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

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An in-depth mechanistic study was undertaken to explain the competition between the homo- and heterocoupling<sup>1</sup> reactions in the case of iron-catalyzed aryl-aryl cross-couplings<sup>2</sup> in the presence of C<sub>6</sub>F<sub>5</sub>Cl as an organic sacrificial oxidant. The formation of the homocoupling product is explained by a crucial iron-to-magnesium transmetalation of a C<sub>6</sub>F<sub>5</sub><sup>-</sup> anion arising from the bielectronic reduction of C<sub>6</sub>F<sub>5</sub>Cl. This mechanism is discussed and supported by experimental results, including <sup>1</sup>H paramagnetic NMR and <sup>57</sup>Fe-Mössbauer spectroscopies.<sup>3</sup> 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.

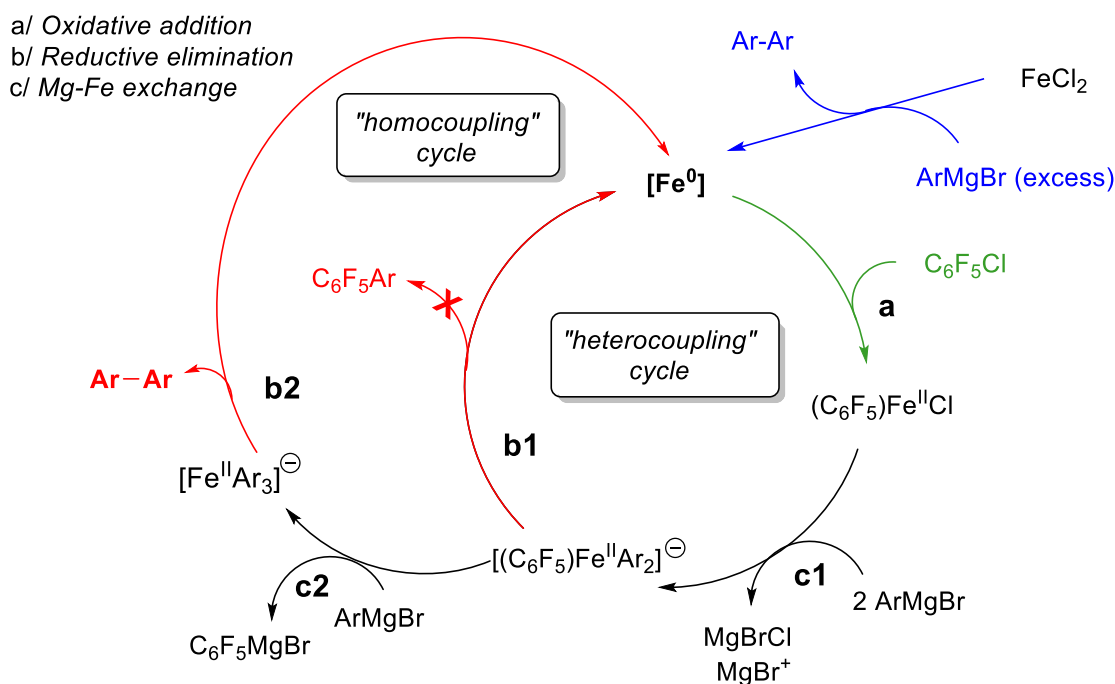


Figure 1: Fe-catalyzed reaction of ArMgBr with C<sub>6</sub>F<sub>5</sub>Cl: homo- and hetero-coupling catalytic cycles

### 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.