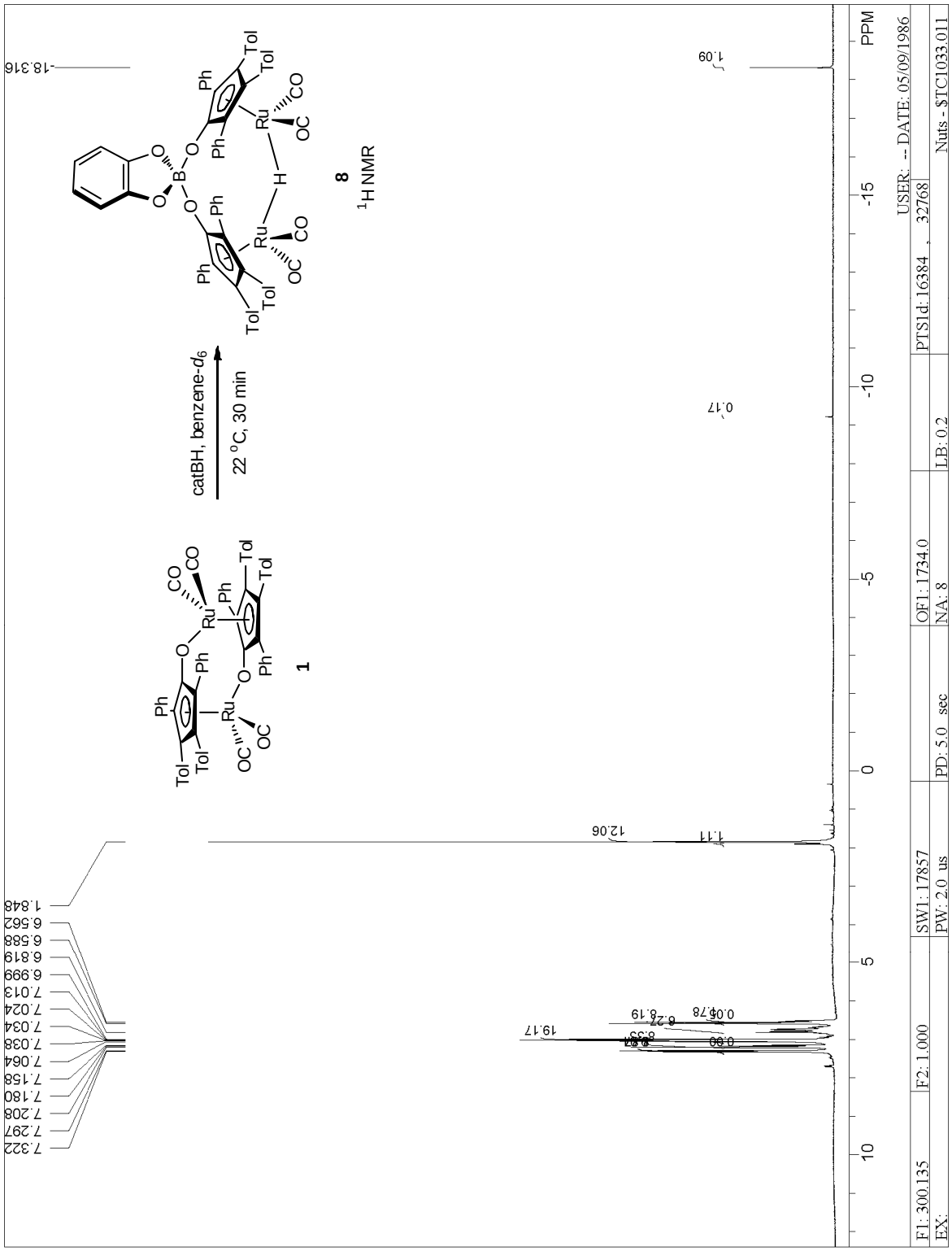
5

^{11}B NMR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22 °C, 30 min
1
8
^{1}H NMR
PPM
USER: -- DATE: 05/09/1986
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F2: 1.000
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LB: 0.2
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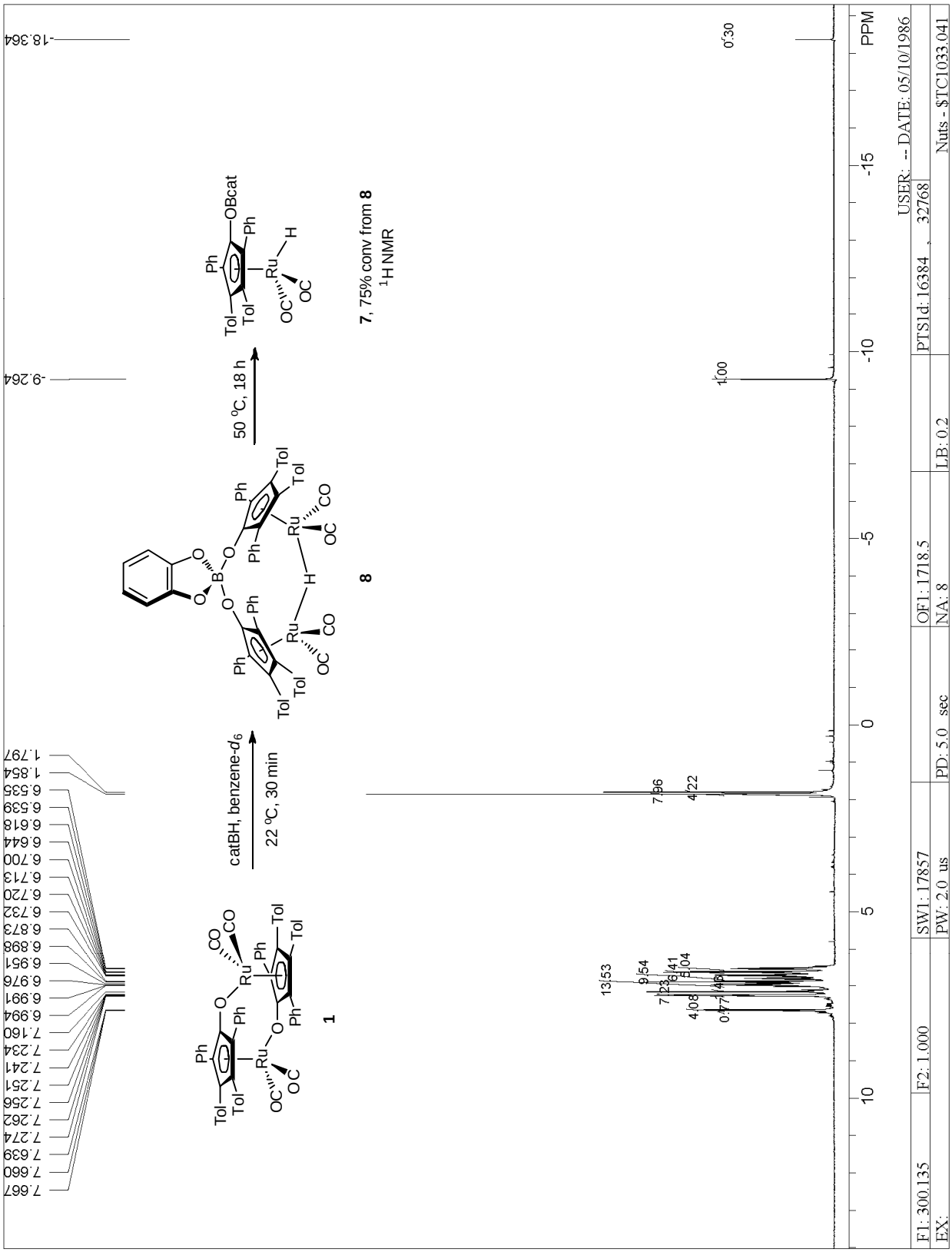
catBH, benzene-d_6
22 °C, 30 min
50 °C, 18 h
1
8
7, 75% conv from 8
^{1}H NMR
PPM
USER: -- DATE: 05/10/1986
F1: 300.135
F2: 1.000
SW1: 17857
OF1: 1718.5
PTS1d: 16384 , 32768
EX:
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LB: 0.2
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Archive directory:
Sample directory:
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512 repetitions
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DECOUPLE H1, 499.8944164 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 32768
Total time 0 min 0 sec
catBH, benzene-d6
22 °C, 30 min
1
8
11B NMR
26.617
20.979
6.548
-5.386
60
40
20
0
-20
-40
-60
ppm

II. X-ray Crystal Data of Complex 5

Data Collection.

A yellow crystal with approximate dimensions 0.35 x 0.20 x 0.20 mm^3 was selected under oil under ambient conditions and attached to the tip of a nylon loop. The crystal was mounted in a stream of cold nitrogen at 100(2) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 4.9 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3º in a 6º range about ω with the exposure time of 10 seconds per frame. A total of 85 reflections were obtained. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 9582 strong reflections from the actual data collection.

The data were collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of a full sphere to a resolution of 0.80 Å. A total of 41042 data were harvested by collecting three sets of frames with 0.25º scans in ω with an exposure time 30 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group *C*2/*c* that yielded chemically reasonable and computationally stable results of refinement [1].

A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation

at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

The final least-squares refinement of 418 parameters against 7745 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0476 and 0.1167, respectively. The final difference Fourier map was featureless.

References

[1] Bruker-AXS. (2000-2003) SADABS V.2.05, SAINT V.6.22, SHELXTL V.6.10 & SMART 5.622 Software Reference Manuals. Bruker-AXS, Madison, Wisconsin, USA.

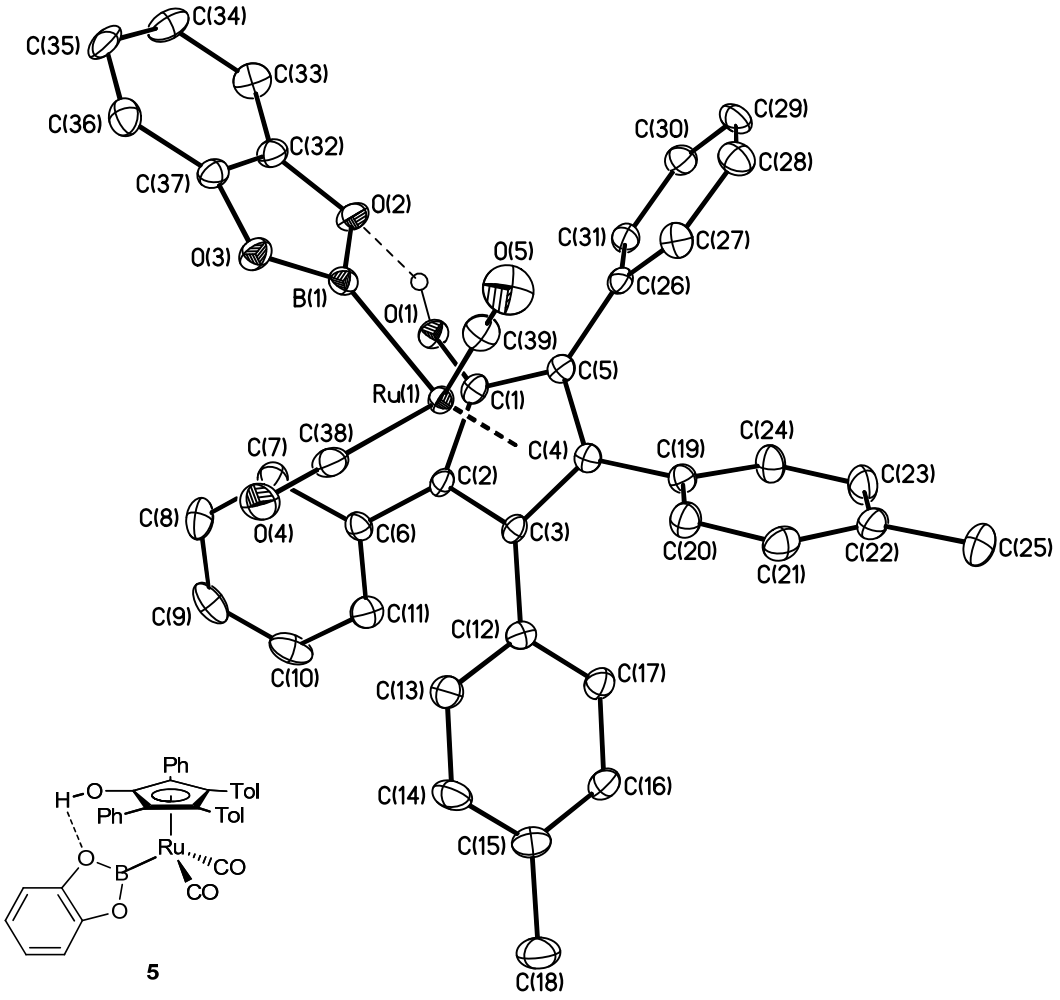

Figure 2: Molecular drawing of **5** shown with 50% probability ellipsoids. All hydrogen atoms except for the O-H are omitted for clarity. The one hydrogen bond is shown as the thin dashed line. The thick dashed line links Ru(1) to the center of the centroid.

Table 1. Crystal data and structure refinement for **5**.

Empirical formula	$C_{39}H_{29}BO_5Ru$	
Formula weight	689.50	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 10.2918(11) Å	α= 90°.
	b = 17.2418(19) Å	β= 98.069(2)°.
	c = 35.581(4) Å	γ = 90°.
Volume	6251.3(12) $Å^3$	
Z	8	
Density (calculated)	1.465 Mg/m^3	
Absorption coefficient	0.547 mm^{-1}	
F(000)	2816	
Crystal size	0.35 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.16 to 28.32°.	
Index ranges	-13<=h<=13, -22<=k<=22, -47<=l<=47	
Reflections collected	41042	
Independent reflections	7745 [R(int) = 0.0719]	
Completeness to theta = 28.32°	99.3 %	
Absorption correction	Multi-scan with SADABS	
Max. and min. transmission	0.8984 and 0.8316	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7745 / 0 / 418	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1061	
R indices (all data)	R1 = 0.0657, wR2 = 0.1167	
Largest diff. peak and hole	0.951 and -1.102 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	3622(1)	520(1)	1174(1)	13(1)
O(1)	4195(2)	1038(1)	2077(1)	18(1)
O(2)	3517(2)	-433(1)	1903(1)	20(1)
O(3)	1993(2)	-884(1)	1424(1)	20(1)
O(4)	892(2)	383(2)	744(1)	33(1)
O(5)	4577(3)	-799(2)	727(1)	34(1)
B(1)	2996(3)	-340(2)	1515(1)	15(1)
C(1)	4354(3)	1205(2)	1713(1)	16(1)
C(2)	3449(3)	1665(2)	1467(1)	14(1)
C(3)	4053(3)	1821(2)	1128(1)	14(1)
C(4)	5270(3)	1415(2)	1164(1)	14(1)
C(5)	5457(3)	1008(2)	1525(1)	14(1)
C(6)	2217(3)	1993(2)	1571(1)	16(1)
C(7)	1334(3)	1525(2)	1734(1)	23(1)
C(8)	202(4)	1838(2)	1837(1)	29(1)
C(9)	-67(4)	2615(2)	1779(1)	32(1)
C(10)	773(4)	3080(2)	1623(1)	29(1)
C(11)	1934(3)	2780(2)	1518(1)	22(1)
C(12)	3601(3)	2416(2)	840(1)	16(1)
C(13)	2362(3)	2416(2)	627(1)	21(1)
C(14)	1941(3)	3031(2)	391(1)	25(1)
C(15)	2737(3)	3676(2)	365(1)	22(1)
C(16)	3985(3)	3675(2)	574(1)	21(1)
C(17)	4416(3)	3052(2)	806(1)	21(1)
C(18)	2298(4)	4350(2)	113(1)	32(1)
C(19)	6219(3)	1468(2)	889(1)	16(1)
C(20)	5844(3)	1290(2)	506(1)	20(1)
C(21)	6734(3)	1361(2)	249(1)	21(1)
C(22)	8015(3)	1600(2)	365(1)	21(1)
C(23)	8371(3)	1794(2)	743(1)	25(1)
C(24)	7485(3)	1732(2)	1003(1)	21(1)
C(25)	8975(4)	1629(2)	83(1)	30(1)
C(26)	6642(3)	574(2)	1692(1)	15(1)
C(27)	7325(3)	91(2)	1469(1)	20(1)
C(28)	8468(3)	-286(2)	1624(1)	23(1)
C(29)	8930(3)	-203(2)	2008(1)	23(1)
C(30)	8269(3)	278(2)	2234(1)	21(1)
C(31)	7140(3)	664(2)	2076(1)	18(1)
C(32)	2798(3)	-1025(2)	2046(1)	19(1)
C(33)	2957(4)	-1335(2)	2401(1)	24(1)
C(34)	2125(4)	-1952(2)	2458(1)	26(1)

C(35)	1195(4)	-2224(2)	2164(1)	25(1)
C(36)	1062(3)	-1906(2)	1810(1)	22(1)
C(37)	1889(3)	-1299(2)	1754(1)	18(1)
C(38)	1926(3)	430(2)	901(1)	21(1)
C(39)	4212(3)	-307(2)	895(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for **5**.

Ru(1)-C(38)	1.881(3)	C(15)-C(16)	1.391(5)
Ru(1)-C(39)	1.886(3)	C(15)-C(18)	1.499(5)
Ru(1)-B(1)	2.075(4)	C(16)-C(17)	1.388(4)
Ru(1)-C(2)	2.250(3)	C(16)-H(16)	0.9500
Ru(1)-C(5)	2.275(3)	C(17)-H(17)	0.9500
Ru(1)-C(1)	2.286(3)	C(18)-H(18A)	0.9800
Ru(1)-C(3)	2.296(3)	C(18)-H(18B)	0.9800
Ru(1)-C(4)	2.297(3)	C(18)-H(18C)	0.9800
Ru(1)-centroid	1.925(3)	C(19)-C(24)	1.386(4)
O(1)-C(1)	1.361(3)	C(19)-C(20)	1.397(4)
O(1)-H(1)	0.8400	C(20)-C(21)	1.388(4)
O(2)-C(32)	1.397(4)	C(20)-H(20)	0.9500
O(2)-B(1)	1.419(4)	C(21)-C(22)	1.388(5)
O(3)-C(37)	1.392(4)	C(21)-H(21)	0.9500
O(3)-B(1)	1.399(4)	C(22)-C(23)	1.386(5)
O(4)-C(38)	1.134(4)	C(22)-C(25)	1.505(4)
O(5)-C(39)	1.132(4)	C(23)-C(24)	1.390(4)
C(1)-C(2)	1.425(4)	C(23)-H(23)	0.9500
C(1)-C(5)	1.435(4)	C(24)-H(24)	0.9500
C(2)-C(3)	1.457(4)	C(25)-H(25A)	0.9800
C(2)-C(6)	1.482(4)	C(25)-H(25B)	0.9800
C(3)-C(4)	1.425(4)	C(25)-H(25C)	0.9800
C(3)-C(12)	1.479(4)	C(26)-C(31)	1.400(4)
C(4)-C(5)	1.454(4)	C(26)-C(27)	1.403(4)
C(4)-C(19)	1.479(4)	C(27)-C(28)	1.389(5)
C(5)-C(26)	1.482(4)	C(27)-H(27)	0.9500
C(6)-C(11)	1.394(5)	C(28)-C(29)	1.389(5)
C(6)-C(7)	1.401(5)	C(28)-H(28)	0.9500
C(7)-C(8)	1.380(5)	C(29)-C(30)	1.396(5)
C(7)-H(7)	0.9500	C(29)-H(29)	0.9500
C(8)-C(9)	1.377(6)	C(30)-C(31)	1.387(4)
C(8)-H(8)	0.9500	C(30)-H(30)	0.9500
C(9)-C(10)	1.355(6)	C(31)-H(31)	0.9500
C(9)-H(9)	0.9500	C(32)-C(33)	1.363(4)
C(10)-C(11)	1.400(5)	C(32)-C(37)	1.380(4)
C(10)-H(10)	0.9500	C(33)-C(34)	1.398(5)
C(11)-H(11)	0.9500	C(33)-H(33)	0.9500
C(12)-C(13)	1.389(4)	C(34)-C(35)	1.396(5)
C(12)-C(17)	1.396(4)	C(34)-H(34)	0.9500
C(13)-C(14)	1.383(5)	C(35)-C(36)	1.362(5)
C(13)-H(13)	0.9500	C(35)-H(35)	0.9500
C(14)-C(15)	1.392(5)	C(36)-C(37)	1.382(5)
C(14)-H(14)	0.9500	C(36)-H(36)	0.9500

C(38)-Ru(1)-C(39)	90.55(14)	C(4)-C(3)-C(2)	107.9(3)
C(38)-Ru(1)-B(1)	84.27(14)	C(4)-C(3)-C(12)	126.1(3)
C(39)-Ru(1)-B(1)	85.21(14)	C(2)-C(3)-C(12)	125.0(3)
C(38)-Ru(1)-C(2)	100.60(13)	C(4)-C(3)-Ru(1)	71.94(17)
C(39)-Ru(1)-C(2)	163.57(13)	C(2)-C(3)-Ru(1)	69.60(17)
B(1)-Ru(1)-C(2)	107.71(12)	C(12)-C(3)-Ru(1)	132.9(2)
C(38)-Ru(1)-C(5)	162.38(13)	C(3)-C(4)-C(5)	108.7(3)
C(39)-Ru(1)-C(5)	105.38(13)	C(3)-C(4)-C(19)	124.4(3)
B(1)-Ru(1)-C(5)	104.18(12)	C(5)-C(4)-C(19)	126.7(3)
C(2)-Ru(1)-C(5)	62.26(11)	C(3)-C(4)-Ru(1)	71.90(17)
C(38)-Ru(1)-C(1)	130.39(13)	C(5)-C(4)-Ru(1)	70.64(16)
C(39)-Ru(1)-C(1)	137.64(13)	C(19)-C(4)-Ru(1)	127.5(2)
B(1)-Ru(1)-C(1)	88.36(12)	C(1)-C(5)-C(4)	106.4(3)
C(2)-Ru(1)-C(1)	36.60(10)	C(1)-C(5)-C(26)	126.4(3)
C(5)-Ru(1)-C(1)	36.68(11)	C(4)-C(5)-C(26)	126.6(3)
C(38)-Ru(1)-C(3)	102.67(12)	C(1)-C(5)-Ru(1)	72.09(17)
C(39)-Ru(1)-C(3)	128.44(13)	C(4)-C(5)-Ru(1)	72.29(16)
B(1)-Ru(1)-C(3)	144.91(12)	C(26)-C(5)-Ru(1)	127.3(2)
C(2)-Ru(1)-C(3)	37.37(10)	C(11)-C(6)-C(7)	118.7(3)
C(5)-Ru(1)-C(3)	61.58(10)	C(11)-C(6)-C(2)	120.6(3)
C(1)-Ru(1)-C(3)	60.74(10)	C(7)-C(6)-C(2)	120.7(3)
C(38)-Ru(1)-C(4)	132.99(12)	C(8)-C(7)-C(6)	120.4(3)
C(39)-Ru(1)-C(4)	101.93(13)	C(8)-C(7)-H(7)	119.8
B(1)-Ru(1)-C(4)	141.23(12)	C(6)-C(7)-H(7)	119.8
C(2)-Ru(1)-C(4)	61.64(11)	C(9)-C(8)-C(7)	120.1(3)
C(5)-Ru(1)-C(4)	37.08(10)	C(9)-C(8)-H(8)	120.0
C(1)-Ru(1)-C(4)	60.62(10)	C(7)-C(8)-H(8)	120.0
C(3)-Ru(1)-C(4)	36.15(11)	C(10)-C(9)-C(8)	120.7(3)
C(1)-O(1)-H(1)	109.5	C(10)-C(9)-H(9)	119.7
C(32)-O(2)-B(1)	106.8(2)	C(8)-C(9)-H(9)	119.7
C(37)-O(3)-B(1)	106.9(2)	C(9)-C(10)-C(11)	120.6(3)
O(3)-B(1)-O(2)	108.4(3)	C(9)-C(10)-H(10)	119.7
O(3)-B(1)-Ru(1)	128.6(2)	C(11)-C(10)-H(10)	119.7
O(2)-B(1)-Ru(1)	123.0(2)	C(6)-C(11)-C(10)	119.6(3)
O(1)-C(1)-C(2)	123.1(3)	C(6)-C(11)-H(11)	120.2
O(1)-C(1)-C(5)	127.0(3)	C(10)-C(11)-H(11)	120.2
C(2)-C(1)-C(5)	109.8(3)	C(13)-C(12)-C(17)	118.0(3)
O(1)-C(1)-Ru(1)	128.4(2)	C(13)-C(12)-C(3)	123.6(3)
C(2)-C(1)-Ru(1)	70.32(17)	C(17)-C(12)-C(3)	118.0(3)
C(5)-C(1)-Ru(1)	71.22(16)	C(14)-C(13)-C(12)	121.0(3)
C(1)-C(2)-C(3)	107.0(3)	C(14)-C(13)-H(13)	119.5
C(1)-C(2)-C(6)	124.7(3)	C(12)-C(13)-H(13)	119.5
C(3)-C(2)-C(6)	127.9(3)	C(13)-C(14)-C(15)	121.1(3)
C(1)-C(2)-Ru(1)	73.08(17)	C(13)-C(14)-H(14)	119.5
C(3)-C(2)-Ru(1)	73.03(17)	C(15)-C(14)-H(14)	119.5
C(6)-C(2)-Ru(1)	125.2(2)	C(16)-C(15)-C(14)	118.1(3)

C(16)-C(15)-C(18)	120.0(3)
C(14)-C(15)-C(18)	121.9(3)
C(17)-C(16)-C(15)	120.9(3)
C(17)-C(16)-H(16)	119.6
C(15)-C(16)-H(16)	119.6
C(16)-C(17)-C(12)	120.9(3)
C(16)-C(17)-H(17)	119.6
C(12)-C(17)-H(17)	119.6
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(24)-C(19)-C(20)	118.5(3)
C(24)-C(19)-C(4)	120.5(3)
C(20)-C(19)-C(4)	120.9(3)
C(21)-C(20)-C(19)	120.4(3)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	121.2(3)
C(22)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(23)-C(22)-C(21)	118.0(3)
C(23)-C(22)-C(25)	122.1(3)
C(21)-C(22)-C(25)	119.8(3)
C(22)-C(23)-C(24)	121.3(3)
C(22)-C(23)-H(23)	119.4
C(24)-C(23)-H(23)	119.4
C(19)-C(24)-C(23)	120.6(3)
C(19)-C(24)-H(24)	119.7
C(23)-C(24)-H(24)	119.7
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(31)-C(26)-C(27)	118.2(3)
C(31)-C(26)-C(5)	120.2(3)
C(27)-C(26)-C(5)	121.6(3)
C(28)-C(27)-C(26)	121.2(3)
C(28)-C(27)-H(27)	119.4
C(26)-C(27)-H(27)	119.4
C(27)-C(28)-C(29)	119.7(3)
C(27)-C(28)-H(28)	120.2
C(29)-C(28)-H(28)	120.2
C(28)-C(29)-C(30)	120.0(3)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	120.0(3)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(26)	120.8(3)
C(30)-C(31)-H(31)	119.6
C(26)-C(31)-H(31)	119.6
C(33)-C(32)-C(37)	123.1(3)
C(33)-C(32)-O(2)	128.5(3)
C(37)-C(32)-O(2)	108.4(3)
C(32)-C(33)-C(34)	115.8(3)
C(32)-C(33)-H(33)	122.1
C(34)-C(33)-H(33)	122.1
C(35)-C(34)-C(33)	121.2(3)
C(35)-C(34)-H(34)	119.4
C(33)-C(34)-H(34)	119.4
C(36)-C(35)-C(34)	121.8(3)
C(36)-C(35)-H(35)	119.1
C(34)-C(35)-H(35)	119.1
C(35)-C(36)-C(37)	117.1(3)
C(35)-C(36)-H(36)	121.4
C(37)-C(36)-H(36)	121.4
C(32)-C(37)-C(36)	121.0(3)
C(32)-C(37)-O(3)	109.5(3)
C(36)-C(37)-O(3)	129.4(3)
O(4)-C(38)-Ru(1)	178.4(3)
O(5)-C(39)-Ru(1)	179.3(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	12(1)	15(1)	12(1)	1(1)	1(1)	-2(1)
O(1)	21(1)	20(1)	12(1)	1(1)	2(1)	-1(1)
O(2)	23(1)	16(1)	19(1)	4(1)	2(1)	-3(1)
O(3)	22(1)	21(1)	16(1)	4(1)	1(1)	-4(1)
O(4)	24(1)	29(2)	41(2)	9(1)	-13(1)	-8(1)
O(5)	43(2)	33(2)	27(1)	-12(1)	9(1)	4(1)
B(1)	15(2)	15(2)	16(2)	0(1)	3(1)	2(1)
C(1)	17(2)	15(2)	14(1)	-2(1)	2(1)	-4(1)
C(2)	14(1)	16(2)	13(1)	2(1)	1(1)	-5(1)
C(3)	14(1)	13(2)	14(1)	-1(1)	1(1)	-4(1)
C(4)	14(1)	15(2)	13(1)	-2(1)	1(1)	-2(1)
C(5)	15(1)	15(2)	12(1)	-1(1)	-1(1)	-3(1)
C(6)	14(2)	20(2)	14(1)	0(1)	0(1)	1(1)
C(7)	21(2)	20(2)	30(2)	0(1)	8(1)	1(1)
C(8)	21(2)	35(2)	35(2)	-1(2)	13(2)	-5(2)
C(9)	19(2)	41(2)	35(2)	-7(2)	4(2)	12(2)
C(10)	33(2)	27(2)	25(2)	-3(1)	3(1)	16(2)
C(11)	25(2)	22(2)	22(2)	0(1)	5(1)	1(1)
C(12)	19(2)	15(2)	15(1)	0(1)	3(1)	1(1)
C(13)	19(2)	17(2)	26(2)	0(1)	-2(1)	-4(1)
C(14)	24(2)	23(2)	26(2)	4(1)	-8(1)	1(1)
C(15)	29(2)	20(2)	17(2)	1(1)	2(1)	2(1)
C(16)	23(2)	19(2)	21(2)	2(1)	4(1)	-4(1)
C(17)	19(2)	25(2)	17(2)	4(1)	0(1)	-5(1)
C(18)	35(2)	23(2)	35(2)	9(2)	-4(2)	-1(2)
C(19)	15(2)	16(2)	16(1)	0(1)	4(1)	1(1)
C(20)	19(2)	24(2)	18(2)	0(1)	3(1)	-2(1)
C(21)	26(2)	24(2)	15(1)	2(1)	5(1)	0(1)
C(22)	23(2)	21(2)	23(2)	6(1)	10(1)	4(1)
C(23)	16(2)	34(2)	25(2)	3(1)	2(1)	-3(1)
C(24)	16(2)	29(2)	17(1)	-3(1)	1(1)	-4(1)
C(25)	26(2)	38(2)	29(2)	8(2)	13(2)	0(2)
C(26)	14(1)	14(2)	17(1)	2(1)	1(1)	-3(1)
C(27)	19(2)	22(2)	17(1)	-4(1)	0(1)	-2(1)
C(28)	23(2)	18(2)	27(2)	-4(1)	1(1)	2(1)
C(29)	14(2)	19(2)	34(2)	1(1)	-5(1)	2(1)
C(30)	20(2)	22(2)	20(2)	4(1)	-3(1)	-2(1)
C(31)	17(2)	20(2)	18(1)	2(1)	2(1)	-1(1)
C(32)	21(2)	13(2)	22(2)	1(1)	6(1)	1(1)
C(33)	29(2)	26(2)	17(2)	-2(1)	2(1)	0(2)
C(34)	40(2)	20(2)	21(2)	4(1)	11(1)	-2(2)

C(35)	29(2)	12(2)	37(2)	2(1)	14(2)	-6(1)
C(36)	20(2)	21(2)	27(2)	-6(1)	3(1)	-2(1)
C(37)	20(2)	16(2)	17(1)	2(1)	6(1)	1(1)
C(38)	24(2)	16(2)	21(2)	4(1)	-2(1)	-4(1)
C(39)	24(2)	24(2)	15(1)	-1(1)	1(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **5**.

	x	y	z	U(eq)
H(1)	4227	556	2110	26
H(7)	1515	988	1773	28
H(8)	-392	1518	1948	35
H(9)	-849	2827	1850	38
H(10)	572	3614	1584	34
H(11)	2526	3110	1412	27
H(13)	1794	1986	643	25
H(14)	1095	3014	245	30
H(16)	4551	4105	558	25
H(17)	5277	3059	943	25
H(18A)	2245	4192	-153	48
H(18B)	2928	4776	164	48
H(18C)	1432	4524	163	48
H(20)	4974	1120	421	24
H(21)	6461	1245	-11	26
H(23)	9237	1972	827	30
H(24)	7750	1872	1260	25
H(25A)	9514	2098	126	45
H(25B)	8494	1638	-175	45
H(25C)	9541	1170	114	45
H(27)	6998	21	1208	24
H(28)	8933	-599	1468	28
H(29)	9695	-474	2117	28
H(30)	8594	342	2495	25
H(31)	6700	994	2231	22
H(33)	3593	-1143	2599	29
H(34)	2193	-2190	2701	31
H(35)	641	-2643	2212	30
H(36)	427	-2094	1611	27

Table 6. Torsion angles [°] for **5**.

C(37)-O(3)-B(1)-O(2)	0.7(3)
C(37)-O(3)-B(1)-Ru(1)	-176.0(2)
C(32)-O(2)-B(1)-O(3)	-1.3(3)
C(32)-O(2)-B(1)-Ru(1)	175.7(2)
C(38)-Ru(1)-B(1)-O(3)	23.4(3)
C(39)-Ru(1)-B(1)-O(3)	-67.7(3)
C(2)-Ru(1)-B(1)-O(3)	122.7(3)
C(5)-Ru(1)-B(1)-O(3)	-172.4(3)
C(1)-Ru(1)-B(1)-O(3)	154.2(3)
C(3)-Ru(1)-B(1)-O(3)	127.3(3)
C(4)-Ru(1)-B(1)-O(3)	-170.8(2)
C(38)-Ru(1)-B(1)-O(2)	-152.9(3)
C(39)-Ru(1)-B(1)-O(2)	116.0(3)
C(2)-Ru(1)-B(1)-O(2)	-53.6(3)
C(5)-Ru(1)-B(1)-O(2)	11.3(3)
C(1)-Ru(1)-B(1)-O(2)	-22.1(3)
C(3)-Ru(1)-B(1)-O(2)	-49.0(4)
C(4)-Ru(1)-B(1)-O(2)	12.9(4)
C(38)-Ru(1)-C(1)-O(1)	75.0(3)
C(39)-Ru(1)-C(1)-O(1)	-87.2(3)
B(1)-Ru(1)-C(1)-O(1)	-6.1(3)
C(2)-Ru(1)-C(1)-O(1)	117.2(3)
C(5)-Ru(1)-C(1)-O(1)	-122.8(4)
C(3)-Ru(1)-C(1)-O(1)	156.5(3)
C(4)-Ru(1)-C(1)-O(1)	-161.8(3)
C(38)-Ru(1)-C(1)-C(2)	-42.2(2)
C(39)-Ru(1)-C(1)-C(2)	155.6(2)
B(1)-Ru(1)-C(1)-C(2)	-123.29(19)
C(5)-Ru(1)-C(1)-C(2)	120.1(3)
C(3)-Ru(1)-C(1)-C(2)	39.33(17)
C(4)-Ru(1)-C(1)-C(2)	81.03(19)
C(38)-Ru(1)-C(1)-C(5)	-162.29(18)
C(39)-Ru(1)-C(1)-C(5)	35.6(3)
B(1)-Ru(1)-C(1)-C(5)	116.65(19)
C(2)-Ru(1)-C(1)-C(5)	-120.1(3)
C(3)-Ru(1)-C(1)-C(5)	-80.73(19)
C(4)-Ru(1)-C(1)-C(5)	-39.03(17)
O(1)-C(1)-C(2)-C(3)	170.7(3)
C(5)-C(1)-C(2)-C(3)	-5.1(3)
Ru(1)-C(1)-C(2)-C(3)	-65.7(2)
O(1)-C(1)-C(2)-C(6)	-2.2(5)
C(5)-C(1)-C(2)-C(6)	-178.0(3)
Ru(1)-C(1)-C(2)-C(6)	121.5(3)
O(1)-C(1)-C(2)-Ru(1)	-123.7(3)

C(5)-C(1)-C(2)-Ru(1)	60.5(2)
C(38)-Ru(1)-C(2)-C(1)	148.61(19)
C(39)-Ru(1)-C(2)-C(1)	-79.4(5)
B(1)-Ru(1)-C(2)-C(1)	61.3(2)
C(5)-Ru(1)-C(2)-C(1)	-35.75(17)
C(3)-Ru(1)-C(2)-C(1)	-114.4(2)
C(4)-Ru(1)-C(2)-C(1)	-77.97(18)
C(38)-Ru(1)-C(2)-C(3)	-97.03(18)
C(39)-Ru(1)-C(2)-C(3)	35.0(5)
B(1)-Ru(1)-C(2)-C(3)	175.65(17)
C(5)-Ru(1)-C(2)-C(3)	78.61(18)
C(1)-Ru(1)-C(2)-C(3)	114.4(2)
C(4)-Ru(1)-C(2)-C(3)	36.39(16)
C(38)-Ru(1)-C(2)-C(6)	27.8(3)
C(39)-Ru(1)-C(2)-C(6)	159.8(4)
B(1)-Ru(1)-C(2)-C(6)	-59.6(3)
C(5)-Ru(1)-C(2)-C(6)	-156.6(3)
C(1)-Ru(1)-C(2)-C(6)	-120.8(3)
C(3)-Ru(1)-C(2)-C(6)	124.8(3)
C(4)-Ru(1)-C(2)-C(6)	161.2(3)
C(1)-C(2)-C(3)-C(4)	3.6(3)
C(6)-C(2)-C(3)-C(4)	176.1(3)
Ru(1)-C(2)-C(3)-C(4)	-62.1(2)
C(1)-C(2)-C(3)-C(12)	-165.5(3)
C(6)-C(2)-C(3)-C(12)	7.0(5)
Ru(1)-C(2)-C(3)-C(12)	128.8(3)
C(1)-C(2)-C(3)-Ru(1)	65.7(2)
C(6)-C(2)-C(3)-Ru(1)	-121.8(3)
C(38)-Ru(1)-C(3)-C(4)	-151.30(18)
C(39)-Ru(1)-C(3)-C(4)	-50.3(2)
B(1)-Ru(1)-C(3)-C(4)	110.5(2)
C(2)-Ru(1)-C(3)-C(4)	117.8(2)
C(5)-Ru(1)-C(3)-C(4)	37.15(16)
C(1)-Ru(1)-C(3)-C(4)	79.25(18)
C(38)-Ru(1)-C(3)-C(2)	90.94(19)
C(39)-Ru(1)-C(3)-C(2)	-168.05(18)
B(1)-Ru(1)-C(3)-C(2)	-7.2(3)
C(5)-Ru(1)-C(3)-C(2)	-80.61(18)
C(1)-Ru(1)-C(3)-C(2)	-38.51(16)
C(4)-Ru(1)-C(3)-C(2)	-117.8(2)
C(38)-Ru(1)-C(3)-C(12)	-28.4(3)
C(39)-Ru(1)-C(3)-C(12)	72.6(3)
B(1)-Ru(1)-C(3)-C(12)	-126.6(3)
C(2)-Ru(1)-C(3)-C(12)	-119.3(4)
C(5)-Ru(1)-C(3)-C(12)	160.1(3)
C(1)-Ru(1)-C(3)-C(12)	-157.8(3)

C(4)-Ru(1)-C(3)-C(12)	122.9(4)
C(2)-C(3)-C(4)-C(5)	-0.7(3)
C(12)-C(3)-C(4)-C(5)	168.2(3)
Ru(1)-C(3)-C(4)-C(5)	-61.4(2)
C(2)-C(3)-C(4)-C(19)	-175.8(3)
C(12)-C(3)-C(4)-C(19)	-6.9(5)
Ru(1)-C(3)-C(4)-C(19)	123.6(3)
C(2)-C(3)-C(4)-Ru(1)	60.6(2)
C(12)-C(3)-C(4)-Ru(1)	-130.5(3)
C(38)-Ru(1)-C(4)-C(3)	39.8(2)
C(39)-Ru(1)-C(4)-C(3)	141.99(18)
B(1)-Ru(1)-C(4)-C(3)	-120.7(2)
C(2)-Ru(1)-C(4)-C(3)	-37.61(16)
C(5)-Ru(1)-C(4)-C(3)	-118.2(2)
C(1)-Ru(1)-C(4)-C(3)	-79.62(18)
C(38)-Ru(1)-C(4)-C(5)	158.1(2)
C(39)-Ru(1)-C(4)-C(5)	-99.78(19)
B(1)-Ru(1)-C(4)-C(5)	-2.5(3)
C(2)-Ru(1)-C(4)-C(5)	80.62(18)
C(1)-Ru(1)-C(4)-C(5)	38.61(17)
C(3)-Ru(1)-C(4)-C(5)	118.2(2)
C(38)-Ru(1)-C(4)-C(19)	-80.0(3)
C(39)-Ru(1)-C(4)-C(19)	22.1(3)
B(1)-Ru(1)-C(4)-C(19)	119.4(3)
C(2)-Ru(1)-C(4)-C(19)	-157.5(3)
C(5)-Ru(1)-C(4)-C(19)	121.9(3)
C(1)-Ru(1)-C(4)-C(19)	160.5(3)
C(3)-Ru(1)-C(4)-C(19)	-119.9(3)
O(1)-C(1)-C(5)-C(4)	-170.9(3)
C(2)-C(1)-C(5)-C(4)	4.7(3)
Ru(1)-C(1)-C(5)-C(4)	64.6(2)
O(1)-C(1)-C(5)-C(26)	0.8(5)
C(2)-C(1)-C(5)-C(26)	176.4(3)
Ru(1)-C(1)-C(5)-C(26)	-123.6(3)
O(1)-C(1)-C(5)-Ru(1)	124.4(3)
C(2)-C(1)-C(5)-Ru(1)	-60.0(2)
C(3)-C(4)-C(5)-C(1)	-2.3(3)
C(19)-C(4)-C(5)-C(1)	172.5(3)
Ru(1)-C(4)-C(5)-C(1)	-64.5(2)
C(3)-C(4)-C(5)-C(26)	-174.1(3)
C(19)-C(4)-C(5)-C(26)	0.8(5)
Ru(1)-C(4)-C(5)-C(26)	123.7(3)
C(3)-C(4)-C(5)-Ru(1)	62.2(2)
C(19)-C(4)-C(5)-Ru(1)	-122.9(3)
C(38)-Ru(1)-C(5)-C(1)	50.0(5)
C(39)-Ru(1)-C(5)-C(1)	-156.01(19)

B(1)-Ru(1)-C(5)-C(1)	-67.1(2)
C(2)-Ru(1)-C(5)-C(1)	35.66(17)
C(3)-Ru(1)-C(5)-C(1)	78.24(19)
C(4)-Ru(1)-C(5)-C(1)	114.5(3)
C(38)-Ru(1)-C(5)-C(4)	-64.5(5)
C(39)-Ru(1)-C(5)-C(4)	89.53(19)
B(1)-Ru(1)-C(5)-C(4)	178.39(18)
C(2)-Ru(1)-C(5)-C(4)	-78.80(18)
C(1)-Ru(1)-C(5)-C(4)	-114.5(3)
C(3)-Ru(1)-C(5)-C(4)	-36.23(17)
C(38)-Ru(1)-C(5)-C(26)	172.5(4)
C(39)-Ru(1)-C(5)-C(26)	-33.5(3)
B(1)-Ru(1)-C(5)-C(26)	55.4(3)
C(2)-Ru(1)-C(5)-C(26)	158.2(3)
C(1)-Ru(1)-C(5)-C(26)	122.6(3)
C(3)-Ru(1)-C(5)-C(26)	-159.2(3)
C(4)-Ru(1)-C(5)-C(26)	-123.0(3)
C(1)-C(2)-C(6)-C(11)	128.5(3)
C(3)-C(2)-C(6)-C(11)	-42.8(5)
Ru(1)-C(2)-C(6)-C(11)	-138.4(3)
C(1)-C(2)-C(6)-C(7)	-49.6(4)
C(3)-C(2)-C(6)-C(7)	139.0(3)
Ru(1)-C(2)-C(6)-C(7)	43.5(4)
C(11)-C(6)-C(7)-C(8)	0.5(5)
C(2)-C(6)-C(7)-C(8)	178.6(3)
C(6)-C(7)-C(8)-C(9)	0.2(5)
C(7)-C(8)-C(9)-C(10)	-0.3(6)
C(8)-C(9)-C(10)-C(11)	-0.3(6)
C(7)-C(6)-C(11)-C(10)	-1.0(5)
C(2)-C(6)-C(11)-C(10)	-179.2(3)
C(9)-C(10)-C(11)-C(6)	1.0(5)
C(4)-C(3)-C(12)-C(13)	132.0(3)
C(2)-C(3)-C(12)-C(13)	-60.9(4)
Ru(1)-C(3)-C(12)-C(13)	33.1(5)
C(4)-C(3)-C(12)-C(17)	-54.4(4)
C(2)-C(3)-C(12)-C(17)	112.7(3)
Ru(1)-C(3)-C(12)-C(17)	-153.3(2)
C(17)-C(12)-C(13)-C(14)	-0.8(5)
C(3)-C(12)-C(13)-C(14)	172.8(3)
C(12)-C(13)-C(14)-C(15)	-1.1(5)
C(13)-C(14)-C(15)-C(16)	1.9(5)
C(13)-C(14)-C(15)-C(18)	-179.8(3)
C(14)-C(15)-C(16)-C(17)	-1.0(5)
C(18)-C(15)-C(16)-C(17)	-179.2(3)
C(15)-C(16)-C(17)-C(12)	-0.9(5)
C(13)-C(12)-C(17)-C(16)	1.7(5)

C(3)-C(12)-C(17)-C(16)	-172.2(3)
C(3)-C(4)-C(19)-C(24)	120.1(3)
C(5)-C(4)-C(19)-C(24)	-54.0(5)
Ru(1)-C(4)-C(19)-C(24)	-147.0(3)
C(3)-C(4)-C(19)-C(20)	-56.7(4)
C(5)-C(4)-C(19)-C(20)	129.1(3)
Ru(1)-C(4)-C(19)-C(20)	36.2(4)
C(24)-C(19)-C(20)-C(21)	1.4(5)
C(4)-C(19)-C(20)-C(21)	178.4(3)
C(19)-C(20)-C(21)-C(22)	0.8(5)
C(20)-C(21)-C(22)-C(23)	-2.3(5)
C(20)-C(21)-C(22)-C(25)	176.7(3)
C(21)-C(22)-C(23)-C(24)	1.7(5)
C(25)-C(22)-C(23)-C(24)	-177.3(3)
C(20)-C(19)-C(24)-C(23)	-2.0(5)
C(4)-C(19)-C(24)-C(23)	-179.0(3)
C(22)-C(23)-C(24)-C(19)	0.5(6)
C(1)-C(5)-C(26)-C(31)	-34.6(5)
C(4)-C(5)-C(26)-C(31)	135.5(3)
Ru(1)-C(5)-C(26)-C(31)	-129.3(3)
C(1)-C(5)-C(26)-C(27)	148.1(3)
C(4)-C(5)-C(26)-C(27)	-41.7(5)
Ru(1)-C(5)-C(26)-C(27)	53.5(4)
C(31)-C(26)-C(27)-C(28)	-0.3(5)
C(5)-C(26)-C(27)-C(28)	177.0(3)
C(26)-C(27)-C(28)-C(29)	1.8(5)
C(27)-C(28)-C(29)-C(30)	-2.2(5)
C(28)-C(29)-C(30)-C(31)	1.0(5)
C(29)-C(30)-C(31)-C(26)	0.5(5)
C(27)-C(26)-C(31)-C(30)	-0.8(5)
C(5)-C(26)-C(31)-C(30)	-178.2(3)
B(1)-O(2)-C(32)-C(33)	178.3(3)
B(1)-O(2)-C(32)-C(37)	1.3(3)
C(37)-C(32)-C(33)-C(34)	-0.6(5)
O(2)-C(32)-C(33)-C(34)	-177.1(3)
C(32)-C(33)-C(34)-C(35)	-0.1(5)
C(33)-C(34)-C(35)-C(36)	0.4(6)
C(34)-C(35)-C(36)-C(37)	0.0(5)
C(33)-C(32)-C(37)-C(36)	1.1(5)
O(2)-C(32)-C(37)-C(36)	178.2(3)
C(33)-C(32)-C(37)-O(3)	-178.0(3)
O(2)-C(32)-C(37)-O(3)	-0.9(4)
C(35)-C(36)-C(37)-C(32)	-0.7(5)
C(35)-C(36)-C(37)-O(3)	178.2(3)
B(1)-O(3)-C(37)-C(32)	0.1(3)
B(1)-O(3)-C(37)-C(36)	-178.9(3)

C(39)-Ru(1)-C(38)-O(4)	156(12)
B(1)-Ru(1)-C(38)-O(4)	71(12)
C(2)-Ru(1)-C(38)-O(4)	-36(12)
C(5)-Ru(1)-C(38)-O(4)	-49(12)
C(1)-Ru(1)-C(38)-O(4)	-12(12)
C(3)-Ru(1)-C(38)-O(4)	-74(12)
C(4)-Ru(1)-C(38)-O(4)	-97(12)
C(38)-Ru(1)-C(39)-O(5)	136(25)
B(1)-Ru(1)-C(39)-O(5)	-140(25)
C(2)-Ru(1)-C(39)-O(5)	3(25)
C(5)-Ru(1)-C(39)-O(5)	-36(25)
C(1)-Ru(1)-C(39)-O(5)	-57(25)
C(3)-Ru(1)-C(39)-O(5)	30(25)
C(4)-Ru(1)-C(39)-O(5)	2(25)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)	0.84	1.96	2.680(3)	143.6

Symmetry transformations used to generate equivalent atoms: