Accepted Manuscript

Research paper

Isolation and Identification of the Pre-Catalyst in Iron-Catalyzed Direct Arylation of Pyrrole with Phenylboronic Acid

Samantha M. Brewer, Philip M. Palacios, Hannah M. Johnston, Brad S. Pierce, Kayla N. Green

PII:	S0020-1693(18)30215-9
DOI:	https://doi.org/10.1016/j.ica.2018.03.036
Reference:	ICA 18181

To appear in: Inorganica Chimica Acta

Received Date:5 February 2018Revised Date:21 March 2018Accepted Date:22 March 2018



Please cite this article as: S.M. Brewer, P.M. Palacios, H.M. Johnston, B.S. Pierce, K.N. Green, Isolation and Identification of the Pre-Catalyst in Iron-Catalyzed Direct Arylation of Pyrrole with Phenylboronic Acid, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.03.036

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Isolation and Identification of the Pre-Catalyst in Iron-Catalyzed Direct

Arylation of Pyrrole with Phenylboronic Acid

Samantha M. Brewer,^a Philip M. Palacios,^b Hannah M. Johnston,^a Brad S. Pierce,^b and Kayla N. Green^a*

^a Department of Chemistry and Biochemistry, Texas Christian University, Fort Worth, TX, USA ^b Department of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX, USA

Abstract. Herein we describe the synthesis, charcterization, and role of three dichloric iron(III) complexes, [L1Fe(III)(Cl)₂]ClO₄ (L1Fe), [L2Fe(III)(Cl)₂]ClO₄ (L2Fe), and [L3Fe(III)(Cl)₂]ClO₄ (L3Fe) [L1 (Pyclen)=1,4,7,10-tetra-aza-2,6-pyridinophane; L2 =3,6,9,15-tetraazabicyclo[9.3.1]penta-deca-

1(15),11,13-trien-13-ol; L3 =3,6,9,15-tetra-azabicyclo[9.3.1]penta-deca-1(15),11,13-trien-12-ol], in the coupling of pyrrole and phenylboronic acid to form 2-phenylpyrrole. The oxidation state and spin state of the iron complexes were characterized using X-ray crystallography, UV-vis absorbance spectroscopy, electron paramagnetic resonance spectroscopy, cyclic voltammetry, and mass spectrometry. Electrochemistry results rank ligand L1-L3 as moderate tetra-azamacrocycle donors to iron between cyclen and Me₂EBC-12. Characterization of the iron(III) complexes and subsequent catalytic testing indicates that the complexes enter the C-C coupling catalytic cycle in the high-spin iron(III) oxidation state. Furthermore, the results indicate that the iron(III) complexes are essential for catalytic and regioselective production of the 2-phenylpyrrole product.

KEYWORDS: Iron, cross-coupling, direct Suzuki-Miyaura, heterocycle, catalysis, pyrrole

Download English Version:

https://daneshyari.com/en/article/7750446

Download Persian Version:

https://daneshyari.com/article/7750446

Daneshyari.com