

## Supporting Information

### Stereoselective Synthesis of Bicyclo[6.1.0]nonene Precursors of the Bioorthogonal Reagents sTCO and BCN

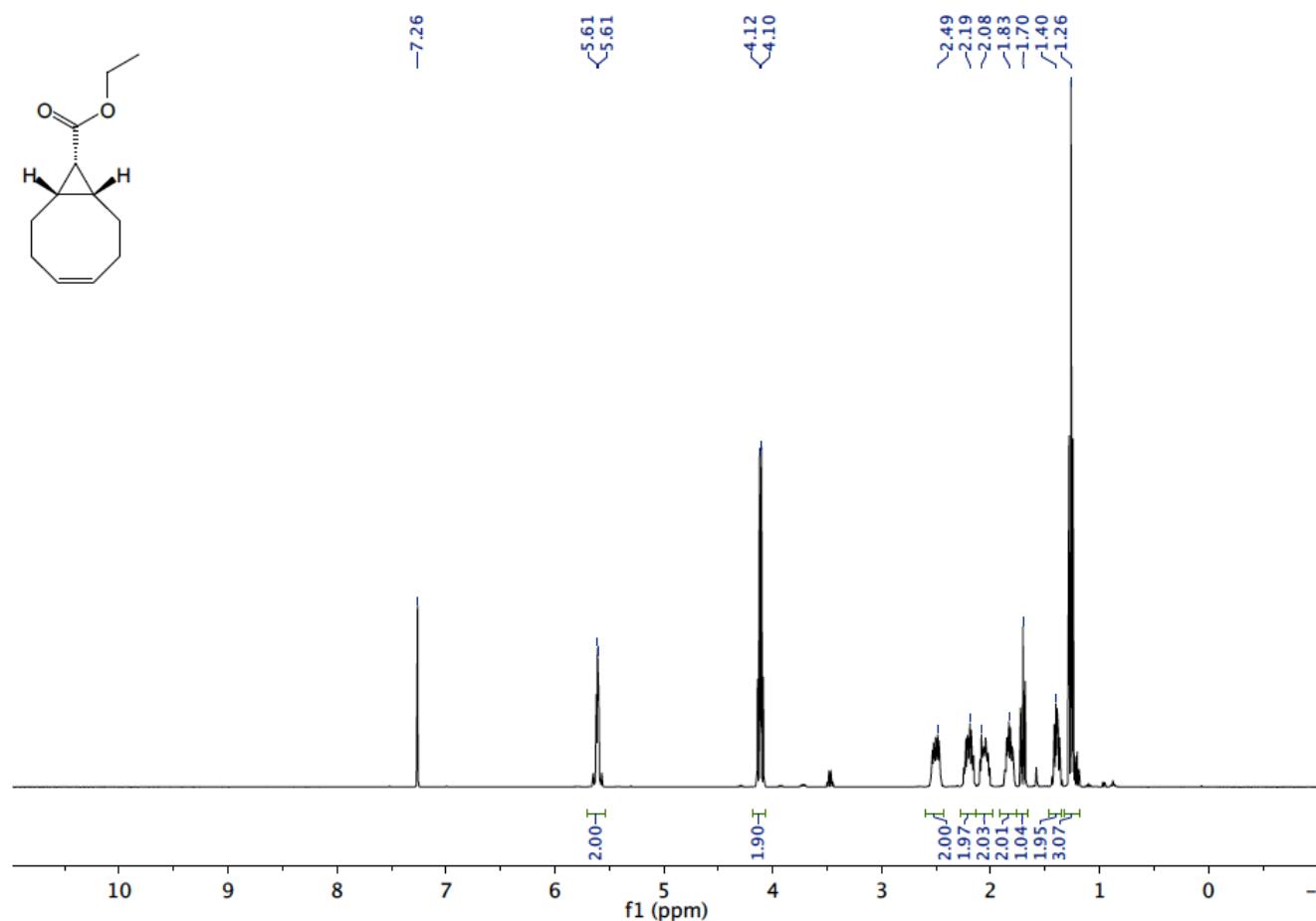
Jessica G. K. O'Brien, Srinivasa Chintala, Joseph M. Fox\*

Brown Laboratories, Department of Chemistry and Biochemistry, University of Delaware, Newark, Delaware, 19716, USA

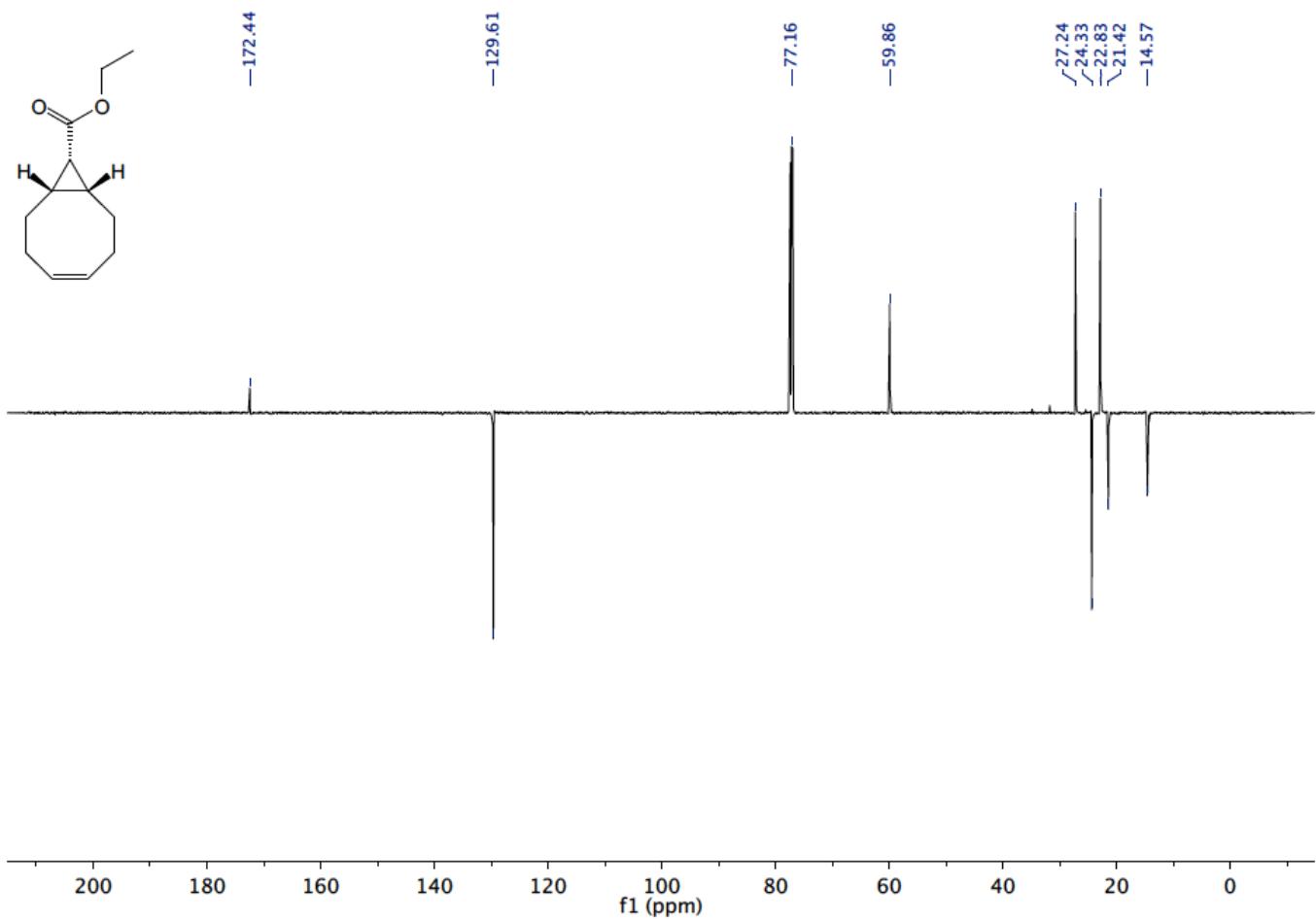
#### Table of Contents

<sup>1</sup> H NMR of <b>3-syn</b>	S-2
<sup>13</sup> C NMR of <b>3-syn</b>	S-3
<sup>1</sup> H NMR of <b>3-anti</b>	S-4
<sup>13</sup> C NMR of <b>3-anti</b>	S-5
<sup>1</sup> H NMR of <b>5</b>	S-6
<sup>13</sup> C NMR of <b>5</b>	S-7
<sup>1</sup> H NMR of <b>6</b>	S-8
<sup>13</sup> C NMR of <b>6</b>	S-9
<sup>1</sup> H NMR of <b>4</b>	S-10
<sup>13</sup> C NMR of <b>4</b>	S-11
<sup>1</sup> H NMR ( <i>S</i> )- <b>BHTL</b>	S-12
<sup>13</sup> C NMR of ( <i>S</i> )- <b>BHTL</b>	S-13
<sup>1</sup> H NMR of <b>Rh<sub>2</sub>(S-BHTL)<sub>4</sub></b>	S-14
<sup>13</sup> C NMR of <b>Rh<sub>2</sub>(S-BHTL)<sub>4</sub></b>	S-16
X-ray Crystal Structure of <b>Rh<sub>2</sub>(S-BHTL)<sub>4</sub></b>	S-17

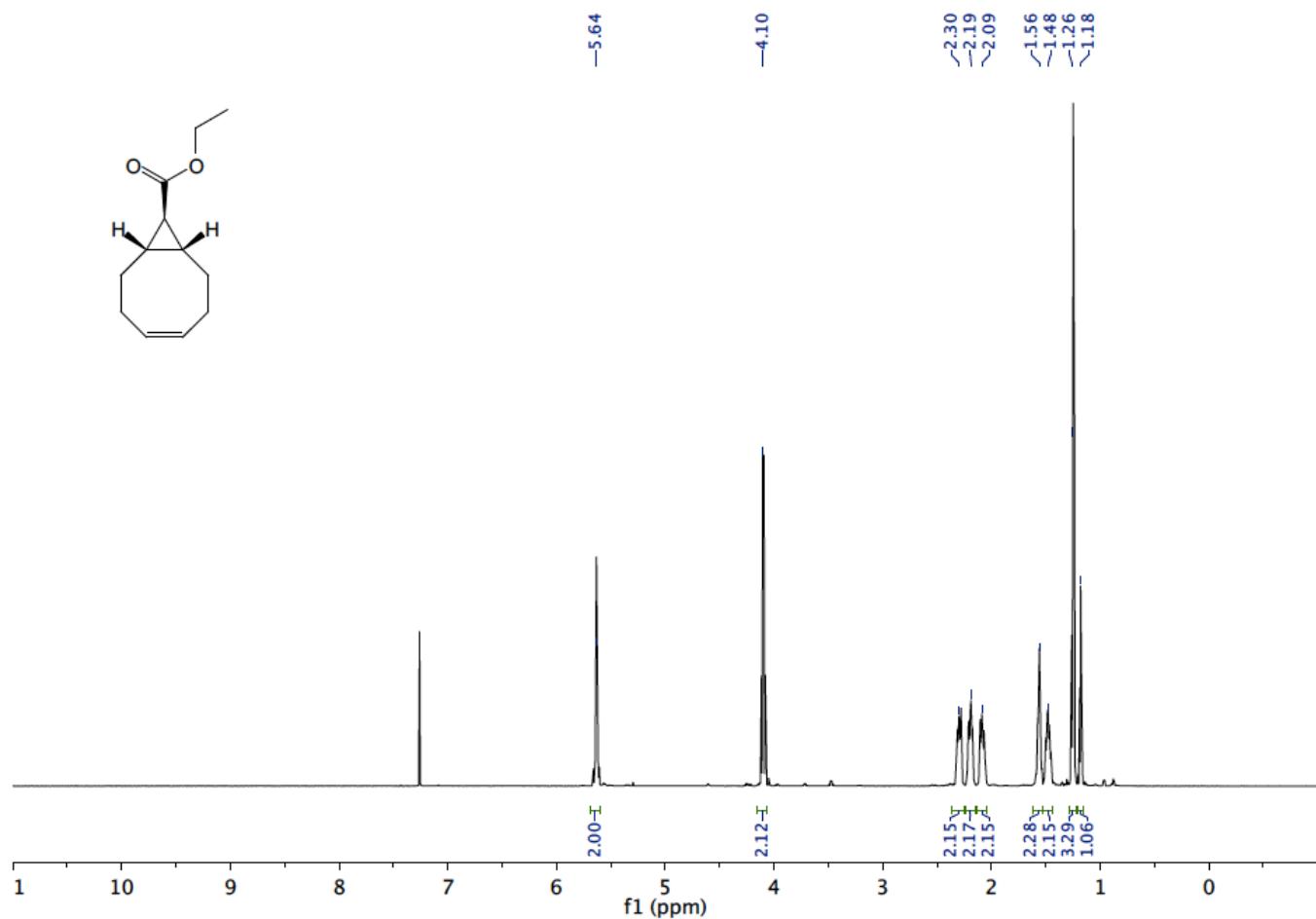
<sup>1</sup>H NMR spectrum of **3-syn** (400 MHz, CDCl<sub>3</sub>)



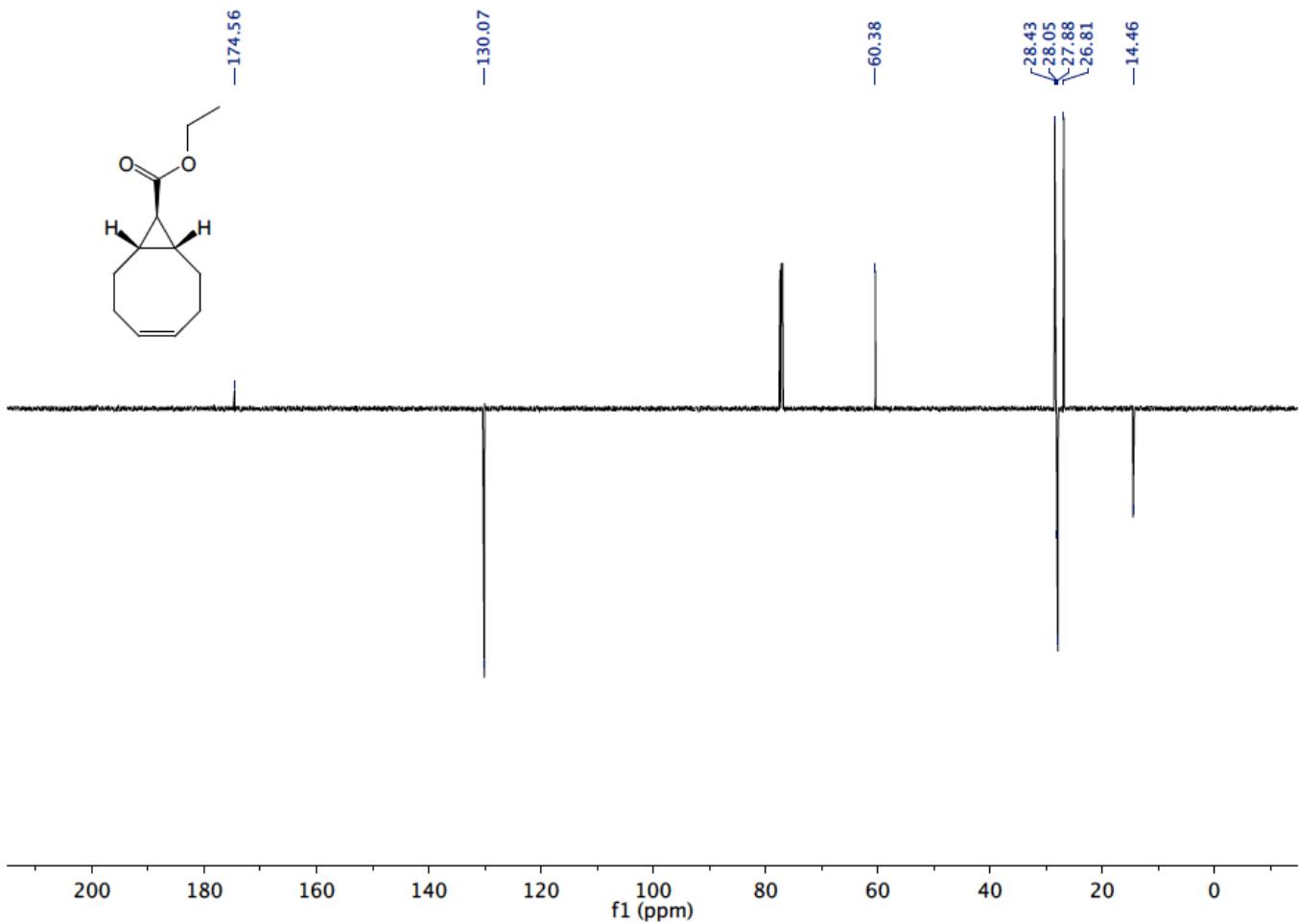
$^{13}\text{C}$  NMR spectrum of **3-syn** (150 MHz,  $\text{CDCl}_3$ )



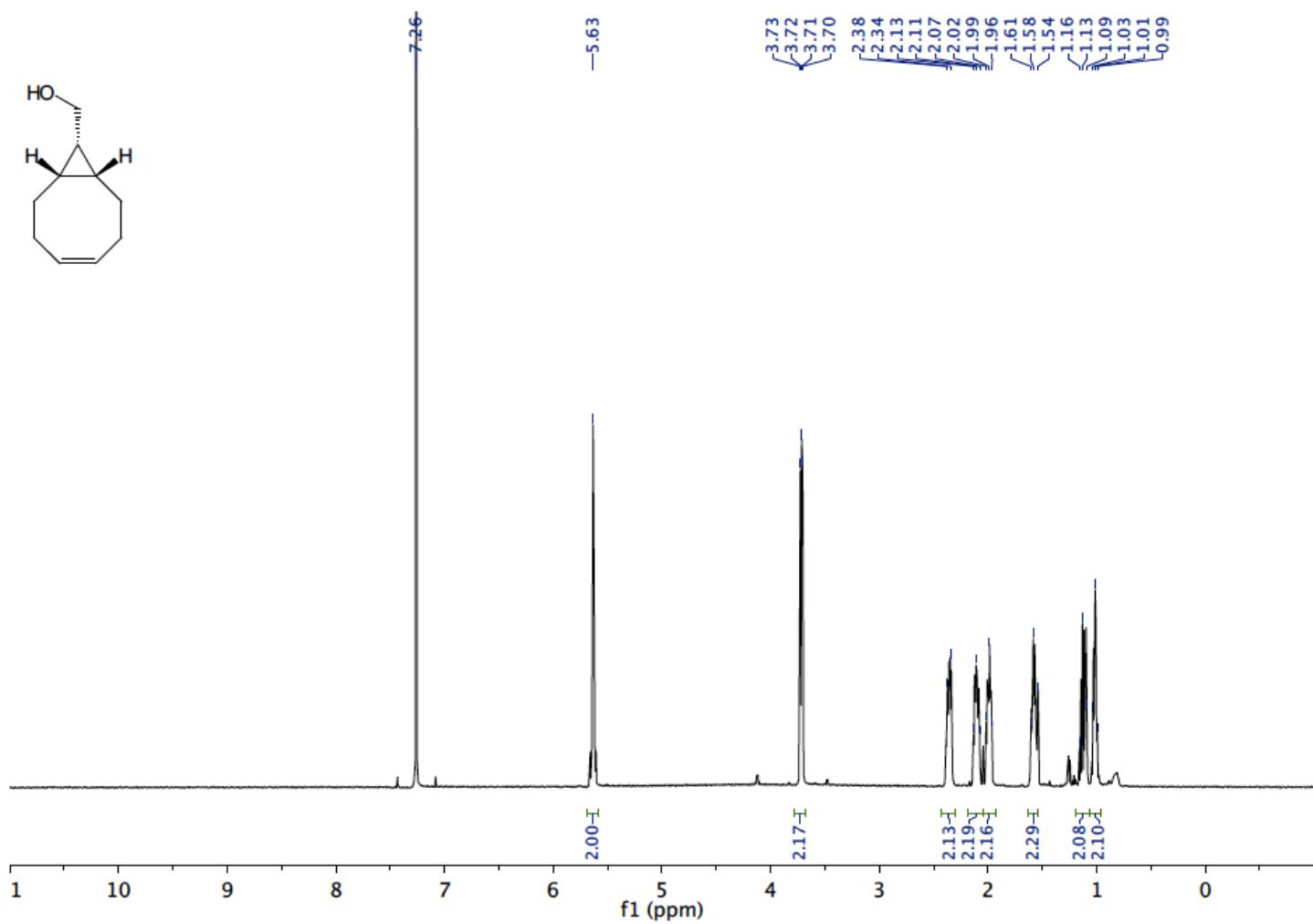
<sup>1</sup>H NMR spectrum of **3-anti** (600 MHz, CDCl<sub>3</sub>)



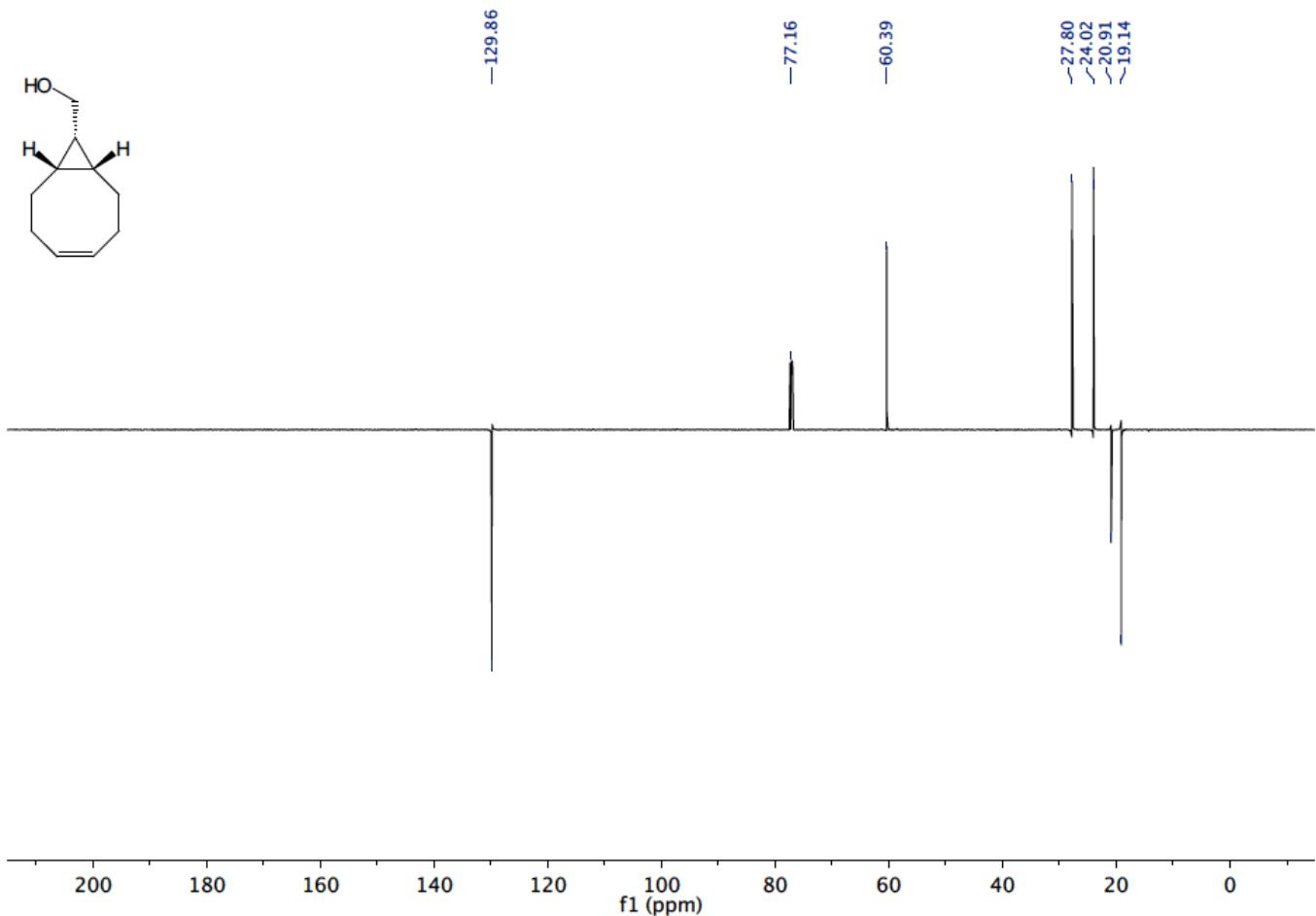
$^{13}\text{C}$  NMR spectrum of **3-anti** (150 MHz,  $\text{CDCl}_3$ )



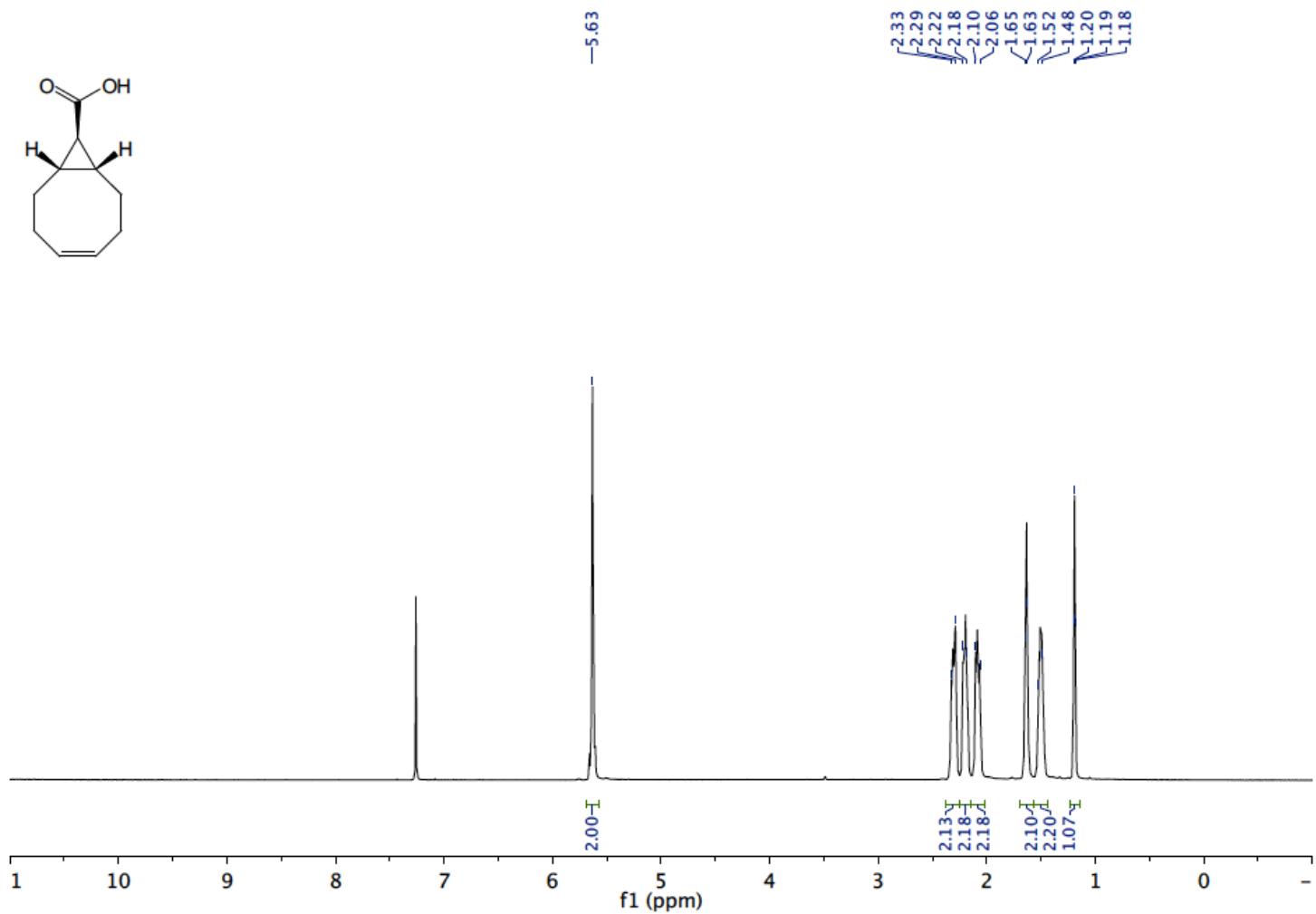
<sup>1</sup>H NMR spectrum of **5** (600 MHz, CDCl<sub>3</sub>)



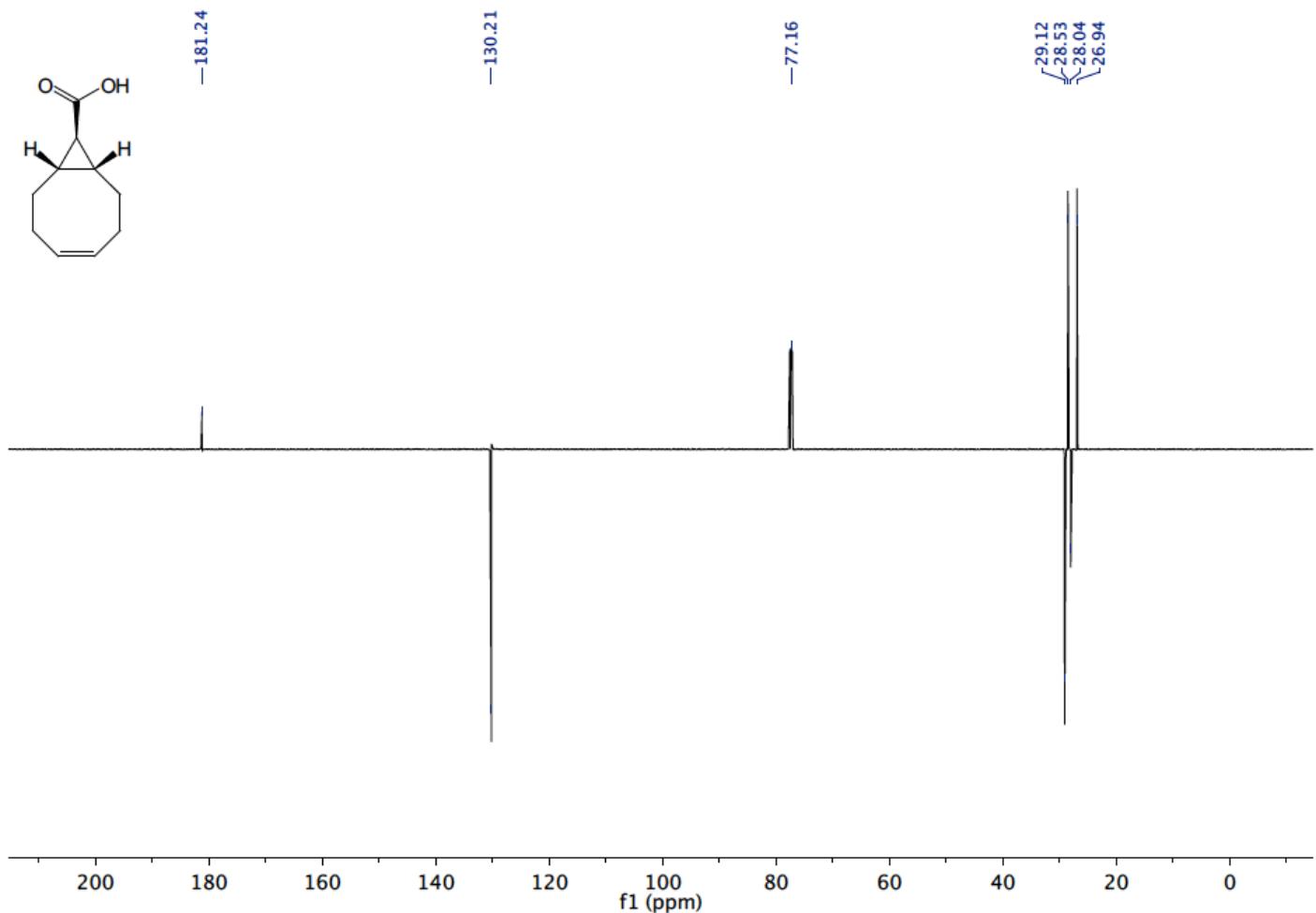
<sup>13</sup>C NMR spectrum of **5** (150 MHz, CDCl<sub>3</sub>)



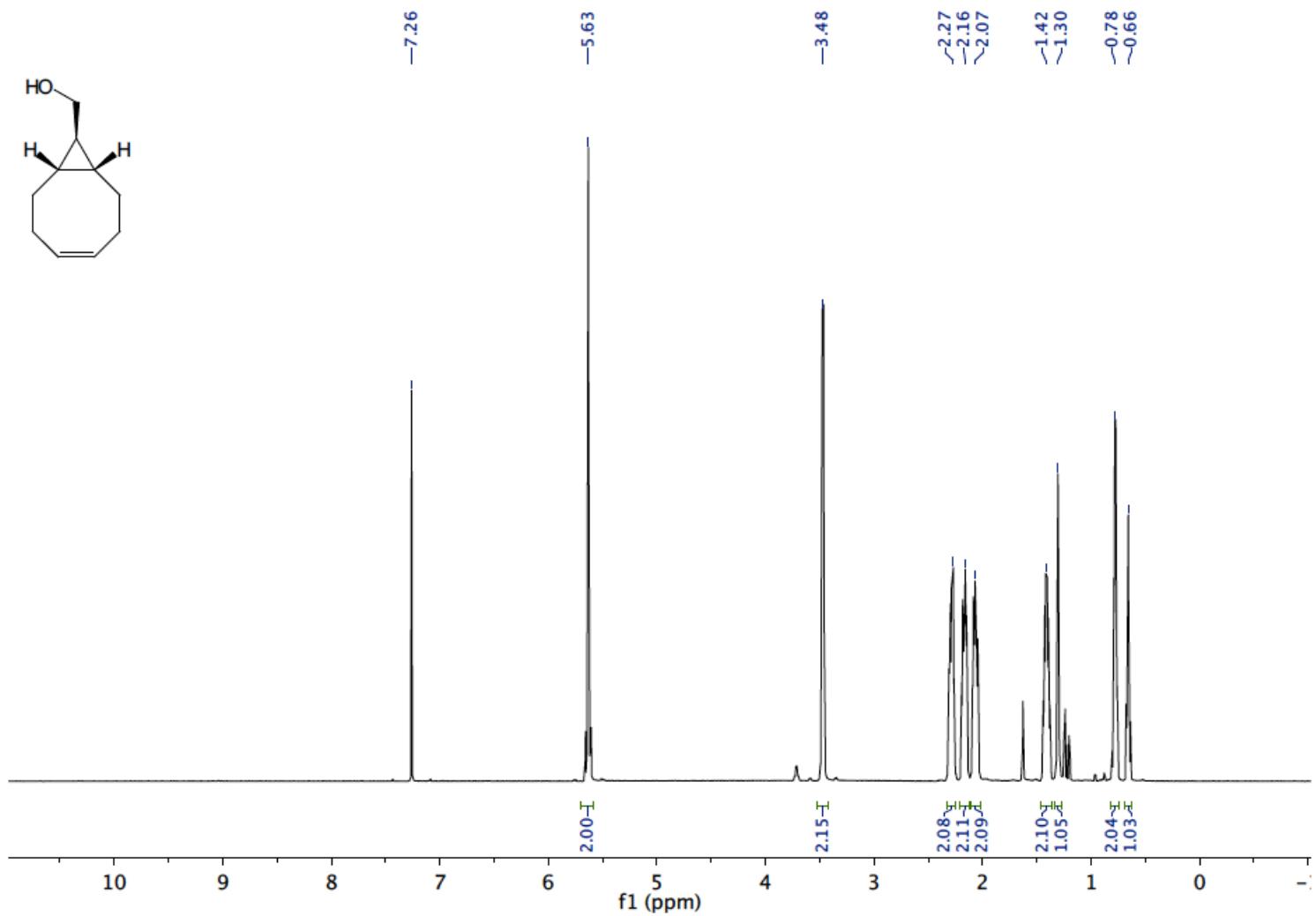
<sup>1</sup>H NMR spectrum of **6** (600 MHz, CDCl<sub>3</sub>)



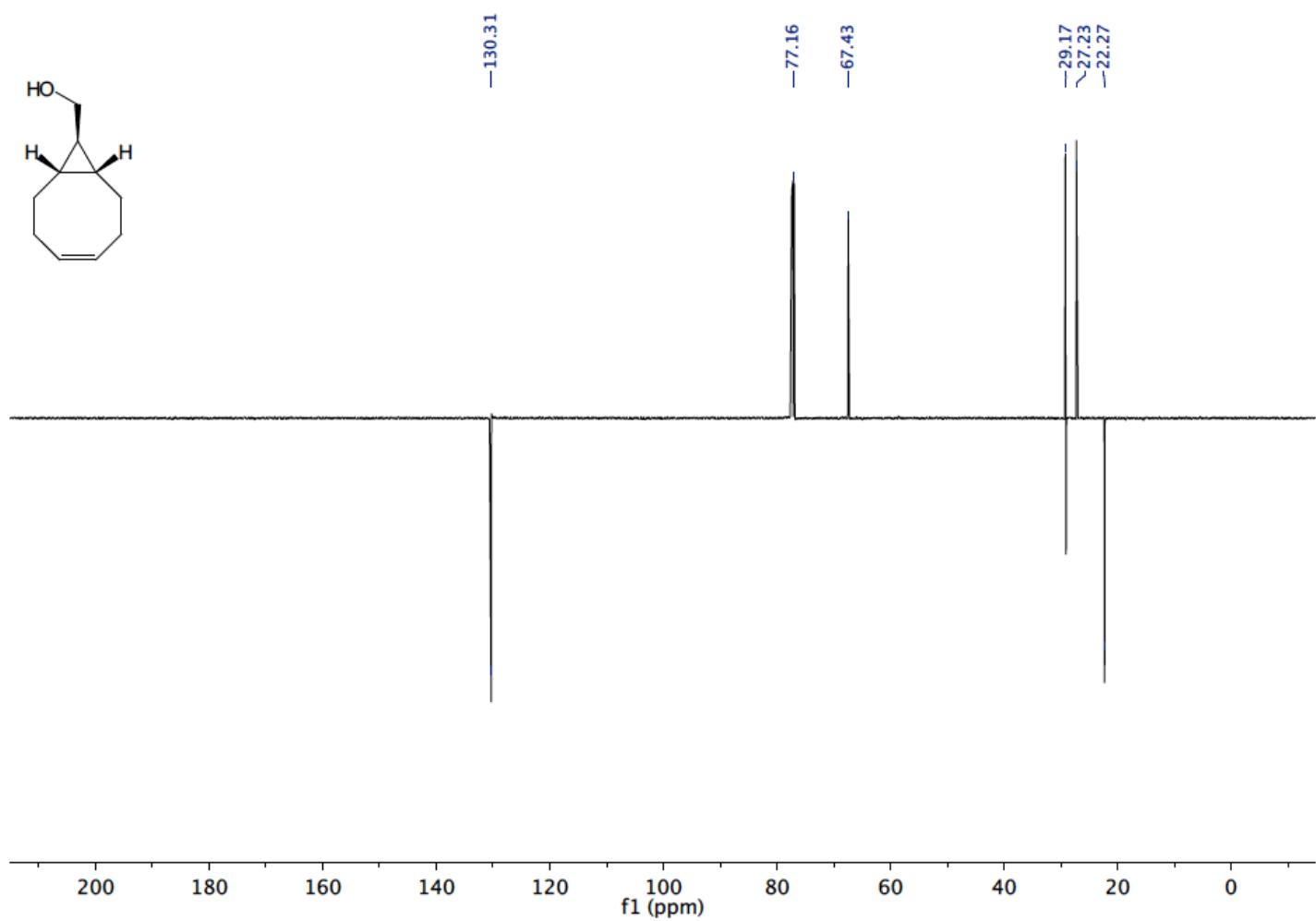
<sup>13</sup>C NMR spectrum of **6** (150 MHz, CDCl<sub>3</sub>)



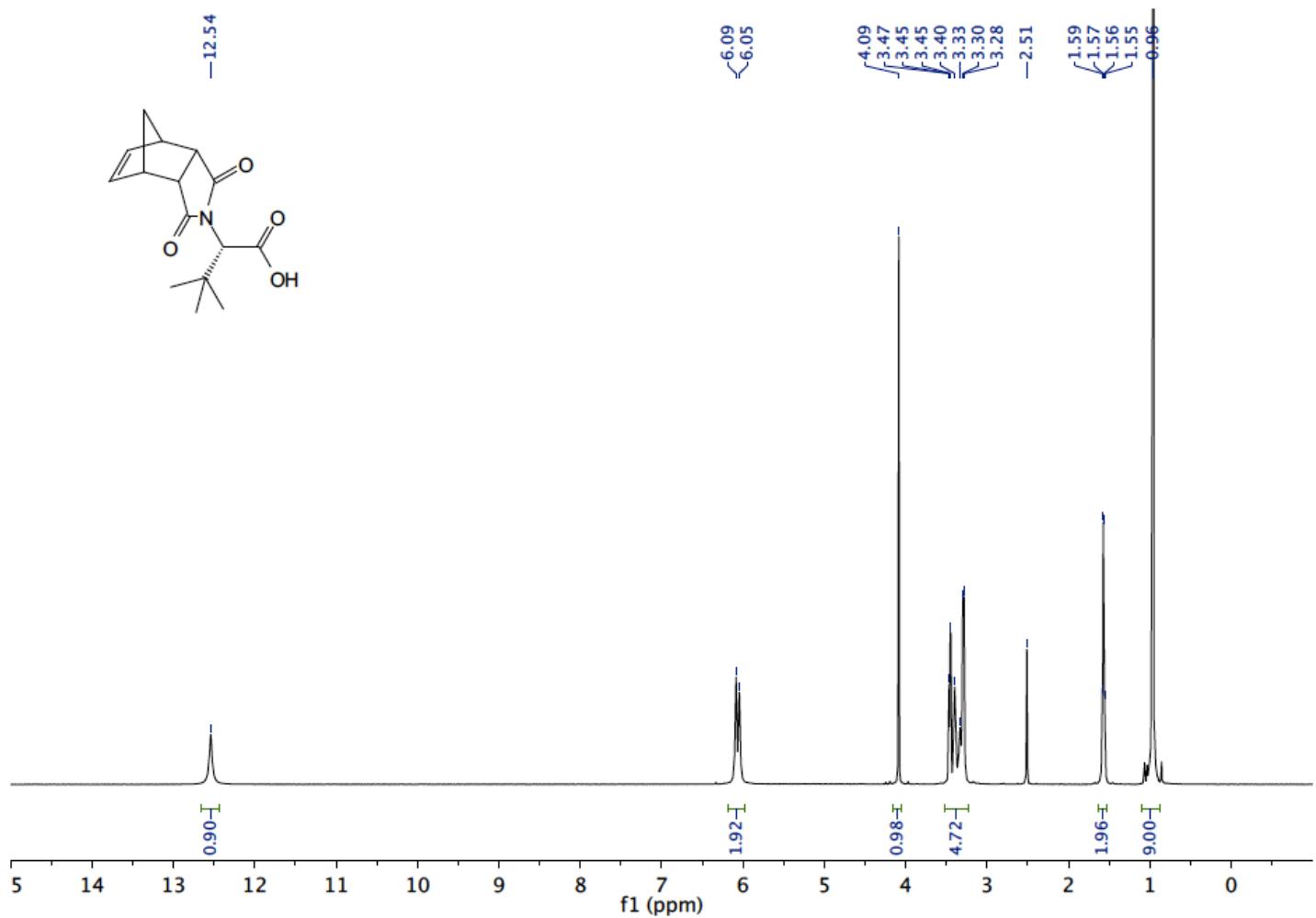
<sup>1</sup>H NMR spectrum of **4** (600 MHz, CDCl<sub>3</sub>)



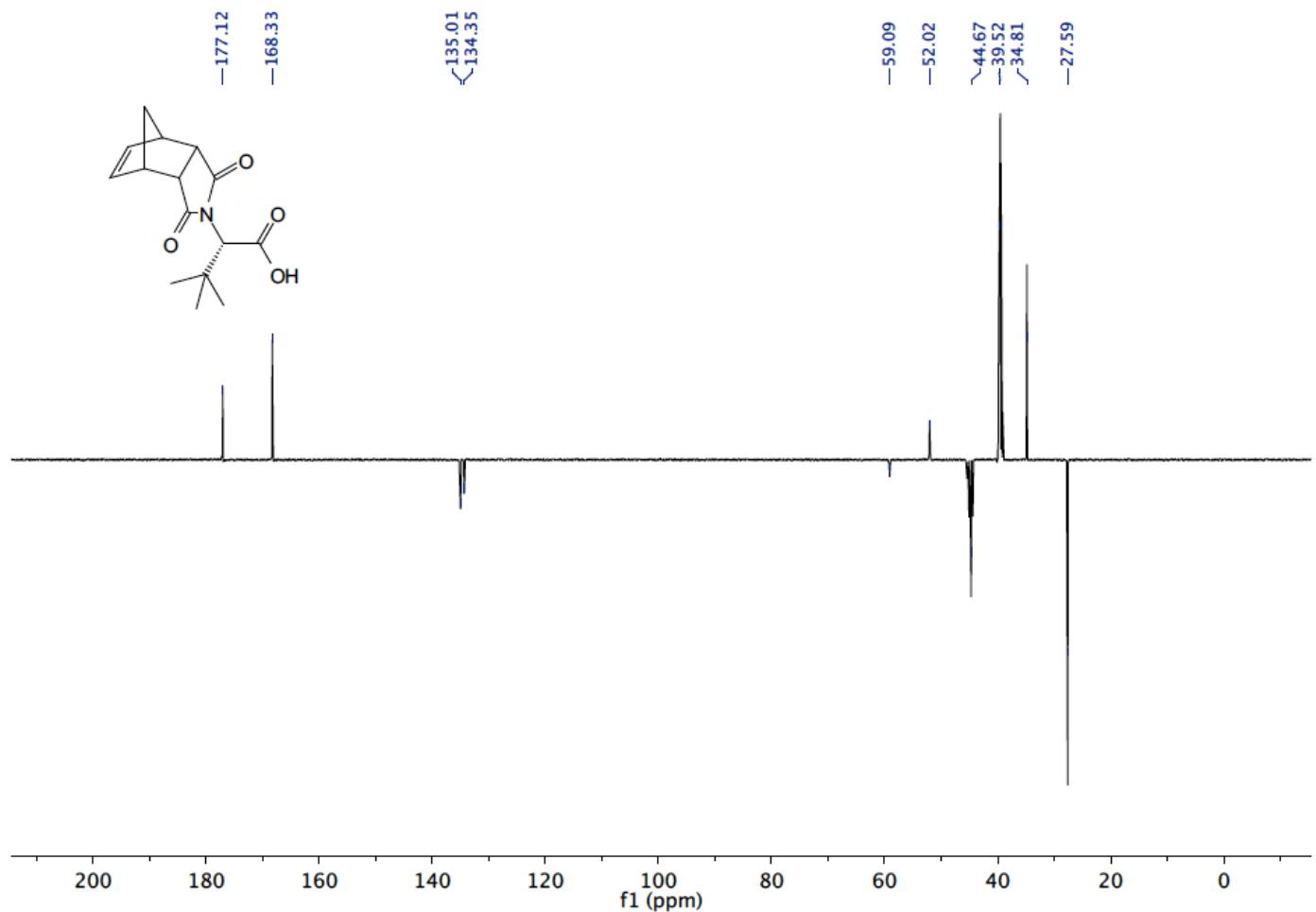
$^{13}\text{C}$  NMR spectrum of **4** (150 MHz,  $\text{CDCl}_3$ )



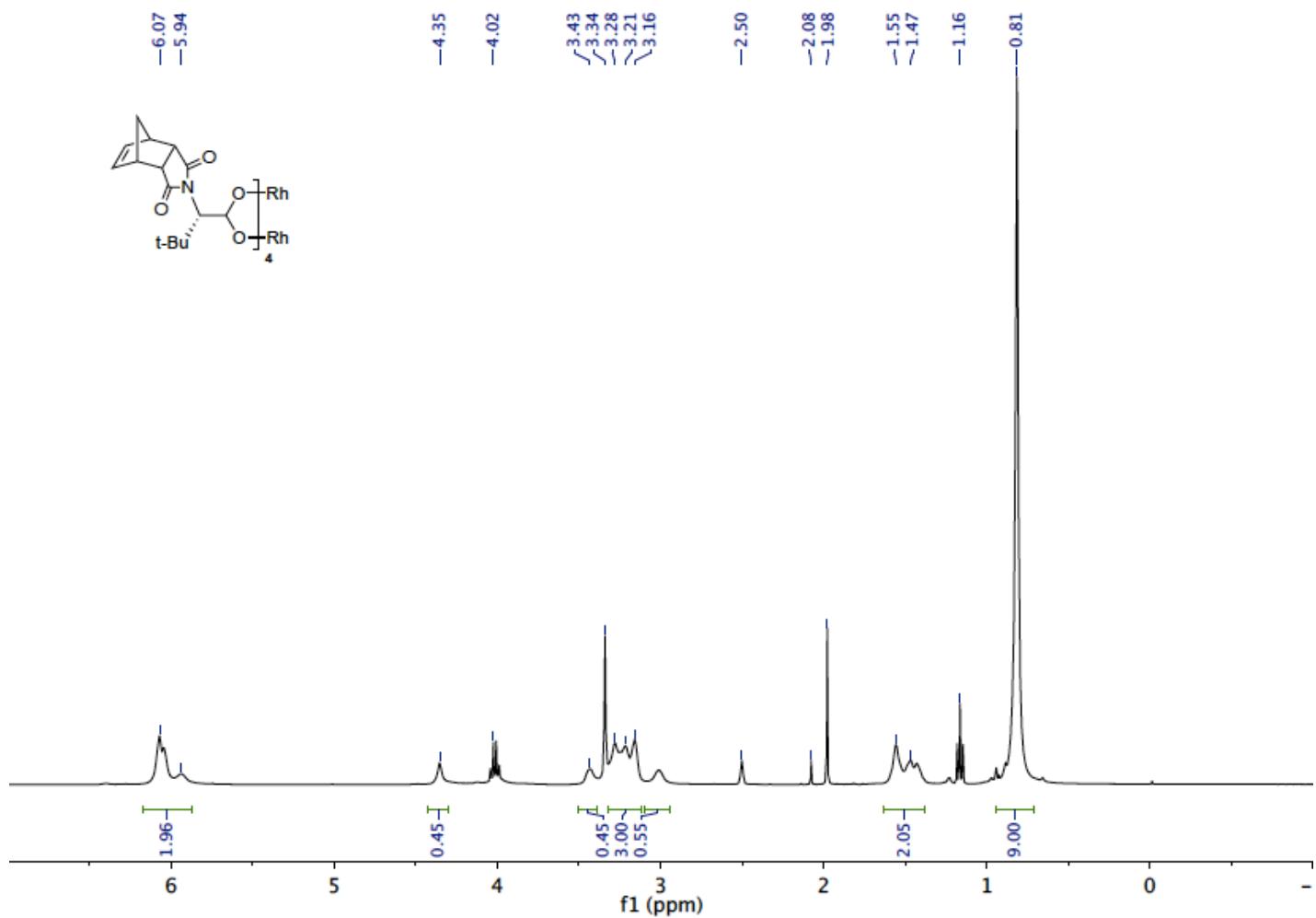
<sup>1</sup>H NMR spectrum of (*S*)-BHTL (600 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)



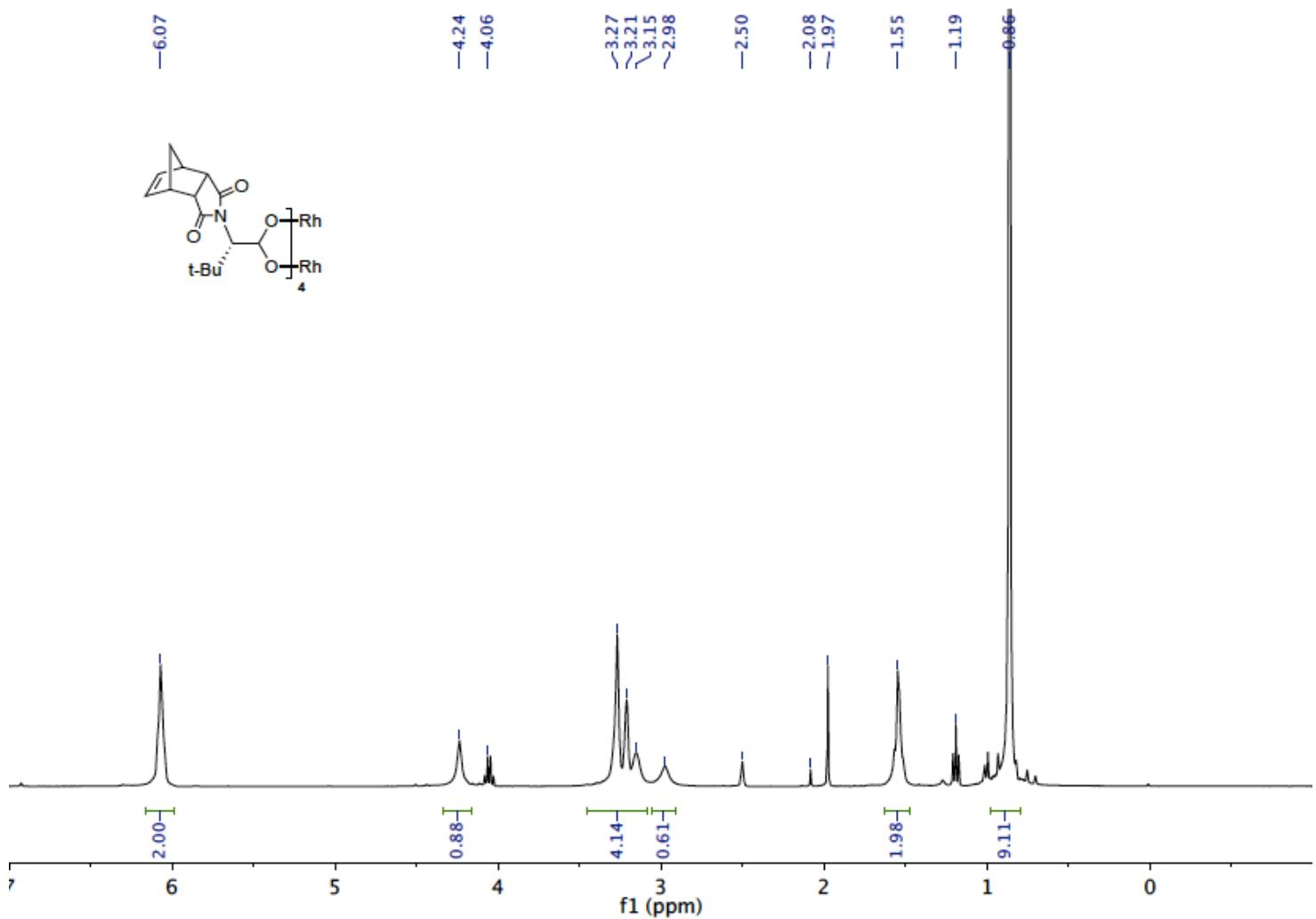
<sup>13</sup>C NMR spectrum of (*S*)-BHTL (150 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)



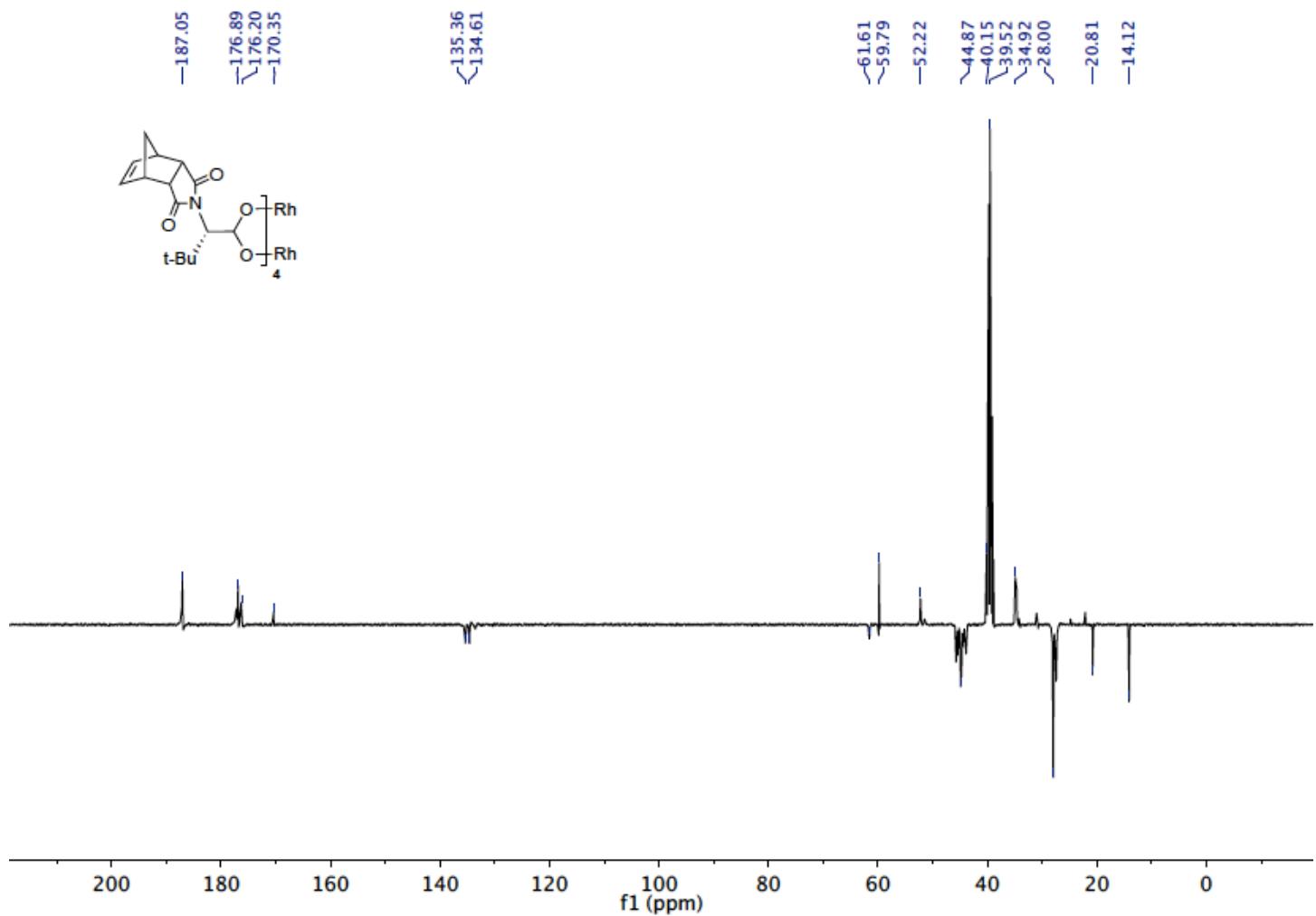
<sup>1</sup>H NMR spectrum of **Rh<sub>2</sub>(S-BHTL)<sub>4</sub>**, room temperature (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)



<sup>1</sup>H NMR spectrum of **Rh<sub>2</sub>(S-BHTL)<sub>4</sub>** 360K (400MHz, (CD<sub>3</sub>)<sub>2</sub>SO)



$^{13}\text{C}$  NMR spectrum of  $\text{Rh}_2(\text{S-BHTL})_4$  (600MHz,  $(\text{CD}_3)_2\text{SO}$ )



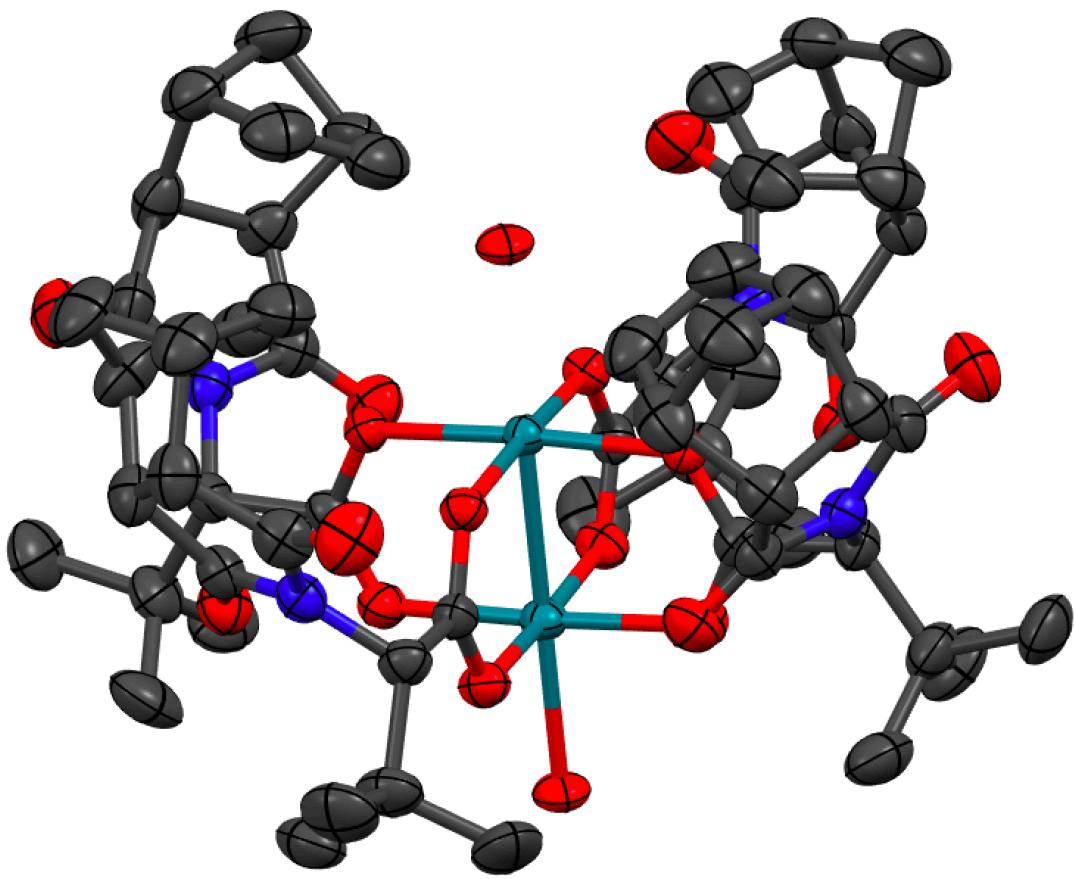


Fig S1. X-ray structure of  $\text{Rh}_2(\text{S-BHTL})_4$  (50% probability ellipsoids)