

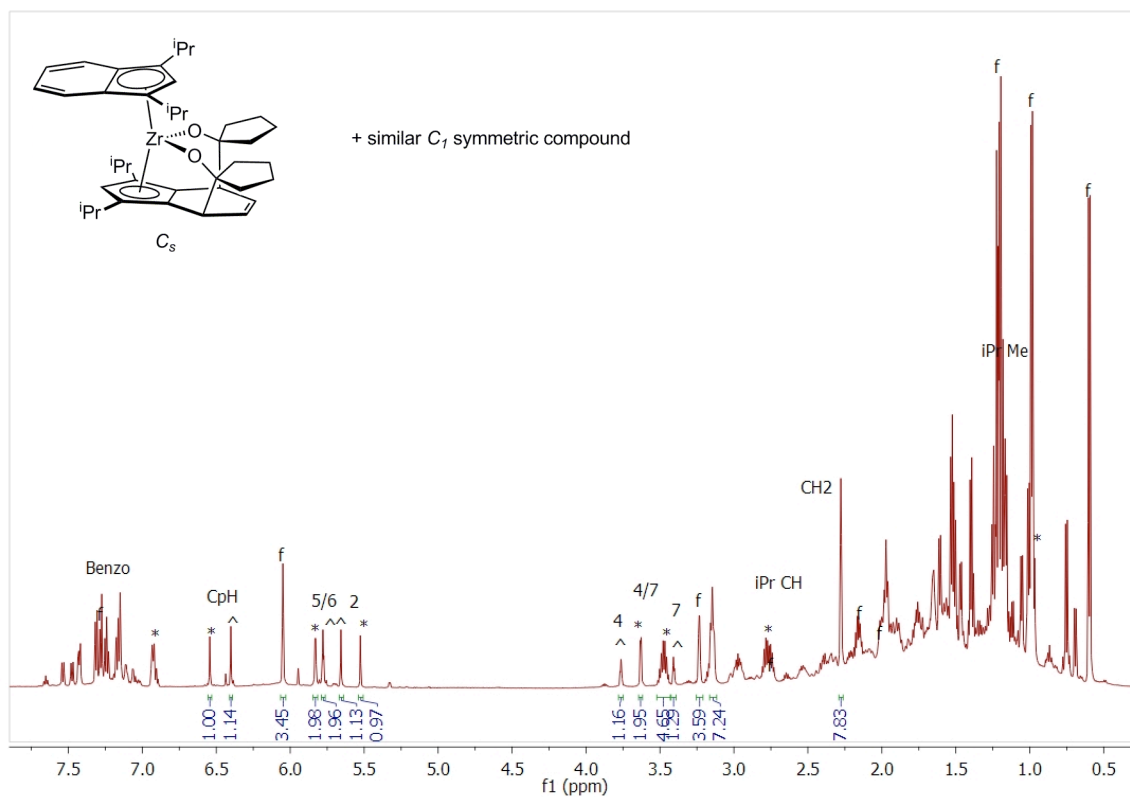
# Cyclopentanone Insertion into $\eta^9, \eta^5$ - Bis(indenyl) Zirconium Sandwich Complexes.

*Doris Pun, Emil Lobkovsky, Ivan Keresztes and Paul J. Chirik\**

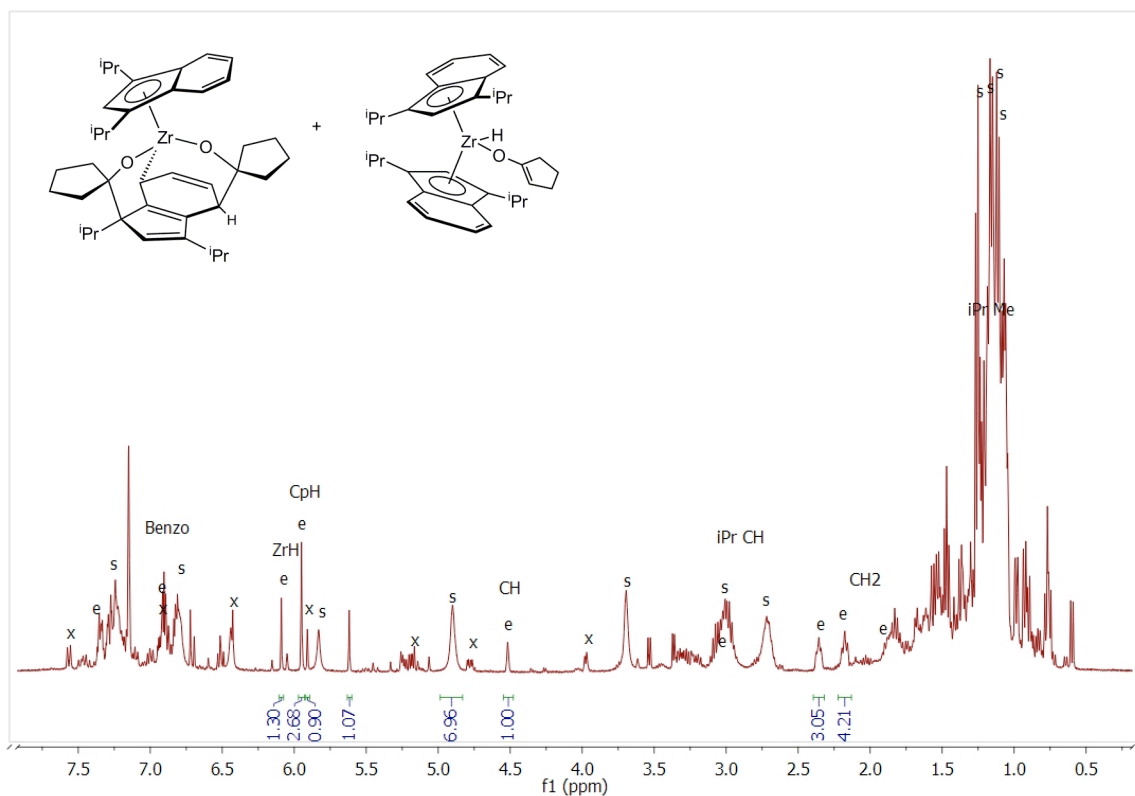
Department of Chemistry and Chemical Biology, Baker Laboratory, Cornell University,  
Ithaca, New York, 14853, U. S. A.

[pc92@cornell.edu](mailto:pc92@cornell.edu)

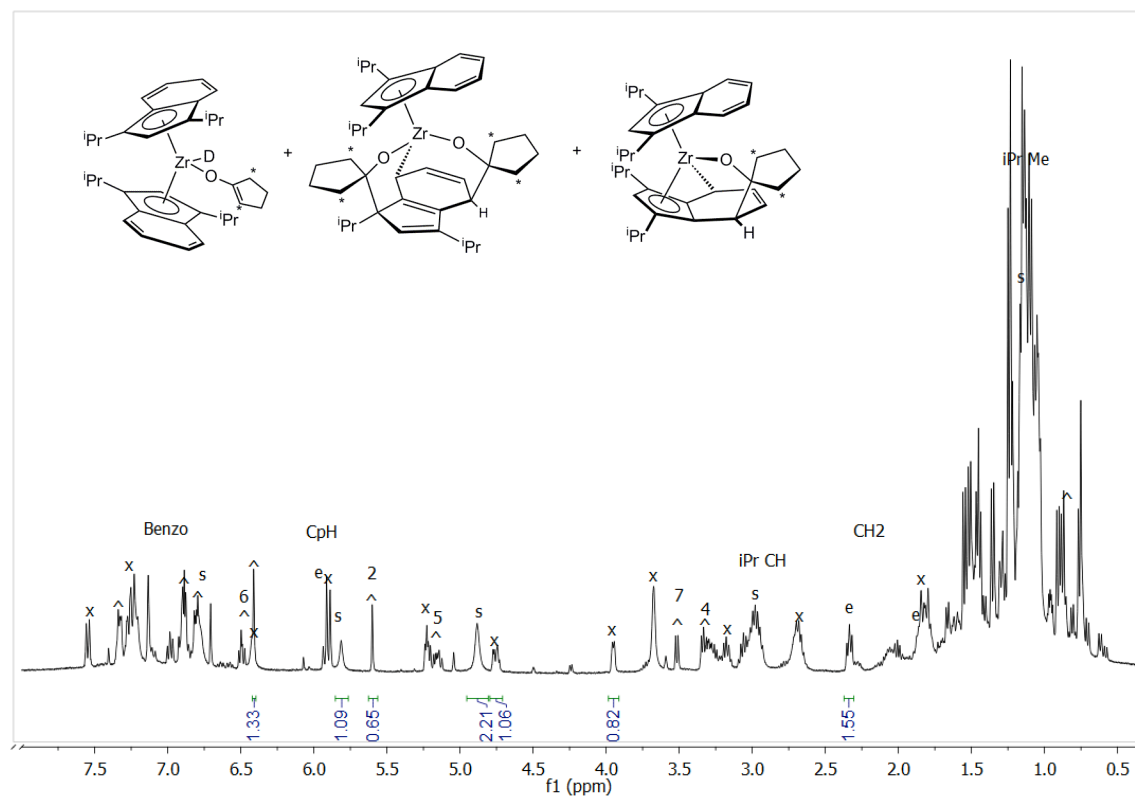
-- Supporting Information --



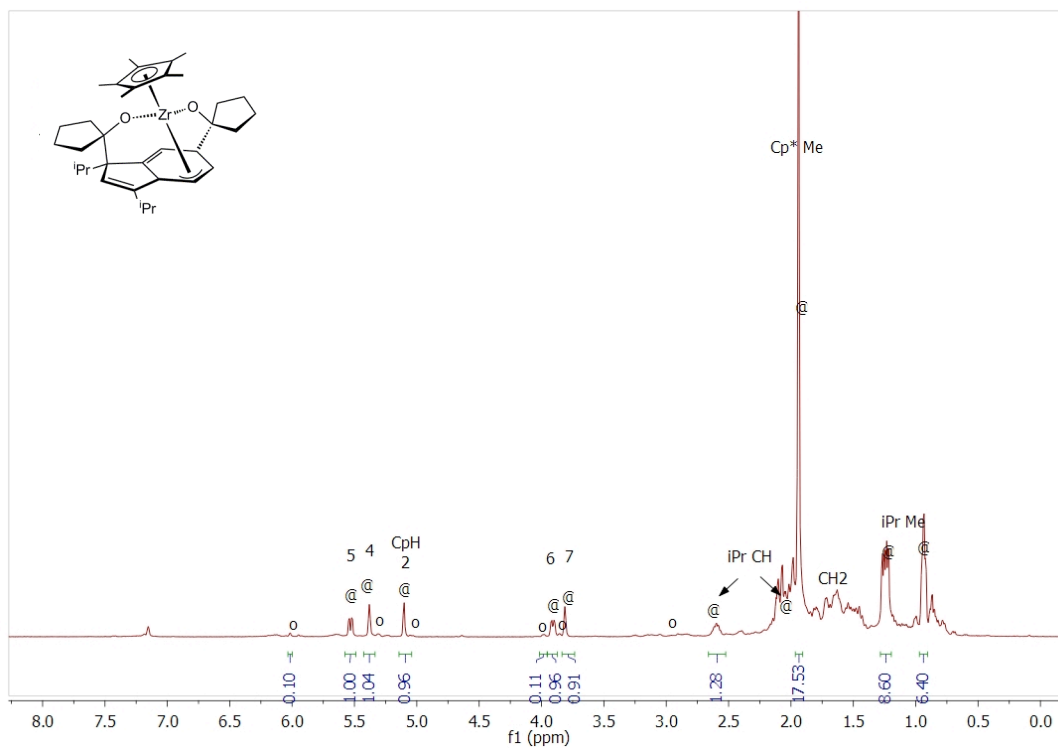
**Figure S1.**  $^1\text{H}$  NMR spectrum of a benzene- $d_6$  solution of **1-(O<sup>c</sup>Pent)<sub>2</sub>-1,4** after heating 90 °C for 1 week affording both  $C_1$  (\*) and  $C_s$  (^) symmetric isomers of **1-(O<sup>c</sup>Pent)<sub>2</sub>-4,7**, along with free ligand (f) in a 1 : 1 : 2.7 ratio. The IUPAC numbering system presented in Chart 1 (full text) is used.



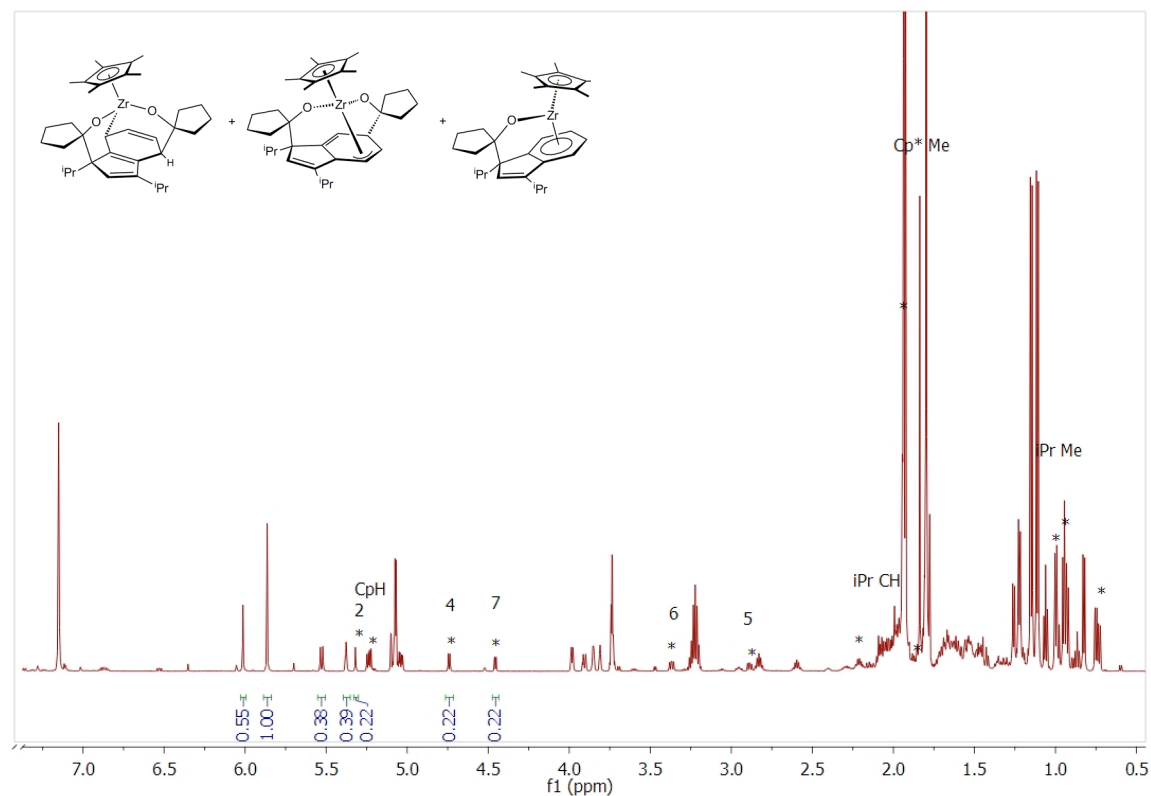
**Figure S2.**  $^1\text{H}$  NMR spectrum of a benzene- $d_6$  solution of **1** (s) after addition of 0.5 equivalents of cyclopentanone and allowing it to stand at 22 °C for 24 hours, forming both **1-(O<sup>c</sup>Pent)<sub>2</sub>-1,4** (x) and **1-(O<sup>c</sup>Pentenyl)H** (e) in a 0.9 : 1 ratio.



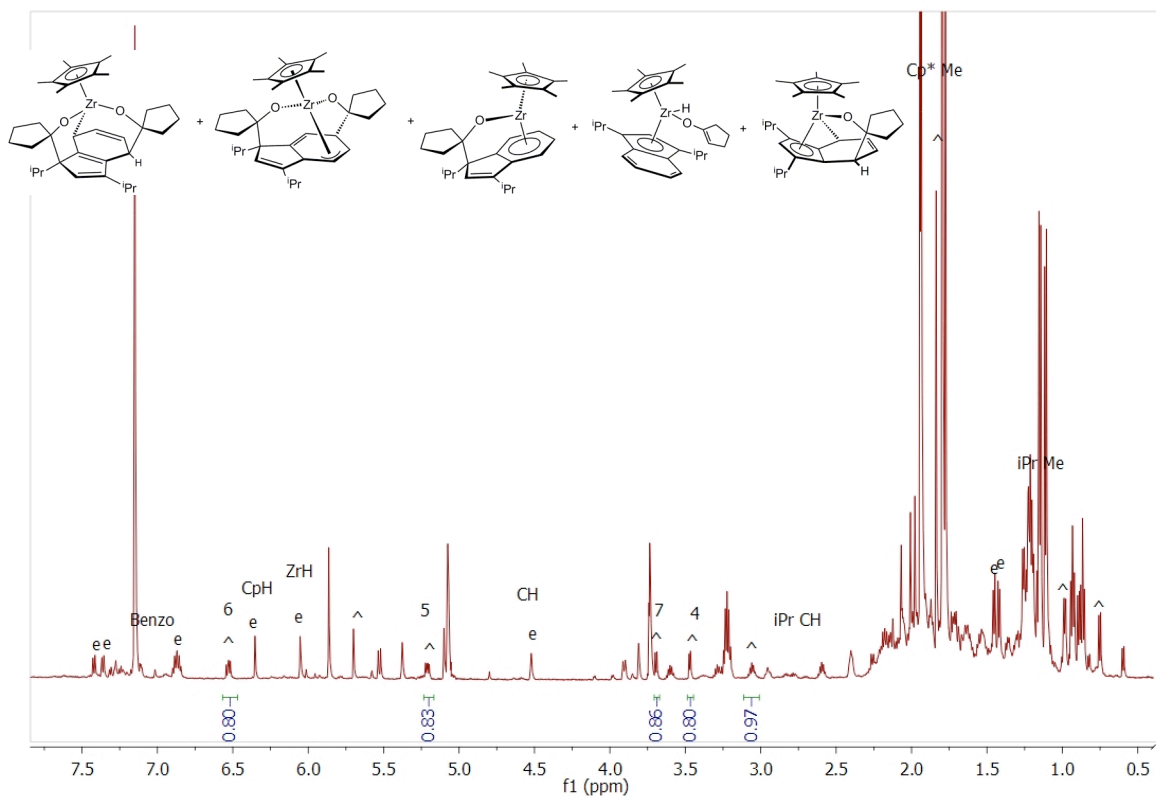
**Figure S3.**  $^1\text{H}$  NMR spectrum of a benzene- $d_6$  solution of **1** (s) after addition of 0.5 equivalents of cyclopentanone- $d_4$  and allowing it to stand at 22 °C for 24 hours, forming **1-(O<sup>c</sup>Pent)<sub>2</sub>-1,4** (x), **1-(O<sup>c</sup>Pentenyl)H** (e) and **1-(O<sup>c</sup>Pent)-4** (^) in a 1.1 : 1 : 0.7 ratio. The IUPAC numbering system presented in Chart 1 is used for **1-(O<sup>c</sup>Pent)-4** (^).



**Figure S4.** <sup>1</sup>H NMR spectrum of a benzene-*d*<sub>6</sub> solution of **2-(O<sup>c</sup>Pent)<sub>2</sub>-1,6 (@)**. Trace quantities of **2-(O<sup>c</sup>Pent)<sub>2</sub>-1,4 (o)** are also present. The IUPAC numbering system presented in Chart 1 is used.



**Figure S5.**  $^1\text{H}$  NMR spectrum of a benzene- $d_6$  solution of **2** initially after addition of 0.5 equivalents of cyclopentanone, affording **2-(O<sup>c</sup>Pent)<sub>2</sub>-1,4**, **2-(O<sup>c</sup>Pent)<sub>2</sub>-1,6** and **2-(O<sup>c</sup>Pent)-1** (\*), along with **2** in a 0.21 : 0.16 : 0.16 : 1.0 ratio. The IUPAC numbering system presented in Chart 1 is used for **2-(O<sup>c</sup>Pent)-1** (\*).



**Figure S6.**  $^1\text{H}$  NMR spectrum of a benzene- $d_6$  solution of **2** 24 hours after addition of 0.5 equivalents of cyclopentanone, resulting in a the ratio of 1 : 0.06 : 0.19 : 0.32 : 0.19 for **2** : **2-(O<sup>c</sup>Pent)<sub>2</sub>-1,4** : **2-(O<sup>c</sup>Pent)<sub>2</sub>-1,6** : **2-(O<sup>c</sup>Pentenyl)H (e)** : **2-(O<sup>c</sup>Pent)-4 (^)**. The IUPAC numbering system presented in Chart 1 is used for **2-(O<sup>c</sup>Pent)-4 (^)**.