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"Green and Efficient Synthesis of Cyclopentanone through Furfural Hydrogenation Using Ni-Cu Bimetallic Catalyst on MOF-5 Support from Biomass-Derived Feedstock"

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1. Introduction

Utilizing bio-derived furfural is essential to identify alternatives for petroleum-based chemicals and establish environmentally friendly, cost-effective, and energy-efficient procedures. The selective conversion of furfural to cyclopentanone through hydrogenation holds significant commercial appeal. Metal Organic Frameworks (MOFs) exhibit distinctive properties and structural versatility, while Cu-Ni bimetallic catalysts are recognized for enhancing cyclopentanone selectivity during furfural hydrogenation in aqueous conditions. Cyclopentanone plays a crucial role in the pharmaceutical, rubber, and insecticide sectors. Hence, employing biomass as the source material, the preferred approach involves producing cyclopentanone from furfural.

2. Material and Methods

2.1. Materials

The following reagents were procured from reputed vendors and used per se: Zinc nitrate hexahydrate (purity > 98%, Sigma Aldrich), N, N-dimethylformamide (purity \geq 98.5 %, Sigma Aldrich), furfural (purity > 98%, S.D. Fine Chemicals. Mumbai, India), Terephthalic acid (purity > 98%, Thomas Baker. Munmbau), Nickel nitrate hexahydrate (purity > 98%, Sigma Aldrich), n-decane (purity 97%, S.D. Fine Chemicals), Ethyl acetate (purity \geq 98.5 %, Sigma Aldrich), Cupric nitrate trihydrate (purity > 98%, Sigma Aldrich)

2.2. Catalyst preparation and characterization

The selection of a Metal Organic Framework (MOF-5) support was based on its notable attributes of elevated temperature stability and expansive surface area. Employing a wet impregnation technique, concurrent doping of nickel and copper onto the MOF support surface was executed. Comprehensive catalyst analysis encompassing assessments of structure, functional groups, acidity, and elemental composition was conducted using a range of techniques, including XRD, TGA-DSC, FESEM-EDAX, HR-TEM, FTIR, NH3-TPD, and XPS.

2.3. Reaction conditions and analysis

A comprehensive investigation of diverse reaction parameters including agitation speed, metal loading, catalyst loading, substrate concentration, pressure impact, and temperature variation was undertaken through a sequence of reactions, leading to their optimization for this specific reaction. Periodic sample collection was performed, followed by analysis utilizing Chemito GC with an OV1701 column with FID detector.

3. Significant Results and Discussion

The MOF support exhibited notable characteristics of high surface area and effective dispersion, prompting an exploration of the catalyst's performance when coupled with the metal moiety in the conversion of Furfural, emphasizing selectivity towards cyclopentanone. The distinctive contributions of the MOF support, as well as the individual roles of copper and nickel components, were comprehended by analyzing their separate impacts on the reaction. The collaborative effect of nickel and copper, when supported on the MOF, demonstrated remarkable selectivity and efficiency in the transformation of Furfural into cyclopentanone.

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Table 1: Catalyst screening

Catalyst	% Conversion	% Selectivity
MOF-5 support	50	40
5 % NiCu(1:1)@MOF-5	100	96
5 % NiCu(2:1)@MOF-5	98	82
5 % NiCu(1:2)@MOF-5	94	75

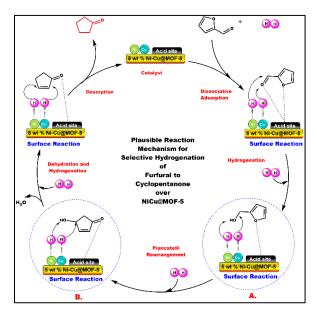


Figure 1: Proposed reaction mechanism

4. Conclusion

The conversion of furfural to furfuryl alcohol and subsequently to cyclopentanone was effectively accomplished utilizing a newly developed NiCu@MOF-5 catalyst and molecular hydrogen gas. This innovative catalytic process aligns with environmentally friendly principles, as it requires significantly reduced metal loading in contrast to conventional catalysts and eliminates the need for precious metals like Pt, Pd, Rh, or Ru. The potential application of MOF as a support in biomass conversion processes could be expanded by the successful and dependable catalytic hydrogenation of furfural, yielding high efficiency and reusability. This approach signifies environmentally conscious and eco-friendly process.

5. References

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