

Antimicrobial Activity of Ba-MOF †

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Abstract: Increasing the tolerance and resistance of pathogens to conventional antibiotics is a global health issue and there is a need to use effective and new substances. MOFs are highly functional materials with antimicrobial properties come from their composition, structure, and high internal volume, which could be a source for antimicrobial guest molecules integrated in the pore. In addition, MOF can contain more than one type of metal ion in the same structure. In this work, a metal-organic framework, $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ was synthesized by the deposition method using benzene-1,2,4,5-tetracarboxylic acid (H₄btec) and Ba(NO₃)₂. Characterization of MOF was performed using XRD, XRF, FTIR, SEM analyses. The metal-organic framework used against gram-positive and gram-negative bacteria including Keleb pneumonia, Staph coccus aureus, Staph saprophyticus, Esherichia coli.

Keywords: MOF; antibacterial; barium

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1. Introduction

Metal-organic frameworks (MOFs) are a class of porous hybrid materials constructed from metal ions and organic ligands, linked through coordination bonds. On the other hand, MOFs have been in focus of consideration due to their unique porous structure with significant characteristics like high surface area, tunable chemical composition as well as various pore size distribution. One of their important properties is antibacterial activity that can be increased by choosing metal ions and/or linkers with antibacterial properties [1,2]. MOFs can contain more than one type of metal ion in the same structure and the use of several metals with antibacterial properties intensifies this feature. Also, the ligand used to prepare the framework can have antibacterial properties and the accumulation of the MOFs can cause the destruction of the bacteria wall and destroy the bacteria [1]. The important point in the synthesis of MOFs that show antibacterial properties is to pay attention to Pearson's hard and soft acid and base theory. In order to have MOFs with antibacterial properties, metal ions must be able to separate easily, if the acid and base are both hard types or both soft types, the bond between them will be very strong and metal ions cannot be released and show antibacterial properties. In the synthesized MOF ($[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$), the linker used (benzene-1,2,4,5-tetrakis carboxylic acid) is hard but barium metal is not considered as a hard acid and can show antibacterial properties.[3]

2. Experimental

2.1. Preparation of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$

The amount of 1 mol benzene-1,2,4,5-tetracarboxylic acid (H₄btec) was dissolved in 20 cc water and 10 cc ethanol then stirred in room temperature until dissolved completely. Afterwards, 2 mol Ba(NO₃)₂ was dissolved in 10 cc water. Then the two solutions were mixed on stirring at 100 °C and 700 rpm for 2h, then cooled in room temperature. The white powder was dried in room temperature for 1 day [4].

2.2. Characterization

The obtained powder, $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ was characterized by XRD, XRF, FTIR and SEM methods.

The XRD pattern of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ is compared with the simulated pattern in Figure 1. It shows that it is correctly synthesized.

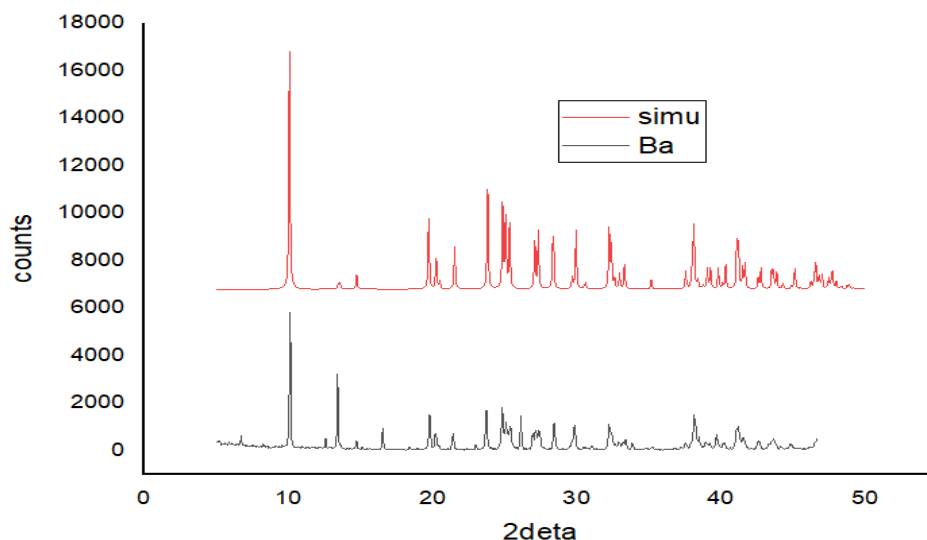


Figure 1. XRD Pattern of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

In XRF analysis of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ shown in Table 1, can be seen the percentage of BaO equal to 100% which confirms the presence of only Barium in the MOF.

Table 1. The XRF result of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

Elements	<u>Na₂O</u>	<u>MgO</u>	<u>Al₂O₃</u>	<u>SiO₂</u>	<u>P₂O₅</u>	<u>SO₃</u>	<u>K₂O</u>	<u>CaO</u>	<u>TiO₂</u>
wt %	-	-	-	-	-	-	-	-	-
Elements	<u>Fe₂O₃</u>	<u>V₂O₅</u>	<u>MnO</u>	<u>Cr₂O₃</u>	<u>La</u>	<u>Sr</u>	<u>Zn</u>	<u>BaO</u>	<u>Pb</u>
wt %	-	-	-	-	-	-	-	100.000	-
Elements	<u>F</u>	<u>Zr</u>	<u>Cl</u>	<u>Ce</u>	<u>Co</u>	<u>Mo</u>	<u>Ca</u>	<u>Cu</u>	<u>Ho</u>
wt %	-	-	-	-	-	-	-	-	-

The FTIR spectrum of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ is shown in Fig 2. The spectrum shows a sharp peak at 1500 cm^{-1} which is related to the carbon-carbon double bond in the aromatic ring, the peak in 1700 cm^{-1} is related to the symmetric stretching bond of carboxylic groups, and the short and broad peak at 3000 cm^{-1} is related to the C–H bond of the aromatic ring.

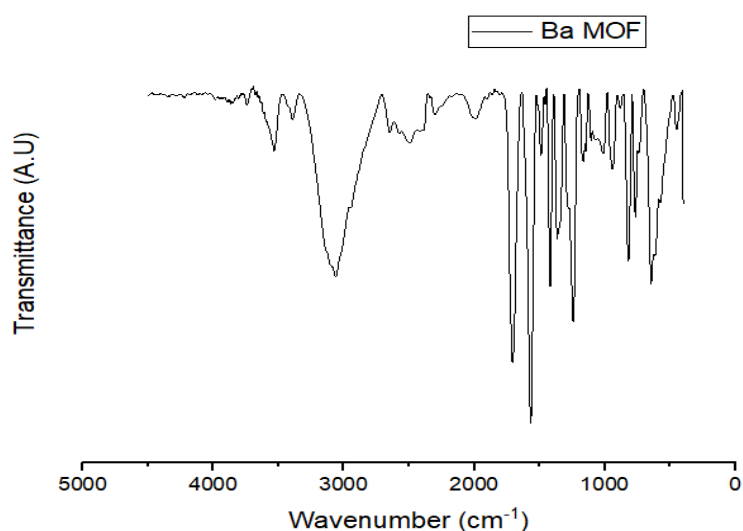


Figure 2. FTIR spectrum of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

The SEM micrographs of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ were shown in Figure 3, in which the rod shape with average particles of MOF has the size of 1 μm to 3 μm .

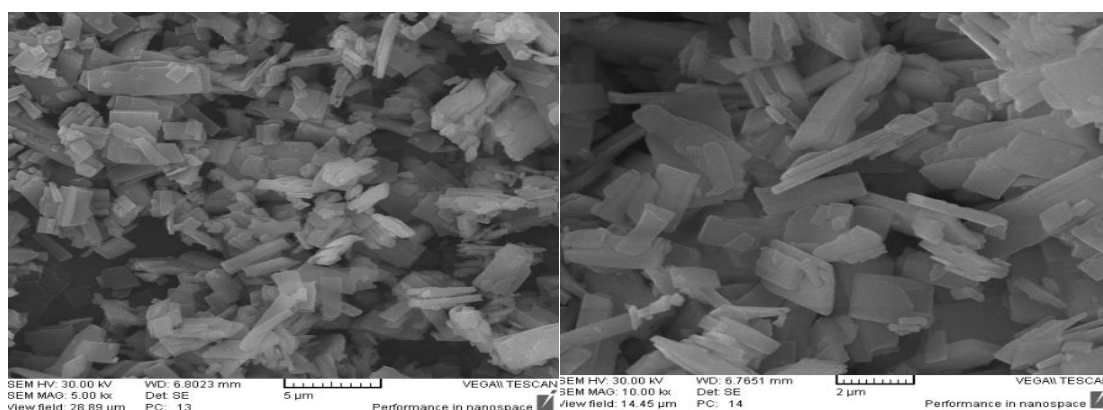


Figure 3. SEM of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

2.3. Antibacterial Activity

Antibacterial Activity of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ against gram positive and gram negative bacteria were tested. The bacteria including Keleb pneumonia, Staph coccus aureus, Staph saprophyticus, Esherichia coli. The results are shown in Figure 4a-e and summarized in Table 2. In all cases was defined the inhibition zone diameter from $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

Table 2. The behavior of $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

Test bacteria with $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$	Inhibition Zone diameter (mm)
Ps. Aeruginosa	10.725
Keleb Pneumonia	11.31
Staph Coccus aureus	13.527
Staph Saprophyticus	12.712
Ecoli	14.360

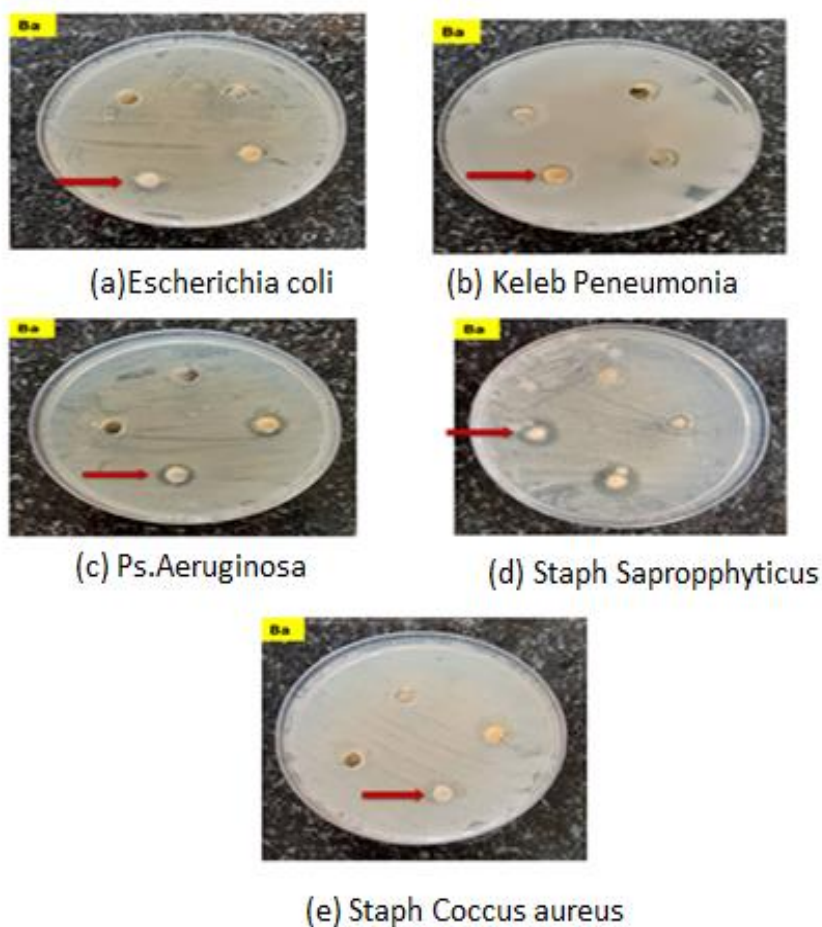


Figure 4. Images of antibacterial test results for gram-negative (a-c) and gram-positive (d,e) bacteria on $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$.

3. Conclusions

In this research, $[\text{Ba}(\text{H}_2\text{btec})\cdot\text{H}_2\text{O}]_n$ was synthesized using benzene-1,2,4,5-tetracarboxylic acid as linker and $\text{Ba}(\text{NO}_3)_2$ as metal source, and they were applied against gram positive and gram negative bacteria and it has shown relatively good performance against both groups. To the best of our knowledge, the title MOF is applied against bacteria for the first time, it is also synthesized by green chemistry and environmentally friendly solvents.

Institutional Review Board Statement:

Informed Consent Statement:

Data Availability Statement:

Conflicts of Interest:

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