Copper-Catalyzed Trifluoromethylation of Aryl Halides via Concurrent Tandem Catalysis

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Introduction

- Goal: To test concurrent tandem catalysis (CTC) methods to render aryl chlorides (ArCl) and aryl bromides (ArBr) equivalent in reactivity to aryl iodides (ArI).

Development of CTC Trifluoromethylation

- Reaction A: Halide Exchange
  - Cu-catalyzed halide exchange of aryl bromides and chlorides form aryl iodides under microwave heating:
  - Equilibrium-limited
  - Aryl halides are widely used as starting materials in synthesis

- Reaction B: Various Possibilities
  - Order of reactivity in coupling reactions: ArCl < ArBr < ArI

Quantifying the Product by 19F NMR

- Reaction Under Investigation
  - Hydrodehalogenation product
  -Highest product yield by GC seen thus far (98%)
  - Two side products formed

- Reproducibility Issues Investigated
  - Same vendor, different batches
  - 25 g bottle had ≈20% less CF3

- CTC Trifluoromethylation of ArBr
  - Proposed trifluoromethylation of less reactive aryl bromides using CTC methodology
  - Initial attempt resulted in a small amount of desired product

Reproducibility

- Conclusions & Future Work
  - Lack of reproducibility was observed