

Correction to Impact of d-Orbital Occupation on Metal–Carbon Bond Functionalization

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In the course of other research in our group, two typographical errors were found for this paper. These do not change the conclusions of the manuscript but are noted here for completeness.

Page 7793 (left column, third paragraph). In the sentence “From separated reactants, the coordination of PyO is exergonic by 22.6 kcal/mol to form the MCI, $^1[\text{Ti}](\text{OPy})\text{-(Me)}$, Figure 7.”, the superscript “1” should be a superscript “3” to denote a triplet ground state.

Page 7794 (right column, bottom). The sentence “Though triplet ($\Delta G_{\text{rel}} = 29.6$ kcal/mol) and quintet ($\Delta G_{\text{rel}} = 20.1$ kcal/mol) OMBV transition states were found, iron was calculated to preferentially oxy-insert via an OAT/MM pathway.” should read “Though a triplet ($\Delta G_{\text{rel}} = 29.6$ kcal/mol) OMBV transition state was found, iron was calculated to preferentially oxy-insert via an OAT/MM pathway.”

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