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Identification of some crystallographic features of several MOFs (ZIF-8, ZIF-67, UiO-66) via ToposPro

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INTRODUCTION & AIM

❑ Metal-Organic Frameworks (MOFs) are porous crystalline materials. They include both organic and inorganic components simultaneously. As shown in Fig. 1, their structure covers coordination bonds between metal ions and organic linkers with voids [1].

❑ Because of its unique properties, such as high porosity and surface area, adjustable topography, MOFs have a wide range of application areas (Fig. 2) [1].

❑ There are more than 75,000 types of MOF recorded in the Cambridge Crystallographic Data Center [2]. Some examples can be seen in Fig. 3.

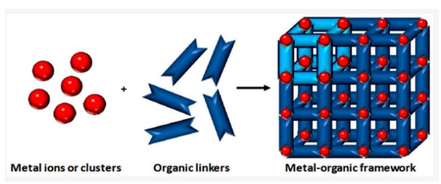


Figure 1. General scheme for MOF synthesis [1]

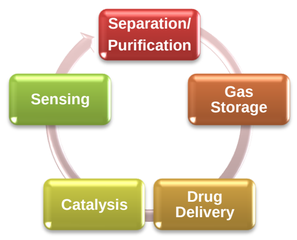


Figure 2. A scheme for MOF applications

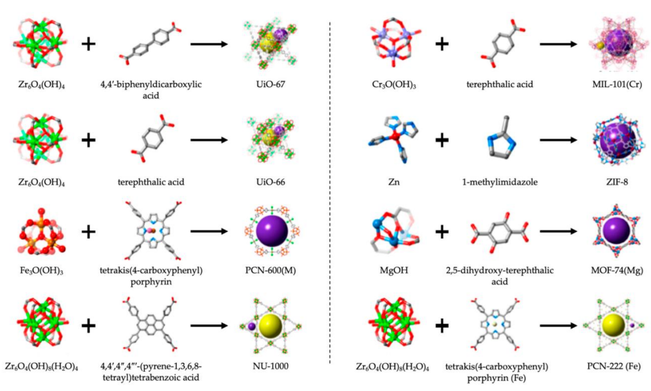


Figure 3. Several MOF structures with their precursors [2]

❑ MOFs are regarded as one of the topologically engineered materials. It is possible to improve MOFs' energy-related performance, like hydrogen storage and hydrogen evaluation, by analyzing their topological features [3]. ToposPro is a tool to detect the topology of a given MOF [4]. Crystal data, bond length and angles, and crystal structure of an MOF can be determined by using ToposPro [5]. Besides that, it can be possible to make simplifications on the topology of a given crystal by utilizing ToposPro software [6]. ToposPro is a new topology tool ,so research is scarce about this topic for MOFs.

❑ *This study aimed to determine some MOF topological features. All of the studies were based on computational studies.*

METHOD

❑ Topological Analysis was carried out on ZIF-67, ZIF-8, and UiO-66 via ToposPro software.

❑ The Isocryst tool in ToposPro was used to draw the unit cell of the MOF.

❑ Identifier Codes for ZIF-8, ZIF-67, and UiO-66 were OFERUN, GITTOT, and RUBTAK, respectively, in the Cambridge Crystal Database (CSD). Their CIF files are used to conduct this study in ToposPro.

RESULTS & DISCUSSION

❑ As shown in Table 1, ZIF-8, ZIF-67, and UiO-66 were cubic because of their unit cell properties.

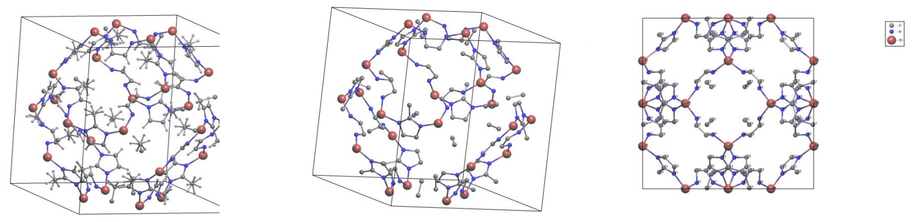
❑As seen in Table 2, Space groups such as I-43m for ZIF-8 and ZIF-67 meant that these MOFs had body-centered cubes. Besides that regarding Fm-3m notification, UiO-66 had each face-centered cubic topology [7].

Table 1. Crystal Unit Cell Dimensions and Angles for selected MOFs

MOF	ToposPro					
	a (Å)	b (Å)	c (Å)	α (º)	β (º)	γ (º)
ZIF-8	16.8815	16.8815	16.8815	90	90	90
ZIF-67	16.9077	16.9077	16.9077	90	90	90
UiO-66	20.7430	20.7430	20.7430	90	90	90

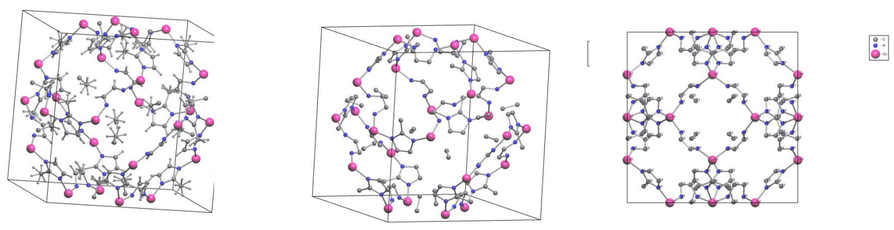
Table 2. Crystallographic Features of selected MOFs

MOF	Formula	Composition	Z-value	Space Group	Cell Volume (Å^3)	Pearson Code
ZIF-8	$0.08(C_{96}H_{120}N_{48}Zn_{12})$	$C_8H_{10}N_4Zn$	12	I-43m	4810.98	cI348-72
ZIF-67	$C_4H_4CoNO_2$	$C_8CoH_{10}N_4$	12	I-43m	4833.41	cI348-72
UiO-66	$Zr_{24}O_{128}C_{192}$	$C_{24}O_{16}Zr_3$	8	Fm-3m	8925.13	cF344



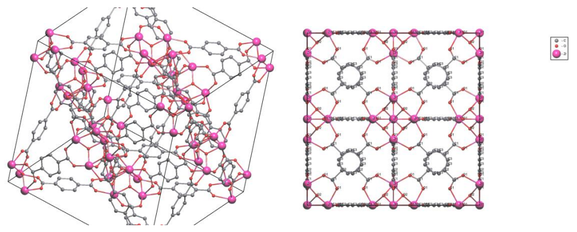
a. b. c.

Figure 4. ZIF-8 unit cell structure original (a), simplified (b), and crossection (c)



a. b. c.

Figure 5. ZIF-67 unit cell structure original (a), simplified (b), and crossection (c)



a. b.

Figure 6. UiO-66 unit cell structure original (a) and crossection (b)

❑Simplification was made by removing hydrogen bonds from the unit cell for this study (Fig. 4-6). Because the UiO-66 crystal had no hydrogen bond, its unit cell was not simplified.

CONCLUSION & FUTURE WORK

❑ The topological Analysis for selected MOFs was conducted via ToposPro software. Unit cells of UiO-66, ZIF-8, and ZIF-67 were drawn. Simplification was done to reach a clear appearance. Crystallographic information, like Pearson code, was obtained.

❑ Especially, there is scarce information about topological analysis for crystalline materials. This analysis can be conducted on any crystalline structures in the future.

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