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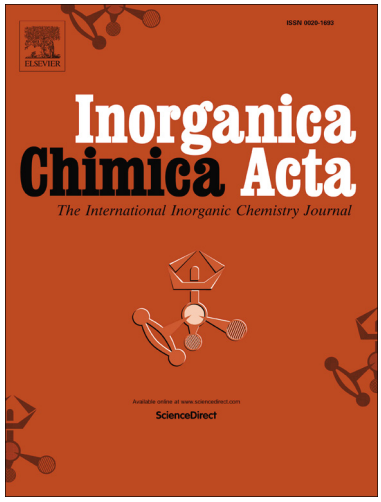

$Ti(\eta^5\text{-}1\text{-}SiMe_3\text{-}C_9H_6)(Cl)_2(OR)$: Structure and Bonding

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$Ti(\eta^5\text{-}1\text{-}SiMe_3\text{-}C_9H_6)(Cl)_2(OR)$: Structure and Bonding

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Abstract. Treatment of $Ti(\eta^5\text{-}1\text{-}SiMe_3C_9H_6)Cl_3$ (**1**) with LiOR (**2a**, R = 2,6-^{t}Bu$_2$C$_6$H$_3$; **2b**, R = 2,6-Ph$_2$C$_6$H$_3$; **2c**, R = ^{i}C$_3$H$_7$; **2d**, R = ^{t}C$_4$H$_9$) in a 1:1 molar ratio produced half-sandwich compounds $Ti(\eta^5\text{-}1\text{-}SiMe_3C_9H_6)(Cl)_2(OR)$ (**3a**, R = 2,6-^{t}Bu$_2$C$_6$H$_3$; **3b**, R = 2,6-Ph$_2$C$_6$H$_3$; **3c**, R = ^{i}C$_3$H$_7$; **3d**, R = ^{t}C$_4$H$_9$) in high yield. Compounds **3c**,**d** were also accessible, when **1** was reacted with a one-fold excess of HOR (**2c**, R = ^{i}C$_3$H$_7$; **2d**, R = ^{t}C$_4$H$_9$) 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-