Group 3 Dialkyl Complexes with Tetradequate (L, L, N, O; L = N, O, S)
Monoanionic Ligands – Synthesis and Reactivity

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Supporting Information

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Figure 1. $^1$H NMR spectra of 7a and 8a at room temperature.

Figure 2. Variable temperature $^1$H NMR spectroscopy studies of 7a.
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Figure 9. Kinetic studies of the conversion of 11 to 12 in toluene-$d_8$ at 0°C. Both the disappearance of 11 (blue squares) and the formation of 12 (red circles) were followed over time by measuring the integrals for baseline separated proton peaks at δ 8.08 ppm (2H), and δ 5.01 ppm (1H), respectively. Equation used: $y = I_f + (I_i - I_f)\exp(-kt)$. 
Figure 10. $^1$H NMR spectroscopy studies of $^{15}$.
**Figure 11.** $^1$H NMR spectroscopy studies of 15 in the presence of ethylene.

![Diagram](image)

**MAO = methyl aluminum oxide**

<table>
<thead>
<tr>
<th>No.</th>
<th>Compound</th>
<th>Productivity (Kg PE·mol M$^{-1}$·h$^{-1}$·bar$^{-1}$)</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>M = Y, L = OCH$_3$, R = CH$_2$Si(CH$_3$)$_2$Ph (7a)</td>
<td>1.4, 2.0</td>
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<tr>
<td>2</td>
<td>M = Y, L = NEt$_2$, R = CH$_2$Si(CH$_3$)$_2$Ph (7b)</td>
<td>1.1, 0.9</td>
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<tr>
<td>3</td>
<td>M = Sc, L = OCH$_3$, R = CH$_2$Si(CH$_3$)$_2$Ph (8a)</td>
<td>0.9, 0.8</td>
</tr>
<tr>
<td>4</td>
<td>M = Sc, L = SCMe$_3$, R = CH$_2$Si(CH$_3$)$_2$Ph (8b)</td>
<td>2.5, 2.5</td>
</tr>
<tr>
<td>5</td>
<td>M = Y, L = OCH$_3$, R = CH$_2$Si(CH$_3$)$_3$ (9)</td>
<td>0.9, 1.0</td>
</tr>
<tr>
<td>6</td>
<td>M = Sc, L = OCH$_3$, R = CH$_2$Si(CH$_3$)$_3$ (10)</td>
<td>1.3, 0.6</td>
</tr>
</tbody>
</table>

**Table 1.** Polymerization trials of the metal dialkyl complexes. Conditions: 1.67 μmol catalyst, 500 equiv. MAO, 5 mL solvent (chlorobenzene), 5 bar, 1 h.
Figure 12. $^1$H NMR spectrum of 10.

Figure 13. Eyring plot for Si(CH$_3$)$_3$ in 10 (toluene-$d_8$, 300 MHz).
Figure 14. Eyring plot for OCH$_3$ in 10 (toluene-$d_8$, 300 MHz).