THESIS INFORMATION

Title: **Cu-BASED ORGANIC FRAMEWORKS AS CATALYSTS FOR C–C AND C–N COUPLING REACTIONS**

Major: **Organic Chemical Technology**

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Contributions of this thesis

The overarching goal of this thesis is to use four Cu-MOFs as catalysts for direct C–C and C–N coupling reactions to synthesize propargylamines and quinoxalines. These compounds are found as the versatile intermediates for the synthesis of many nitrogen-containing biologically active compounds. Herein, the following are the main research contributions of this thesis.

- $Cu_3(BTC)_2$, $Cu_2(BDC)_2(DABCO)$, $Cu_2(BPDC)_2(BPY)$ and Cu(BDC) were synthesized successfully by solvothermal methods. These Cu-MOFs were characterized by characterized by PXRD, FT-IR, SEM, TEM, TGA, ICP-MS, H_2TPR and nitrogen physisorption measurements.

- It is first time to use these Cu-MOFs as heterogeneous catalysts for the reactions: i) the $Cu_3(BTC)_2$ was used as a heterogeneous catalyst for the direct oxidative C–C coupling reaction *via* C–H functionalization between *N*,*N*-dimethylanilines and terminal alkynes (reaction **1**); ii) the $Cu_2(BDC)_2(DABCO)$ was used as a heterogeneous catalyst for the direct C–C coupling reaction *via* C–H functionalization between *N*-methylanilines and terminal alkynes (reaction **2**); iii) the $Cu_2(BPDC)_2(BPY)$ could be used as a heterogeneous catalyst for the copper-catalyzed A^3 reaction of tetrahydroisoquinoline, aldehydes, and alkynes (reaction **3**); iv) the Cu(BDC) was employed as a heterogeneous catalyst for the oxidative cyclization reaction between α-hydroxyacetophenone and phenylenediamine derivatives (reaction **4**).

- $Cu_3(BTC)_2$, $Cu_2(BDC)_2(DABCO)$, $Cu_2(BPDC)_2(BPY)$ and Cu(BDC) showed high catalytic activities for those C–C and C–N coupling reactions and the optimal conditions of the these reactions have been found.

- These Cu-MOFs can be reused and recycled several times without a significant degradation in catalytic activities. Fresh Cu-MOFs and reused Cu-MOFs were also compared by PXRD and FT-IR.

- All major products from the reaction **1**, **2**, **3**, **4** were confirmed by ^{1}H NMR and ^{13}C NMR. Besides, the isolated yields of those reactions were calculated.

- The most prominent point of this thesis the reaction of *N*-methylanilines and terminal alkynes (reaction **2**). To the best of our knowledge, the reaction **2** has not been previously reported. Based on direct C–C coupling reactions, it is contributed to provide a new way to get propargylamines with the aldehyde-free from secondary amines and terminal alkynes. The mechanism of this reaction was also proposed.

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