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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 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 transmetalation 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.

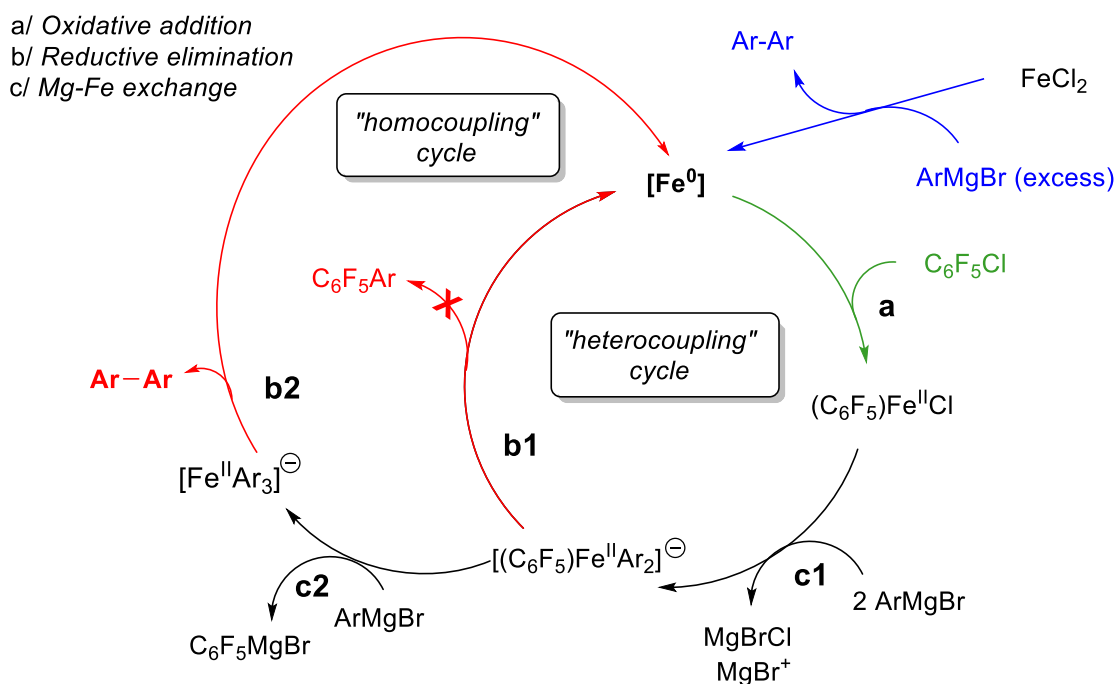


Figure 1: Fe-catalyzed reaction of ArMgBr with C₆F₅Cl: homo- and hetero-coupling catalytic cycles

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