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

Nini Ding, a Wenhua Zhang a and T. S. Andy Hor a,b

a Department of Chemistry, National University of Singapore, 3 Science Drive 3, 117543, Singapore; b Institute of Materials Research and Engineering, Agency for Science, Technology and Research, 3 Research Link, 117602, Singapore.

1H, 13C, 31P NMR spectra

Electronic Supplementary Material (ESI) for Dalton Transactions
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**Colorless Ligand /CD2Cl2 13C AMX500**

1.0000 4.0992 2.2384 1.0853 1.0841 3.2085

**Integral**


(ppm)

**NSCH2C(CH3)=CH2--1H AMX500**

N  S

1

N  S

2

Br

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**Current Data Parameters**

**NAME**: dnn0814  
**EXPNO**: 6  
**PROCNO**: 1  

**Acquisition Parameters**

**LOCNUC**: 2H  
**NS**: 64  
**NUCLEUS**: off  
**O1**: 13204.57 Hz  
**PULPROG**: zgpg30  
**SFO1**: 125.7709936 MHz  
**SOLVENT**: CD2Cl2  
**SW**: 238.7675 ppm  
**TD**: 65536  
**TE**: 297.3 K  

**Processing Parameters**

**LB**: 1.00 Hz  
**SF**: 125.7577890 MHz  

**1D NMR Plot Parameters**

**NUCLEUS**: off

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**Current Data Parameters**

**NAME**: dnn0814  
**EXPNO**: 7  
**PROCNO**: 1  

**Acquisition Parameters**

**LOCNUC**: 2H  
**NS**: 8  
**NUCLEUS**: off  
**O1**: 3088.51 Hz  
**PULPROG**: zg30  
**SFO1**: 500.1330885 MHz  
**SOLVENT**: CD2Cl2  
**SW**: 20.6557 ppm  
**TD**: 32768  
**TE**: 296.9 K  

**Processing Parameters**

**LB**: 0.30 Hz  
**SF**: 500.1300300 MHz  

**1D NMR Plot Parameters**

**NUCLEUS**: off

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### Current Data Parameters

**NAME**: dnn0814  
**EXPNO**: 8  
**PROCNO**: 1

### Acquisition Parameters

**LOCNUC**: 2H  
**NS**: 800  
**NUCLEUS**: off  
**O1**: 13204.57 Hz  
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**SFO1**: 125.7709936 MHz  
**SOLVENT**: CDCl3  
**SW**: 132.4875 ppm  
**TD**: 65536  
**TE**: 297.0 K

### Processing Parameters

**LB**: 1.0 Hz  
**SF**: 125.7577890 MHz

### 1D NMR Plot Parameters

**NUCLEUS**: off

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### Current Data Parameters

**NAME**: dnn0606  
**EXPNO**: 11  
**PROCNO**: 1

### Acquisition Parameters

**LOCNUC**: 2H  
**NS**: 8  
**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

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### Current Data Parameters

**NAME**: dnn0606  
**EXPNO**: 11  
**PROCNO**: 1

### Acquisition Parameters

**LOCNUC**: 2H  
**NS**: 8  
**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

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### Current Data Parameters

**NAME**: dnn0606  
**EXPNO**: 11  
**PROCNO**: 1

### Acquisition Parameters

**LOCNUC**: 2H  
**NS**: 8  
**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

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### Current Data Parameters

**NAME**: dnn0606  
**EXPNO**: 11  
**PROCNO**: 1

### Acquisition Parameters

**LOCNUC**: 2H  
**NS**: 8  
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**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

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### Current Data Parameters

**NAME**: dnn0606  
**EXPNO**: 11  
**PROCNO**: 1

### Acquisition Parameters

**LOCNUC**: 2H  
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**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
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Ru\(\text{NCH}_2\text{C}(\text{CH}_3)\text{=CH}_2\) 1H NMR 500MHz

![RuNCH2C(CH3)=CH2 NMR Spectrum](image)

**Current Data Parameters**

- **NAME**: dnn0605
- **EXPNO**: 1
- **PROCNO**: 1

**Acquisition Parameters**

- **LOCNUC**: 2H
- **NS**: 32
- **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
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<th>Formula</th>
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<tbody>
<tr>
<td>Fw</td>
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<tr>
<td>cryst. Syst.</td>
<td>Monoclinic</td>
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<tr>
<td>space group</td>
<td>P2(1)/c</td>
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<td>a (Å)</td>
<td>15.6472(18)</td>
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<tr>
<td>b (Å)</td>
<td>8.6894(10)</td>
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<tr>
<td>c (Å)</td>
<td>36.182(4)</td>
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<tr>
<td>α (°)</td>
<td>90</td>
</tr>
<tr>
<td>β (°)</td>
<td>101.388(3)</td>
</tr>
<tr>
<td>γ (°)</td>
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</tr>
<tr>
<td>V (Å³)</td>
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<tr>
<td>Z</td>
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<td>no. of unique reflns</td>
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<td>no. of observed reflns</td>
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<td>Parameters</td>
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<td>T (K)</td>
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<td>R1 (all data)</td>
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<td>wR2 (all data)</td>
<td>0.2768</td>
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<tr>
<td>GOF</td>
<td>1.133</td>
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</tbody>
</table>

Table Summary of crystallographic parameters and refinement results for complexes 6
$\Delta \rho_{\text{max}}$ (e Å$^{-3}$) \hspace{1cm} 1.545

$\Delta \rho_{\text{min}}$ (e Å$^{-3}$) \hspace{1cm} -1.686

$^a R_1 = \Sigma |F_o|-|F_c|/|\Sigma F_o|.$  
$^b wR_2 = \{w \Sigma (|F_o|-|F_c|)^2/\Sigma w|F_o|^2\}^{1/2}.$  
$^c \text{GOF} = \{\Sigma w(|F_o|-|F_c|)^2/(n- p)\}^{1/2},$ 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°