Supporting Information

Conformation controlled stepwise hydride shuffling from the metal to the ligand backbone

Nicholas R. Wiedmaier, Hansjörg Speth, Georg Leistikow, Klaus Eichele, Hartmut Schubert, Hermann A. Mayer*, Lars Wesemann*

Content

Crystallographic Details

Table 1S. Selected crystallographic data for compound **2**, **3**.

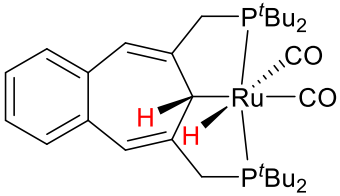
	syn-**2**	**3**
Empirical formula	$C_{31}H_{48}O_2P_2Ru$	$C_{32}H_{51}BCl_2F_4O_2P_2Ru$ $[C_{31}H_{49}O_2P_2Ru]\ BF_4 \times CH_2Cl_2$
M [g·mol^{-1}]	615.70	788.45
λ [Å]	0.71073	0.71073
T [K]	100(2)	100(2)
Crystal system	triklin	monoklin
Space group	$P\bar{1}$	$P2_1/c$
Z	2	4
a [Å]	11.7759(2)	11.9110(3)
b [Å]	12.0484(2)	12.8598(3)
c [Å]	13.1386(2)	23.6570(5)
α [°]	100.4810 (10)	90
β [°]	106.2420(10)	98.8350(10)
γ [°]	117.2990(10)	90
V [Å^3]	1481.55(4)	3580.62(14)
D_c [g·cm^{-3}]	1.380	1.463
μ [mm^{-1}]	0.663	0.725
F(000)	948	1632
Crystal size [mm]	0.26 x 0.13 x 0.10	0.11 x 0.15 x 0.17
Θ range [°]	2.56 – 27.14	2.35 – 29.15
Limiting indices	–15 ≤ h ≤ 15 –15 ≤ k ≤ 15 –16 ≤ l ≤ 16	–16 ≤ h ≤ 16 –17 ≤ k ≤ 17 –32 ≤ l ≤ 32
Reflections collected	14133	140096
Independent	13333	9631
R_{int}	0.0218	0.0248
Completeness	99.9	99.6
Absorption correction	Numerisch	multi-scan
Max. , Min.	0.935, 0.844	0.7458, 0.6860
Parameters/ restraints	345/ 0	417/ 1
R_1, wR_2 [I>2σI]	0.0201, 0.0473	0.0360, 0.0766
R_1, wR_2 (all data)	0.0239, 0.0488	0.0380, 0.0775
GooF on F^2	1.039	1.253
Peak/ hole [e·Å^{-3}]	0.442, –0.414	0.785, –0.709
CCDC	1982522	1982525

Table 2S. Selected crystallographic data for compound **5**, **6**.

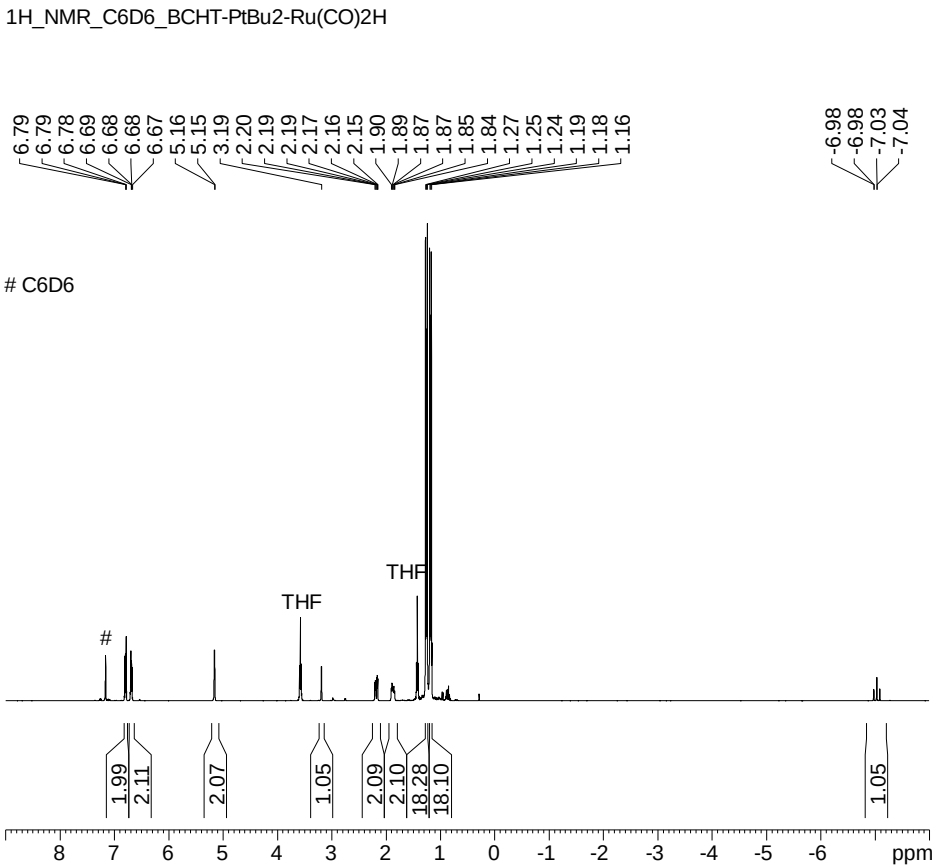
	5	*syn*-**6**
Empirical formula	$C_{67}H_{63}BF_{24}O_2P_2Ru$	$C_{33}H_{56}O_{2.5}P_2Ru$
	$[C_{31}H_{51}O_2P_2Ru]C_{36}H_{12}BF_{24}$	$C_{31}H_{52}O_2P_2Ru$ x 0.5 THF
M [g·mol^{-1}]	1481.86	655.78
λ [Å]	0.71073	0.71073
T [K]	100(2)	100(2)
Crystal system	monoklin	monoklin
Space group	$P2_1/n$	$P2_1/c$
Z	8	4
a [Å]	12.9706(3)	10.5466(8)
b [Å]	16.5597(3)	11.6310(8)
c [Å]	31.8663(7)	27.2772(19)
α [°]	90	90
β [°]	99.5240(10)	98.329(3)
γ [°]	90	90
V [Å^3]	6750.2(2)	3310.7(4)
D_c [g·cm^{-3}]	1.458	1.316
μ [mm^{-1}]	0.387	0.599
F(000)	3008	1392
Crystal size [mm]	0.18 x 0.16 x 0.14	0.20 x 0.19 x 0.17
Θ range [°]	2.46 – 28.67	3.82 – 27.88
Limiting indices	$-17 \le h \le 14$	$-13 \le h \le 9$
	$-22 \le k \le 22$	$-15 \le k \le 14$
	$-36 \le l \le 43$	$-35 \le l \le 35$
Reflections collected	107737	21639
Independent	17376	7811
R_{int}	0.0310	0.0175
Completeness	99.8	98.7
Absorption correction	multi-scan	multi-scan
Max. , Min.	0.7458, 0.6940	0.7456, 0.7044
Parameters/ restraints	882/ 0	362/ 8
R_1, wR_2 [I>2σI]	0.0418, 0.1026	0.0251, 0.0564
R_1, wR_2 (all data)	0.0532, 0.1098	0.0297, 0.0584
GooF on F^2	1.028	1.026
Peak/ hole [e·Å^{-3}]	1.675, –1.348	0.634, –0.957
CCDC	1982524	1982523

NMR data

^{1}H NMR spectrum of compound **2**



syn-**2**



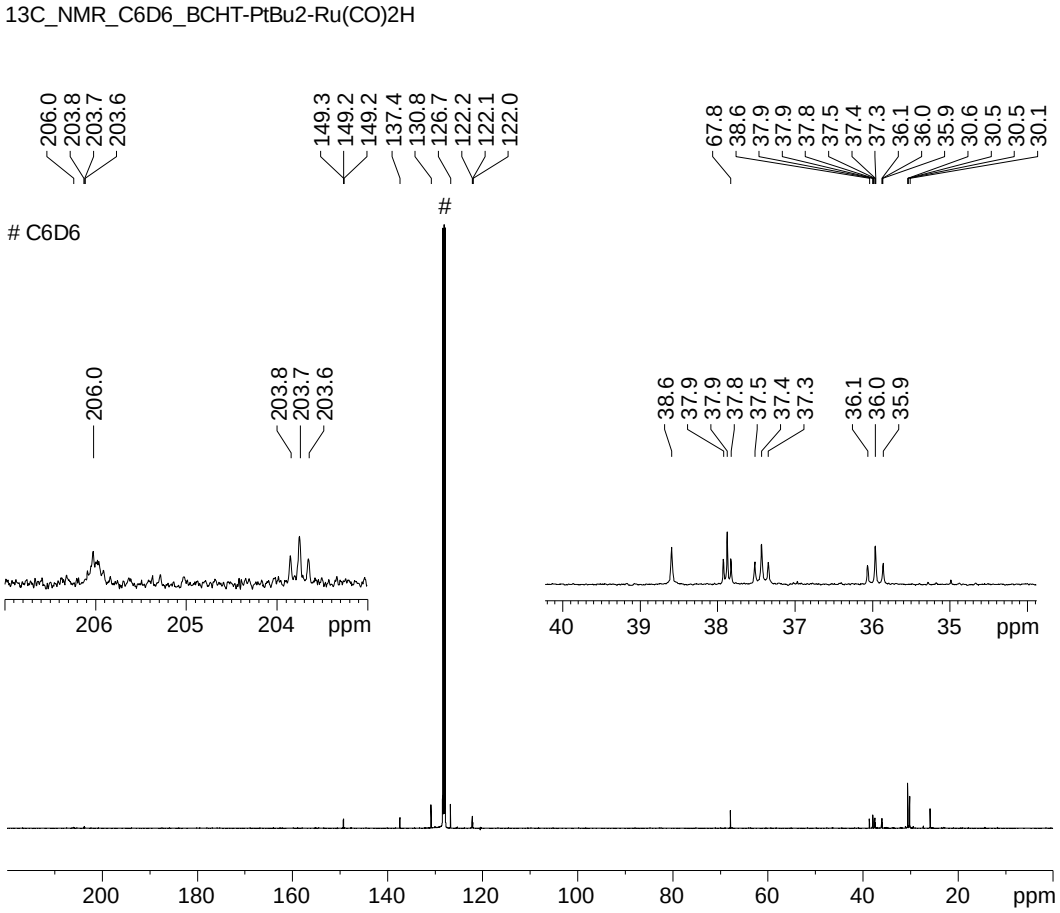
Current Data Parameters
NAME GL1-060618-Nacht
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180606
Time 20.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 52656
SOLVENT C6D6
NS 32
DS 0
SWH 12019.230 Hz
FIDRES 0.228259 Hz
AQ 2.1904895 sec
RG 161
DW 41.600 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.60 usec
PL1 -3.00 dB
PL1W 16.03799057 W
SFO1 400.1100000 MHz

F2 - Processing parameters
SI 65536
SF 400.1099934 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

$^{13}C\{^{1}H\}$ NMR spectrum of compound **2**



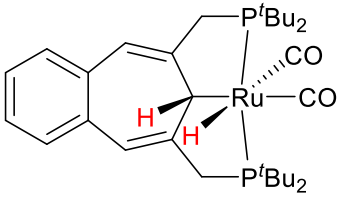
Current Data Parameters
NAME GL1-060618-Nacht_2
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180607
Time 7.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 53700
SOLVENT C6D6
NS 15000
DS 0
SWH 30864.197 Hz
FIDRES 0.574752 Hz
AQ 0.8699400 sec
RG 32800
DW 16.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
PL1 -4.16 dB
PL1W 78.55633545 W
SFO1 100.6198135 MHz

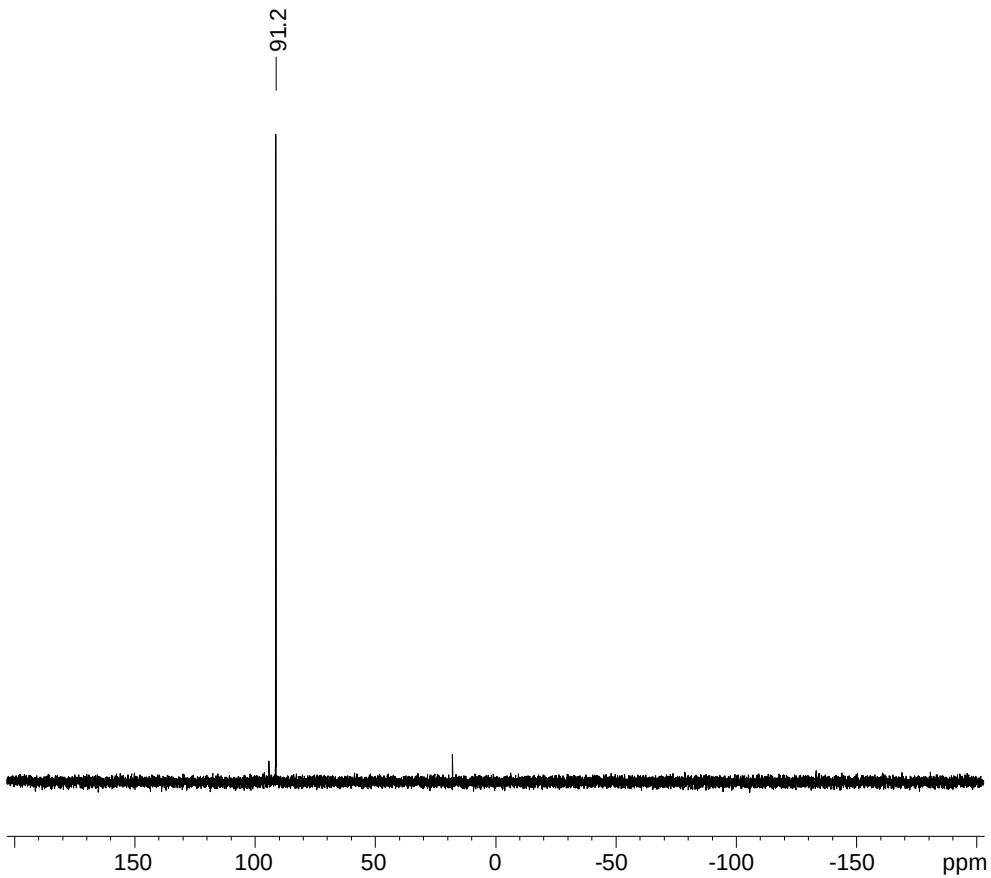
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 65536
SF 100.6077005 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



syn-**2**

$^{31}P\{^{1}H\}$ NMR spectrum of compound **2**



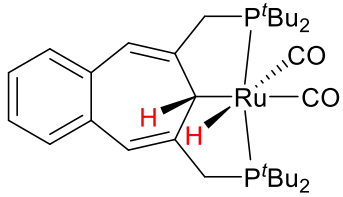
Current Data Parameters
NAME GL1-060618-Nacht
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180606
Time 20.07
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 88150
SOLVENT C6D6
NS 64
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 31P
P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

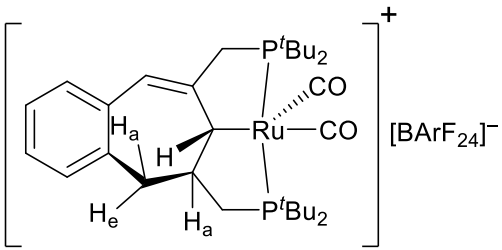
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

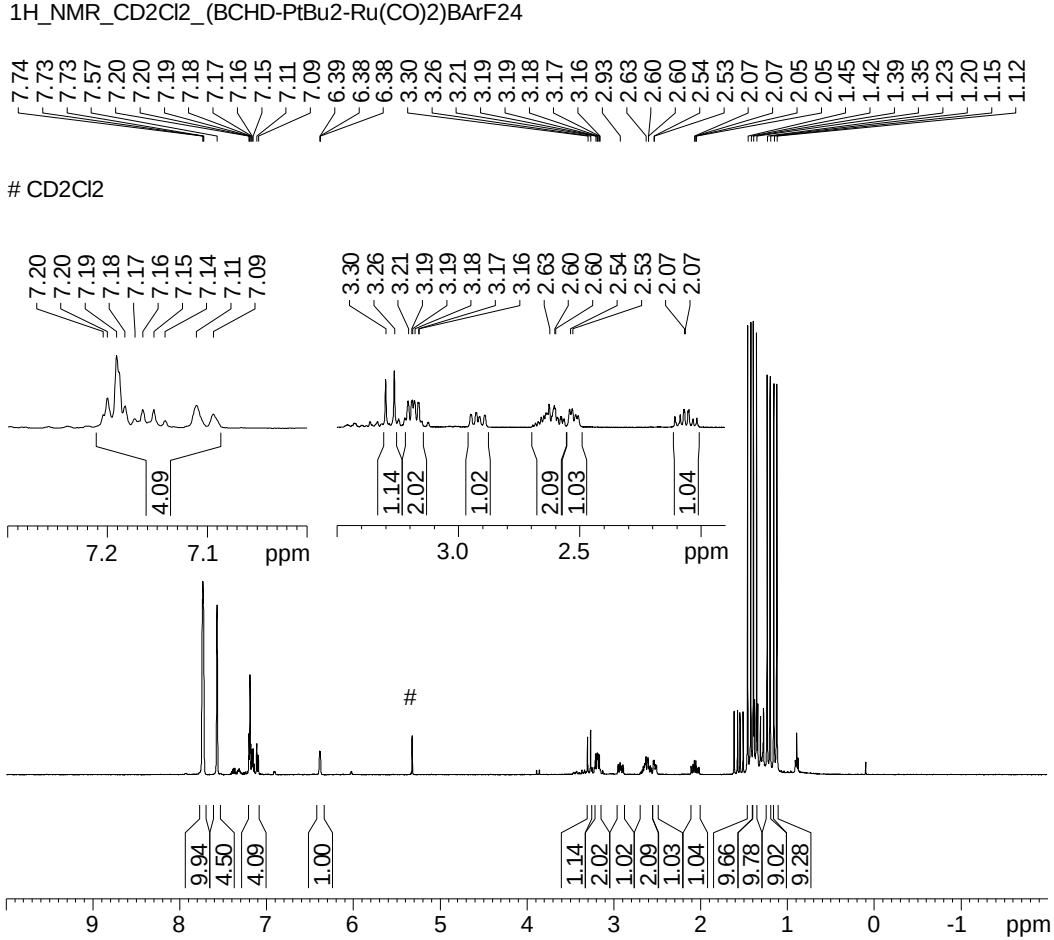


syn-**2**

^{1}H NMR spectrum of compound **3**



3



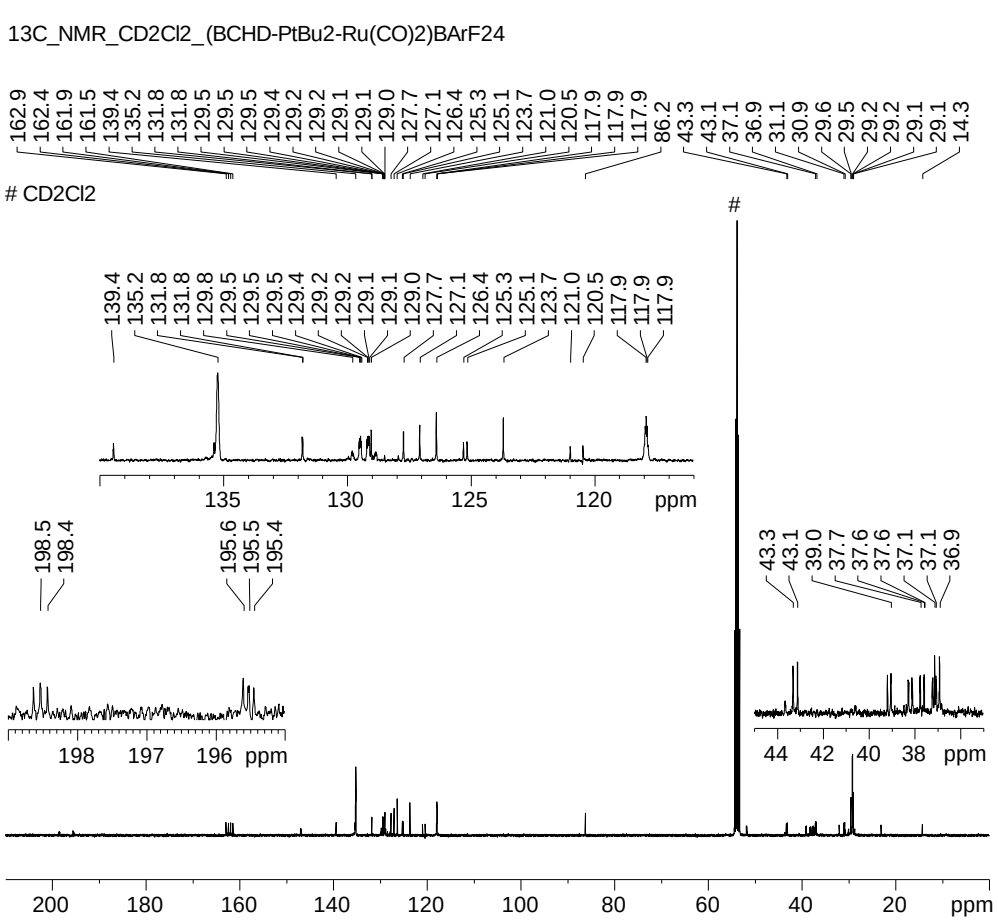
Current Data Parameters
NAME NW53-130718-Nacht
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180713
Time 20.05
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 52656
SOLVENT CD2Cl2
NS 16
DS 0
SWH 16025.641 Hz
FIDRES 0.304346 Hz
AQ 1.6428672 sec
RG 228
DW 31.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.60 usec
PL1 -3.00 dB
PL1W 16.03799057 W
SFO1 400.1100000 MHz

F2 - Processing parameters
SI 65536
SF 400.1100114 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

$^{13}C\{^{1}H\}$ NMR spectrum of compound **3**



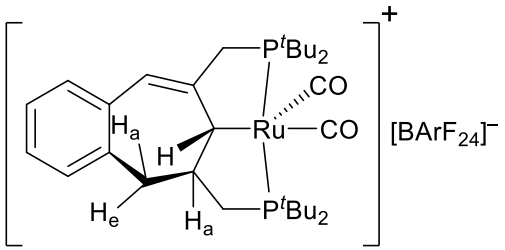
Current Data Parameters
NAME NW53-130718-Nacht
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180714
Time 7.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 53700
SOLVENT CD2Cl2
NS 15000
DS 0
SWH 30864.197 Hz
FIDRES 0.574752 Hz
AQ 0.8699400 sec
RG 32800
DW 16.200 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
PL1 -4.16 dB
PL1W 78.55633545 W
SFO1 100.6198135 MHz

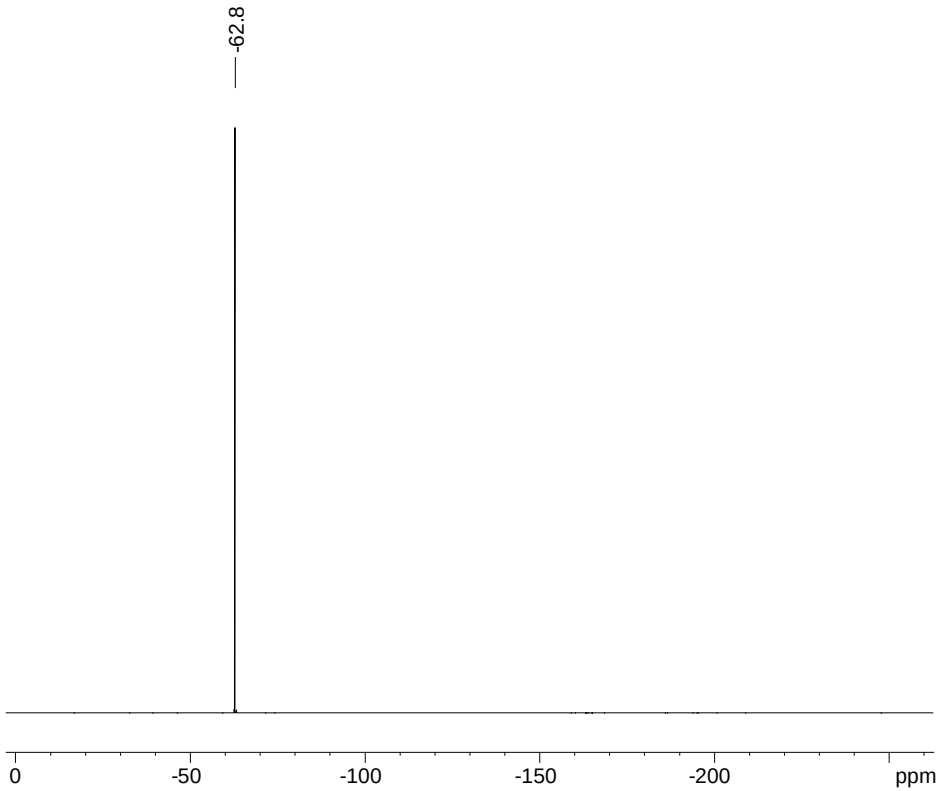
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 65536
SF 100.6076933 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



3

$^{19}F\{^{1}H\}$ NMR spectrum of compound 3



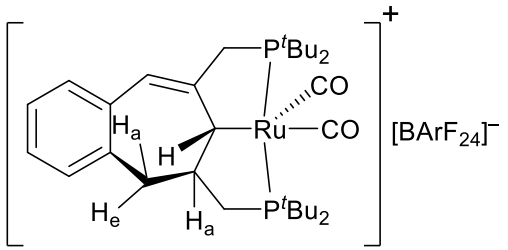
Current Data Parameters
NAME NW53-130718-Nacht
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180713
Time 20.07
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgfhigqn
TD 131072
SOLVENT CD2Cl2
NS 32
DS 0
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6553600 sec
RG 4100
DW 5.000 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 19F
P1 18.75 usec
PL1 -2.92 dB
PL1W 30.50645256 W
SFO1 376.4306030 MHz

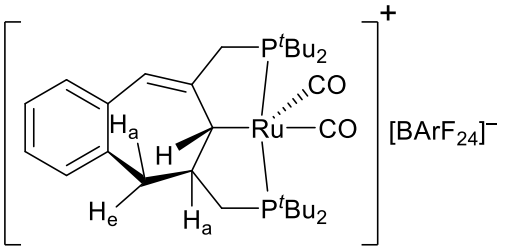
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 262144
SF 376.4795470 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

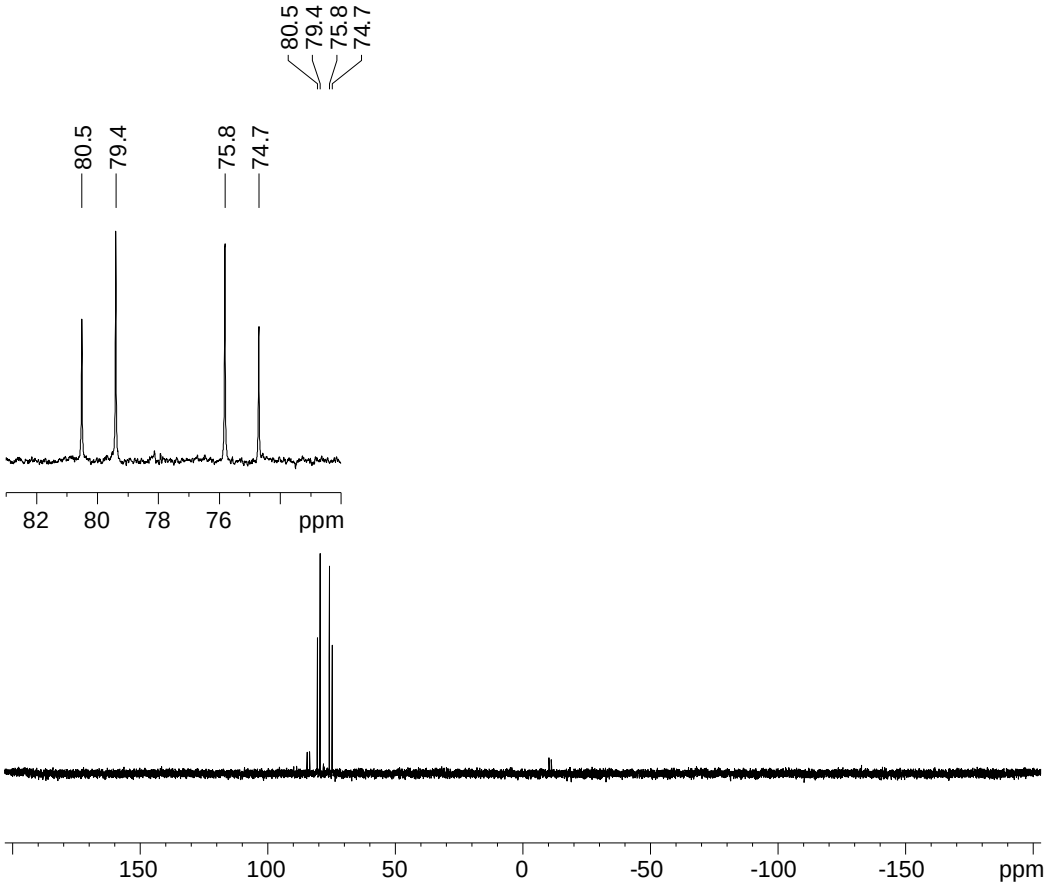


3

$^{31}P\{^{1}H\}$ NMR spectrum of compound **3**



3



Current Data Parameters
NAME NW53-130718-Nacht
EXPNO 11
PROCNO 1

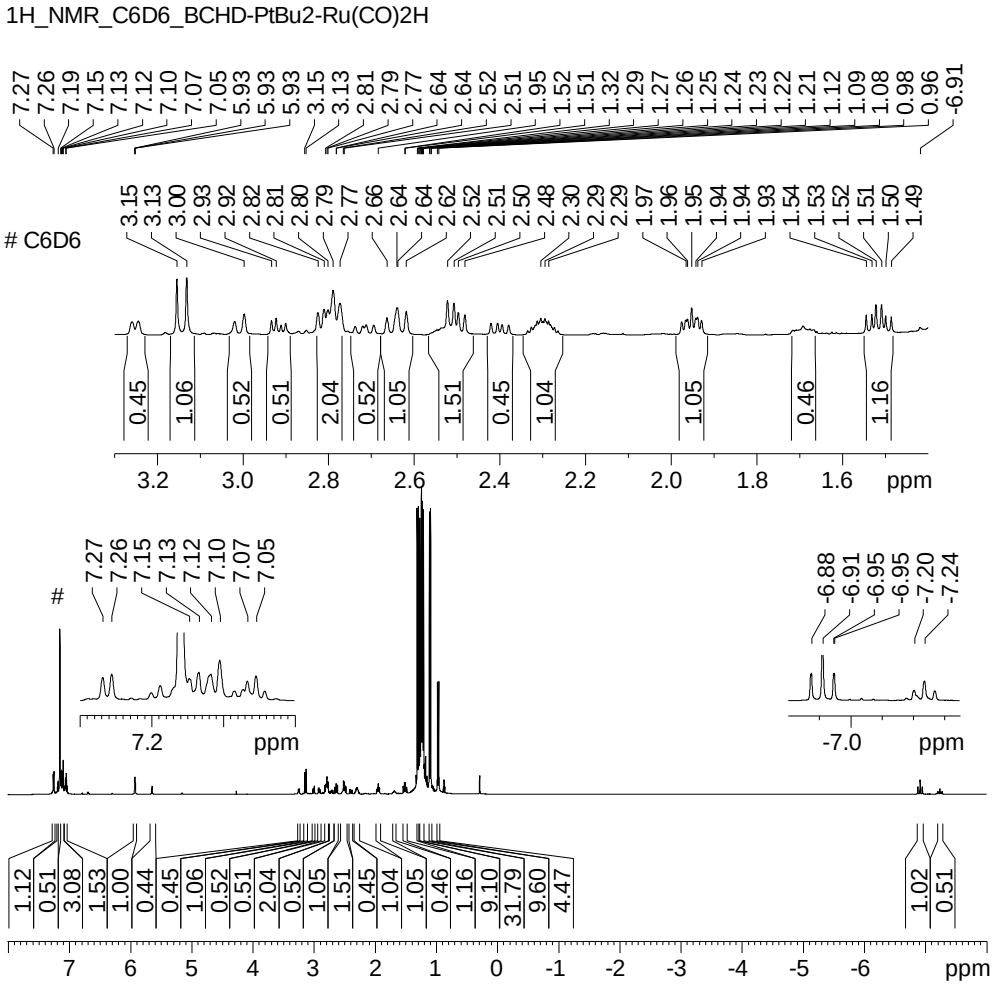
F2 - Acquisition Parameters
Date_ 20180713
Time 20.06
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 88150
SOLVENT CD2Cl2
NS 32
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 300.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 31P
P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

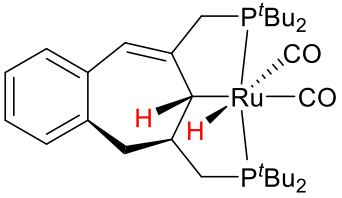
^{1}H NMR spectrum of **4**



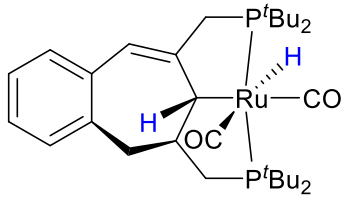
Current Data Parameters
NAME NW103-29112018-600-Nacht
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181129
Time 14.30 h
INSTRUM spect
PROBHD Z126545_0027 (
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 64
DS 0
SWH 9615.385 Hz
FIDRES 0.293438 Hz
AQ 3.4078720 sec
RG 17.08
DW 52.000 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1300000 MHz
NUC1 1H
P1 12.00 usec
PLW1 23.41200066 W

F2 - Processing parameters
SI 65536
SF 600.1299951 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

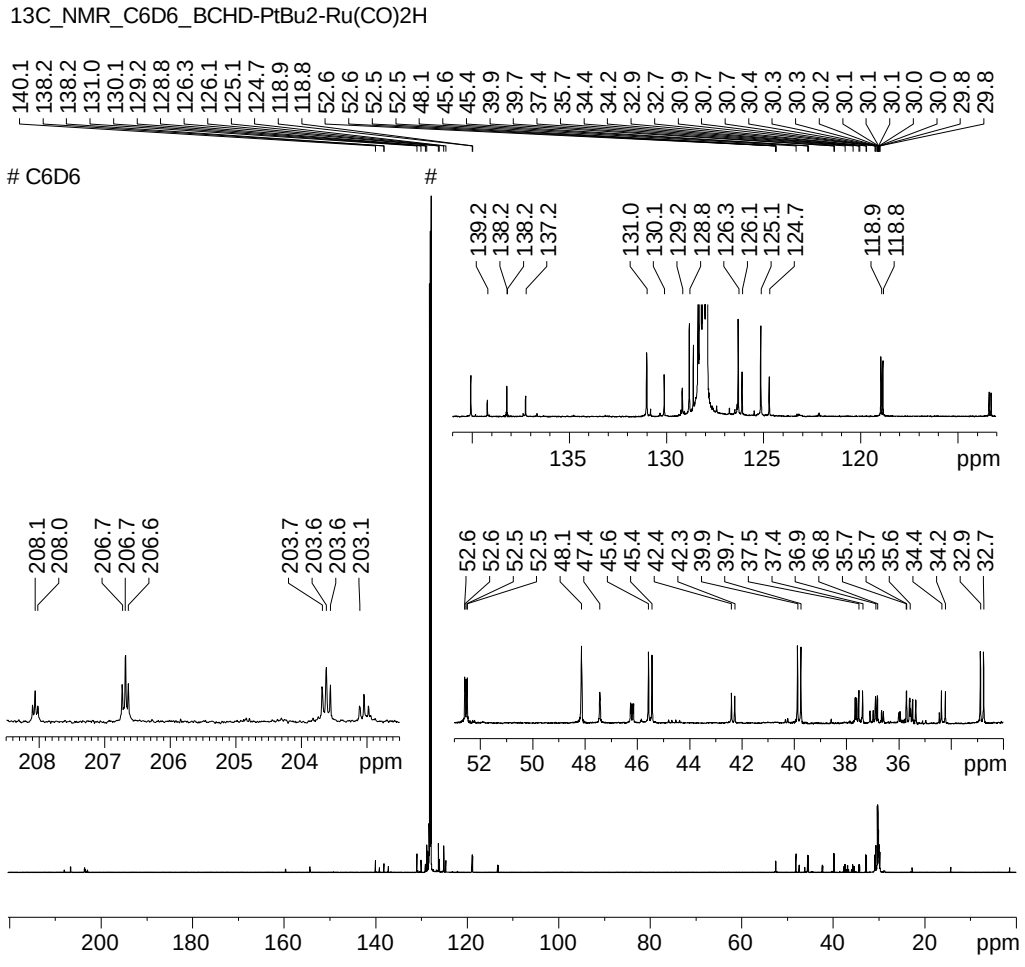


syn-**4**



anti-**4**

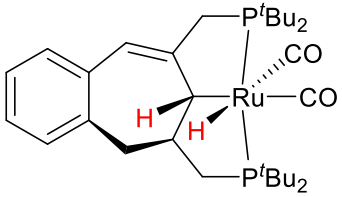
$^{13}C\{^{1}H\}$ NMR spectrum of 4



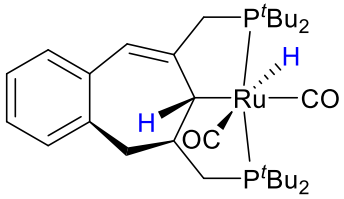
Current Data Parameters
NAME NW103-29112018-600-Nacht
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181129
Time 18.36 h
INSTRUM spect
PROBHD Z126545_0027 (
PULPROG udeft
TD 25902
SOLVENT C6D6
NS 3072
DS 0
SWH 36231.883 Hz
FIDRES 2.797613 Hz
AQ 0.3574476 sec
RG 189.6
DW 13.800 usec
DE 18.00 usec
TE 298.0 K
D1 4.00000000 sec
D12 0.00002000 sec
D20 25.00000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 10.00 usec
P13 2000.00 usec
P26 500.00 usec
PLW1 57.02700043 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 8.71310043 W
SPNAM[8] Crp60,0.5,20.1
SPOAL8 0.500
SPOFFS8 0 Hz
SPW8 8.71310043 W
SFO2 600.1300000 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 23.41200066 W
PLW12 0.68803000 W

F2 - Processing parameters
SI 32768
SF 150.9027515 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

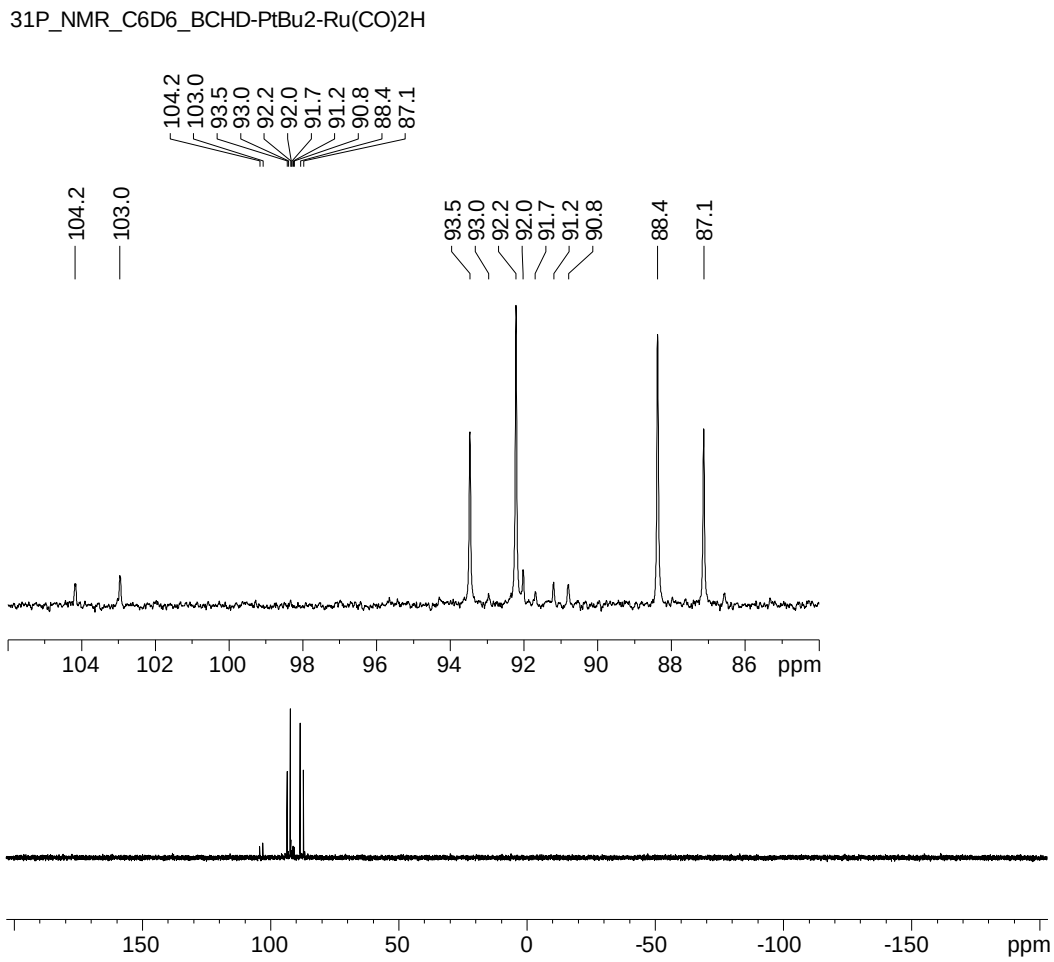


syn-**4**



anti-**4**

$^{31}P\{^{1}H\}$ NMR spectrum of 4



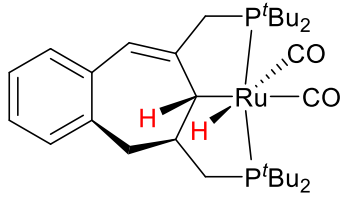
Current Data Parameters
NAME NW103-231118-1
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181123
Time 15.31
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 88150
SOLVENT C6D6
NS 64
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

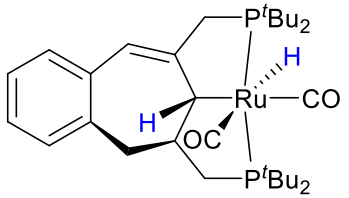
======== CHANNEL f1 ========
NUC1 31P
P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

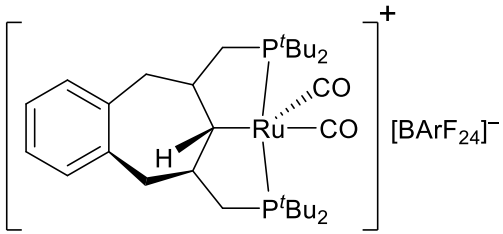


syn-**4**

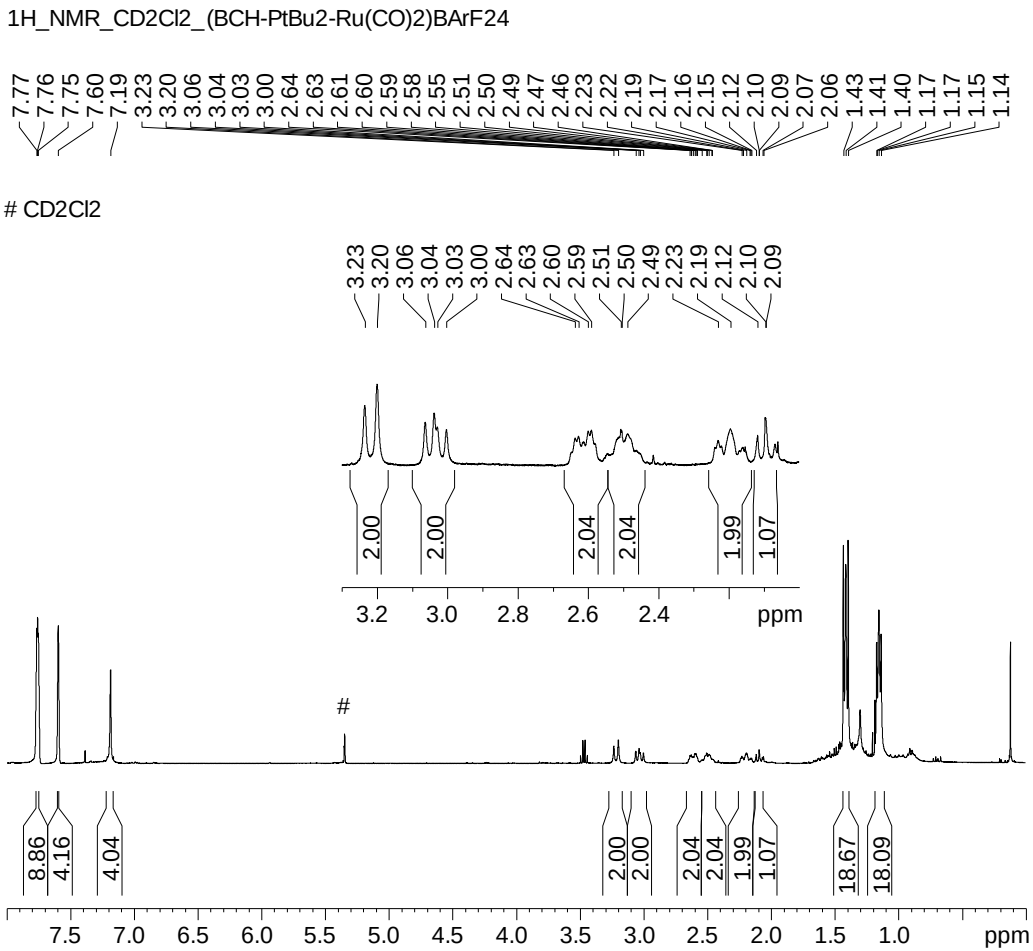


anti-**4**

^{1}H NMR spectrum of compound **5**



5



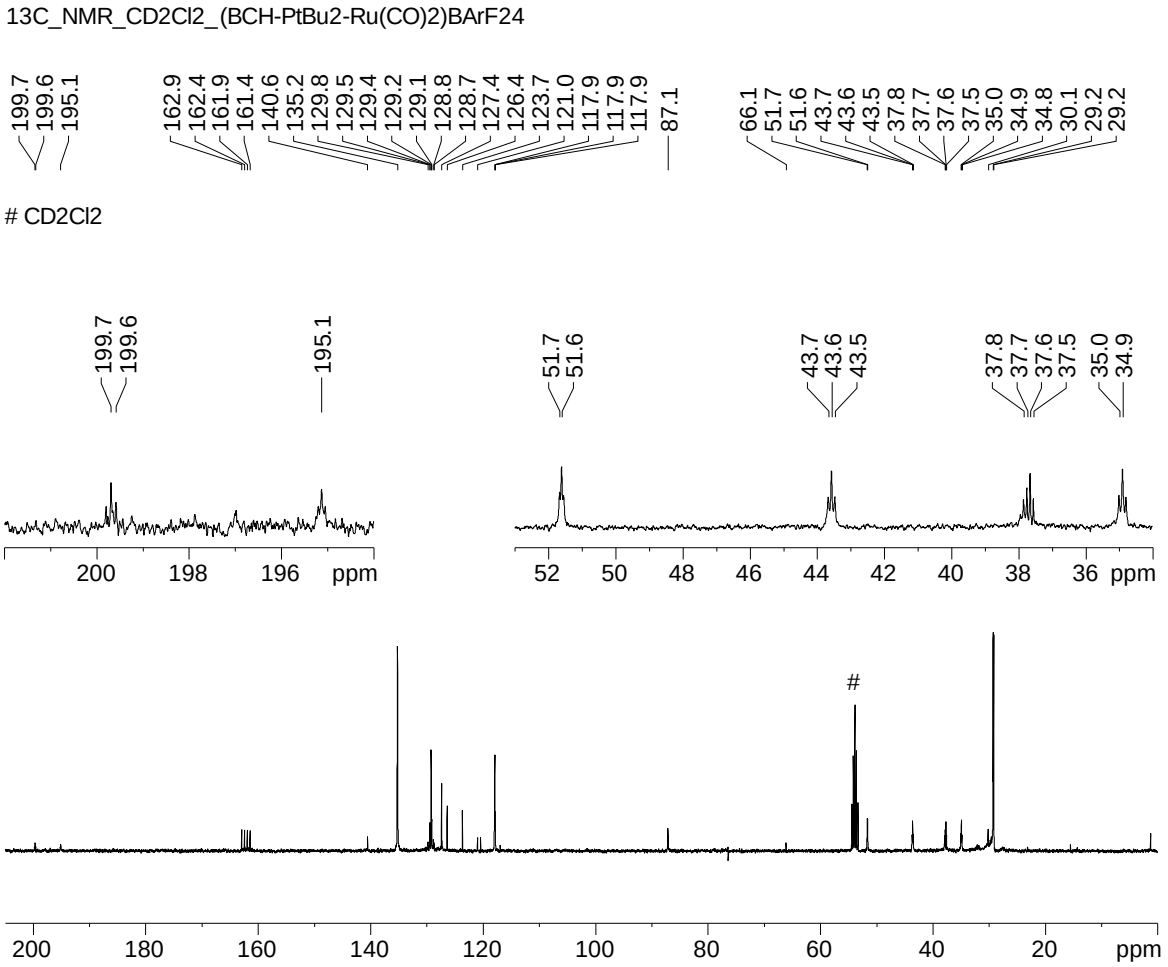
Current Data Parameters
NAME NW88-041218-Nacht
EXPNO 10
PROCNO 1

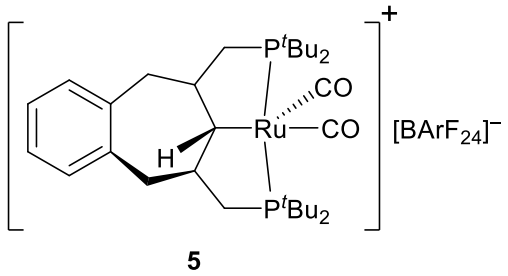
F2 - Acquisition Parameters
Date_ 20181204
Time 20.12
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 52656
SOLVENT CD2Cl2
NS 64
DS 0
SWH 4000.000 Hz
FIDRES 0.075965 Hz
AQ 6.5819998 sec
RG 228
DW 125.000 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.60 usec
PL1 -3.00 dB
PL1W 16.03799057 W
SFO1 400.1120006 MHz

F2 - Processing parameters
SI 65536
SF 400.1100000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

$^{13}C\{^{1}H\}$ NMR spectrum of compound **5**





5

Current Data Parameters
NAME NW88-091218-Nacht_2
EXPNO 14
PROCNO 1

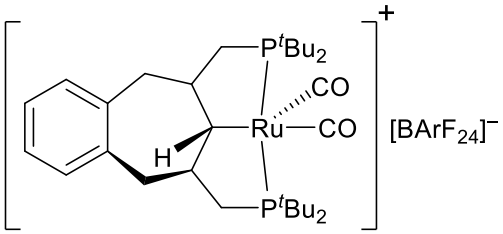
F2 - Acquisition Parameters
Date_ 20181210
Time 7.47
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG udeft
TD 22218
SOLVENT CD2Cl2
NS 11300
DS 0
SWH 30864.197 Hz
FIDRES 1.389153 Hz
AQ 0.3599316 sec
RG 32800
DW 16.200 usec
DE 6.00 usec
TE 299.2 K
D1 3.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D20 100.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
P13 2000.00 usec
P26 500.00 usec
PL1 -4.16 dB
PL1W 78.55633545 W
SFO1 100.6198135 MHz
SP8 1.39 dB
SP13 1.39 dB
SPNAM[8] Crp60,0.5,20.1
SPNAM[13 Crp60comp.4
SPOAL8 0.500
SPOAL13 0.500
SPOFFS8 0 Hz
SPOFFS13 0 Hz

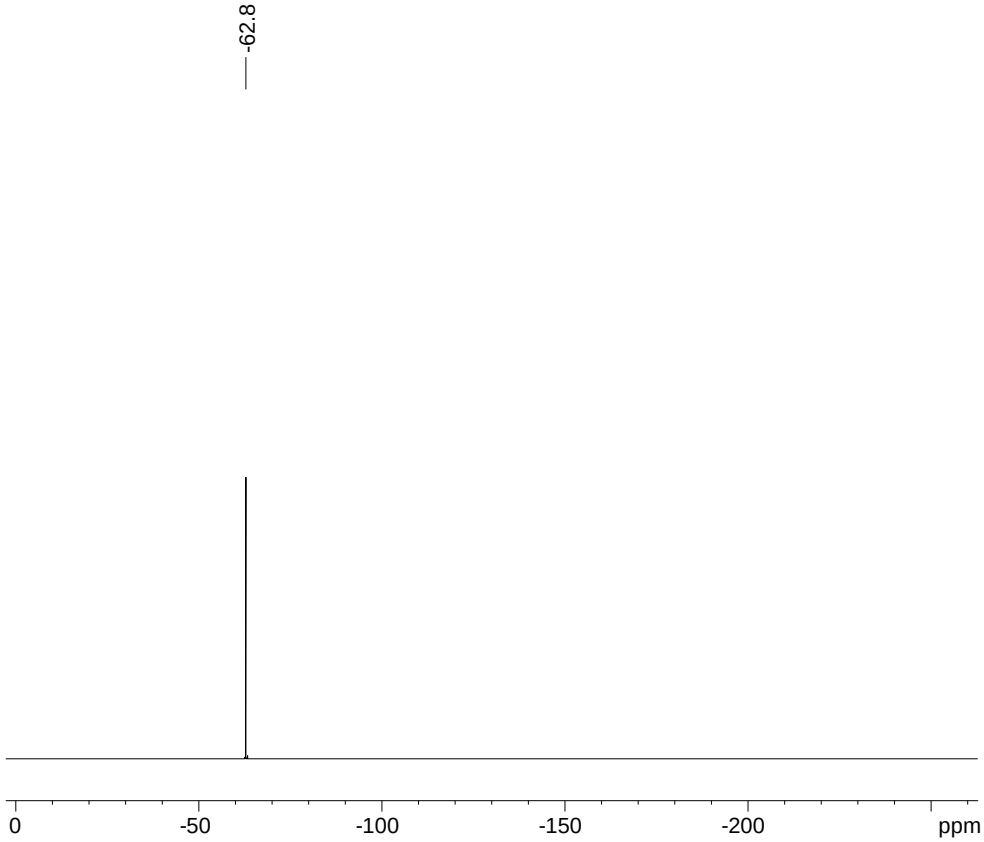
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 100.6076941 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

$^{19}F\{^{1}H\}$ NMR spectrum of compound **5**



5



Current Data Parameters
NAME NW88-041218-Nacht
EXPNO 18
PROCNO 1

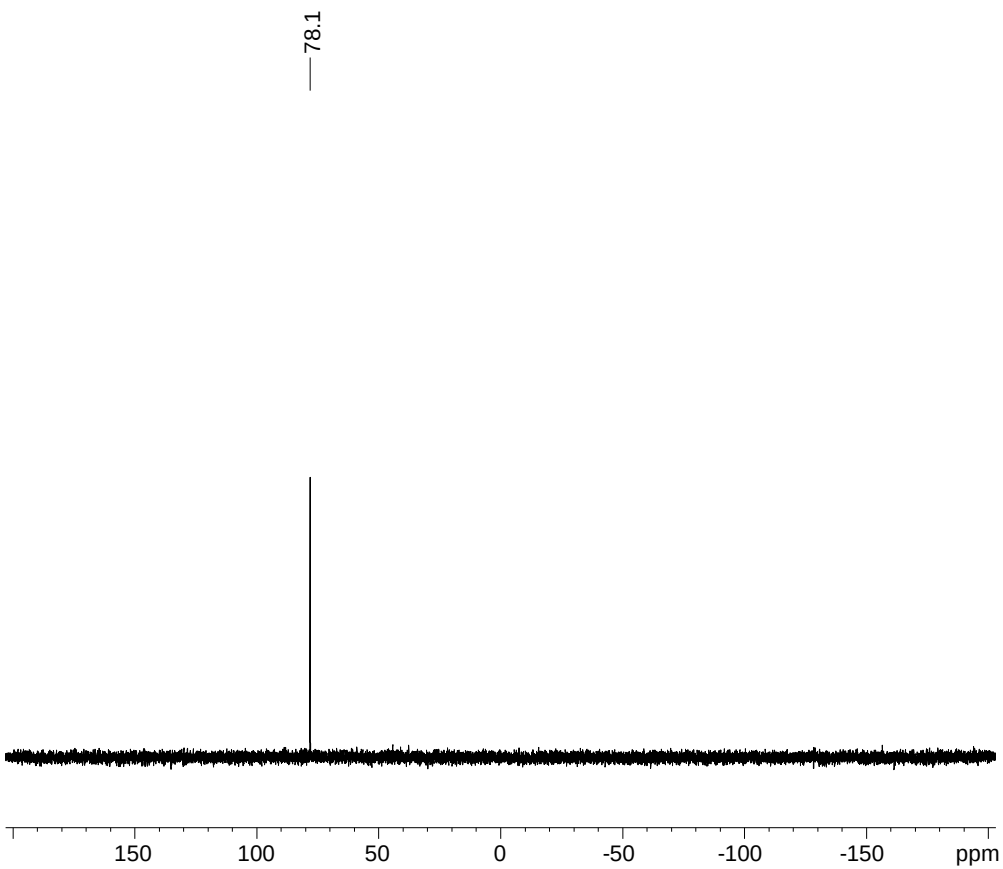
F2 - Acquisition Parameters
Date_ 20180903
Time 16.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgfhigqn
TD 131072
SOLVENT CD2Cl2
NS 32
DS 0
SWH 100000.000 Hz
FIDRES 0.762939 Hz
AQ 0.6553600 sec
RG 4100
DW 5.000 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 19F
P1 18.75 usec
PL1 -2.92 dB
PL1W 30.50645256 W
SFO1 376.4306030 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 262144
SF 376.4795470 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

$^{31}P\{^{1}H\}$ NMR spectrum of compound **5**



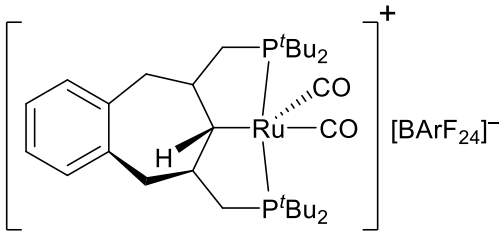
Current Data Parameters
NAME NW88-041218-Nacht
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181204
Time 20.14
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 88150
SOLVENT CD2Cl2
NS 64
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 31P
P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

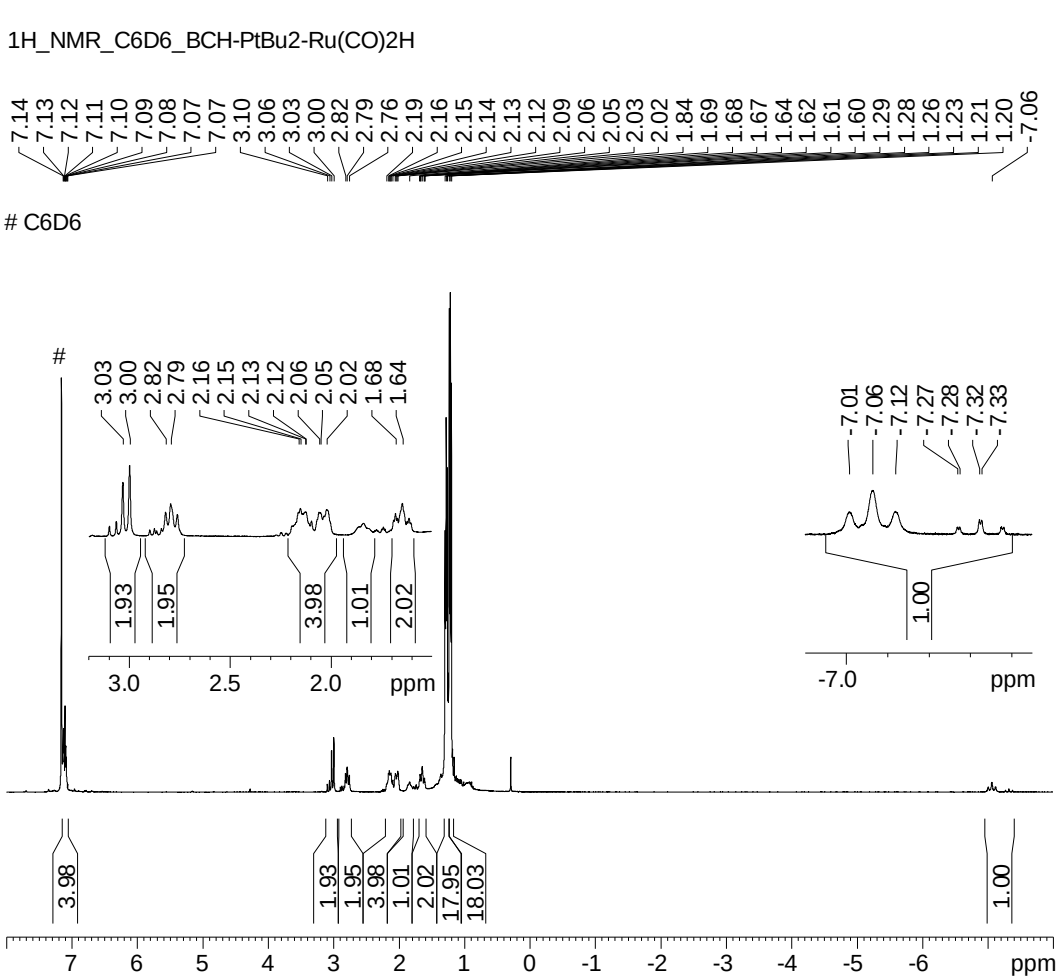
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



5

^{1}H NMR spectrum of **6**

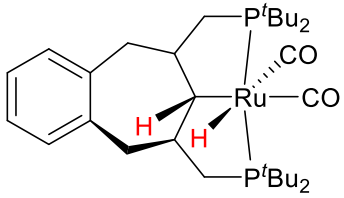


Current Data Parameters
NAME NW159-131218-Nacht
EXPNO 10
PROCNO 1

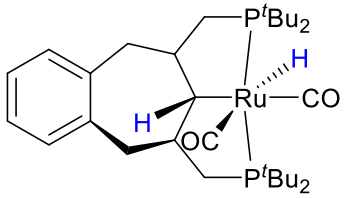
F2 - Acquisition Parameters
Date_ 20181213
Time 20.06
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 52656
SOLVENT C6D6
NS 32
DS 0
SWH 8305.647 Hz
FIDRES 0.157734 Hz
AQ 3.1698911 sec
RG 161
DW 60.200 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.60 usec
PL1 -3.00 dB
PL1W 16.03799057 W
SFO1 400.1100000 MHz

F2 - Processing parameters
SI 65536
SF 400.1099924 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

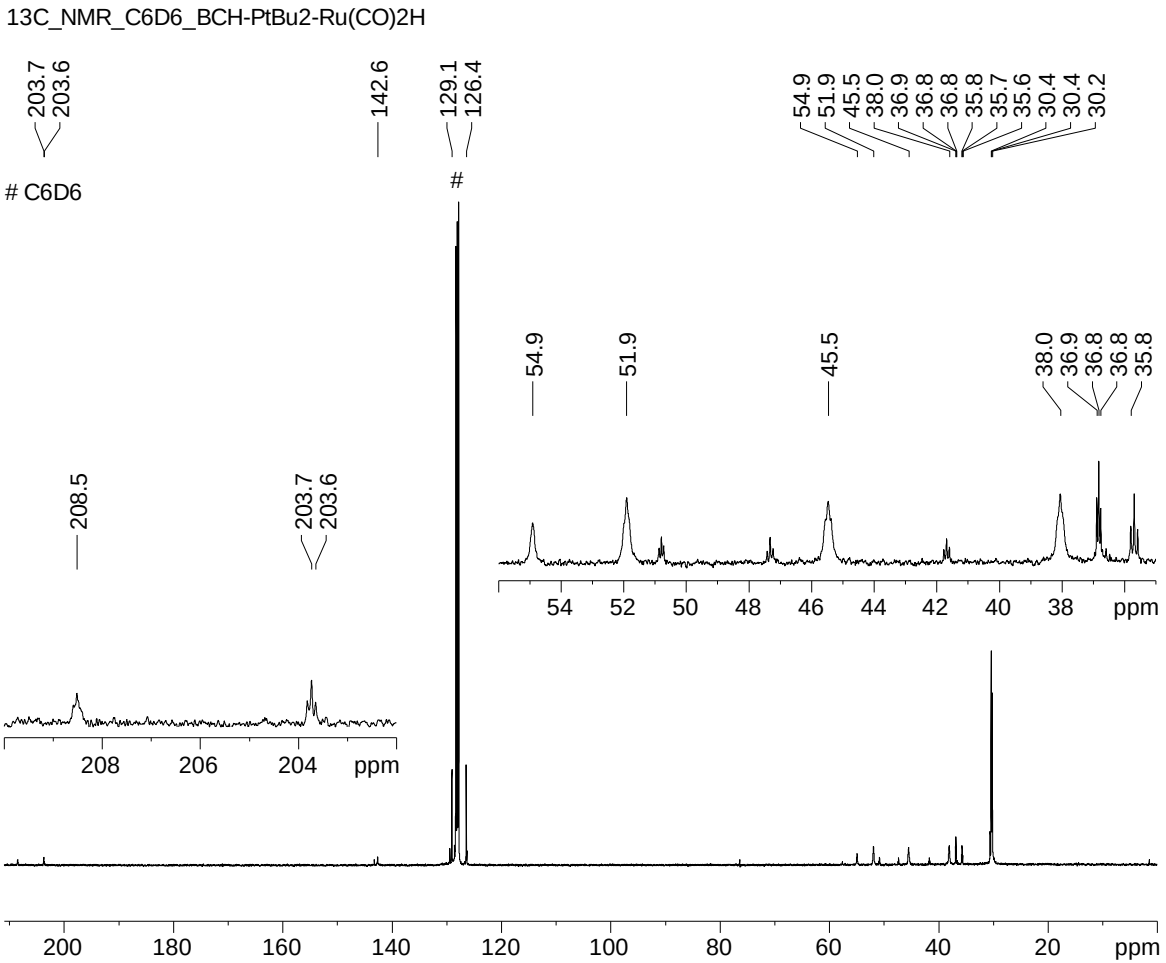


syn-**6**



anti-**6**

^{13}C {^{1}H} NMR spectrum of **6**



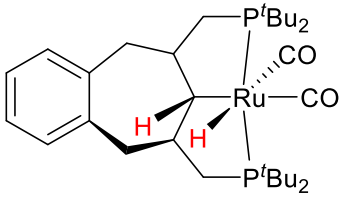
Current Data Parameters
NAME NW159-131218-Nacht_2
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181214
Time 4.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG udeft
TD 22218
SOLVENT C6D6
NS 7500
DS 0
SWH 30864.197 Hz
FIDRES 1.389153 Hz
AQ 0.3599316 sec
RG 32800
DW 16.200 usec
DE 6.00 usec
TE 299.2 K
D1 3.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D20 100.00000000 sec
TD0 1

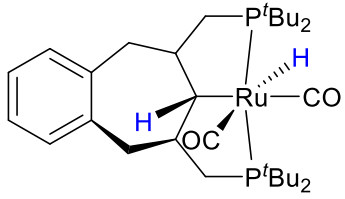
======== CHANNEL f1 ========
NUC1 13C
P1 13.50 usec
P13 2000.00 usec
P26 500.00 usec
PL1 -4.16 dB
PL1W 78.55633545 W
SFO1 100.6198135 MHz
SP8 1.39 dB
SP13 1.39 dB
SPNAM[8] Crp60,0.5,20.1
SPNAM[13 Crp60comp.4
SPOAL8 0.500
SPOAL13 0.500
SPOFFS8 0 Hz
SPOFFS13 0 Hz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 100.6077013 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

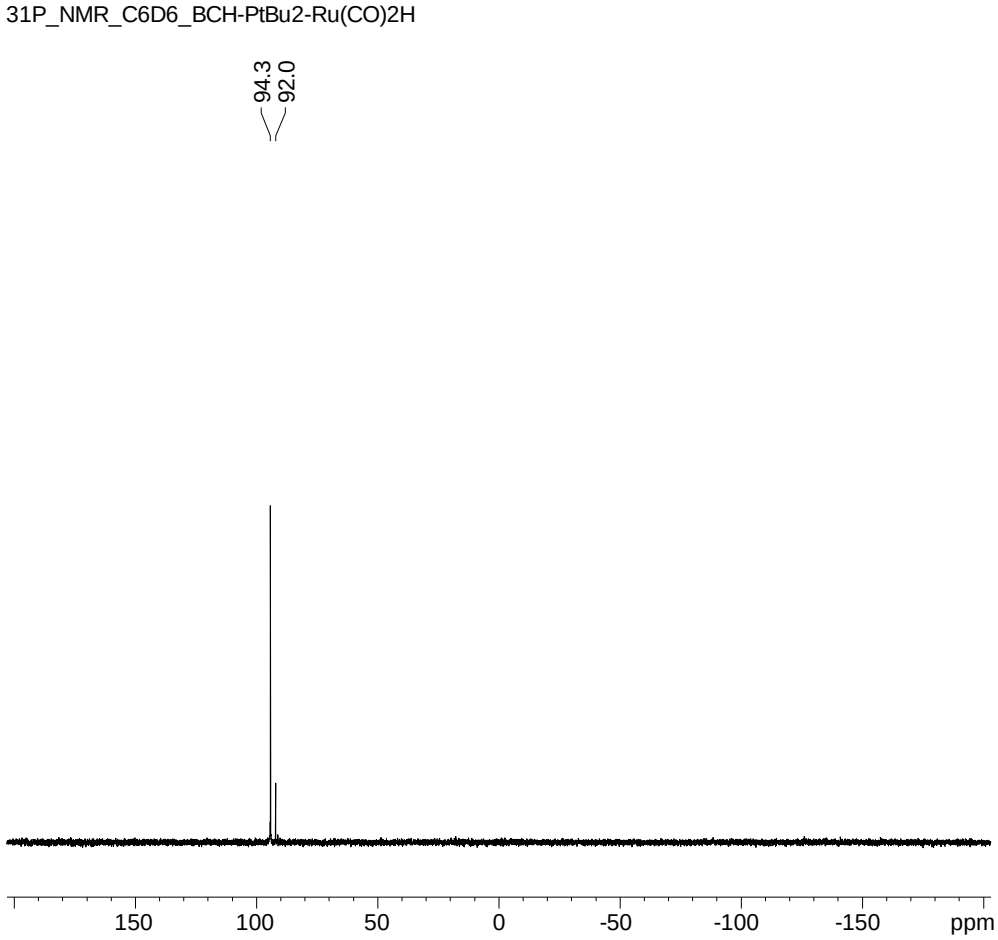


syn-**6**



anti-**6**

$^{31}P\{^{1}H\}$ NMR spectrum of **6**



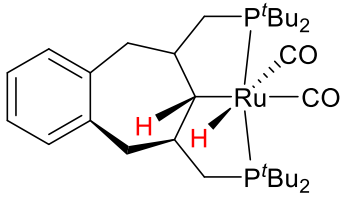
Current Data Parameters
NAME NW159-131218-Nacht
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181213
Time 20.08
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 88150
SOLVENT C6D6
NS 64
DS 0
SWH 65789.477 Hz
FIDRES 0.746336 Hz
AQ 0.6699400 sec
RG 23100
DW 7.600 usec
DE 6.00 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

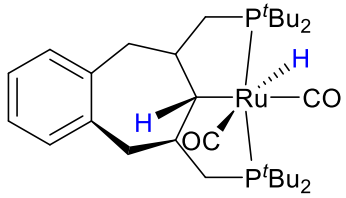
======== CHANNEL f1 ========
NUC1 31P
P1 11.00 usec
PL1 -3.00 dB
PL1W 45.10684967 W
SFO1 161.9674970 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.77 dB
PL13 13.14 dB
PL2W 16.03799057 W
PL12W 0.53474891 W
PL13W 0.39007664 W
SFO2 400.1120007 MHz

F2 - Processing parameters
SI 131072
SF 161.9674970 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



syn-**6**



anti-**6**