

Iron-Catalyzed Aryl-Aryl Cross-Coupling Reaction: Homo-versus Hetero-Coupling Reactions

E. Zhou, Lidie Rousseau, M. Ahr, M. Clemancey, J.-M Latour, G. Blondin, G. Lefèvre, G. Cahiez

► **To cite this version:**

E. Zhou, Lidie Rousseau, M. Ahr, M. Clemancey, J.-M Latour, et al.. Iron-Catalyzed Aryl-Aryl Cross-Coupling Reaction: Homo-versus Hetero-Coupling Reactions. International Symposium on Synthesis and Catalysis (ISYSYCAT 2019), Sep 2019, Evora, Portugal. cea-02339520

HAL Id: cea-02339520

<https://hal-cea.archives-ouvertes.fr/cea-02339520>

Submitted on 30 Oct 2019

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Iron-Catalyzed Aryl-Aryl Cross-Coupling Reaction: Homo- versus Hetero-Coupling Reactions

E. Zhou ^a, L. Rousseau ^{a,b}, M. Ahr ^a, N. Lefèvre ^a, M. Clémancey ^c, J.-M. Latour ^c, G. Blondin ^c, G. Lefèvre* ^{a,b} and G. Cahiez* ^a

^a CSB2D, Institute of Chemistry for Life and Health Sciences, Chimie ParisTech, PSL University, CNRS, 75005 Paris, France ;

^b LCMCE, NIMBE, CEA, CNRS, Univ. Paris-Saclay, 91191 Gif, France ; ^c LCBM, pmb, Univ. Grenoble Alpes, CEA, CNRS, 38000 Grenoble, France

Email: lidie.rousseau@chimieparitech.psl.eu

An in-depth mechanistic study was undertaken to explain the competition between the homo- and heterocoupling¹ reactions in the case of iron-catalyzed aryl-aryl cross-couplings² in the presence of C₆F₅Cl as an organic sacrificial oxidant. The formation of the homocoupling product is explained by a crucial iron-to-magnesium transmetallation of a C₆F₅⁻ anion arising from the bielectronic reduction of C₆F₅Cl. This mechanism is discussed and supported by experimental results, including ¹H paramagnetic NMR and ⁵⁷Fe-Mössbauer spectroscopies.³ These results enlighten the mechanistic features of iron-catalyzed Grignard oxidative homocoupling, and can provide guidance in the choice of suitable sacrificial oxidants for such systems.

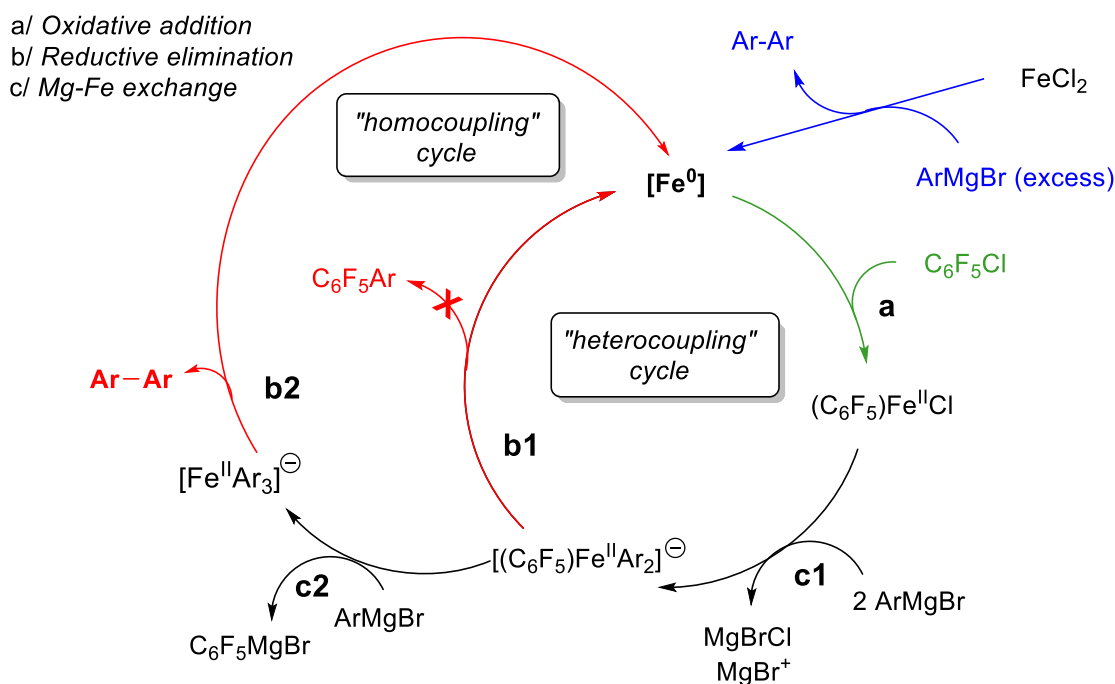


Figure 1: Fe-catalyzed reaction of ArMgBr with C₆F₅Cl: homo- and hetero-coupling catalytic cycles

References:

- Hatakeyama T., Nakamura M. *J. Am. Chem. Soc.* **2007**, 129, 9844.
- Kuzmina O. M., Steib A. K., Moyeux A., Cahiez G., Knochel P., *Synthesis* **2015**, 47, 1696.
- Clémancey M., Cantat T., Blondin G., Latour J.-M., Dorlet P., Lefèvre G. *Inorg. Chem.*, **2017**, 56, 3834.