

METAL-ORGANIC FRAMEWORK FOR THE SYNTHESIS OF FINE CHEMICALS

THESIS

submitted in partial fulfilment of the requirements for the award of

MASTER OF SCIENCE IN CHEMISTRY

BY

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DEPARTMENT OF CHEMISTRY

SCHOOL OF SCIENCE AND HUMANITIES

SATHYABAMA

INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)

Accredited with Grade "A" by NAAC I 12B Status by UGC
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MAY, 2023



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DEPARTMENT OF CHEMISTRY

BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of V. SANDHIYA (41910015) who carried out the project entitled "**METAL ORGANIC FRAMEWORK FOR THE SYNTHESIS OF FINE CHEMICALS**" project under my supervision from 04/01/2023 to 05/05/2023.

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ABSTRACT

This project is about the metal-organic framework (MOF) for the synthesis of fine chemicals. The MOFs consist of metal ions and organic ligands, is a highly porous materials with an ultrahigh surface area. The various structure of MOFs can be synthesized depending on the kind of metal ions and organic ligands. MOFs are crystalline porous materials. Basically synthesised by Di/Tri carboxylic acids with bi/tri valent metals such as Zr, Cu, Zn, Ni, Fe, Al and Cr. Zirconyl Nitrate is used as a base metal in Metal-Organic Frameworks (MOFs), and Copper Chloride is inserted using Schiff base to provide a catalyst. Benzaldehyde is created via a subsequent reaction employing the Zr(MOF) catalyst. Finding tuneable qualities, a large surface area, stability, biocompatibility, and cost-effectiveness is made.

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LIST OF ABBREVIATIONS AND SYMBOLS

S.NO.	ABBREVIATIONS AND SYMBOLS	DEFINITION
1	Zr	Zirconium
2	BDC	1,4, benzene dicarboxylic acid
3	DMF	Dimethyl formamide
4	CuCl ₂	Copper chloride
5	°C	Degree Celcius

CHAPTER 1

INTRODUCTION

1.1. METAL-ORGANIC FRAMEWORKS (MOFs):

Metal-organic frameworks (MOFs) are a type of crystalline material that consists of metal ions and organic linkers, which are bound together by strong coordinate bonds to create an open framework with high permanent porosity. Due to their unique properties, such as ultrahigh porosity, high thermal stability, and adaptable surface chemistry, MOFs have numerous potential applications, including gas storage, separations, catalysis, energy conversion, and sensing technology. However, the randomness of structural behaviour resulting from the combination of metal nodes and ligands can be a challenge for MOFs.

1.2. POST-SYNTHETIC MODIFICATION (PSM):

Post-synthesis modification (PSM) is a promising technique that can address the limitations of de novo synthesis by modifying synthesized MOFs to create new frameworks with improved properties. PSM provides greater control over the results and can introduce new chemical and physical properties to MOFs, opening up new possibilities for various applications. Although obtaining identical topological networks for specific ligands with diverse sets of metal ions, counter anions, and guest molecules can be challenging, PSM can combine the components of MOFs with the surrounding medium by easily exchanging them, leading to new structures with the desired properties. PSM does not alter the original topology and structure of the compound through a single crystal-to-single crystal transformation (SCSC). MOFs are particularly well-suited for PSM due to the labile nature of the coordination bond between the metal and ligand units, which enables easy detachment and bond formation, as well as the porous nature and accessibility of guest molecules to the framework, which influences the stability of parent MOFs towards PSM.

MOFs are porous hybrid inorganic–organic parts made of metal–oxo clusters connected by ligands that are organic in nature. An organic substance and a metal core make up their structure; the former serves as a "strut" and the latter as a "joint."

Three main elements of MOFs are their framework topology, inorganic metal centres, and organic ligands. As created with an extended zeolite topology, MOFs have larger pores and higher porosity as compared to zeolites. Inorganic SBUs and organic ligands are mixed to create MOFs. To create materials with certain physical and chemical qualities, these can be altered. High porosity and huge pore sizes in the resulting 3D structures make them perfect for a variety of uses, including the immobilisation of molecular catalysts, selective chemical processes, and electrochemical energy storage systems.

1.3. POST-SYNTHESIS MODIFIED-MOF (PSM-MOF) CATALYSTS ANCHORED WITH SCHIFF BASE COMPLEXES:

Coupling, epoxidation, oxidation, and hydrogenation are examples of catalytic reactions that are crucial to the production of organic compounds and other industrial processes. In particular, Schiff base complex-anchored MOFs have been found as promising post-synthesis-modified MOF (PSM-MOF) catalysts. Through strong binding to heterogeneous MOF supports, Schiff-base ligands can effectively scatter active metals and improve the recyclability and reusability of catalytically active metals. Because they combine the best features of heterogeneous and homogeneous catalysts, Schiff base complex-anchored MOF catalysts are very effective and selective. (Manpreet Kaur and others, 2021)

1.4. APPLICATION:

1.4.1. MOFs FOR BIOMEDICAL APPLICATIONS:

MOFs are potentially efficient drug delivery materials as they can modify their properties by adjusting the functional groups of the frameworks and by finely tuning the pore size.

1.4.2. CATALYTIC APPLICATIONS OF MOFs:

MOFs can be considered an alternative approach to heterogeneous catalysts emulating the catalytic properties of homogeneous complexes.

Zirconium: The catalytic properties of zirconium are favourably applied in a number of applications including biodiesel production, Knoevenagel condensation, and Friedel–Crafts acylation reactions.

1.4.3. LUMINESCENCE PROPERTIES OF MOFs:

The majority of luminescent MOF materials are based on active substances, such as the light-emitting rare earth europium and terbium, or on reactions speed up by an organic chromophore that is both the excitation source and the emission source. By substituting metal and organic ligands, it is possible to adjust the luminescence of MOFs.

MOF materials are of great interest to the chemical industry. Promising fields of applications are gas storage, gas purification, separations and catalysis. Gas storage, gas purification and separation are the most mature fields of research. Therefore, it is most likely that the first application will come from one of these fields. However, research on the catalytic properties of MOFs is gaining momentum.

Due to their unique properties, MOFs are likely to give new impulses to catalysis research as a whole and may also be beneficial for existing processes. All in all, as an emerging class of porous materials, MOFs are being investigated more and more. Consequently, an increasing number of new materials are being discovered and novel applications are being identified.

CHAPTER 2

LITERATURE SURVEY

1. Metal-organic frameworks based on Schiff base condensation reaction as battery-type electrodes for super capacitor: Xuedong Ma, et al, the year 2021:

Xuedong Ma describes the use of organometallic frameworks (MOFs) synthesized by Schiff base condensation reactions as potential electrode materials for supercapattery applications. MOFs exhibit high specific capacitance, excellent cycling stability, and excellent rate performance, demonstrating their potential as high-performance electrode materials. The authors suggest that further research is needed to optimize MOF performance for supercapattery applications.

2. Synthesis, Structure and Characterization of Some Metal-Organic Framework Based on 4-Aminobenzoic Acid Schiff Base Linker Reem G. Deghadi, et al, the year 2020:

The production of the Schiff base ligand, creation of the MOF, characterization of its structure and properties, and assessment of its potential applications all play a role in the synthesis, structure, and characterisation of MOFs based on 4-aminobenzoic acid Schiff base linker.

3. A nanoscale Cu-Metal organic framework with Schiff base ligand: Synthesis, characterization, and investigation catalytic activity in the oxidation of alcohol Sima Aryanejad, et al, the year 2017:

Sima Aryanejad describes the synthesis, characterization, and catalytic activity of nanoscale Cu-metal organic frameworks (MOF) functionalized with Schiff base ligands in the oxidation of alcohols. Cu-MOF showed high catalytic activity and stability in the presence of hydrogen peroxide as an oxidant. The authors studied the effects of various reaction parameters on the catalytic activity of Cu-MOF and found it has the potential as an effective and recyclable catalyst for the oxidation of alcohols.

4. Novel Synthesis of Cu-Schiff Base Complex @Metal-Organic Framework MIL 101 via a Mild Method: A Comparative Study for Rapid Catalytic Effect

Dr. Yun Wu, et al, year 2019:

Yun Wu describes the synthesis and characterization of novel Cu-Schiff base complexes anchored on metal-organic frameworks (MOFs) MIL-101 using a mild method. The authors compared the catalytic activity of the synthesized Cu Schiff base@MIL-101 with Cu Schiff base complexes under different reaction conditions. The results showed that Cu Schiff base@MIL-101 exhibited superior catalytic activity and stability in the oxidation of various substrates. The authors attribute the improved catalytic performance to a synergistic effect between the Schiff base ligand and the MOF structure. Overall, the results suggest that the mildly synthesized Cu-Schiff base@MIL-101 has potential as an efficient and stable catalyst for various catalytic reactions.

5. Post synthetic modification of metal–organic frameworks—a progress report Kristine K. Tanabe and Seth M. Cohen 2010:

Kristine provides a progress report on the post-synthesis modification (PSM) of metal-organic frameworks (MOFs) for various applications. The authors described various methods of PSM, including functionalization, encapsulation, and replacement, and highlighted recent advances in each method. They also discussed potential applications of PSM-MOFs in areas such as catalysis, sensing, and drug delivery. The authors emphasized the importance of PSM in tailoring the properties of MOFs for specific applications and discussed challenges and future directions in this area. Overall, this whitepaper provides a comprehensive overview of MOF's PSM progress and its potential applications.

6. Post-Synthesis modification of metal-organic frameworks using Schiff base complexes for various catalytic applications Manpreet Kaur, et al 2021:

Manpreet Kaur describes the use of Schiff base complexes in the post-synthesis modification (PSM) of metal-organic frameworks (MOFs) for various catalytic applications. The authors described various PSM methods using Schiff base ligands, including encapsulation, functionalization, and exchange. They also highlighted recent advances in this field and discussed potential applications of Schiff base-modified MOFs in catalytic reactions such as oxidation, reduction, and coupling

reactions. The authors emphasized the importance of Schiff base-modified MOFs for enhancing MOF catalytic activity and selectivity and discussed challenges and future directions in this field. Overall, this paper provides a comprehensive overview of the use of Schiff base complexes in his PSM MOFs for catalytic applications.

7. Synthesis of MOF-199 and application to CO₂ adsorptionThuy Van Nguyen Thi, et al 2013:

Thuy Van Nguyen Thi describes the synthesis and application of MOF-199 for CO₂ adsorption. The authors used the solvothermal method to synthesize his MOF-199 and characterize its structural features. They examined his CO₂ adsorption capacity of MOF-199 and compared it to his other MOFs. As a result, MOF-199 showed high CO₂ adsorption capacity and selectivity, and was found to be a promising material for CO₂ capture and storage. The authors also explained the factors that affect the CO₂ adsorption performance of MOF-199, such as temperature, pressure and surface area. Overall, this paper provides a comprehensive understanding of the synthesis and application of MOF-199 for CO₂ adsorption.

8. Nanoporous metal-organic framework (MOF-199): Synthesis, characterization and photocatalytic degradation of Basic Blue 41 Niyaz Mohammad Mahmoodie, et al 2019:

Niyaz Mohammad Mahmoodi describes the synthesis, characterization, and photocatalytic activity of MOF-199 for the degradation of Basic Blue 41. The authors synthesized his MOF-199 using hydrothermal methods and characterized its structural properties. They studied the photocatalytic activity of MOF-199 and compared it with other his MOFs. The results showed that MOF-199 exhibited high photocatalytic activity for the degradation of Basic Blue 41 under UV light irradiation. The authors attribute the enhanced photocatalytic activity to the nanoporous structure of MOF-199. This provides a large surface area for adsorption and degradation of Basic Blue 41. Overall, this publication provides a comprehensive understanding of the synthesis, characterization, and photocatalytic activity of his MOF-199 for the degradation of organic dyes.

CHAPTER 3

AIM AND SCOPE

3.1. AIM:

The aim of the study focused on the Metal-organic framework of the synthesis of chemicals.

3.2. SCOPE:

Metal-organic frameworks (MOFs) are a class of porous materials composed of metal ions or clusters connected by organic ligands. Zirconyl nitrate is one of the metal sources used in the synthesis of zirconium-based MOFs.

The scope of zirconyl nitrate-based MOFs is broad, as these materials possess unique properties such as high surface area, tuneable pore size, and thermal stability. These properties make them attractive for a wide range of applications, including gas storage and separation, catalysis, drug delivery, and sensing.

Zirconyl nitrate and 1,4 benzene dicarboxylic acid compound were dissolved in dimethyl formamide. It was broken into particles under ultrasonication which is the technique that has been used in this work

CHAPTER 4

MATERIALS AND METHODS

4.1 MATERIALS:

Zirconyl Nitrate $\text{ZrO}(\text{NO}_3)_2 \cdot x\text{H}_2\text{O}$, 1,4-benzene dicarboxylic acid, Dimethylformamide, Salicylaldehyde, Ethanol, Aniline, Copper Chloride, Benzyl alcohol, Hydrogen peroxide. 2,4-dinitrophenyl hydrazine, ether, sodium bicarbonate, and 1,2-benzene dicarboxylic acid are the chemicals used in the entire experiment.

4.2 METHODS:

4.2.1 SYNTHESIS OF ZIRCONYL METAL-ORGANIC FRAMEWORK (MOF):

RATIO 1:1

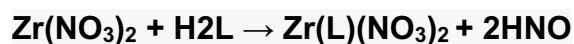
1g of zirconyl nitrate and 1.4g of 1,4-benzene dicarboxylic acid are dissolved in 10 ml of dimethylformamide in a beaker, respectively. They combine it once it has thoroughly dissolved, then sonicate it for 30 minutes. After sonication, the solution is washed with 5 ml of distilled water thrice and 5 ml of ethanol twice. The precipitate will form after washing and it will dry and weighted.

RATIO 1:2

1g of zirconyl nitrate and 2.8g of 1,4-benzene dicarboxylic acid are dissolved in 10 ml of dimethylformamide in a beaker, respectively. They combine it once it has thoroughly dissolved, then sonicate it for 30 minutes. After sonication, the solution is washed with 5 ml of distilled water thrice and 5 ml of ethanol twice. The precipitate will form after washing and it will dry and weighted.

RATIO 1:3

1g of zirconyl nitrate and 4.2g of 1,4-benzene dicarboxylic acid are dissolved in 10 ml of dimethylformamide in a beaker, respectively. They combine it once it has thoroughly dissolved, then sonicate it for 30 minutes. A precipitate will form after the solution has been sonicated and has been rinsed three times with distilled water and twice with ethanol. The precipitate will be dried and weighed when it forms.



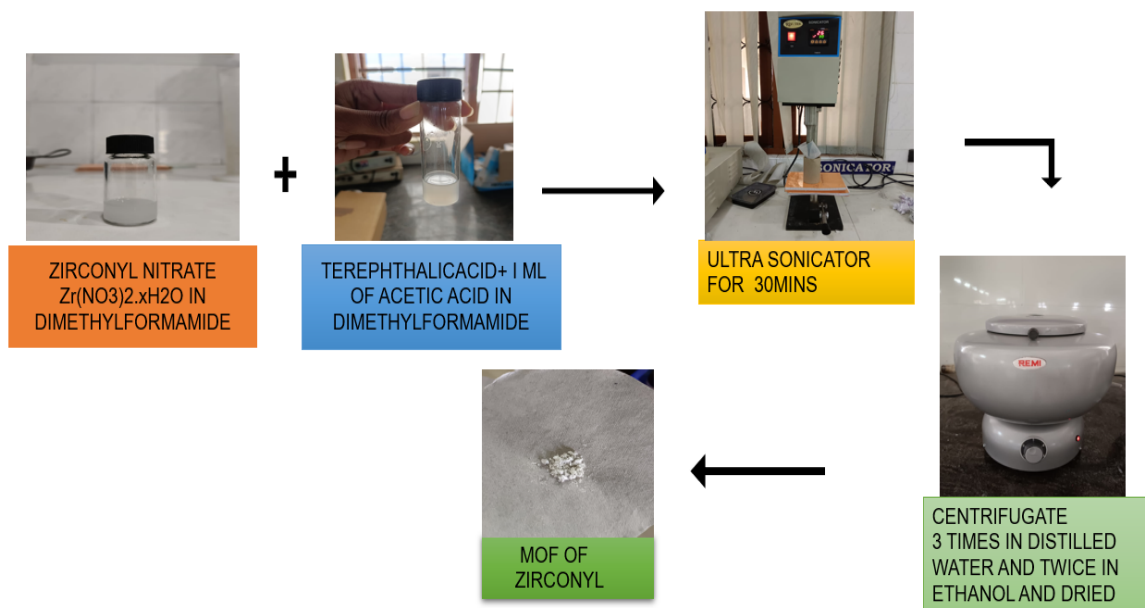


Fig. 4.2. Schematic representation of Zirconyl MOF

4.2.2. SCHIFF BASE:

In a round-bottom flask, add 0.5g of Zr MOF and 2 ml of salicylaldehyde, dissolve them in 5 ml of ethanol, and keep the solution in reflux for 30–40 minutes at 30°C. After refluxing, add 1 ml of aniline and keep it on a magnetic stirrer for 3–4 hours to form yellow crystals. The obtained crystals are dried and weighed. The weight of the Schiff base is 1g.

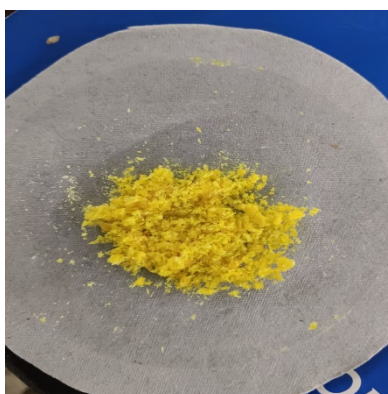


Fig. 4.2.2. Schiff base

4.2.3. PREPARATION OF CATALYST:

0.5g of Schiff's base is dissolved in ethanol and 2 ml of copper chloride is then added which results in the formation of a green precipitate. The precipitate is filtered out and dried, acting as a catalyst for further reaction.



Fig. 4.2. Catalyst

4.2.4. BENZALDEHYDE REACTION:

Benzyl alcohol, hydrogen peroxide, and 0.5g of catalyst are added to a round-bottom flask and refluxed for 4 hours. The solution turns brown in colour. The catalyst will then be separated by dissolving the solution in hot water. After adding the remaining solution to a separating funnel, ether and sodium bicarbonate are added to form two distinct layers - an ether layer and an aqueous layer. These layers are separated, and an aldehyde test is performed.

4.3. INSTRUMENTAL TECHNIQUES:

4.3.1. SONICATOR:

Sonication is a technique that uses sound waves to agitate particles in a solution. To separate substances, it turns an electrical signal into a physical vibration. These disturbances can mix solutions, accelerate the dissolution of a solid into a liquid, and remove dissolved gas from liquids



Fig. 4.3.1.Sonicator

4.4. CHARACTERISATION TECHNIQUES:

4.4.1. FTIR SPECTROSCOPY:

Fourier Transform Infrared Spectroscopy, also known as FTIR Analysis or FTIR Spectroscopy, is an analytical technique used to identify organic, polymeric, and, in some cases, inorganic materials

4.4.2. WORKING PRINCIPLE:

Molecules absorb light in the infrared spectrum, which is why Fourier Transform Infrared Spectroscopy depends on this fact. The bonds in the molecule that are present correspond precisely to this absorption. Wave numbers used to measure frequency typically fall between 4000 and 600 cm^{-1} . It is a method for obtaining an infrared spectrum of a solid, liquid, or gas's absorption or emission. This simultaneously gathers data with great spectral resolution across a broad spectrum. In comparison to a dispersive spectrometer, which measures intensity over a limited spectrum of wavelengths at a time, this offers a significant advantage.

4.5. X-RAY DIFFRACTION:

X-ray diffraction or XRD, is a technique for analysing the atomic or molecular structure of materials. It is non-destructive and works most effectively with materials that are wholly, or part, crystalline. The technique is often known as X-ray powder diffraction because the material being analysed typically is finely ground down to a uniform state.

4.5.1. WORKING:

X-ray diffraction analysis (XRD) is a method used to identify the crystalline structure of a substance. When using XRD, a material is exposed to incident X-rays, and the intensity and scattering angles of the X-rays that are emitted from the material are then measured

CHAPTER 5

RESULT AND DISCUSSION

5.1. PREPARATION OF CATALYST:

In a 1:1 ratio, the total amount of Zr(MOF) is 1g from that 0.5g of Zr(MOF) is taken and used to prepare Schiff base, which has obtained around 1g. This is then dissolved in 5 ml of ethanol and 2 ml of copper chloride to prepare the catalyst. Finally, 0.9g of catalyst is obtained.

In a 1:2 ratio, the total amount of Zr(MOF) is 1.5g from that 1g of Zr(MOF) is taken and used to prepare Schiff base, which has obtained around 1.2g. This is then dissolved in 5 ml of ethanol and 2 ml of copper chloride to prepare the catalyst. Finally, 1g of catalyst is obtained.

In a 1:3 ratio, the total amount of Zr(MOF) is 1.8g from that 1g of Zr(MOF) is taken and used to prepare Schiff base, which has obtained around 1g. This is then dissolved in 7ml of ethanol and 2ml of copper chloride to prepare the catalyst. Finally, 1.2g of catalyst is obtained.

5.2. REACTION FOR ALDEHYDE TEST:

Ether layer: Take 1 ml of the Ether layer and mix it with 2,4 diphenyl hydrazine solution in a test tube. Place the test tube in a water bath, and observe. No orange precipitate was observed, indicating the absence of aldehyde.

Aqueous layer: Take 1 ml of the Ether layer and mix it with 2,4 diphenyl hydrazine solution in a test tube. Place the test tube in a water bath, and observe within a few minutes, an orange precipitation formed, indicating the presence of an aldehyde. After the presence of aldehyde, the remaining is weighted. The final amount of aldehyde is 0.57ml.

To confirm the presence of aldehyde, perform characterization using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR)

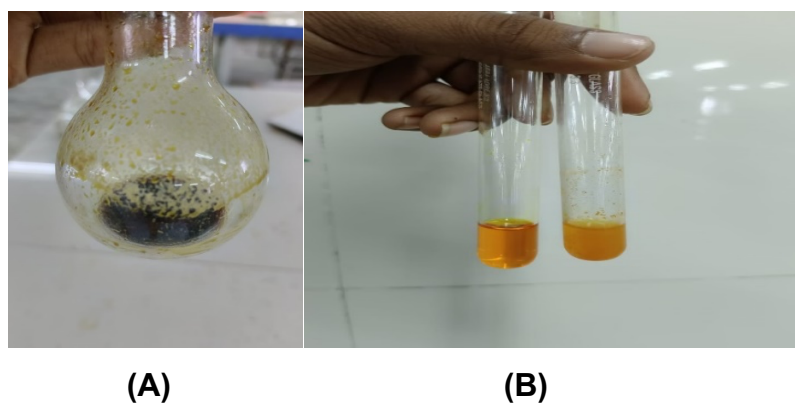


Fig. 5.2. (A) The reaction of catalyst, benzyl alcohol and hydrogen peroxide; (B) Aldehyde Test

5.3. X-RAY DIFFRACTION RESULT FOR CATALYST:

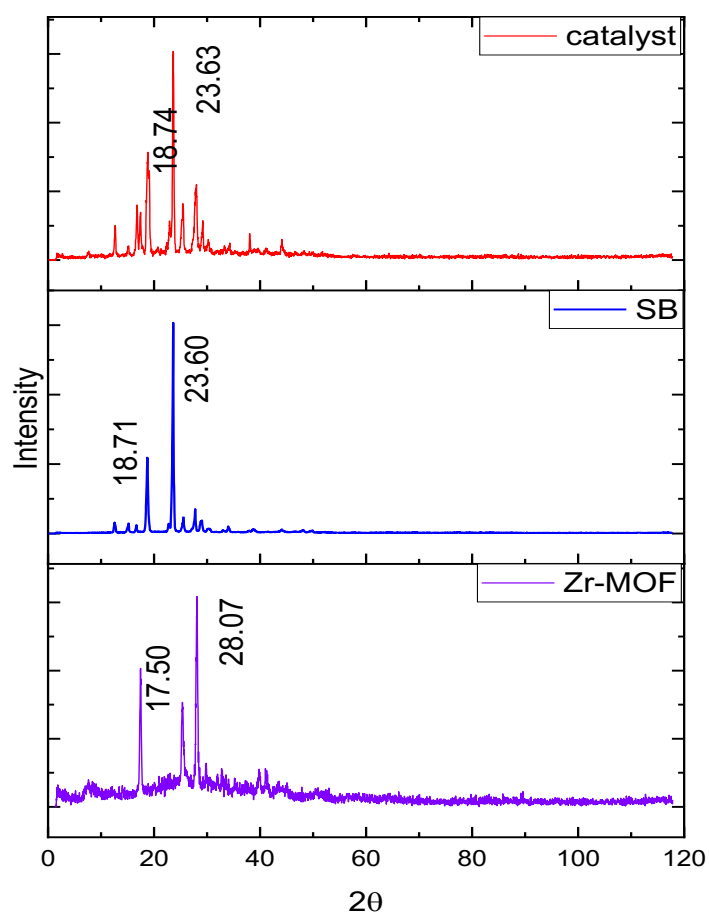


Fig. 5.4. XRD result for Zr MOF, Schiff base and Catalyst

5.4. FOURIER TRANSFORM INFRARED SPECTROSCOPY RESULTS FOR CATALYST:

The result for the catalyst in IR Spectrum, The Zr-O was formed in the range of 500cm⁻¹. In 1500-2000cm⁻¹ Co-ordinated -COOH bond is obtained and stretching O-H is present in the range of 3500-4000cm⁻¹.

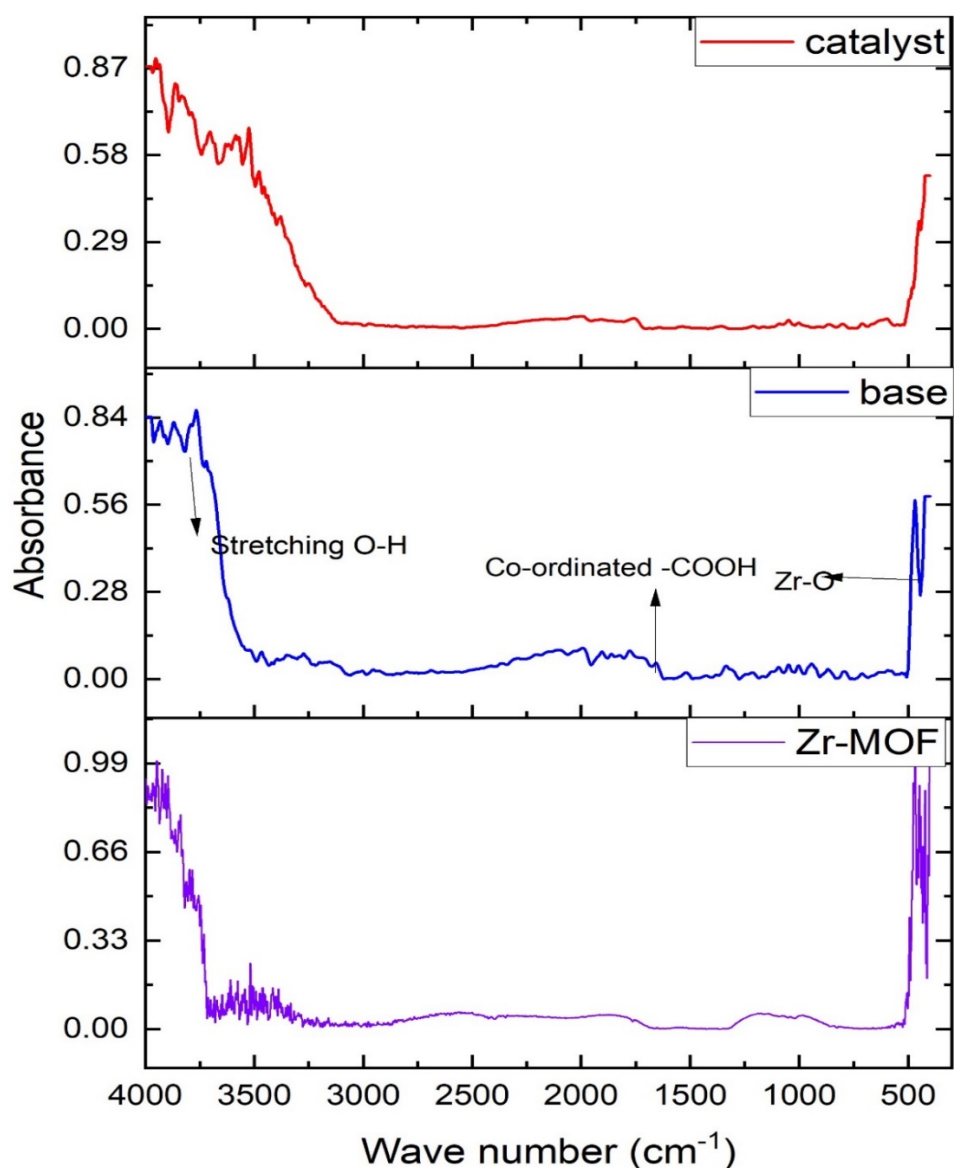


Fig. 5.4. Fourier Transform Infrared spectroscopy results for Catalyst

5.5. FOURIER TRANSFORM INFRARED SPECTROSCOPY RESULTS FOR ALDEHYDE:

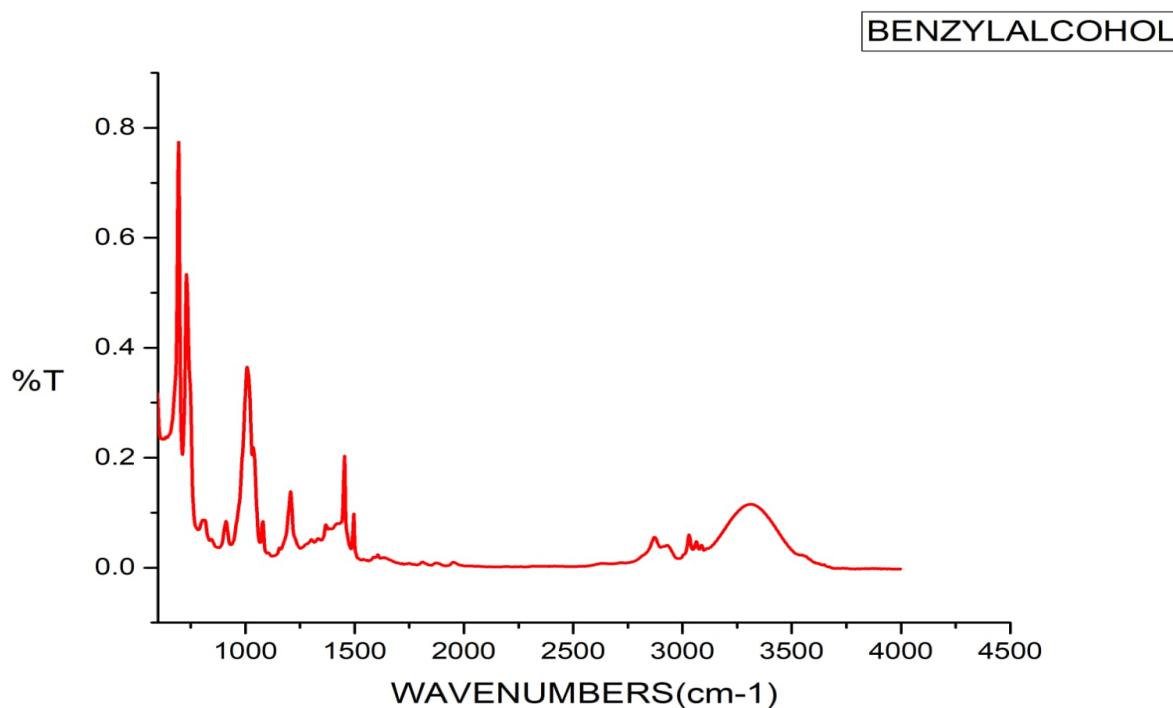


Fig. 5.1.3. FTIR spectrum for Benzyl alcohol

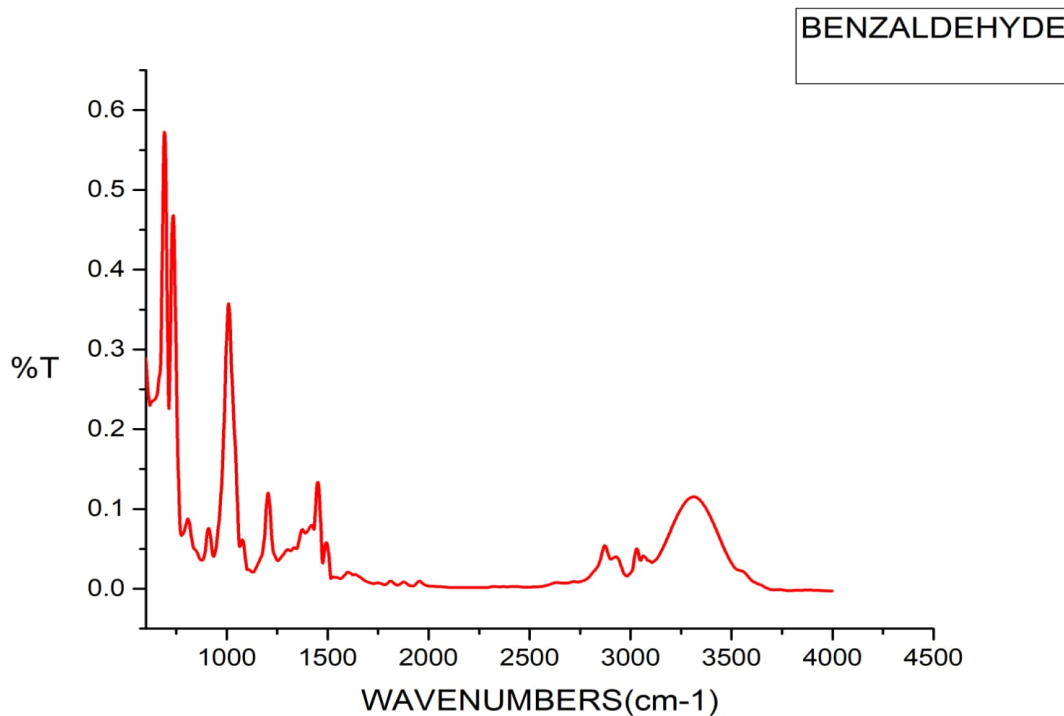


Fig. 5.1.3. FTIR spectrum for Benzaldehyde

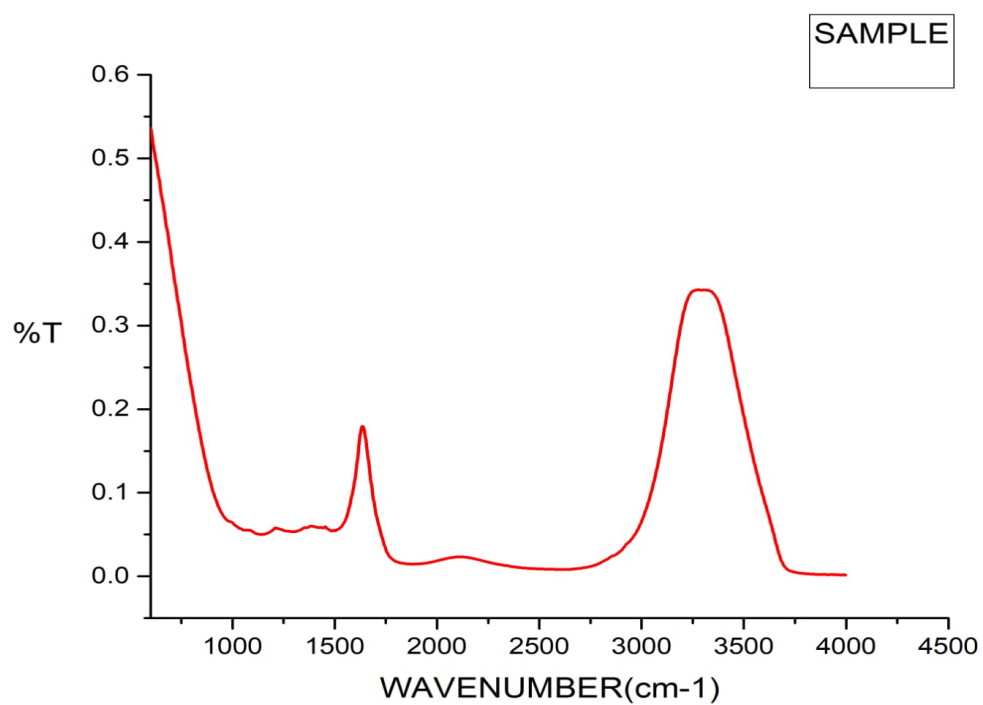


Fig. 5.1.3. FTIR Spectrum for Sample

In the sample, a characteristic peak at 1710-1720cm⁻¹. Indicates the presence of aldehyde while the peak at 3300cm⁻¹. Indicates the presence of aromatic CH stretching. The presence of these characteristic peaks confirms the formation of benzaldehyde from benzyl alcohol.

CHAPTER 6

SUMMARY AND CONCLUSION

Zirconyl nitrate is a metal-organic framework that contains zirconium and nitrate ions. It forms a complex that can be used to locate an aldehyde when combined with a Schiff base, which is a compound that has a functional group with a carbon-nitrogen double bond. The zirconium ion in the zirconyl nitrate can form a connection with the nitrogen atom in the Schiff base molecule. Aldehydes from a mixture of molecules can be selectively captured using this method, which creates a stable complex.

In conclusion, a complex that may be used to specifically detect aldehydes in a mixture of chemicals is formed when a Schiff base and the metal-organic framework of zirconyl nitrate are joined.

The primary method in this project is the use of a Sonicator to create the ZrMOF, Schiff base to form the catalyst, and a reflux condenser along with benzyl alcohol and hydrogen peroxide to produce an aldehyde.

All three ratios used the same methodology, and their characteristics are FTIR and XRD. Benzyl alcohol was oxidised to produce benzaldehyde, according to the data above.

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