

THESIS INFORMATION

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Title: SYNTHESIS OF COBALT AND IRON-BASED METAL-ORGANIC FRAMEWORKS AND THEIR APPLICATIONS

Major: Organic Chemical Technology

Major Code: 62527505

Training institute: Ho Chi Minh City University of Technology, VNU-HCM

Scientific supervisors: Prof. Nam Son Thanh PHAN

The aim of the thesis

In our scope of exploration, we employed the cheap and commercial linkers as well as earth abundant metals such as iron and cobalt to synthesize the novel metal-organic frameworks. Subsequently, the newly discovered crystal structure were employed as standpoint for initially justifying the interesting properties of novel MOFs to use in relevant applications.

Targeted Applications

Application 1: Highlighting the advantage of obtained MOFs with the large pore size and high surface area can be a highly active heterogeneous catalyst for chemical transformation of large organic molecules which cannot be done by smaller pore size MOFs.

Application 2: Synthesis of MOFs that achieve high proton conductivity at elevated temperature ($T \geq 95$ °C) under low humidity ($RH \leq 60\%$).

Scientific Contribution

1. Material Synthesis and Characterization

- Four novel metal organic frameworks, namely, VNU-10, VNU-15, Fe-NH₂-BDC and Fe-BTC have been synthesized and the structure of these compounds was solved by single crystal x-ray diffraction (SC-XRD).
- Full characterization of VNU-10 and VNU-15 was done by various host method, included single and powder X-rays diffraction, Fourier transforms infrared analysis (FT-IR), thermogravimetric analysis (TGA) gas (CO₂, CH₄, N₂), atomic absorption spectroscopy (AAS) and water adsorption at various temperature.

- Preliminary characterization on Fe-NH₂-BDC and Fe-BTC have been done by powder X-rays diffraction, Fourier transforms infrared analysis (FT-IR), thermogravimetric analysis (TGA).

2. Application of VNU-10

- VNU-10 with large pore aperture was found to efficiently catalyze direct amination reactions of oxazoles. Excellent conversions with a variety of amines were obtained. Remarkably, VNU-10 offered significantly higher activity than that of Co₂(BDC)₂(DABCO) with the sql structure as well as other Co-based catalysts.
- VNU-10 was proven to be recyclable without a significant degradation in catalytic activity. Leaching tests indicated no contribution of homogeneous leached active cobalt species.
- Various derivatives from amination of benzoxazole with different amines were also synthesized using VNU-10 catalyst.

3. Application of VNU-15

- VNU-15 exhibited ultrahigh proton conductivity ($2.9 \times 10^{-2} \text{ S cm}^{-1}$) at the practical conditions of 60% RH and 95 °C with low activation energy (0.22 eV) through the wide range temperature.
- Time-dependent proton conductivity at 60% RH and 95 °C indicated the stable conductivity of pelletized VNU-15 with no appreciated loss of conductivity over 40 hours.
- Powder X-rays diffraction, Fourier transforms infrared analysis (FT-IR) revealed the maintenance of long range structural order of VNU-15 after proton conducting measurement.
- The proton conductivity of VNU-15 is amongst the highest reported in MOF chemistry, especially when considering practical operating conditions.

Scientific Advisor

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