Research Article

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Irregular topological indices of certain metal organic frameworks

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Abstract: It is interesting to study the molecular topology that provides a base for relationship of physicochemical property of a definite molecule. The topology of a molecule and the irregularity of the structure plays a vital character in shaping properties of the structure like enthalpy and entropy. In this article, we are interested to calculate some irregular topological indices of two classes of metal organic frameworks (MOFs) namely BHT (Butylated hydroxytoluene) based metal ($M = \text{Co, Fe, Mn, Cr}$) organic frameworks (MBHT) and M1TPyP-M2 (TPyP = 5, 10, 15, 20-tetrakis (4-pyridyl) porphyrin and M1, M2, = Fe and Co) MOFs. Also we compare our results graphically.

Keywords: topological descriptors, irregularity indices, chemical graph theory, metal organic frameworks

1 Introduction

Metal organic frameworks (MOFs) are defined by their three-dimensional frameworks formed of metal ions and organic molecules. In MOFs, all metal ions and organic molecules form networks which can get a variety of guest molecules. MOFs have many applications, such as energy storage devices, gas storage, heterogeneous catalysis, and assessment of chemicals (Awais et al., 2020). In 1959, Kinoshita and coworkers were the first ones to study metal

organic frameworks (Kinoshita, 1959). Due to their design and synthesis, MOFs gain attention rapidly (Hoskins, 1989). Till now a large number of MOFs have been synthesized and used in many applications especially in gas catalysis (Hall et al., 2016; Lee et al., 2009; Roy et al., 2012), delivery of drugs (Horcajada et al., 2008; Mandal et al., 2017; Vallet-Regi et al., 2007), sensing (Sarkisov et al., 2012), separation (Kim et al., 2017; Li et al., 2009), storage (Kennedy et al., 2013; Murray et al., 2009; Rosi et al., 2003), and absorption (Czaja et al., 2009; Geier et al., 2013; Mu et al., 2010; Park et al., 2017; Queen et al., 2014). MOFs are capable of capturing industrial gases, such as CO_2 , SO_2 , NO , CO , NO_2 , etc. (Dietzel et al., 2009; Lee et al., 2015; Wu et al., 2009). These gases are very dangerous for our environment. For example, the CO_2 continuously changing our climate and effects greenhouse (Rodhe, 1990), acid rain, and smog is due to the emission of SO_2 and NO_2 (Singh and Agarwal, 2007), and CO and NO are very harmful for humans (Olson and Phillips, 1997). For a healthy environment, it is necessary to control these dangerous gases. MOFs have ability to reduce the quantity of CO_2 at room temperature and low pressure. We can study the ability of MOFs to reduce flue gases in these articles (Chakarvarty et al., 2016; Howe et al., 2017; Tan et al., 2017; Yu et al., 2012). We can study for degree based topological invariants of metal-organic networks (Hong et al., 2020).

Let $G(V, E)$ with vertex set V and edge set E be a connected graph of order $n = |V(G)|$ and size $m = |E(G)|$. The number of edges associated with a vertex is the degree of that vertex. The quantitative topological categorization of irregularity of graphs has an increasing significance for analyzing the structure of deterministic and arbitrary networks and systems occurring in chemistry, biology and common networks. The idea of topological indices was given by Wiener (1947). He also found a strong relation among weiner index and physicochemical properties of compounds. But mathematicians did not work with interest on it for next 20 years. In the mid of 1970s, Wiener index gain popularity and gave some important research articles. After 1990s, a lot of work has done on other distance based topological indices closely related

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to Wiener index. Till now, thousands of topological indices (distance based and degree based topological indices) have found which plays a vital role in chemical graph theory.

Now we present the irregularity topological indices that is calculated here. Albertson (1997) defined a degree based index called the Albertson index (AL) as $AL(G) = \sum_{uv \in E} |d_u - d_v|$. Vukicevic and Gasparov (2004) defined the irregularity index IRL and IRLU as $IRL(G) = \sum_{uv \in E} |\ln d_u - \ln d_v|$ and $IRLU(G) = \sum_{uv \in E} \frac{\|d_u - d_v\|}{\min(d_u, d_v)}$.

Abdoo et al. (2014) defined the total irregularity index (IRRT) as $IRRT(G) = \frac{1}{2} \sum_{uv \in E} |du - dv|$. Gutman (2018) introduced the IRF(G) irregularity index that is. The Randic index (Li and Gutman, 2006) was described as

$$IRA(G) = \sum_{uv \in E} \left(du^{-\frac{1}{2}} - dv^{-\frac{1}{2}} \right)^2. \text{ We have some more degree based irregularity topological indices that was studied in Reti et al. (2018). These degree based irregularity topological indices are defined as } IRDIF(G) = \sum_{uv \in E} \left| \frac{du}{dv} - \frac{dv}{du} \right|, \\ IRLF(G) = \sum_{uv \in E} \frac{|du - dv|}{\sqrt{(du dv)}}, \quad LA(G) = 2 \sum_{uv \in E} \frac{|du - dv|}{(du + dv)}, \quad IRDI(G) = \sum_{uv \in E} \ln \{1 + |du - dv|\}, \quad IRGA(G) = \sum_{uv \in E} \ln \frac{du + dv}{2\sqrt{du dv}}, \text{ and } \\ IRB(G) = \sum_{uv \in E} \left(du^{\frac{1}{2}} - dv^{\frac{1}{2}} \right)^2.$$

2 Irregularity topolglcal indices of 2D struture Of M1TPyP-M2 metalorganic frameworks

Let $G1(c,d)$ be the graph of 2D structure of M1TPyP-M2 metal organic frameworks, where 'c' and 'd' are the unit cells in a row and column respectively. The molecular graph of $G1(2,2)$ is shown below. We can verified that $G1(c,d)$ has $74cd$ number of vertices and $88cd-2c-2d+1$ number of edges.

Theorem 2.1

Let $G1(c,d)$ be the graph of 2D structure of M1TPyP-M2 metal organic frameworks, then the irregularity indices of $G1(c,d)$ are:

1. $AL(G) = 56cd + 2(c + d)$
2. $IRL(G) = 28.668cd + 1.2822(c + d) - 0.1836$
3. $IRLU(G) = 50.6667cd + 1.6667(c + d) + 0.3333$
4. $IRRT(G) = 28cd + c + d$
5. $IRF(G) = 104cd + 2(c + d) + 2$
6. $IRA(G) = 4.3336cd + 0.088(c + d) + 0.0906$

7. $IRDIF(G) = 68.6672cd + 2.6666(c + d) + 0.0001$
8. $IRLF(G) = 30.0224cd + 1.2944(c + d) - 0.1397$
9. $LA(G) = 26.2858cd + 1.2572(c + d) - 0.2572$
10. $IRDI(G) = 31.9112cd + 1.3862(c + d) - 0.2876$
11. $IRGA(G) = 3.5336cd + 10.8314(c + d) - 10.6876$
12. $IRB(G) = 6.5744cd + 0.3188(c + d) - 0.0688$

Proof: We will use Figure 1 to prove all the above theorems. We can verify the values given in Table 1 for the edges of $G1(c,d)$.

$$\begin{aligned} 1. \quad AL(G) &= \sum_{uv \in E} |d_u - d_v| \\ &= (24cd + 1)|3 - 1| + (6c + 6d - 6)|3 - 2| \\ &\quad + (56cd - 4c - 4d + 2)|3 - 3| \\ &\quad + (8cd - 4c - 4d + 4)|4 - 3| \\ &= 48cd + 2 + 6c + 6d - 6 + 8cd - 4c - 4d + 4 \\ &= 56cd + 2(c + d) \\ 2. \quad IRL(G) &= \sum_{uv \in E} |\ln d_u - \ln d_v| \\ &= (24cd + 1)|\ln 3 - \ln 1| + (6c + 6d - 6)|\ln 3 - \ln 2| \\ &\quad + (56cd - 4c - 4d + 2)|\ln 3 - \ln 3| \\ &\quad + (8cd - 4c - 4d + 4)|\ln 4 - \ln 3| \\ &= 1.0986(24cd + 1) + 0.4055(6c + 6d - 6) \\ &\quad + 0(56cd - 4c - 4d + 2) \\ &\quad + 0.2877(8cd - 4c - 4d + 4) \\ &= 28.668cd + 1.2822(c + d) - 0.1836 \end{aligned}$$

$$\begin{aligned} 3. \quad IRLU(G) &= \sum_{uv \in E} \frac{\|d_u - d_v\|}{\min(d_u, d_v)} \\ &= (24cd + 1) \frac{|3 - 1|}{\min(3, 1)} + (6c + 6d - 6) \frac{|3 - 2|}{\min(3, 2)} \\ &\quad + (56cd - 4c - 4d + 2) \frac{|3 - 3|}{\min(3, 3)} \\ &\quad + (8cd - 4c - 4d + 4) \frac{|4 - 3|}{\min(4, 3)} \\ &= 48cd + 2 + 3c + 3d - 3 \\ &\quad + 2.6667cd - 1.3333c - 1.3333d + 1.3333 \\ &= 50.6667cd + 1.6667(c + d) + 0.3333 \end{aligned}$$

Figure 1: 2×2 supercell of M1TPyP-M2 MOFs (M1, M2 = Fe and Co).

Table 1: Edge partition of 2×2 supercell of M1TPyP-M2 MOFs (M1, M2 = Fe and Co)

$(\deg(x), \deg(y))$ where $xy \in E(G_1(c, d))$	Total number of edges
(1, 3)	$24cd + 1$
(2, 3)	$6c + 6d - 6$
(3, 3)	$56cd - 4c - 4d + 2$
(3, 4)	$8cd - 4c - 4d + 4$

$$\begin{aligned}
 4. \quad IRRT(G) &= \frac{1}{2} \sum_{uv \in E} |du - dv|^2 \\
 &= \frac{1}{2} [(24cd + 1)|3 - 1| + (6c + 6d - 6)|3 - 2| \\
 &\quad + (56cd - 4c - 4d + 2)|3 - 3| \\
 &\quad + (8cd - 4c - 4d + 4)|4 - 3|] \\
 &= \frac{1}{2} [48cd + 2 + 6c + 6d - 6 + 8cd - 4c - 4d + 4] \\
 &= 28cd + c + d
 \end{aligned}$$

$$\begin{aligned}
 5. \quad IRF(G) &= \sum_{uv \in E} |du - dv|^2 \\
 &= (24cd + 1)(3 - 1)^2 + (6c + 6d - 6)(3 - 2)^2 \\
 &\quad + (56cd - 4c - 4d + 2)(3 - 3)^2 \\
 &\quad + (8cd - 4c - 4d + 4)(4 - 3)^2 \\
 &= 96cd + 4 + 6c + 6d - 6 + 8cd - 4c - 4d + 4 \\
 &= 104cd + 2(c + d) + 2
 \end{aligned}$$

$$\begin{aligned}
 6. \quad IRA(G) &= \sum_{uv \in E} \left(du^{\frac{1}{2}} - dv^{\frac{1}{2}} \right)^2 \\
 &= (24cd + 1) \left((3)^{\frac{-1}{2}} - (1)^{\frac{-1}{2}} \right)^2 \\
 &\quad + (6c + 6d - 6) \left((3)^{\frac{-1}{2}} - (2)^{\frac{-1}{2}} \right)^2 \\
 &\quad + (56cd - 4c - 4d + 2) \left((3)^{\frac{-1}{2}} - (3)^{\frac{-1}{2}} \right)^2 \\
 &\quad + (8cd - 4c - 4d + 4) \left((4)^{\frac{-1}{2}} - (3)^{\frac{-1}{2}} \right)^2
 \end{aligned}$$

$$\begin{aligned}
& + (8cd - 4c - 4d + 4) \left((4)^{\frac{-1}{2}} - (3)^{\frac{-1}{2}} \right)^2 \\
& = 0.1786(24cd + 1) + 0.0186(6c + 6d - 6) \\
& \quad + 0.0059(8cd - 4c - 4d + 4) \\
& = 4.3333cd + 0.088(c + d) + 0.0906
\end{aligned}$$

$$\begin{aligned}
7. \quad IRDIF(G) &= \sum_{uv \in E} \left| \frac{du}{dv} - \frac{dv}{du} \right| \\
&= (24cd + 1) \left| \frac{3}{1} - \frac{1}{3} \right| + (6c + 6d - 6) \left| \frac{3}{2} - \frac{2}{3} \right| \\
& \quad + (56cd - 4c - 4d + 2) \left| \frac{3}{3} - \frac{3}{3} \right| \\
& \quad + (8cd - 4c - 4d + 4) \left| \frac{4}{3} - \frac{3}{4} \right| \\
&= 2.6667(24cd + 1) + 0.8333(6c + 6d - 6) \\
& \quad + 0.5833(8cd - 4c - 4d + 4) \\
&= 68.6672cd + 2.6666(c + d) + 0.0001
\end{aligned}$$

$$\begin{aligned}
8. \quad IRLF(G) &= \sum_{uv \in E} \frac{|du - dv|}{\sqrt{(dudv)}} \\
&= (24cd + 1) \frac{|3 - 1|}{\sqrt{(3 \times 1)}} + (6c + 6d - 6) \frac{|3 - 2|}{\sqrt{(3 \times 2)}} \\
& \quad + (56cd - 4d + 2) \frac{|3 - 3|}{\sqrt{(3 \times 3)}} \\
& \quad + (8cd - 4c - 4d + 4) \frac{|4 - 3|}{\sqrt{(4 \times 3)}} \\
&= 1.1547(24cd + 1) + 0.4082(6c + 6d - 6) \\
& \quad + 0.2887(8cd - 4c - 4d + 4) \\
&= 30.0224cd + 1.2944(c + d) - 0.1397
\end{aligned}$$

$$\begin{aligned}
9. \quad LA(G) &= 2 \sum_{uv \in E} \frac{|du - dv|}{(du + dv)} \\
&= 2 \left[(24cd + 1) \frac{|3 - 1|}{(3 + 1)} + (6c + 6d - 6) \frac{|3 - 2|}{(3 + 2)} \right. \\
& \quad + (56cd - 4c - 4d + 2) \frac{|3 - 3|}{(3 + 3)} \\
& \quad \left. + (8cd - 4c - 4d + 4) \frac{|4 - 3|}{(4 + 3)} \right]
\end{aligned}$$

$$\begin{aligned}
&= 2[12cd + 0.5 + 0.2(6c + 6d - 6) \\
& \quad + 0.1429(8cd - 4c - 4d + 4)] \\
&= 26.2858cd + 1.2572(c + d) - 0.2572
\end{aligned}$$

$$\begin{aligned}
10. \quad IRDI(G) &= \sum_{uv \in E} \ln\{1 + |du - dv|\} \\
&= (24cd + 1) \ln\{1 + |3 - 1|\} \\
& \quad + (6c + 6d - 6) \ln\{1 + |3 - 2|\} \\
& \quad + (56cd - 4c - 4d + 2) \ln\{1 + |3 - 3|\} \\
& \quad + (8cd - 4c - 4d + 4) \ln\{1 + |4 - 3|\} \\
&= 1.0986(24cd + 1) + 0.6931(6c + 6d - 6) \\
& \quad + 0.6931(8cd - 4c - 4d + 4) \\
&= 31.9112cd + 1 - 3862(c + d) - 0.2876
\end{aligned}$$

$$\begin{aligned}
11. \quad IRGA(G) &= \sum_{uv \in E} \ln \frac{du + dv}{2\sqrt{(dudv)}} \\
&= (24cd + 1) \ln \frac{3 + 1}{2\sqrt{(3 \times 1)}} \\
& \quad + (6c + 6d - 6) \ln \frac{3 + 2}{2\sqrt{(3 \times 2)}} \\
& \quad + (56cd - 4c - 4d + 2) \ln \frac{3 + 3}{2\sqrt{(3 \times 3)}} \\
& \quad + (8cd - 4c - 4d + 4) \ln \frac{4 + 3}{2\sqrt{(4 \times 3)}} \\
&= 0.1438(24cd + 1) + 1.8121(6c + 6d - 6) \\
& \quad + 0.0103(8cd - 4c - 4d + 4) \\
&= 3.5336cd + 10.8314(c + d) - 10.6876
\end{aligned}$$

$$\begin{aligned}
12. \quad IRB(G) &= \sum_{uv \in E} \left(du^{\frac{1}{2}} - dv^{\frac{1}{2}} \right)^2 \\
&= (24cd + 1) \left((3)^{\frac{1}{2}} - (1)^{\frac{1}{2}} \right)^2 \\
& \quad + (6c + 6d - 6) \left((3)^{\frac{1}{2}} - (2)^{\frac{1}{2}} \right)^2 \\
& \quad + (56cd - 4c - 4d + 2) \left((3)^{\frac{1}{2}} - (3)^{\frac{1}{2}} \right)^2 \\
& \quad + (8cd - 4c - 4d + 4) \left((4)^{\frac{1}{2}} - (3)^{\frac{1}{2}} \right)^2 \\
&= 0.25(24cd + 1) + 0.1010(6c + 6d - 6) \\
& \quad + 0.0718(8cd - 4c - 4d + 4) \\
&= 6.5744cd + 0.3188(c + d) - 0.0688
\end{aligned}$$

Figure 2: 2×2 supercell of 2D CoBHT(CO) lattice.

3 Irregularity topological indices of 2D CoBHT(CO) lattice

Let $G_2(a,b)$ be the graph of 2D CoBHT(CO) lattice, where 'a' and 'b' are the unit cells in a row and column respectively. The molecular graph of $G_2(2,2)$ is shown below. We can verified that $G_2(a,b)$ has $27ab$ number of vertices and $36ab-2a-2b$ number of edges.

Theorem 2

Let $G_2(a,b)$ be the graph of 2D structure of CoBHT(CO) lattice, then the irregularity indices of $G_2(a,b)$ are:

1. $AL(G) = 36ab - 2(a+b)$
2. $IRL(G) = 13.1832ab$
3. $IRLU(G) = 18ab + a + b$
4. $IRRt(G) = 18ab - a - b$
5. $IRF(G) = 60ab - 2(a+b)$
6. $IRA(G) = 0.294ab + 0.3082(a+b)$
7. $IRDIF(G) = 27.9996ab + 0.6668(a+b)$
8. $IRLFO(G) = 13.3836ab + 0.0788(a+b)$
9. $LA(G) = 12.8ab - 0.0667(a+b)$
10. $IRDI(G) = 21.5004ab - 1.3862(a+b)$
11. $IRGA(G) = 22.452ab - 3.4544(a+b)$
12. $IRB(G) = 5.3292ab - 0.3882(a+b)$

Proof: We will use Figure 2 to prove all above theorems. We can verify the values given in Table 2 for the edges of $G_2(a,b)$.

Table 2: Edge partition of 2×2 supercell of 2D CoBHT(CO) lattice

$(\deg(x), \deg(y))$ where $xy \in E(G_2(a, b))$	Total number of edges
(1, 3)	$2a + 2b$
(2, 2)	$2a + 2b$
(2, 3)	$12ab - 2a - 2b$
(2, 4)	$12ab - 2a - 2b$
(3, 3)	$12ab$

1.
$$\begin{aligned}
 AL(G) &= \sum_{uv \in E} |d_u - d_v| \\
 &= (2a+2b)|3-1| + (2a+2b)|2-2| \\
 &\quad + (12ab-2a-2b)|3-2| \\
 &\quad + (12ab-2b-2b)|4-2| + 12ab|3-3| \\
 &= 4a+4b+12ab-2a-2b+24ab-4a-4b \\
 &= 36ab-2(a+b)
 \end{aligned}$$
2.
$$\begin{aligned}
 IRL(G) &= \sum_{uv \in E} |\ln d_u - \ln d_v| \\
 &= (2a+2b)|\ln 3 - \ln 1| + (2a+2b)|\ln 2 - \ln 2| \\
 &\quad + (12ab-2a-2b)|\ln 3 - \ln 2| \\
 &\quad + (12ab-2a-2b)|\ln 4 - \ln 2| + 12ab|\ln 3 - \ln 3| \\
 &= 1.0986(2a+2b) + 0.4055(12ab-2a-2b) \\
 &\quad + 0.6931(12ab-2a-2b) = 13.1832ab
 \end{aligned}$$

$$\begin{aligned}
3. \quad IRL(G) &= \sum_{uv \in E} \frac{\|d_u - d_v\|}{\min(d_u, d_v)} \\
&= (2a+2b) \frac{|3-1|}{\min(3,1)} + (2a+2b) \frac{|2-2|}{\min(2,2)} \\
&\quad + (12ab-2a-2b) \frac{|3-2|}{\min(3,2)} \\
&\quad + (12ab-2a-2b) \frac{|4-2|}{\min(4,2)} + 12ab \frac{|3-3|}{\min(3,3)} \\
&= 4a+4b+6ab-a-b+12ab-2a-2b \\
&= 18ab+a+b
\end{aligned}$$

$$\begin{aligned}
4. \quad IRRT(G) &= \frac{1}{2} \sum_{uv \in E} |du-dv| \\
&= \frac{1}{2} [(2a+2b)|3-1| + (2a+2b)|2-2| \\
&\quad + (12ab-2a-2b)|3-2| \\
&\quad + (12ab-2a-2b)|4-2| + 12ab|3-3|] \\
&= \frac{1}{2} [4a+4b+12ab-2a-2b+24ab-4a-4b] \\
&= 18ab-a-b
\end{aligned}$$

$$\begin{aligned}
5. \quad IRF(G) &= \sum_{uv \in E} (du-dv)^2 \\
&= (2a+2b)(3-1)^2 + (2a+2b)(2-2)^2 \\
&\quad + (12ab-2a-2b)(3-2)^2 \\
&\quad + (12ab-2a-2b)(4-2)^2 + 12ab(3-3)^2 \\
&= 8a+8b+12ab-2a-2b+48ab-8a-8b \\
&= 60ab-2(a+b)
\end{aligned}$$

$$\begin{aligned}
6. \quad IRA(G) &= \sum_{uv \in E} \left(du^{\frac{1}{2}} - dv^{\frac{1}{2}} \right)^2 \\
&= (2a+2b) \left((3)^{\frac{1}{2}} - (1)^{\frac{1}{2}} \right)^2 \\
&\quad + (2a+2b) \left((2)^{\frac{1}{2}} - (2)^{\frac{1}{2}} \right)^2 \\
&\quad + (12ab-2a-2b) \left((3)^{\frac{1}{2}} - (2)^{\frac{1}{2}} \right)^2 \\
&\quad + (12ab-2a-2b) \left((4)^{\frac{1}{2}} - (2)^{\frac{1}{2}} \right)^2 \\
&\quad + 12ab \left((3)^{\frac{1}{2}} - (3)^{\frac{1}{2}} \right)^2 \\
&= 0.1786(2a+2b) + 0.0186(12ab-2a-2b) \\
&\quad + 0.0059(12ab-2a-2b) \\
&= 0.294ab + 0.3082(a+b)
\end{aligned}$$

$$\begin{aligned}
7. \quad IRDIF(G) &= \sum_{uv \in E} \left| \frac{du}{dv} - \frac{dv}{du} \right| \\
&= (2a+2b) \left| \frac{3}{1} - \frac{1}{3} \right| + (2a+2b) \left| \frac{2}{2} - \frac{2}{2} \right| \\
&\quad + (12ab-2a-2b) \left| \frac{3}{2} - \frac{2}{3} \right| \\
&\quad + (12ab-2a-2b) \left| \frac{4}{2} - \frac{2}{4} \right| + 12ab \left| \frac{3}{3} - \frac{3}{3} \right| \\
&= 2.6667(2a+2b) + 0.8333(12ab-2a-2b) \\
&\quad + 1.5(12ab-2a-2b) \\
&= 27.9996ab + 0.6668(a+b)
\end{aligned}$$

$$\begin{aligned}
8. \quad IRLF(G) &= \sum_{uv \in E} \frac{|du-dv|}{\sqrt{(dudv)}} \\
&= (2a+2b) \frac{|3-1|}{\sqrt{(3 \times 1)}} + (2a+2b) \frac{|2-2|}{\sqrt{(2 \times 2)}} \\
&\quad + (12ab-2a-2b) \frac{|3-2|}{\sqrt{(3 \times 2)}} \\
&\quad + (12ab-2a-2b) \frac{|4-2|}{\sqrt{(4 \times 2)}} + 12ab \frac{|3-3|}{\sqrt{(3 \times 3)}} \\
&= 1.1547(2a+2b) + 0.4082(12ab-2a-2b) \\
&\quad + 0.7071(12ab-2a-2b) \\
&= 13.3836ab + 0.0788(a+b)
\end{aligned}$$

$$\begin{aligned}
9. \quad LA(G) &= 2 \sum_{uv \in E} \frac{|du-dv|}{(du-dv)} \\
&= 2 \left[(2a+2b) \frac{|3-1|}{(3+1)} + (2a+2b) \frac{|2-2|}{(2+2)} \right. \\
&\quad + (12ab-2a-2b) \frac{|3-2|}{(3+2)} \\
&\quad + (12ab-2a-2b) \frac{|4-2|}{(4+2)} + 12ab \frac{|3-3|}{(3+3)} \left. \right] \\
&= 2[a+b+2.4ab-0.4a-0.4b \\
&\quad + 4ab-0.6667a-0.6667b] \\
&= 12.8ab-0.0667(a+b)
\end{aligned}$$

$$\begin{aligned}
10. \quad IRDI(G) &= \sum_{uv \in E} \ln\{1+|du-dv|\} \\
&= (2a+2b)\ln\{1+|3-1|\} + (2a+2b)\ln\{1+|2-2|\} \\
&\quad + (12ab-2a-2b)\ln\{1+|3-2|\} \\
&\quad + (12ab-2a-2b)\ln\{1+|4-2|\} \\
&\quad + 12ab\ln\{1+|3-3|\} \\
&= 1.0986(2a+2b) + 0.6931(12ab-2a-2b) \\
&\quad + 1.0986(12ab-2a-2b) \\
&= 21.5004ab - 1.3862(a+b)
\end{aligned}$$

$$\begin{aligned}
11. \quad IRGA(G) &= \sum_{uv \in E} \ln \frac{du+dv}{2\sqrt{(dudv)}} \\
&= (2a+2b)\ln \frac{3+1}{2\sqrt{(3 \times 1)}} + (2a+2b)\ln \frac{2+2}{2\sqrt{(2 \times 2)}} \\
&\quad + (12ab-2a-2b)\ln \frac{3+2}{2\sqrt{(3 \times 2)}} \\
&\quad + (12ab-2a-2b)\ln \frac{4+2}{2\sqrt{(4 \times 2)}} \\
&\quad + 12(ab)\ln \frac{3+3}{2\sqrt{(3 \times 3)}} \\
&= 0.1438(2a+2b) + 1.8121(12ab-2a-2b) \\
&\quad + 0.0589(12ab-2a-2b) \\
&= 22.452ab - 3.4544(a+b)
\end{aligned}$$

$$\begin{aligned}
12. \quad IRB(G) &= \sum_{uv \in E} \left(du^{\frac{1}{2}} - dv^{\frac{1}{2}} \right)^2 \\
&= (2a+2b) \left((3)^{\frac{-1}{2}} - (1)^{\frac{-1}{2}} \right)^2 \\
&\quad + (2a+2b) \left((2)^{\frac{-1}{2}} - (2)^{\frac{-1}{2}} \right)^2 \\
&\quad + (12ab-2a-2b) \left((3)^{\frac{-1}{2}} - (2)^{\frac{-1}{2}} \right)^2 \\
&\quad + (12ab-2a-2b) \left((4)^{\frac{-1}{2}} - (2)^{\frac{-1}{2}} \right)^2 \\
&\quad + 12ab \left((3)^{\frac{-1}{2}} - (3)^{\frac{-1}{2}} \right)^2 \\
&= 0.25(2a+2b) + 0.1010(12ab-2a-2b) \\
&\quad + 0.3431(12ab-2a-2b) \\
&= 5.3292ab - 0.3882(a+b)
\end{aligned}$$

Table 3: Irregularity indices of 2D structure of M1TPyP-M2 metal organic frameworks

Irregularity indices	c = 1, d = 1	c = 2, d = 2
1. $AL(G) = 56cd + 2(c+d)$	60	232
2. $IRL(G) = 28.668cd + 1.2822(c+d) - 0.1836$	31.2324	119.8008
3. $IRLU(G) = 50.6667cd + 1.6667(c+d) + 0.3333$	54.3334	209.6669
4. $IRRt(G) = 28cd + c + d$	30	116
5. $IRF(G) = 104cd + 2(c+d) + 2$	110	426
6. $IRA(G) = 4.3336cd + 0.088(c+d) + 0.0906$	4.6002	17.7770
7. $IRDIF(G) = 68.6672cd + 2.6666(c+d) + 0.0001$	74.0005	285.3354
8. $IRLF(G) = 30.0224cd + 1.2944(c+d) - 0.1397$	32.4715	125.1275
9. $LA(G) = 26.2858cd + 1.2572(c+d) - 0.2572$	28.543	109.9148
10. $IRDI(G) = 31.9112cd + 1.3862(c+d) - 0.2876$	34.3960	132.9020
11. $IRGA(G) = 3.5336cd + 10.8314(c+d) - 10.6876$	14.5088	46.7724
12. $IRB(G) = 6.5744cd + 0.3188(c+d) - 0.0688$	7.1432	27.5040

4 Graphical analysis and conclusions

Here we present the graphical analysis and comparison table (Table 3) of some of the irregularity indices of the graph of 2D structure of M1TPyP-M2 metal organic frameworks. Figure 3 contains the graphical values of Albertson index ($AL(G)$), irregularity $IRL(G)$ and $IRLU(G)$ indices, total irregularity index ($IRRt$), $IRF(G)$ irregularity index, randic index ($IRA(G)$), irregularity index $IRDIF(G)$, irregularity index $IRLF(G)$, irregularity index $LA(G)$, irregularity index $IRDI(G)$, irregularity index $IRGA(G)$, and irregularity index $IRB(G)$. In this table, we can check the values of some irregularity indices for some different values of 'c' and 'd'.

Now we present the graphical analysis and comparison table (Table 4) of some of the irregularity indices of the graph of 2D structure of CoBHT(CO) lattice. Figure 4 contains the graphical values of Albertson index ($AL(G)$), irregularity $IRL(G)$ and $IRLU(G)$ indices, total irregularity index $IRRt(G)$, $IRF(G)$ irregularity index, randic index $IRA(G)$, irregularity index $IRDIF(G)$, irregularity index $IRLF(G)$, irregularity index $LA(G)$, irregularity index $IRDI(G)$, irregularity index $IRGA(G)$, and irregularity index $IRB(G)$. In Table 4 we can check the values of some irregularity indices for some different values of 'a' and 'b'.

Figure 3: Comparison graph of irregularity topological indices of 2D structure of M1TPyP-M2 metal organic frameworks.

Table 4: Irregularity indices of 2D CoBHT(CO) lattice

Irregularity indices	$a = 1, b = 1$	$a = 2, b = 2$
1. $AL(G) = 36ab - 2(a + b)$	32	136
2. $IRL(G) = 13.1832ab$	13.1832	52.7328
3. $IRLU(G) = 18ab + a + b$	20	76
4. $IRRt(G) = 18ab - a - b$	16	68
5. $IRF(G) = 60ab - 2(a + b)$	56	232
6. $IRA(G) = 0.294ab + 0.3082(a + b)$	0.9104	2.4088
7. $IRDIF(G) = 27.9996ab + 0.6668(a + b)$	29.3332	114.6656
8. $IRLF(G) = 13.3836ab + 0.0788(a + b)$	13.5412	53.8496
9. $LA(G) = 12.8ab - 0.0667(a + b)$	12.6666	50.9332
10. $IRDI(G) = 21.5004ab - 1.3862(a + b)$	18.7280	80.4568
11. $IRGA(G) = 22.452ab - 3.4544(a + b)$	15.5432	75.9904
12. $IRB(G) = 5.3292ab - 0.3882(a + b)$	4.5528	19.7640

Figure 4: Comparison graph of irregularity topological indices of 2D CoBHT(CO) lattice.

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