Electronic Supplementary Material (ESI) for Dalton Transactions


# One-Step Entry to Olefin-Tethered *N*,*S*-Heterocyclic Carbene Complexes of Ruthenium with Mixed Ligands

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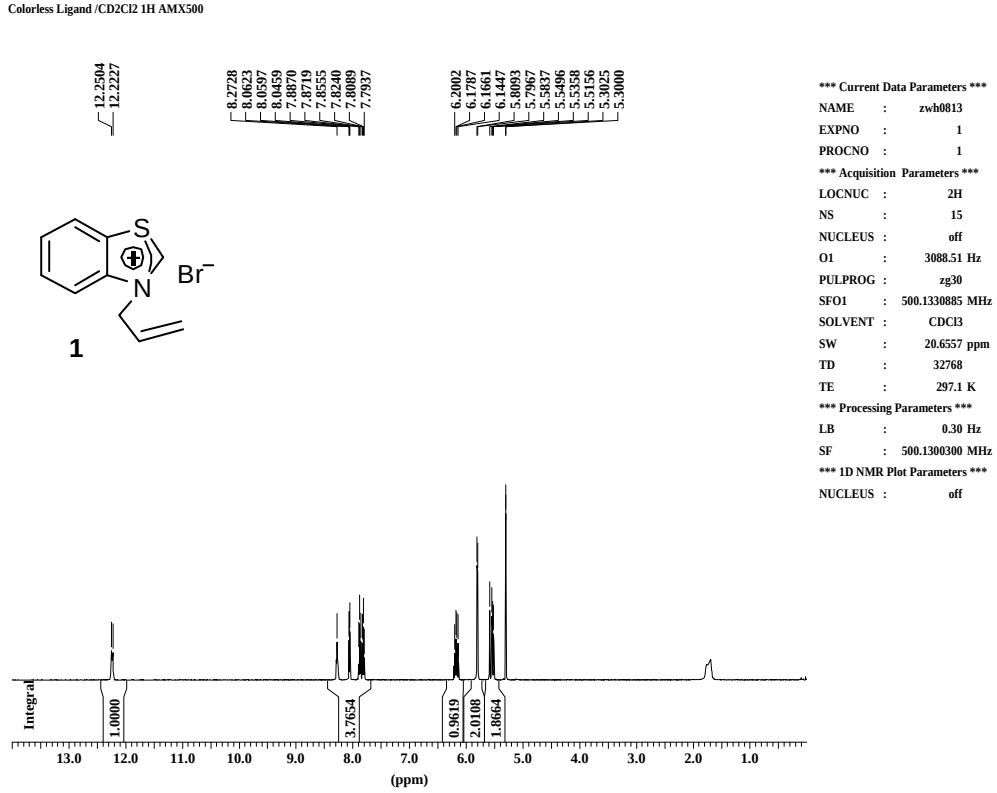
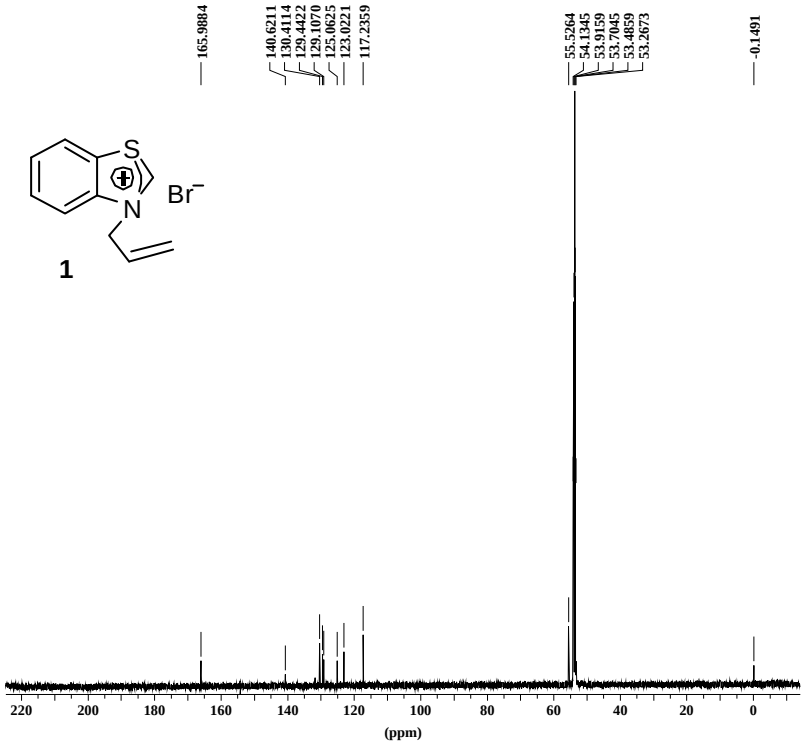
## $^{1}$H, $^{13}$C, $^{31}$P NMR spectra



Colorless Ligand /CD2Cl2 13C AMX500

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PROCNO : 1
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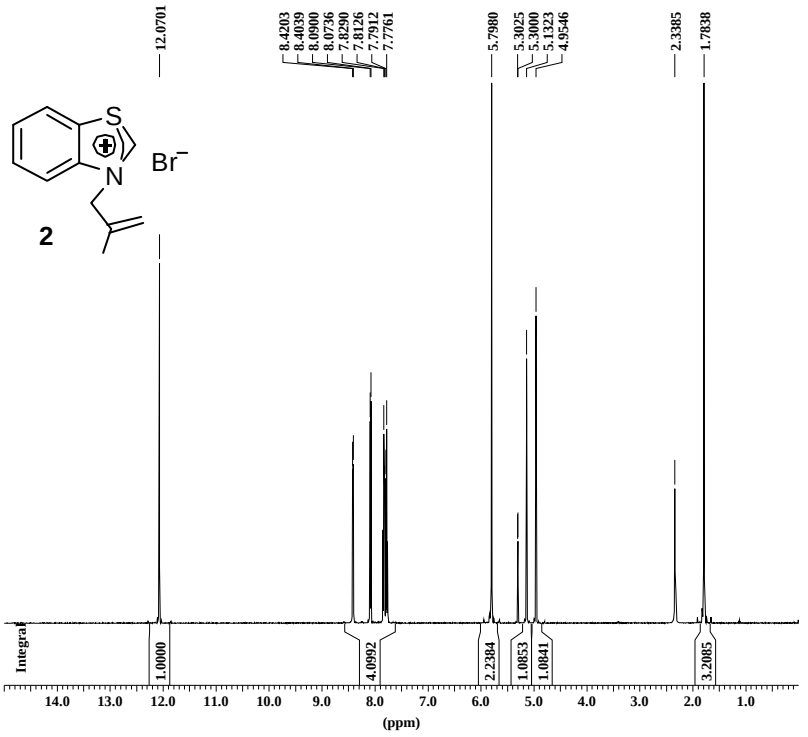
NS : 1324
NUCLEUS : off
O1 : 13204.57 Hz
PULPROG : zgpg30
SFO1 : 125.7709936 MHz
SOLVENT : CD2Cl2
SW : 238.7675 ppm
TD : 65536
TE : 297.6 K
*** Processing Parameters ***
LB : 1.00 Hz
SF : 125.7577514 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off

NSCH2C(CH3)=CH2--1H AMX500

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NS : 8
NUCLEUS : off
O1 : 3088.51 Hz
PULPROG : zg30
SFO1 : 500.1330885 MHz
SOLVENT : CDCl3
SW : 20.6557 ppm
TD : 32768
TE : 296.7 K
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LB : 0.30 Hz
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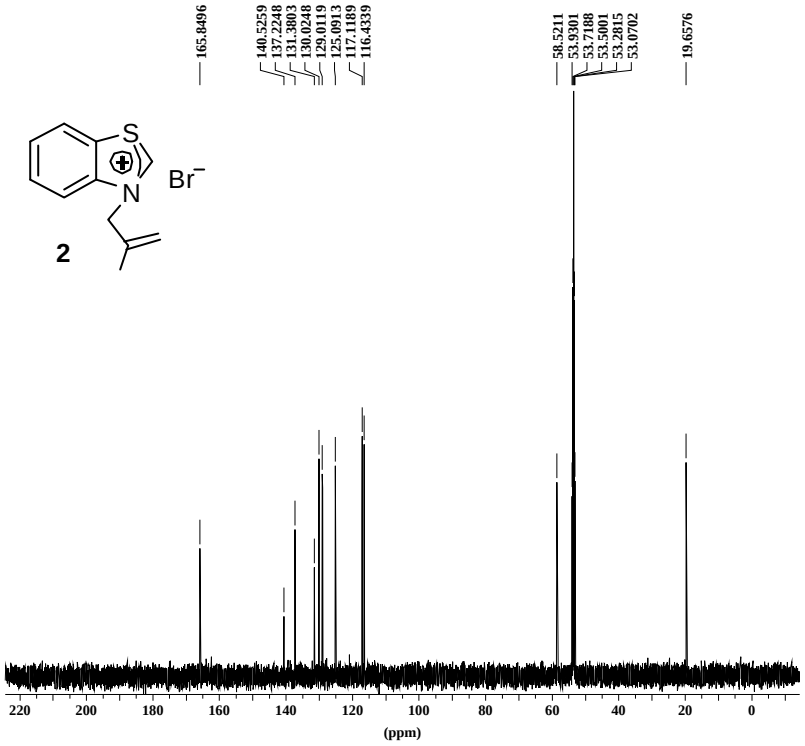
*** 1D NMR Plot Parameters ***
NUCLEUS : off

NSCH2C(CH3)=CH2--13C AMX500

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SOLVENT : CD2Cl2
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TD : 65536
TE : 297.3 K
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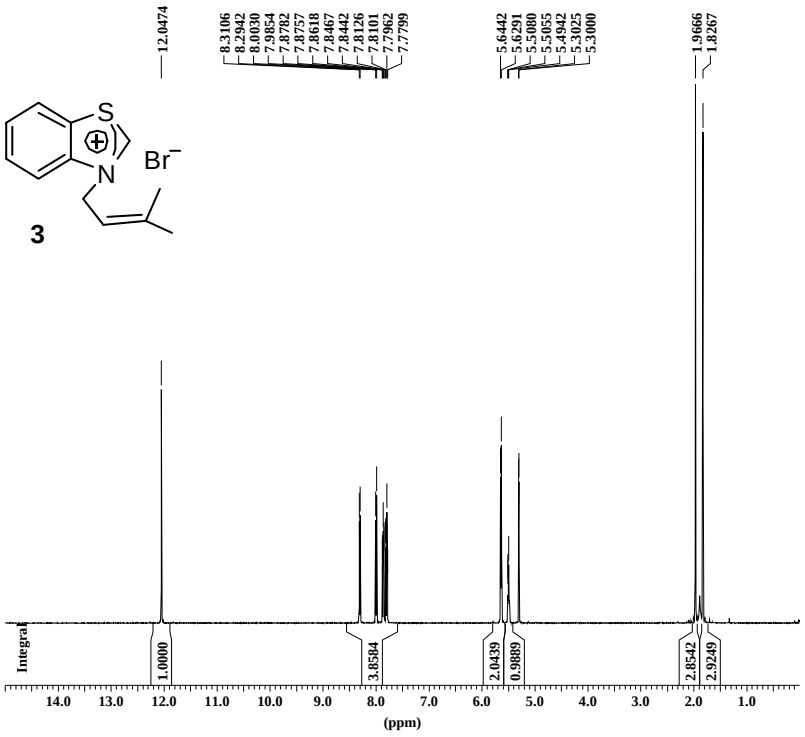
*** 1D NMR Plot Parameters ***
NUCLEUS : off

NSCH2C=C(CH3)2--1H AMX500

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NS : 8
NUCLEUS : off
O1 : 3088.51 Hz
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SFO1 : 500.1330885 MHz
SOLVENT : CD2Cl2
SW : 20.6557 ppm
TD : 32768
TE : 296.9 K
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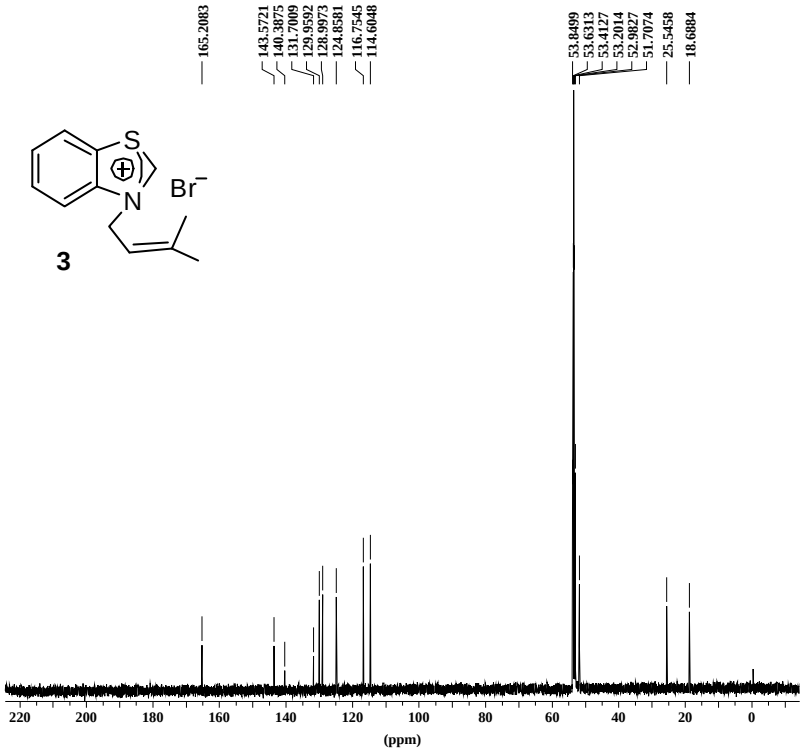
*** 1D NMR Plot Parameters ***
NUCLEUS : off

NSCH2C=C(CH3)2--13C AMX500

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SOLVENT : CDCl3
SW : 238.7675 ppm
TD : 65536
TE : 297.0 K
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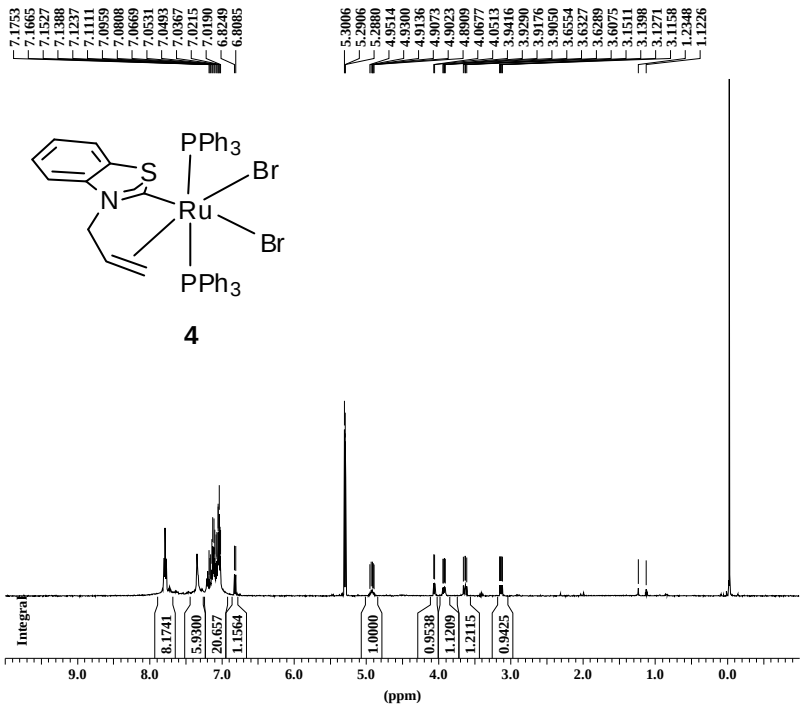
SF : 125.7577890 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off

RuNSCH2CH=CH2 1H AMX500

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SOLVENT : CDCl3
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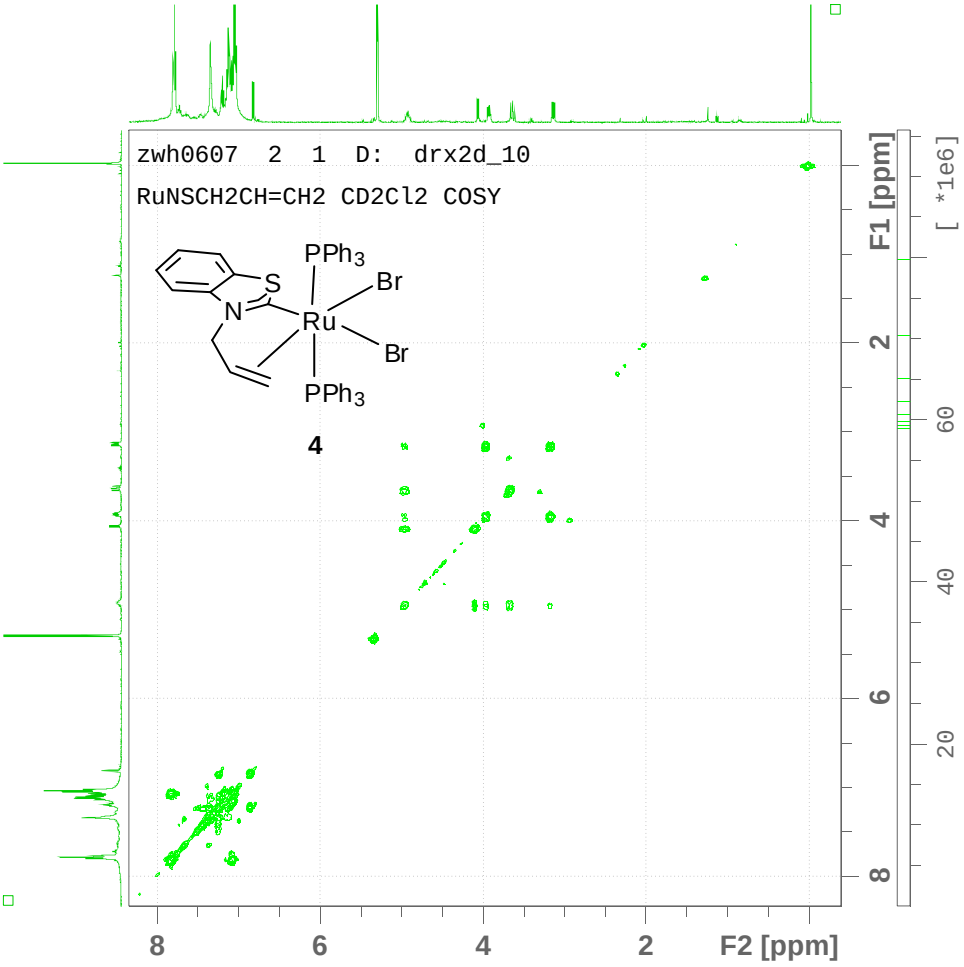
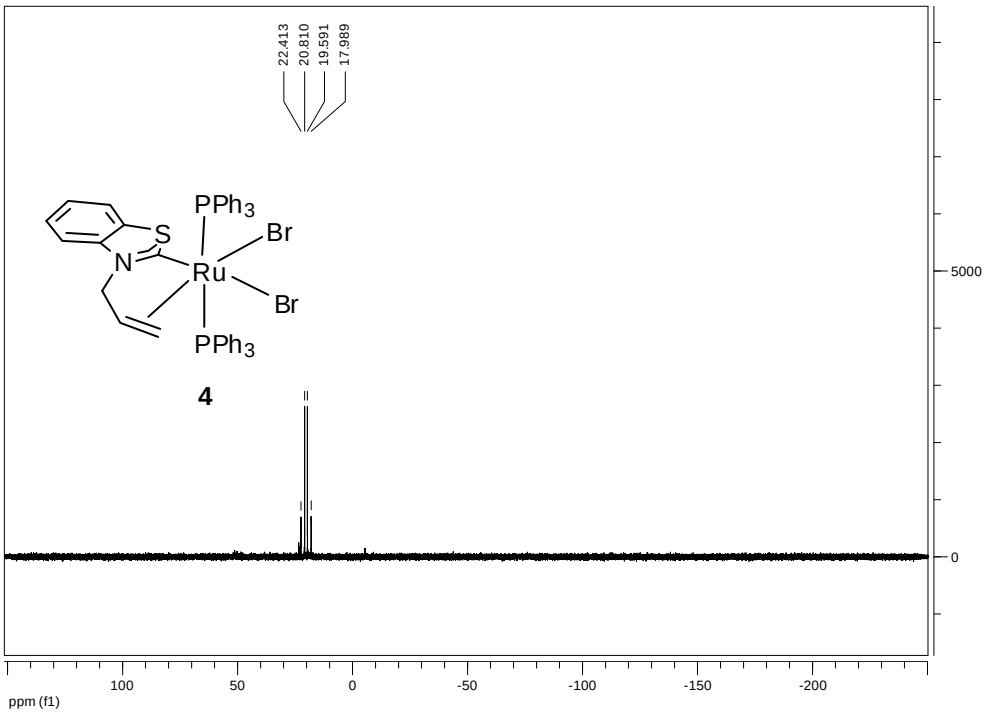
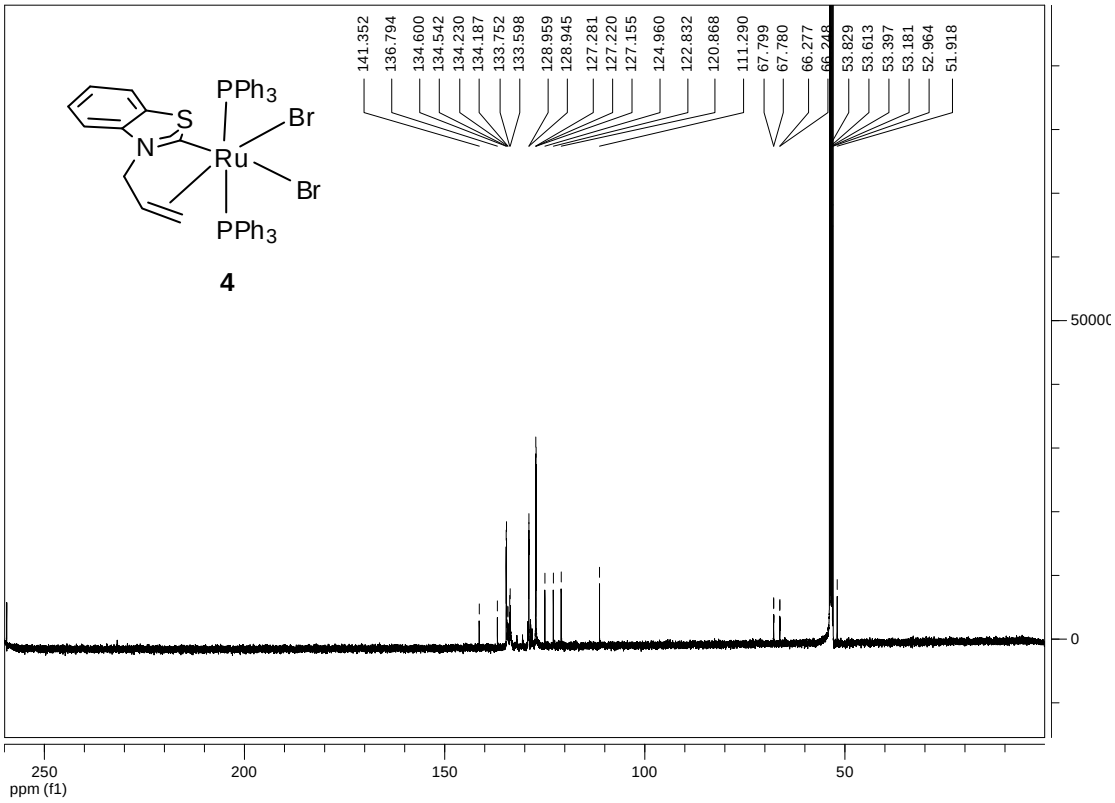
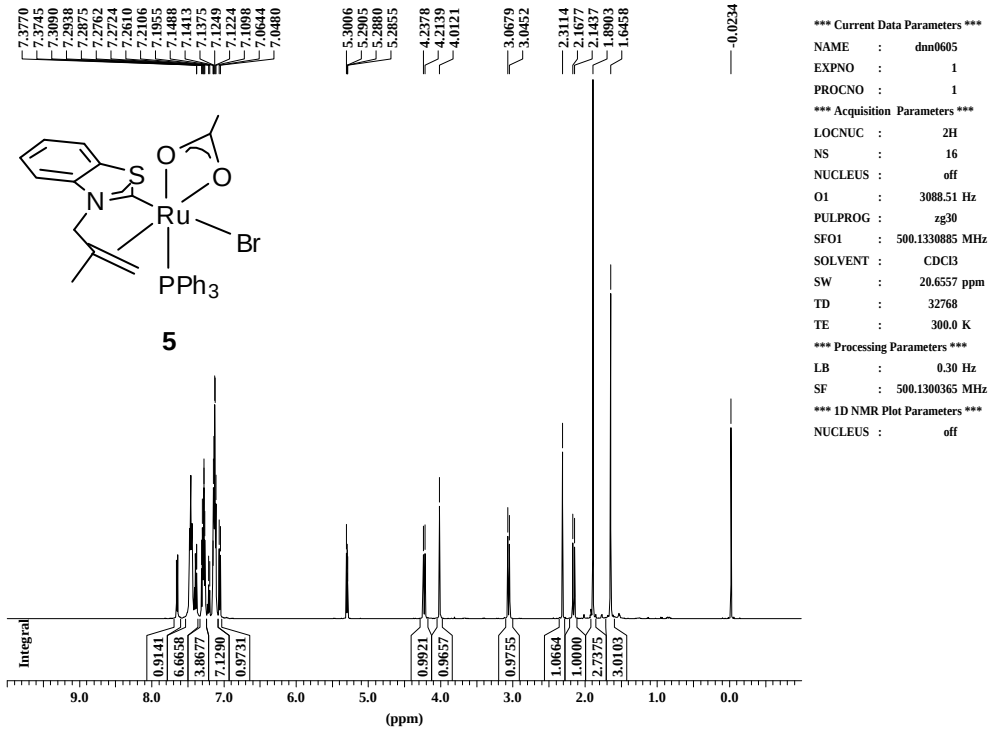
SF : 500.1300365 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off






RuNSCH2C(CH3)=CH2 1H NMR 500MHz




*** Current Data Parameters ***
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PROCNO : 1
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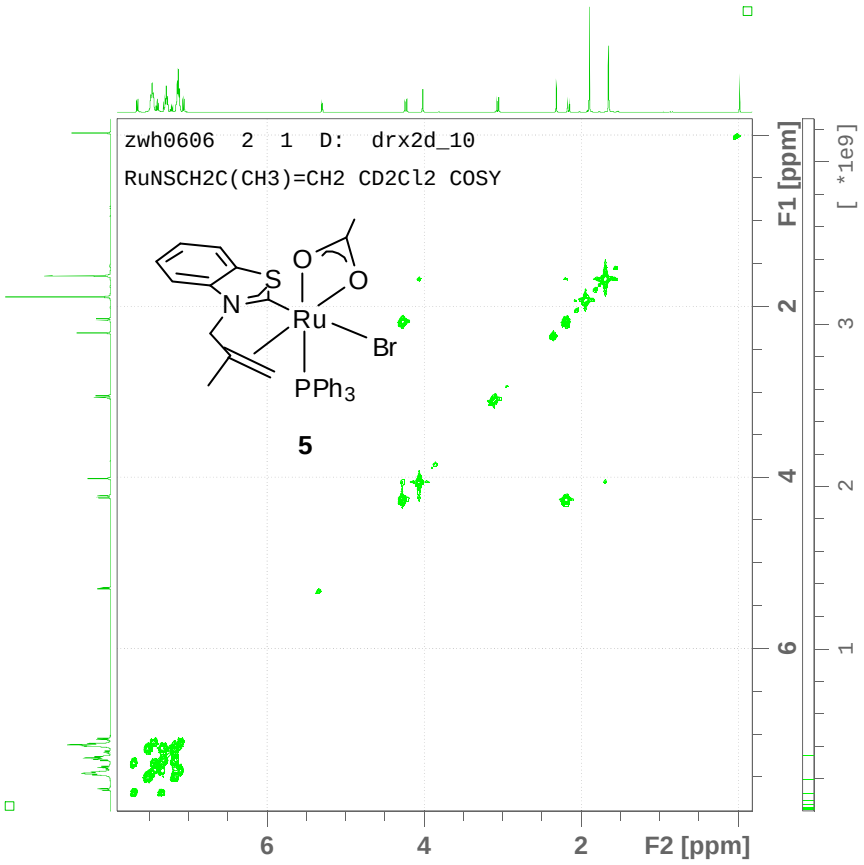
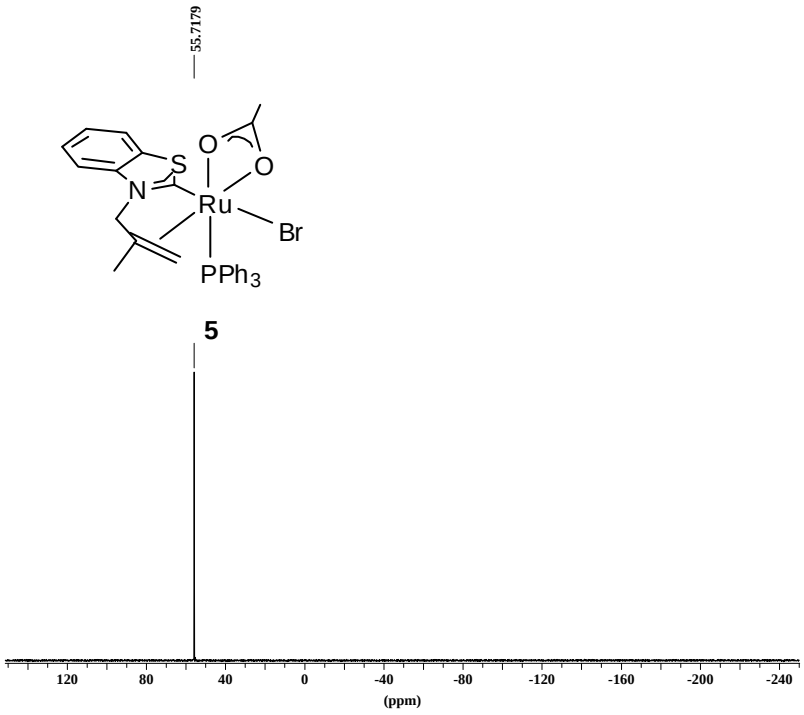
LOCNUC : 2H
NS : 16
NUCLEUS : off
O1 : 3088.51 Hz
PULPROG : zg30
SFO1 : 500.1330885 MHz
SOLVENT : CDCl3
SW : 20.6557 ppm
TD : 32768
TE : 300.0 K
*** Processing Parameters ***
LB : 0.30 Hz
SF : 500.1300365 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off




RuNSCH2C(CH3)=CH2 31p AMX500




*** Current Data Parameters ***
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EXPNO : 2
PROCNO : 1
*** Acquisition Parameters ***
LOCNUC : 2H
NS : 32
NUCLEUS : off
O1 : -10122.85 Hz
PULPROG : zgpg
SFO1 : 202.4462121 MHz
SOLVENT : CD2Cl2
SW : 401.5922 ppm
TD : 65536
TE : 300.0 K
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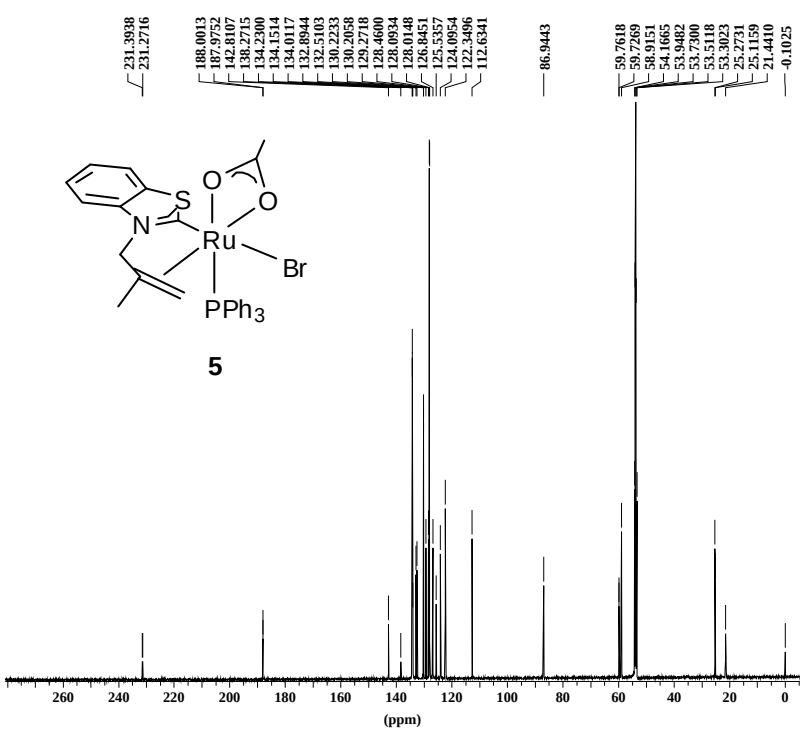
LB : 1.00 Hz
SF : 202.4562171 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off

RuNSCH2C(CH3)=CH2 13C AMX500

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PROCNO : 1
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LOCNUC : 2H
NS : 22536
NUCLEUS : off
O1 : 17291.70 Hz
PULPROG : zgpg30
SFO1 : 125.7750807 MHz
SOLVENT : CDCl3
SW : 285.9964 ppm
TD : 65536
TE : 300.0 K
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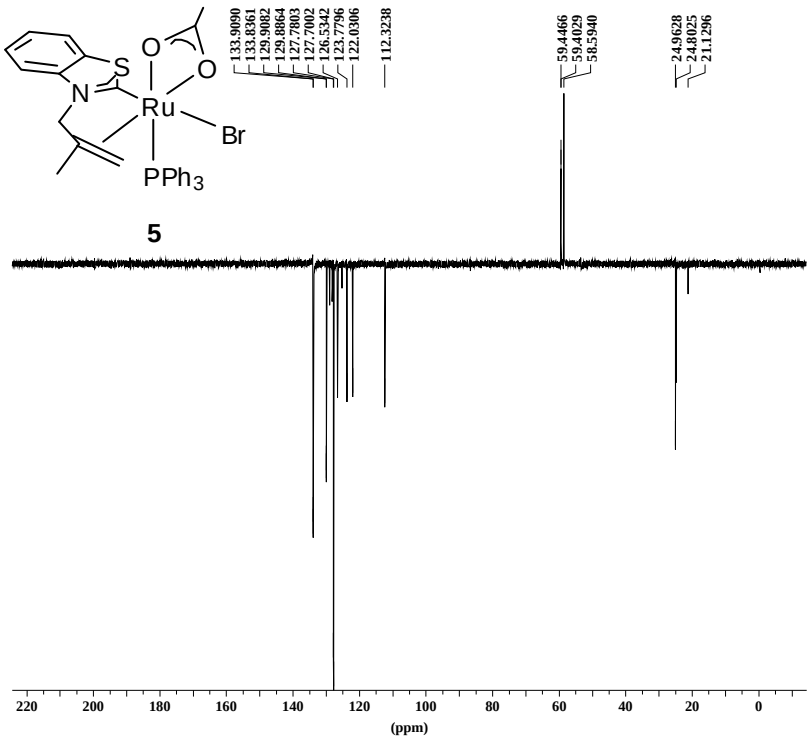
LB : 1.00 Hz
SF : 125.7577490 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off

RuNSCH2C(CH3)=CH2 DEPT135 AMX500

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PROCNO : 1
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LOCNUC : 2H
NS : 936
NUCLEUS : off
O1 : 13204.57 Hz
PULPROG : dept135
SFO1 : 125.7709936 MHz
SOLVENT : CDCl3
SW : 238.7675 ppm
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TE : 300.0 K
*** Processing Parameters ***
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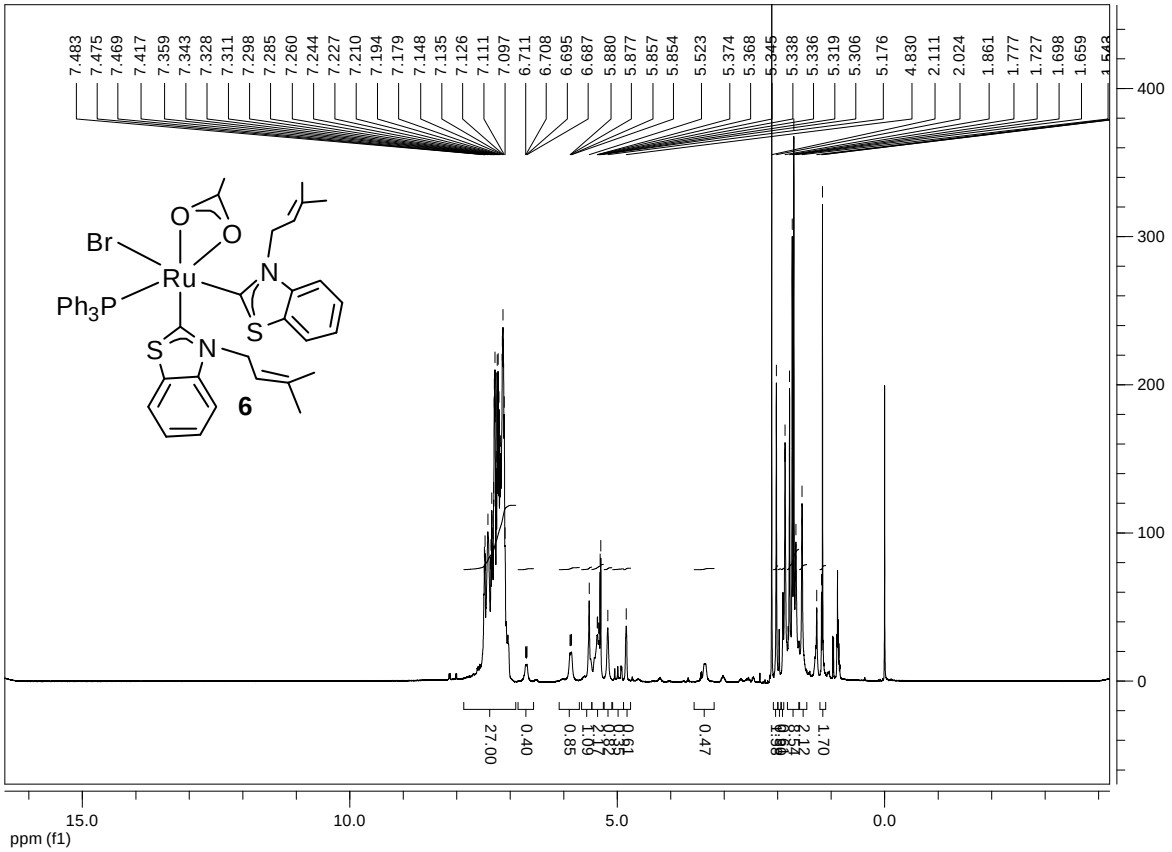
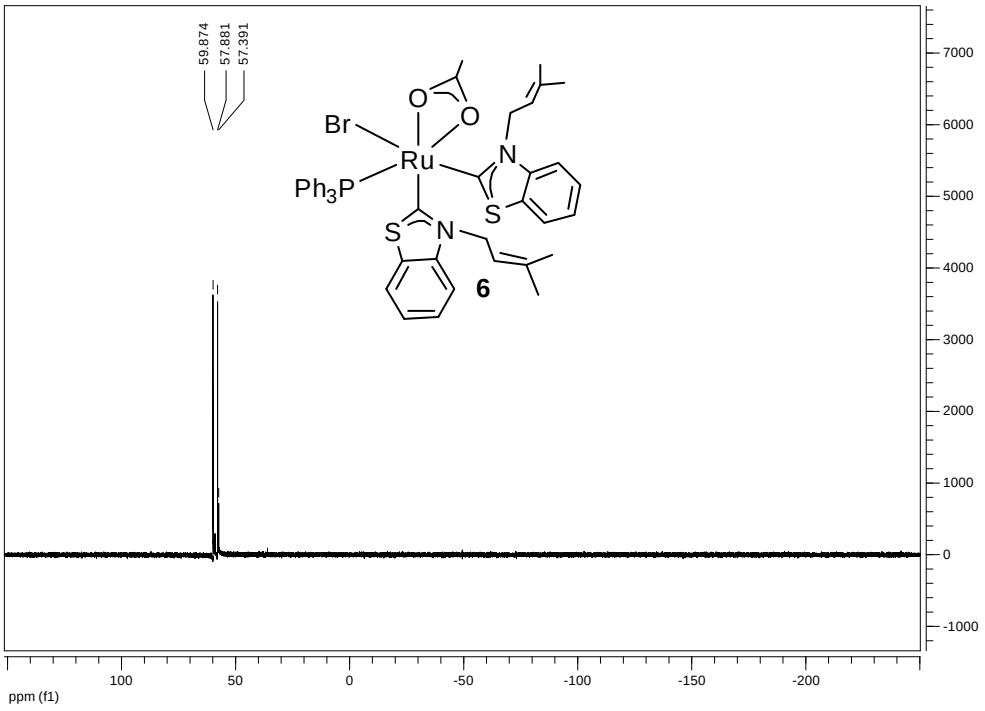
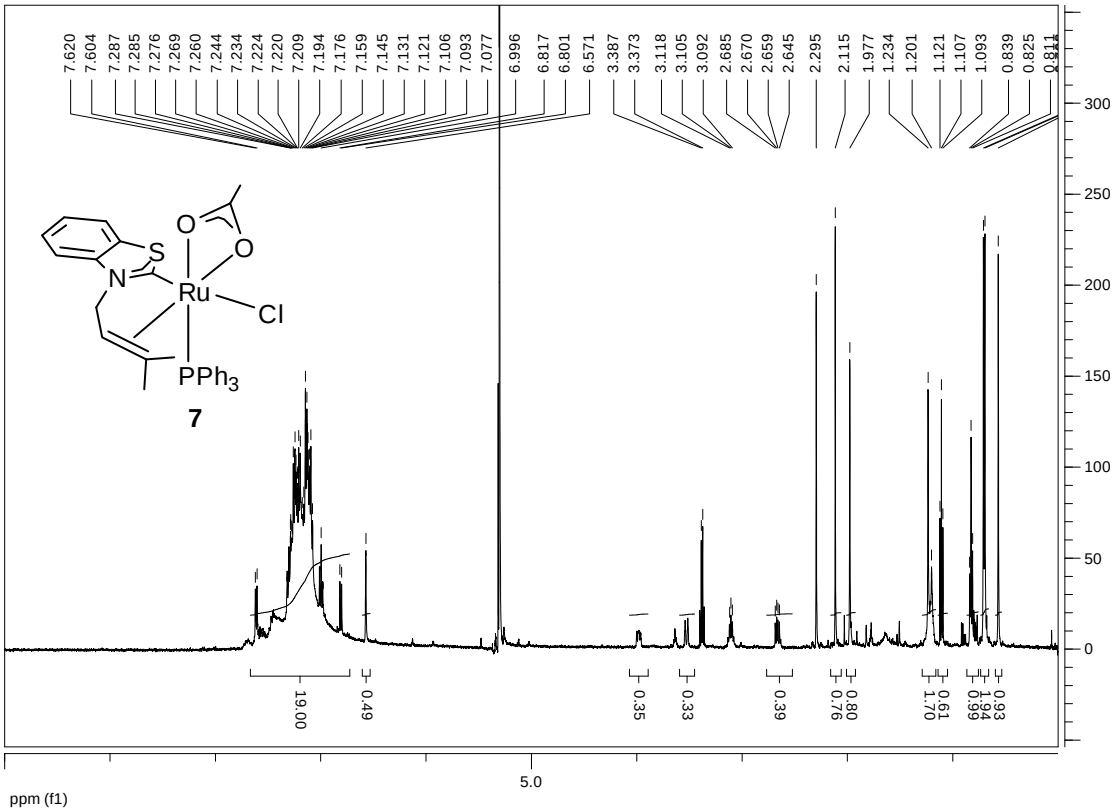
SF : 125.7577890 MHz
*** 1D NMR Plot Parameters ***
NUCLEUS : off





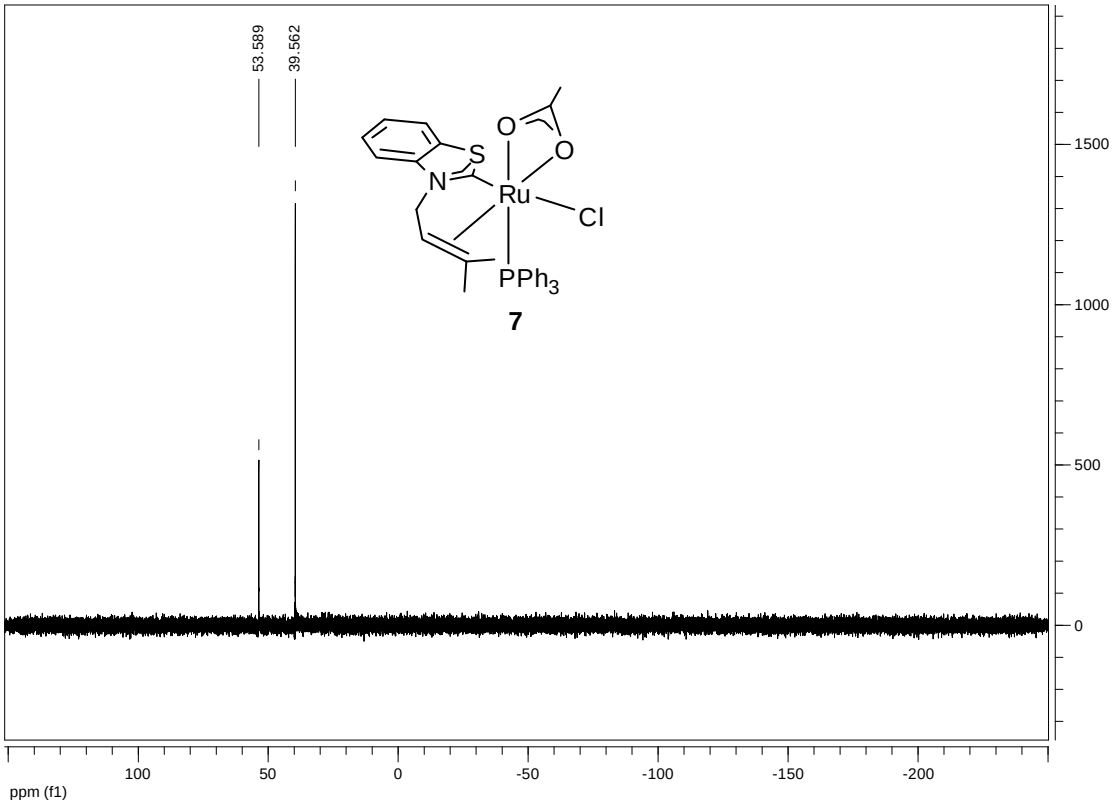
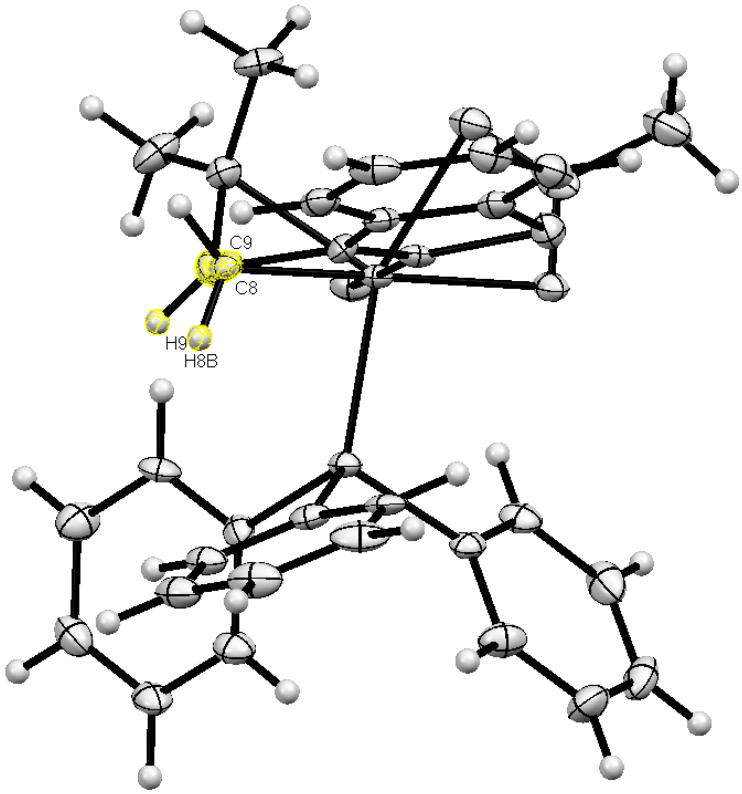



**Table** Summary of crystallographic parameters and refinement results for complexes **6**

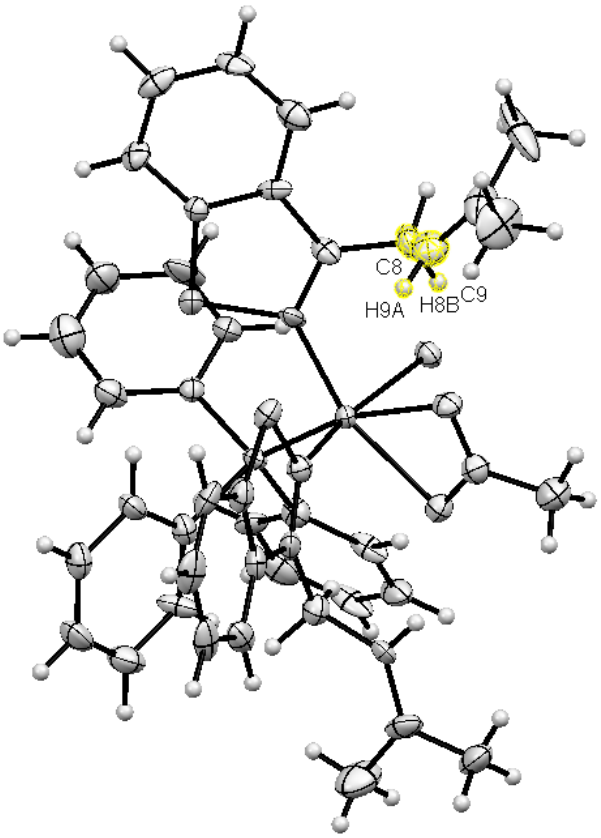
| | Complex **6** |
|---|---|
| Formula | C51H52BrN2O2PRuS2 |
| Fw | 1001.02 |
| cryst. Syst. | Monoclinic |
| space group | *P*2(1)/*c* |
| *a* (Å) | 15.6472(18) |
| *b* (Å) | 8.6894(10) |
| c (Å) | 36.182(4) |
| *α* (°) | 90 |
| *β* (°) | 101.388(3) |
| *γ* (°) | 90 |
| *V* (Å3) | 4822.6(9) |
| *Z* | 4 |
| *D*calcd ($g \cdot cm^{-3}$) | 1.379 |
| *μ* ($mm^{-1}$) | 1.314 |
| *F*(000) | 2056 |
| no. of reflns collected | 27229 |
| no. of unique reflns | 8501 |
| $R_{int}$ | 0.1479 |
| no. of observed reflns | 5367 |
| Parameters | 580 |
| *T* (K) | 100(2) |
| *R*1[a] (all data) | 0.1711 |
| *wR*2[b](all data) | 0.2768 |
| GOF[c] | 1.133 |

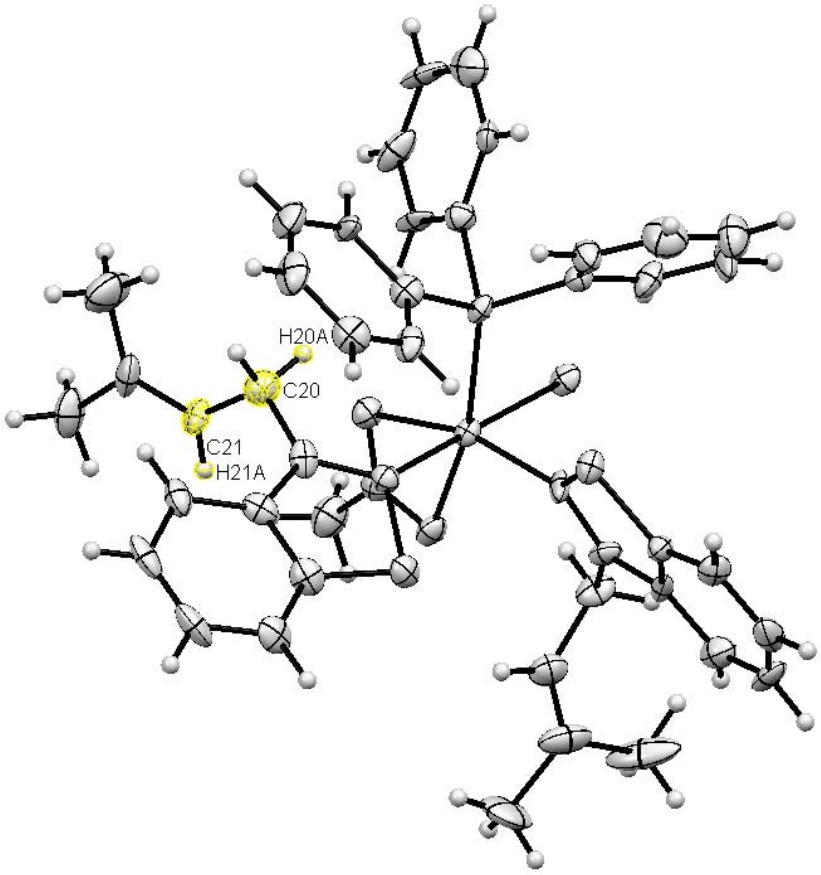
| | |
|---|---|
| $\Delta\rho$max (e Å$^{-3}$) | 1.545 |
| $\Delta\rho$min (e Å$^{-3}$) | -1.686 |

[a] R1 = Σ||Fo|-|Fc||/Σ|Fo|. [b] wR2 = {wΣ(|Fo|-|Fc|)2/Σw|Fo|2}}1/2. [c] GOF = {Σw(|Fo|-|Fc|)2/(n- p)}1/2, where n is the number of reflections and p is total number of parameters refined.




torsion angle in complex **7**: H8B-C8-C9-H9, 22.71°






torsion angle in complex **6**: H8B-C8-C9-H9A, -79.93°
torsion angle in complex **6**: H20A-C20-C21-H21A, 94.13°