

Supplementary Materials

# Novel Allyl Cobalt Phosphine Complexes: Synthesis, Characterization and Behavior in the Polymerization of Allene and 1,3-Dienes

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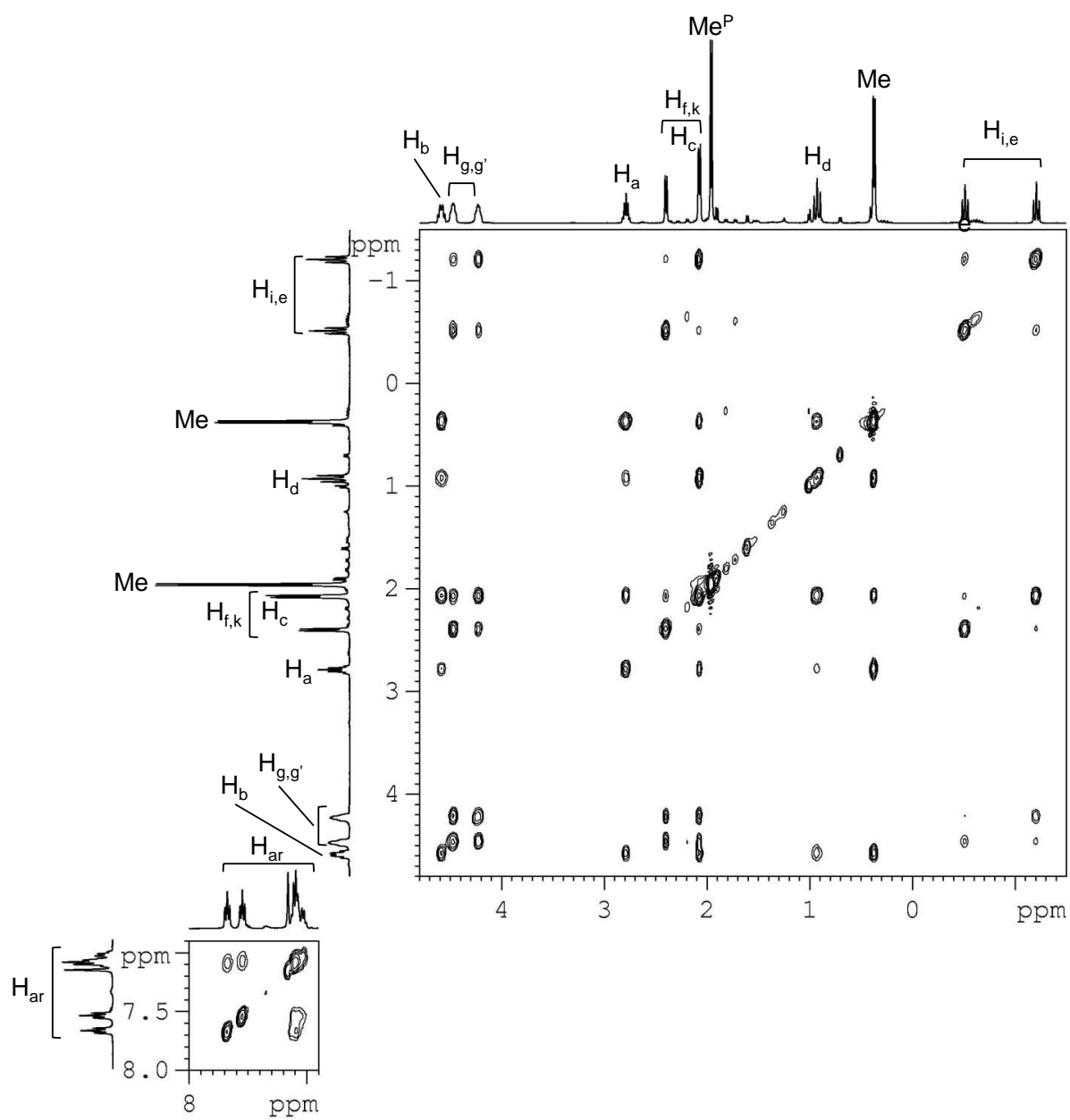
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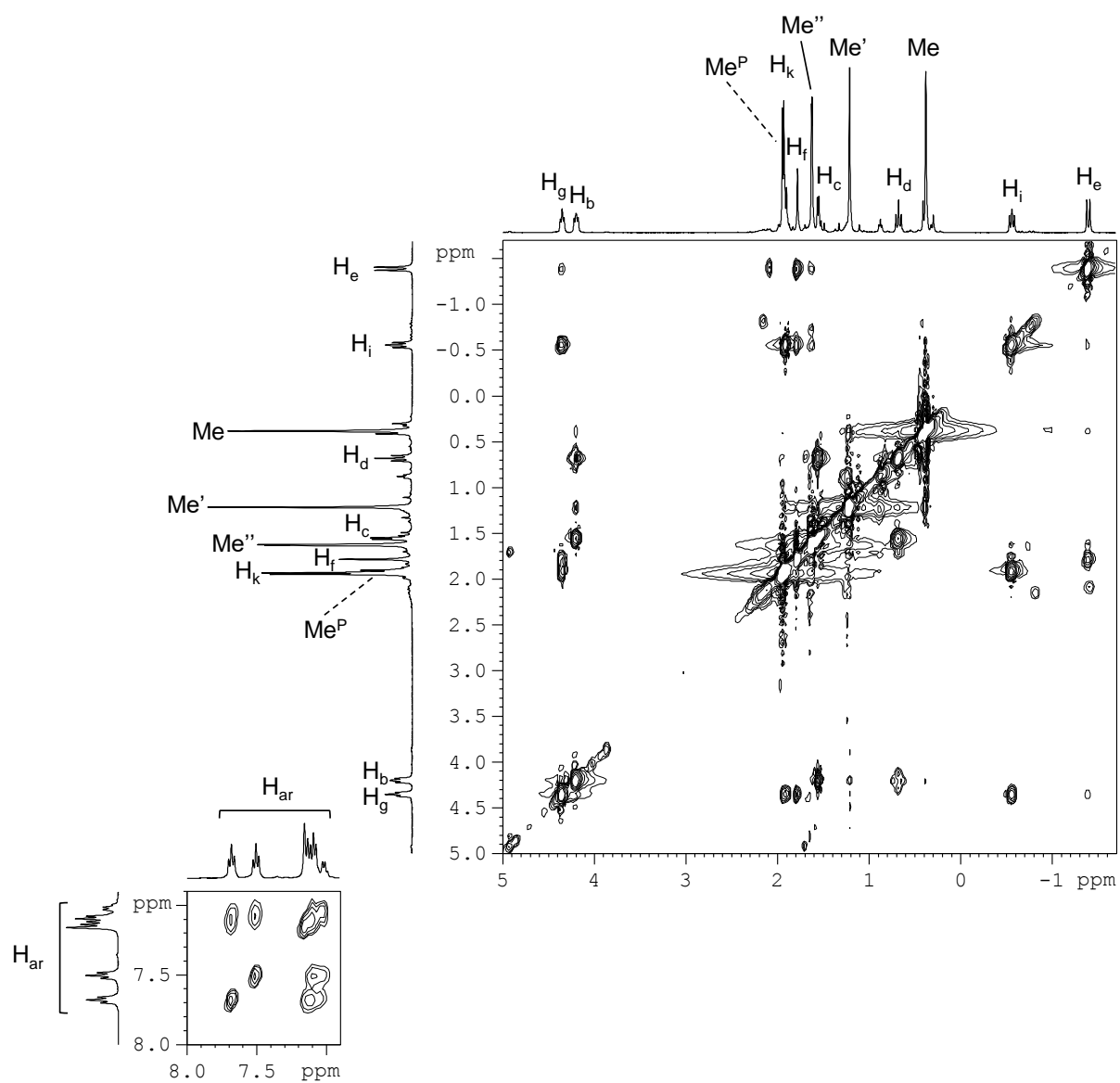
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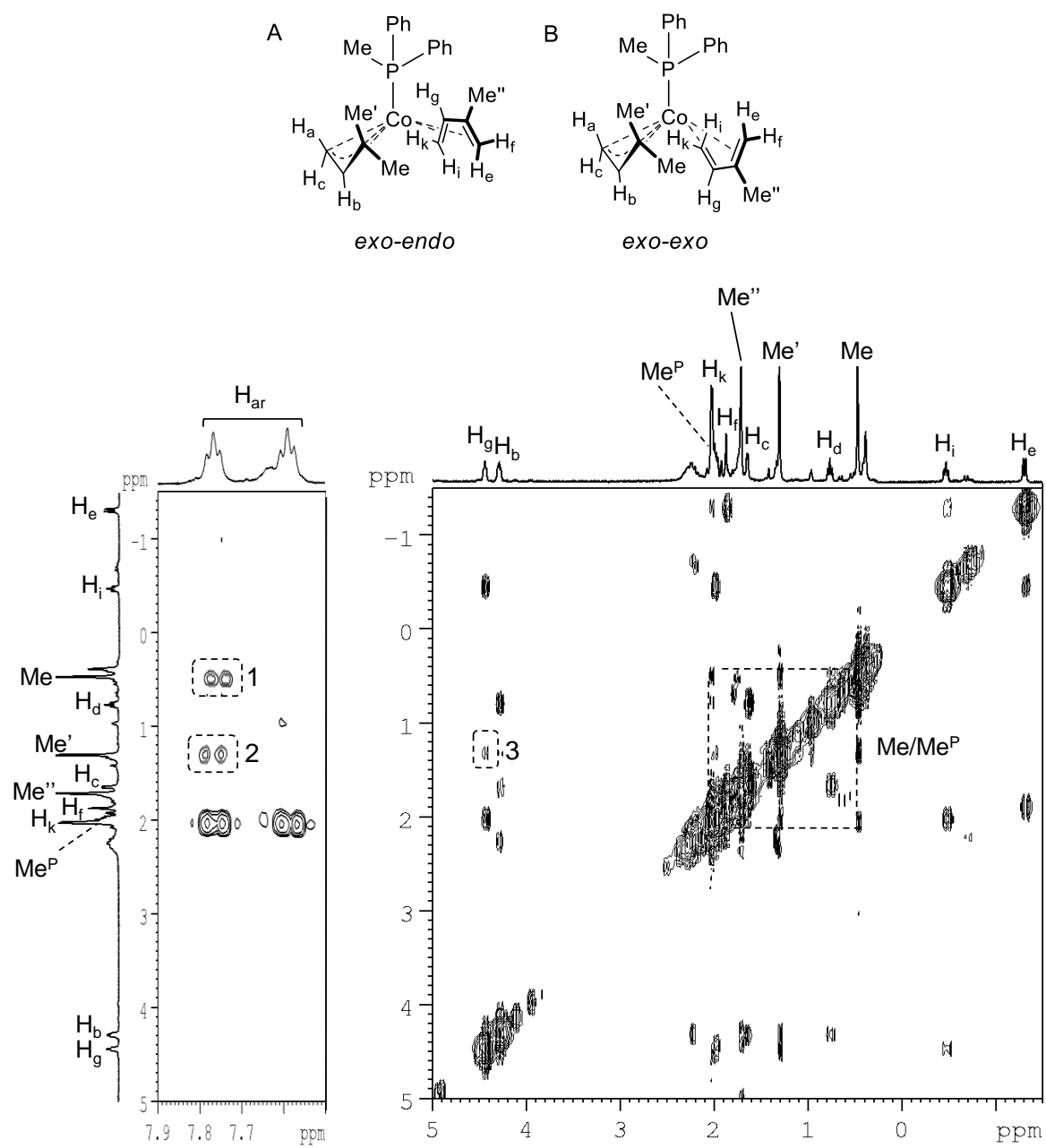
- **Table S1:** Crystallographic data and results of structure refinement for (PCyPh<sub>2</sub>)Co(η<sup>3</sup>-C<sub>4</sub>H<sub>7</sub>)(η<sup>4</sup>-C<sub>4</sub>H<sub>6</sub>) (**1**).
- **Figure S1:** TOCSY NMR spectrum of (PMePh<sub>2</sub>)Co(η<sup>3</sup>-C<sub>4</sub>H<sub>7</sub>)(η<sup>4</sup>-C<sub>4</sub>H<sub>6</sub>) (**2**).
- **Figure S2:** TOCSY NMR spectrum of (PMePh<sub>2</sub>)Co(η<sup>3</sup>-C<sub>5</sub>H<sub>9</sub>)(η<sup>4</sup>-C<sub>5</sub>H<sub>8</sub>) (**3**).
- **Figure S3:** ROESY NMR spectrum of (PMePh<sub>2</sub>)Co(η<sup>3</sup>-C<sub>5</sub>H<sub>9</sub>)(η<sup>4</sup>-C<sub>5</sub>H<sub>8</sub>) (**3**).
- **Figure S4:** ROESY NMR spectrum of (PMePh<sub>2</sub>)Co(η<sup>3</sup>-C<sub>4</sub>H<sub>7</sub>)(η<sup>4</sup>-C<sub>4</sub>H<sub>6</sub>) (**2**).

**Table S1:** Crystallographic data and results of structure refinement for (PCyPh<sub>2</sub>)Co(η<sup>3</sup>-C<sub>4</sub>H<sub>7</sub>)(η<sup>4</sup>-C<sub>4</sub>H<sub>6</sub>) (**1**).

Chemical Formula	C <sub>26</sub> H <sub>34</sub> CoP
Molecular weight	436.43
<i>T</i> (K)	90(2)
Crystal system	Monoclinic
space group	<i>C2/c</i>
<i>a</i> (Å)	17.649(4)
<i>b</i> (Å)	13.587(3)
<i>c</i> (Å)	18.801(4)
α(°)	90
β(°)	101.559(3)
γ(°)	90
<i>V</i> (Å <sup>3</sup> )	4417.2(17)
<i>Z</i>	8
<i>D</i> <sub>calcd</sub> (g cm <sup>-3</sup> )	1.313
μ (mm <sup>-1</sup> )	0.859
Crystal size (mm)	0.28 x 0.20 x 0.10
Color, habit	Orange, prism
2θ <sub>max</sub> , °	55.14
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	30850/5103/4160
( <i>R</i> <sub>int</sub> )/( <i>R</i> <sub>σ</sub> )	0.0471/0.0361
data/restraints/params	5103/0/283
R[ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], wR( <i>F</i> <sup>2</sup> ), S	0.0833, 0.2298, 1.121
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	1.209, -1.350

**Figure S1:** TOCSY NMR spectrum of  $(\text{PMePh}_2\text{Co})(\eta^3\text{-C}_4\text{H}_7)(\eta^4\text{-C}_4\text{H}_6)$  (**2**).

**Figure S2:** TOCSY NMR spectrum of  $(\text{PMePh}_2)\text{Co}(\eta^3\text{-C}_5\text{H}_9)(\eta^4\text{-C}_5\text{H}_8)$  (**3**).

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