IOSR Journal of Applied Chemistry (IOSR-JAC)
e-ISSN: 2278-5736.Volume 18, Issue 9 Ser. I (September. 2025), PP 01-07
www.iosrjournals.org

Application Of Metal-Organic Frameworks (MOF) To Capture Carbon Dioxide (CO_2)

C. Shobha Devi, M. Sunita
(Department Of Chemistry, Telangana Tribal Welfare Residential Degree College (Girls) (TGTWRDC), Mahabubabad, Telangana, India.
(Department Of Chemistry, Government Polytechnic, Nalgonda, Telangana, India)

Abstract:
Since carbon dioxide (CO_2) is one of the main contributors to global warming, its continuous increase in the atmosphere is a serious environmental concern. Therefore, CO_2 gas capture is essential. To address this global issue, industries have proposed and implemented a variety of approaches and technologies, including CO_2 capture, conversion, and reduction, using various materials, such as zeolitic adsorption, porous membranes, and amine solution absorption. Nevertheless, these technologies are costly and energy-intensive. A novel family of porous materials called Metal-Organic Frameworks (MOFs) exhibits remarkable performance in removing carbon dioxide. MOFs are crystallized permeable substances composed of coordinating organic ligands and metal clusters, or nodes. From functionality and shape to large surface area and porosity, MOFs have a number of outstanding qualities. It has been demonstrated that MOFs have great potential for CO_2 separation applications because of these special qualities. In the present work, we report the preparation and CO_2 absorption of $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$. The MOF mentioned above is characterised using SEM, XRD and thermogravimetric analysis. In order to develop novel useful and effective CO_2 mitigation strategies, the applications of this MOF in adsorption of carbon dioxide were also examined.

***Materials and Methods**: Chemicals and reagents of analytical grade were employed without additional purification. 4-Nitrobenzoic acid, Trans-1,2-bis(4-pyridyl)ethylene, zinc nitrate hexahydrate,methanol, acetic acid, dimethylformamide (DMF), sodium hydroxide and glucose were purchased from Tia chemicals Mumbai. The Powder X-ray Diffraction (XRD) was analysed on a Rigaku diffractometer (Cu $K\alpha$, $\lambda=1.5406$ Å, and angle range of $2\theta = 10°$ to $80°$). Thermogravimetric Analysis (TGA) was performed on a simultaneous thermal analyser (Model: STA6000) Perkin Elmer using Pyris manager software. Scanning electron microscopy (SEM) (PMP03960AHipace10) was used to analyze the morphologies of MOF at a 15 kV accelerating voltage. To produce high-quality micrographs with a resolution of 1–10 µm, the sample was pre-conditioned with a thin layer of gold film as the conductive material by ionsputter and mounted with maximum focus.*

***Results**: The XRD results indicate that the material is crystalline, and the SEM results indicate that the surface of the material contains cavities. It adsorbed very little CO_2 in the adsorption experiment, which may have been caused by improper activation, which prevents the solvent from evaporating correctly, thereby reducing its adsorbent properties. Additional research is being conducted on the material to improve its performance in the adsorption phenomenon. The conclusion is that the material absorbed CO_2 but at a very low absorption efficiency.*

***Key Word:** CO_2 capture, Metal-Organic Frameworks (MOF), Zn $(AzDC)(4,4'\text{-}BPE)_{0.5}$, Thermogravimetry*

Date of Submission: 27-08-2025 Date of Acceptance: 07-09-2025

I. Introduction

Global warming and environmental constraints are inescapable in the minds of environmental scientists and researchers in the 21st century due to the rapid growth of the world's population and the rising energy cost abroad. The Energy Information Administration (EIA) predicts that by 2050, energy expenditures will increase to 50% of total expenditures [1]. Many environmentalists believe that greenhouse gas emissions are the primary cause of environmental concerns and global warming. Carbon dioxide (CO_2) is the most dangerous greenhouse gas. According to estimates, CO_2 emissions account for 60% of global warming effects [2].

The major sources of CO_2 emissions are industrial processes, fossil-fueled power plants, decarbonisation and transportation. Although fossil fuel power plants are regarded as one of the most damaging sources of greenhouse gas emissions, there are other sources of greenhouse gas emissions than 81% of the world's industrial energy needs are satisfied by fossil fuels[3]. Approximately 34 billion tones (Gt) of CO_2 are emitted annually from the combustion of fossil fuels worldwide. Approximately 45% is contributed by coal, 35% by oil, and 20% by gas[4]. The atmospheric concentration of CO_2 is rising by 2 parts per million annually. The IPCC (Intergovernmental Panel on Climate Change) claims that, there will be up to 570 ppm of CO_2 in the atmosphere by 2100, resulting in a net global temperature increase of nearly 1.5°C and a sea level rise of 3.80 m[5].

The atmospheric concentration of CO_2 is rising by 2 parts per million annually. The Intergovernmental Panel on Climate Change (IPCC) claims that Carbon capture storage and utilisation (CCS), also known as CCSU, is used to sequester carbon dioxide by reducing the carbon footprint and increasing energy efficiency. In post-combustion capture, CO_2 is separated from combustion flue gases using CCS technologies such absorption, chemical looping combustion, cryogenic distillation, membrane technology, hydrate-based separation, and micro-algal separation. [6–9]. The majority of CO_2 separation technologies now on the market are still in their infancy and have not yet been tested on a wide scale. Another technology necessitates a considerable amount of energy [10,11]. The absorption method employing liquid amine-based solvents has garnered considerable industrial interest owing to its superior efficiency in separation of CO_2 via chemical processes [12–14].

Usually, power plants spend their energy on amine solvent regeneration, which uses 85 KJ/mol CO_2 which lowers 25% of energy production. According to reports, substituting adsorption by solid materials for amine-based absorption can lower 40% of the heat requirement for the regeneration of amine solvents. Consequently, the use of porous solid materials for adsorption of CO2 is an updated technology that can effectively replace amine-based absorption methods. [15–17].

The regenerative nature of the adsorptive materials used in CO_2 capture techniques is a significant concern. Therefore, global supplies will be depleted if the chemical material is utilised for the first time per batch. Therefore, the energy required for material regeneration is a significant factor in determining the productivity and cost of the procedure. The next crucial factor to consider is the capability of adsorptive materials to remove CO_2 from gas mixtures. The presence of surface forces increases the concentration of dissolved material at the interface of the solid phase. This phenomenon is called adsorption[18].The adsorbate forms chemical bonds, typically covalent, to the surface of the adsorbent's pores, resulting in the formation of monolayers on the surface of the adsorbent due to the nature of the interactions is referred as chemisorption. Generally speaking, chemisorption is a dissociative process in which bonds within the adsorbate molecules are broken to form chemical bonds with the adsorbent.

The class of crystalline solids known as metal-organic frameworks (MOFs) has shown promise in CO_2 capture and separation applications [19]. MOFs are porous crystalline materials composed of organic ligands and metal clusters (nodes). MOFs are capable of physisorption, a non-dissociative process that typically leaves the electronic structure of both the adsorbate and adsorbent unaltered. Adsorbate and adsorbent are frequently reversible due to long-range interactions associated with electron redistribution[20,21]. The adsorption of a guest molecule onto an adsorbent is heavily influenced by pore size, pore topology, and, most importantly, host-guest interactions [22,23].

Herein we reported the metal-organic framework $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ byusing a simple solvothermal synthesis method [24, 25]. Converting azobenzene to 4,4'-dicarboxylate (AzDC) produces a ligand suitable for use in MOF structures. As a pillar ligand, trans-1,2-bis(4-pyridyl)ethylene (4,4'-BPE) is utilised. MOF $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ is a triply interconnected framework made up of these two ligands and Zn-based MOFs. Pillar ligands AzDC and 4,4'-BPE congregate from paddle wheel dinuclear Zn_2 units. In addition, MOF was characterized by X-ray Diffraction (XRD), scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). The dynamic adsorption of CO_2 onto $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ was investigated experimentally with the aid of a TGA that is discussed in greater detail in the section devoted to experiments.

II. Material And Methods

Materials: Chemicals and reagents of analytical grade were employed without additional purification. 4-Nitrobenzoic acid, Trans-1,2-bis(4-pyridyl)ethylene, zinc nitrate hexahydrate,methanol, acetic acid, dimethylformamide (DMF), sodium hydroxide and glucose were purchased from Tia chemicals Mumbai.

Preparation of AzDC ligand

Liu et al. previously outlined the procedure for preparing the AzDC ligand [26]. In an aqueous sodium hydroxide solution, 10 g (0.06 mol) of 4-nitrobenzoic acid was dissolved by heating the solution (33.87 g, 0.85 mol, in 100 ml water). The yellow precipitate formed instantly and transformed into a brown solution when a hot aqueous glucose solution (66.74 g, 0.37 mol, in 100 ml water) was slowly added to the aforesaid solution at 50 °C. Later, the mixture was turned into a black solution after reacting overnight at room temperature. The aged solution was mixed with methanol until a brilliant brown precipitate appeared. To create a light pink precipitate, the filtered precipitate was dissolved in water and 15 mL of acetic acid was added to acidify it. Then filtration was done, washed to remove excess water, and dried overnight to obtain the final product (3.8 g).

Preparation of $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ Zhou et al. demonstrated a solvothermal preparation method for metal-organic frameworks [27]. A 100 mL suspension of $Zn(NO_3)_2.6H_2O$, 1 and 4,4'-BPE in DMF was heated for 24 hours at 100 °C. The red crystals (**Fig. 1**) that produced were filtered, cleaned with hexane followed by DMF and then dried.

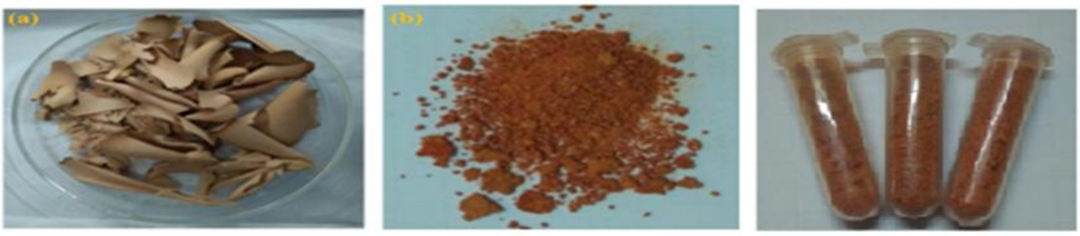

Figure 1. Images of final product a)AzDC ligand and b)$Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ MOF

Materials Characterisation

The Powder X-ray Diffraction (XRD) was analysed on a Rigaku diffractometer (Cu Kα, λ=1.5406 Å, and angle range of 2θ = 10° to 80°). Thermogravimetric Analysis (TGA) was performed on a simultaneous thermal analyser (Model: STA6000) Perkin Elmer using Pyris manager software. Scanning electron microscopy (SEM) (PMP03960AHipace10) was used to analyze the morphologies of MOF at a 15 kV accelerating voltage. To produce high-quality micrographs with a resolution of 1–10 µm, the sample was pre-conditioned with a thin layer of gold film as the conductive material by ionsputter and mounted with maximum focus.

Procedures for the photoreduction of CO_2

CO_2 adsorption experiments were performed using a thermal analyzer (Perkin-Elmer STA 6000)[28]. The setup includes a microbalance with a maximum sensitivity of 0.1 mg, enclosed in a stainless steel high-pressure housing rated up to 210 bar. Feed and exit flows were controlled using ISCO 500D pumps. To minimize external disturbances, the balance and housing were mounted on an active air vibration isolation platform, and the entire setup was enclosed in a temperature-controlled environment. A digital pressure gauge with an accuracy of 0.035% was attached to the chamber to monitor the pressure. Continuous pressure, temperature, and microbalance output monitoring was performed using a built-in data acquisition board. The chamber enabled the sample to be rapidly cooled to room temperature.

The sample was degassed and dehydrated by increasing the temperature to 373 K. After the $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ MOF sample's mass reached a constant value in that inert atmosphere, the environment was changed to CO_2, and the CO_2 flow rate was maintained at 20 mL min^{-1}. The increase in sample mass suggests that $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ was adsorbing CO_2 [29]. The flow of CO_2 gas was maintained at a controlled temperature to evaluate absorption behavior and determine adsorption capacity by varying the holding times. Pyris™ software was used for data acquisition, storage, and numerical analysis of the CO_2 adsorption process.

III. Results And Discussion

The Scanning Electron Microscope (SEM) is one of the versatile instruments used for chemical composition characterisation, microstructure morphology analysis, and examination. The necked eye has a visual angle of 1/60°, corresponding to a resolution of approximately 0.1 mm. The optical resolution of a lens is limited. Instead of a light source, electron microscopy evolved with a beam of high energy. The formation of the tube-shaped MOF has depicted in **Fig. 2**. The low magnification images (a) and (b) of material with internal cavities predict the surface topology. Images (c) and (d) depict high-magnification cavities without agglomeration. The SEM images clearly support the formation of pure $Zn(AzDC)(4,4'\text{-}BPE)_{0.5}$ MOF.

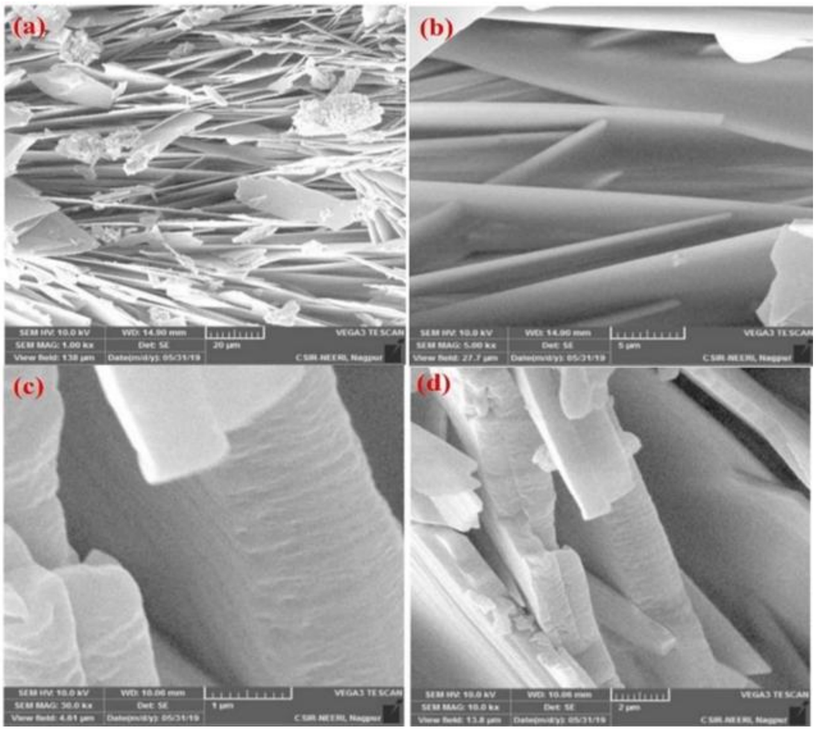

Figure 2.SEM image of Zn(AzDC)(4,4'-BPE)$_{0.5}$MOF

X-Ray Diffraction Analysis: X-ray diffraction analysis is a very useful analytical method for characterising crystalline materials without damaging the sample. It details the crystal structure and orientations, phases, crystallinity and crystal defects. The framework of Zn(AzDC)(4,4'-BPE)$_{0.5}$ is assembled from paddle wheel dinuclear Zn_2 units, bridging AzDC dianions and 4,4'-BPE pillar ligands. As illustrated in **Fig. 3**, the X-ray diffraction peaks obtained were sharp, indicating the crystalline nature of the desolvated phase.

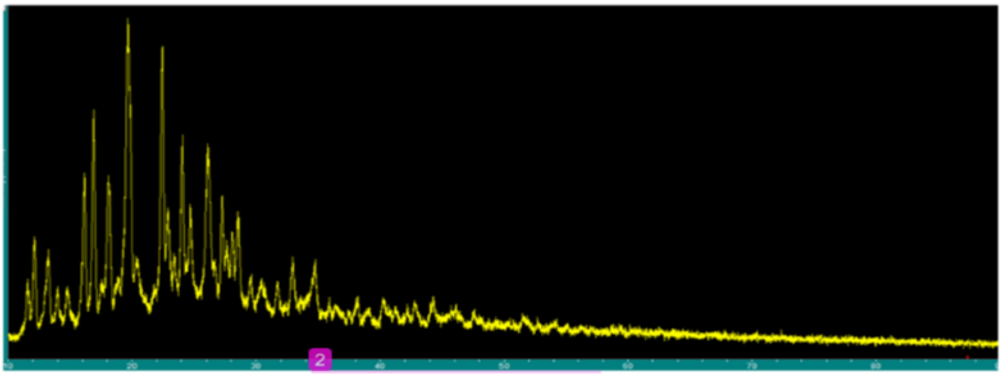

Figure 3. Crystallogram of Zn(AzDC)(4,4'-BPE)$_{0.5}$MOF

Thermogravimetric Analysis (TGA)

Thermogravimetric analysis (TGA) is a technique in which the weight of a substance is recorded as a function of time or temperature. In contrast, a substance sample is subjected to a regulated temperature programme in a regulated atmosphere. TGA consists of a sample pan and a precise balance. This container is cooled or heated in a furnace during the experiment. During the experiment, the sample's mass is determined. In the instrument, purging gases regulate the environment.

The 6.125-gram MOF sample was examined in a programmable temperature range from -30 to 900°Cat 10°C/min. TGA analysis of the given MOF indicates that the material is stable up to 92.1°C (99.7888% by weight) after it begins to decompose at 888.38 °C (16.04142% by weight) and other values. ΔY is calculated using software, where the value of ΔY represents a decrease in the weight percentage due to an increase in temperature (**Fig. 4**).

ΔY =16.113%

X_1=91.1°C, Y_1=99.788%

X_2=261.15°C, Y_2=83.675%
ΔY =24.91%
X_1=281.8° C, Y_1=83.406%
X_2=416.42°C, Y_2=58.495%
ΔY =32.823%
X_1=421.07° C, Y_1=56.835%
X_2=535.75°C, Y_2=24.012%.
Where X_1 and X_2 are the temperature scale on X-axis, Y_1 and Y_2 are the weight percent of material on the Y-axis.

CO_2 adsorption experiment For the CO_2 adsorption experiment, the recording balance is a microbalance on which a Zn(AzDC)(4,4'-BPE)$_{0.5}$ sample was kept for CO_2 adsorption, and the CO_2 gas was purged into the adsorption apparatus.

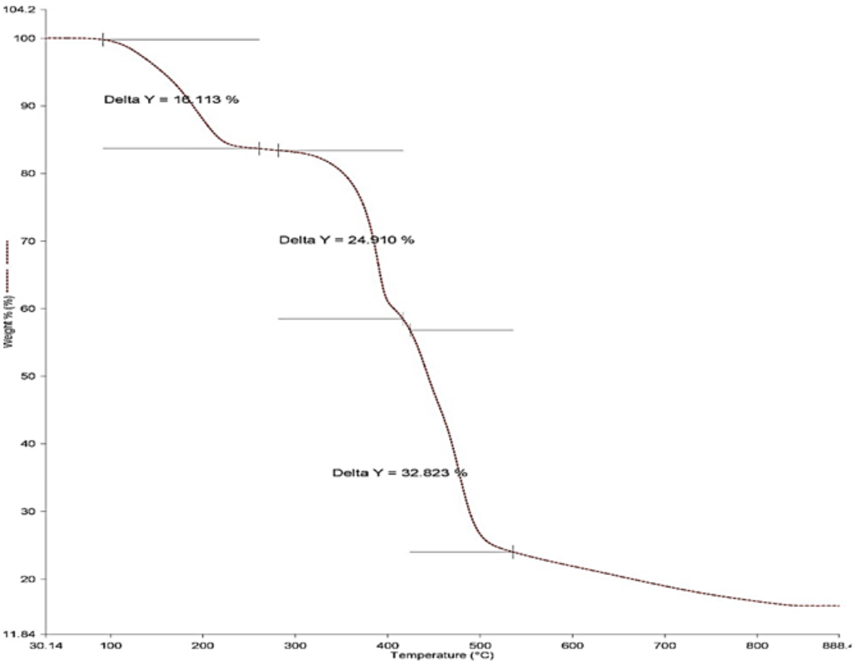

Figure 4.Thermogram of Zn(AzDC)(4,4'-BPE)$_{0.5}$MOF

An initial sample weight of 9.839mg is placed on a thermobalance, and CO_2 is purged into the experimental setup at a constant pressure of 1.3 bar and a temperature range of 30 °C to 100 °C.

The following Observation is shown in the experiment,
Initial Weight= 9.839mg Final Weight=10.0348 mg
Temperature Range= 30-90 °C Pressure Condition=1.3bar
The change in weight of MOF with the application of CO_2 is calculated as follows:
Total mass adsorbed= Final weight - Initial weight
=10.03477mg - 9.839mg =0.19577mg
Weight percentage=1.441%

The metal-organic framework Zn(AzDC)(4,4'-BPE)0.5 absorbed only 0.19577mg (1.441% of its weight) of carbon dioxide on its surface. Nevertheless, because it is a microporous material, it should have a greater CO_2 adsorptive, but only a small amount is absorbed. Monitoring the increase in mass of a metal-organic framework Zn(AzDC)(4,4'-BPE)$_{0.5}$ exposed to a constant flow of carbon dioxide at 1.3 bar pressure was used to generate the CO_2 adsorption graph. The given graph (**Fig. 5**) shows the saturation at 86.9 °C and increasing from 30 °C onwards.

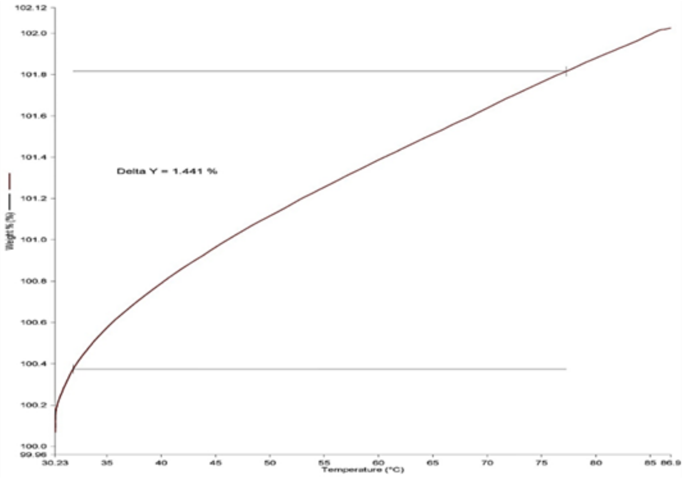

FIGURE 5. Thermogram for CO_2 adsorbed Zn(AzDC)(4,4'-BPE)$_{0.5}$ MOF

IV. Conclusion

The reports indicate that Zn(AzDC)(4,4'-BPE)$_{0.5}$, a metal-organic framework, was successfully synthesised using the solvothermal method. In order to better comprehend the subject matter and characteristics, the characteristics are completed later. The prepared material exhibits thermal stability and adsorption. The XRD results indicate that the material is crystalline, and the SEM results indicate that the surface of the material contains cavities. It adsorbed very little CO_2 in the adsorption experiment, which may have been caused by improper activation, which prevents the solvent from evaporating correctly, thereby reducing its adsorbent properties. Additional research is being conducted on the material to improve its performance in the adsorption phenomenon. The conclusion is that the material absorbed CO_2 but at a very low absorption efficiency.

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