#### Accepted Manuscript

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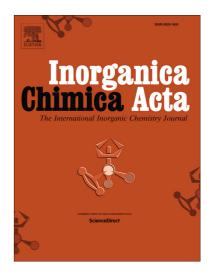
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### **ACCEPTED MANUSCRIPT**

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

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**Abstract**. Treatment of  $Ti(\eta^5-1-SiMe_3C_9H_6)Cl_3$  (1) with LiOR (2a, R=2,6- ${}^tBu_2C_6H_3$ ; 2b, R=2,6- ${}^tPh_2C_6H_3$ ; 2c,  $R={}^tC_3H_7$ ; 2d,  $R={}^tC_4H_9$ ) in a 1:1 molar ratio produced half-sandwich compounds  $Ti(\eta^5-1-SiMe_3C_9H_6)(Cl)_2(OR)$  (3a, R=2,6- ${}^tBu_2C_6H_3$ ; 3b, R=2,6- ${}^tPh_2C_6H_3$ ; 3c,  $R={}^tC_3H_7$ ; 3d,  $R={}^tC_4H_9$ ) in high yield. Compounds 3c,d were also accessible, when 1 was reacted with a one-fold excess of HOR (2c,  $R={}^tC_3H_7$ ; 2d,  $R={}^tC_4H_9$ ) 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-

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