chemistry proceedings

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Proceeding Paper

Antimicrobial Activity of Ba-MOF †

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† Presented at the 26th International Electronic Conference on Synthetic Organic Chemistry, 1–15 November 2022; Available online: https://sciforum.net/event/ecsoc-26.

Abstract: The increasing tolerance and resistance of pathogens to conventional antibiotics is a global health issue, and there is a need to use effective and new substances. Metal–organic frameworks (MOFs) are highly functional materials with antimicrobial properties that come from their composition, structure, and high internal volume, which could be a source for antimicrobial guest molecules integrated into the pores. In addition, MOFs can contain more than one type of metal ion in the same structure. In this work, a metal–organic framework, $[Ba(H_2btec){\cdot}H_2O]_n$, was synthesized by the deposition method using benzene-1,2,4,5-tetracarboxylic acid (H4btec) and $Ba(NO_3)_2$. Characterization of the MOF was performed using Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Fourier Transform Infrared (FTIR) and x-ray fluorescence (XRF) alyses. The metal–organic framework was used against Gram-positive and Gram-negative bacteria including *Keleb peneumonia*, *Staph coccus aureus*, *Staph saprophyticus*, and *Esherichia coli*.

Keywords: MOF; antibacterial; barium

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Citation: Aghaee, M.; Alishahi, M.A.; Manteghi, F. Antimicrobial Activity of Ba-MOF. *Chem. Proc.* **2022**, *12*, 75. https://doi.org/10.3390/ecsoc-26-13725

Academic Editor: Julio A. Seijas

Published: 21 November 2022

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 the focus of consideration due to their unique porous structure with significant characteristics such as high surface area, tunable chemical composition, and varied pore size distribution. One of their important properties is antibacterial activity, which 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. In addition, 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 will not be able to be released and show antibacterial properties. In the synthesized MOF ($[Ba(H_2btec).H_2O]_n$), 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 $[Ba(H_2btec){\cdot}H_2O]_n$

The amount of 1 mol benzene-1,2,4,5-tetracarboxylic acid (H_4btec) was dissolved in 20 cc water and 10 cc ethanol and then stirred at room temperature until dissolved completely. Afterward, 2 mol $Ba(NO_3)_2$ was dissolved in 10 cc water. Then the two solutions were mixed by stirring at 100 °C and 700 rpm for 2 h and then cooled at room temperature. The white powder was dried at room temperature for 1 day [4].

2.2. Characterization

The obtained powder, $[Ba(H_2btec)\cdot H_2O]_n$, was characterized by XRD, XRF, FTIR, and SEM methods.

The XRD pattern of $[Ba(H_2btec)\cdot H_2O]_n$ is compared with the simulated pattern in Figure 1. This comparison shows that $[Ba(H_2btec)\cdot H_2O]_n$ was correctly synthesized.

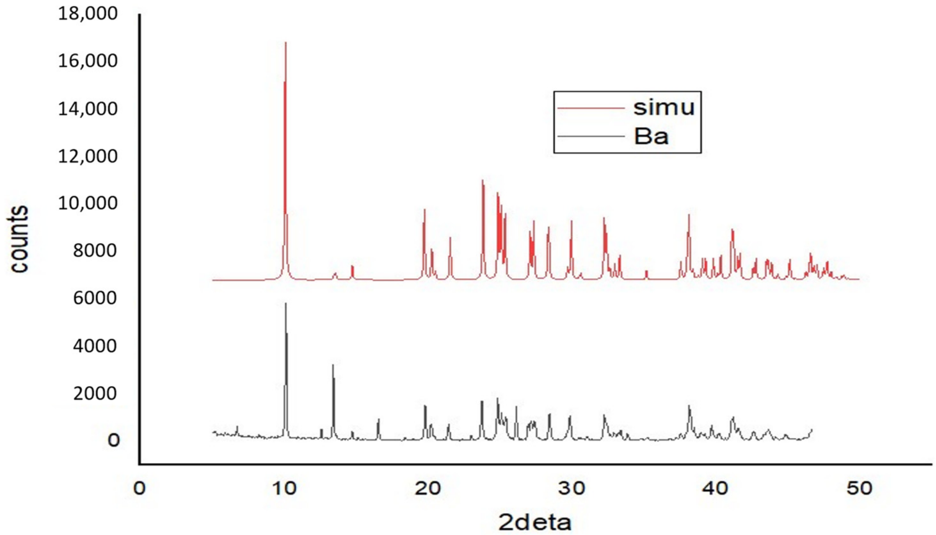

Figure 1. XRD pattern of $[Ba(H_2btec)\cdot H_2O]_n$.

The FTIR spectrum of $[Ba(H_2btec)\cdot H_2O]_n$ is shown in Figure 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 at 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 CH bond of the aromatic ring.

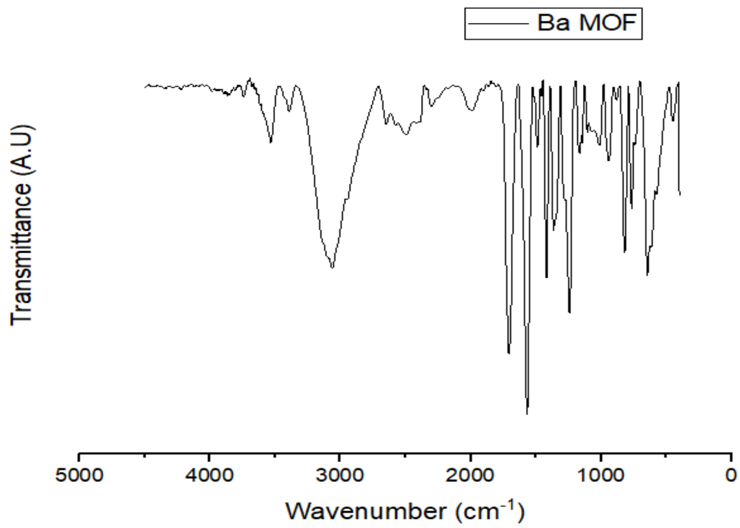

Figure 2. FTIR spectrum of $[Ba(H_2btec)\cdot H_2O]_n$.

The SEM micrographs of $[Ba(H_2btec)\cdot H_2O]_n$ are presented in Figure 3, showing that the rod-shaped average particles of the MOF have the size of 1 µm to 3 µm.

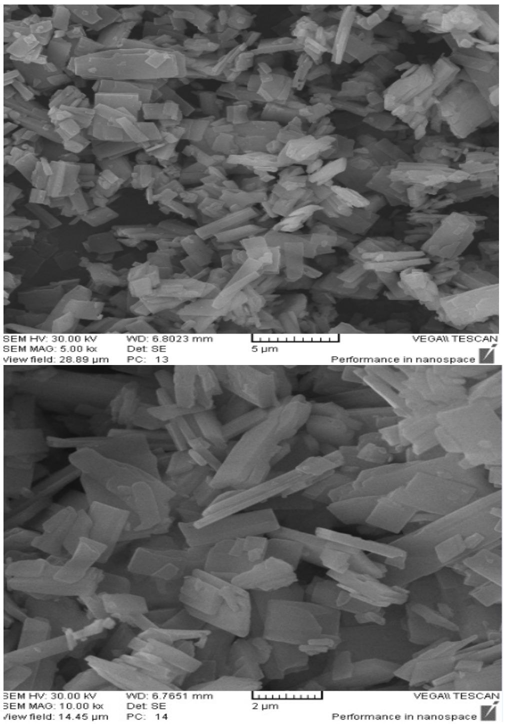

Figure 3. SEM of $[Ba(H_2btec){\cdot}H_2O]_n$.

2.3. Antibacterial Activity

The antibacterial activity of $[Ba(H_2btec){\cdot}H_2O]_n$ was tested against Gram-positive and Gram-negative bacteria. The bacteria included *Keleb peneumonia*, *Staph coccus aureus*, *Staph sapropphyticus*, and *Esherichia coli*. The results are shown in Figure 4a–e and summarized in Table 1. In all cases, the inhibition zone diameter from $[Ba(H_2btec){\cdot}H_2O]_n$ was defined.

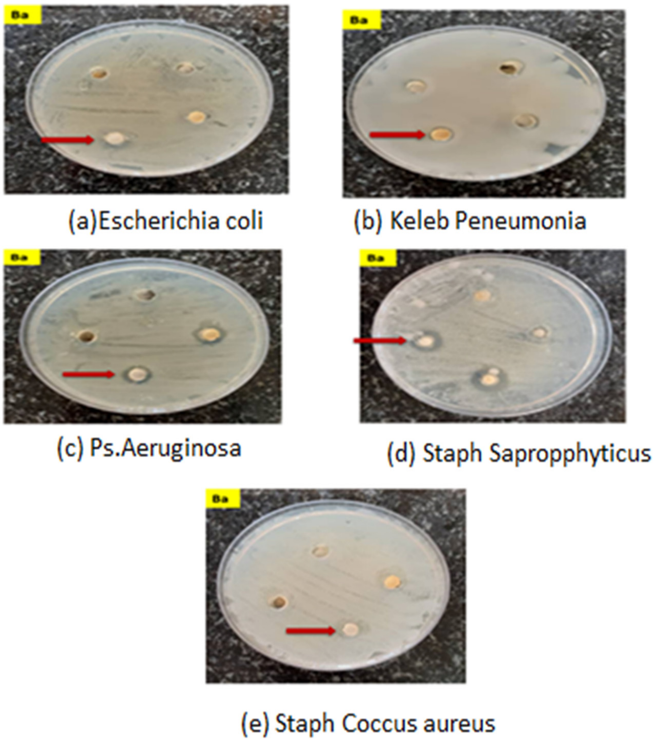

Figure 4. Images of antibacterial test results for Gram-negative (**a**–**c**) and Gram-positive (**d**,**e**) bacteria on $[Ba(H_2btec){\cdot}H_2O]_n$.

Table 1. The behavior of $[Ba(H_2btec)\cdot H_2O]_n$.

Bacteria Tested with $[Ba(H_2btec)\cdot H_2O]_n$	Inhibition Zone Diameter (mm)
Ps. seruginosa	10.725
Keleb seneumonia	11.31
Staph soccus aureus	13.527
Staph sapropphyticus	12.712
E. coli	14.360

3. Conclusions

In this research, $[Ba(H_2btec)\cdot H_2O]_n$ was synthesized using benzene-1,2,4,5-tetracarboxylic acid as a linker and $Ba(NO_3)_2$ as a metal source; it was applied against Gram-positive and Gram-negative bacteria and showed relatively good performance against both groups. To the best of our knowledge, the considered MOF has been applied against bacteria for the first time; it was also synthesized using green chemistry and environmentally friendly solvents.

Author Contributions: M.A., M.A.A. and F.M. contributed equally to this manuscript. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Conflicts of Interest: The authors declare no conflict of interest.

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