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Ti( $\eta^5$ -1-SiMe<sub>3</sub>-C<sub>9</sub>H<sub>6</sub>)(Cl)<sub>2</sub>(OR): Structure and Bonding

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# Ti( $\eta^5$ -1-SiMe<sub>3</sub>-C<sub>9</sub>H<sub>6</sub>)(Cl)<sub>2</sub>(OR): Structure and Bonding

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**Abstract.** Treatment of Ti( $\eta^5$ -1-SiMe<sub>3</sub>C<sub>9</sub>H<sub>6</sub>)Cl<sub>3</sub> (**1**) with LiOR (**2a**, R = 2,6-<sup>t</sup>Bu<sub>2</sub>C<sub>6</sub>H<sub>3</sub>; **2b**, R = 2,6-Ph<sub>2</sub>C<sub>6</sub>H<sub>3</sub>; **2c**, R = <sup>i</sup>C<sub>3</sub>H<sub>7</sub>; **2d**, R = <sup>t</sup>C<sub>4</sub>H<sub>9</sub>) in a 1:1 molar ratio produced half-sandwich compounds Ti( $\eta^5$ -1-SiMe<sub>3</sub>C<sub>9</sub>H<sub>6</sub>)(Cl)<sub>2</sub>(OR) (**3a**, R = 2,6-<sup>t</sup>Bu<sub>2</sub>C<sub>6</sub>H<sub>3</sub>; **3b**, R = 2,6-Ph<sub>2</sub>C<sub>6</sub>H<sub>3</sub>; **3c**, R = <sup>i</sup>C<sub>3</sub>H<sub>7</sub>; **3d**, R = <sup>t</sup>C<sub>4</sub>H<sub>9</sub>) in high yield. Compounds **3c,d** were also accessible, when **1** was reacted with a one-fold excess of HOR (**2c**, R = <sup>i</sup>C<sub>3</sub>H<sub>7</sub>; **2d**, R = <sup>t</sup>C<sub>4</sub>H<sub>9</sub>) in refluxing benzene. The molecular structure of **3b** in the solid state was determined by single-crystal X-ray diffraction studies, confirming the piano-stool geometry. Quantum chemical calculations at the B3LYP/6-

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