Research Article

Irregularity Measures for Metal-Organic Networks

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Topological index plays an important role in predicting physicochemical properties of a molecular structure. With the help of the topological index, we can associate a single number with a molecular graph. Drugs and other chemical compounds are frequently demonstrated as different polygonal shapes, trees, graphs, etc. In this paper, we will compute irregularity indices for metal-organic networks.

1. Introduction

Every planet is a blend of various kinds of parts, and every part has a significant commitment in the composition of the earth. The most significant parts in the earth are hydrogen, oxygen, and nitrogen. Subatomic hydrogen is one of the segments that has cordial situation and is a cutting edge wellspring of vitality [1, 2]. As a gas, it can likewise be used in energy units to control engines. Among the various kinds of gases, hydrogen needs smell that makes any hole acknowledgment practically difficult to human creatures. The ongoing standards settled by the United States Vitality Sector put emphasis on the speed proficient of the gadget that can detect one percent by volume of drab and also scent-free atomic hydrogen in climate in less than sixty seconds in particular [3–6].

Jang et al. [7] presented an exceptionally quick hydrogen recognizing device comprising organic ligands and metals recognized with the assistance of palladium nanowires which can perceive hydrogen stages lower than 1 percent in just seven seconds. Moreover, other than distinguishing and detecting, the MONs appear exceptionally valuable with synthetic and physical properties, for example, grafting active groups [8], changing natural ligands [9], impregnating reasonable active materials [10], postsynthetic ligands, ion trade [11], and getting ready composites with useable substance [12].

Graph theory provides the interesting appliance in mathematical chemistry that is used to compute the various kinds of chemical compounds by means of graph theory and predict their various properties [13–19]. One of the most important tools in the chemical graph theory is a topological index, which is useful in predicting the chemical and physical properties of the underlying chemical compound, such as boiling point, strain energy, rigidity, heat of evaporation, and tension [20, 21]. A graph having no loop or multiple edge is known as a simple graph. A molecular graph is a simple graph in which atoms and bounds are represented by the vertex and edge sets, respectively. The degree of the vertex is the number of edges attached with that vertex. These properties of various objects is of primary interest. Winner, in 1947, introduced the concept of the first topological index while finding the boiling point. In 1975, Gutman gave a remarkable identity [22] about Zagreb indices. Hence, these two indices are among the oldest degree-based descriptors, and their properties are extensively investigated. The mathematical formulae of these indices are
Theorem 1. Let $G$ be the metal-organic network $E(MON_1(p))$. The irregularity indices are

\begin{align*}
M_1(G) &= \sum_{uv \in E(G)} (d_u + d_v), \\
M_2(G) &= \sum_{uv \in E(G)} (d_u \times d_v). \\
\end{align*}

A topological index is known as the irregularity index [23] if the value of the topological index of the graph is greater than or equal to zero, and the topological index of the graph is equal to zero if and only if the graph is regular. The irregularity indices are given in Table 1. Most of the irregularity indices are from the family of degree-based topological indices and are used in quantitative structure activity relationship modeling.

For more about topological indices, one can read [24–31].

2. Irregularity Indices for Metal-Organic Networks

In this section, we discuss metal-organic networks by means of a graph. The unit cell of the metal-organic network is given in Figure 1. We give computational results of irregularity indices for two types of metal-organic networks $MON_1(p)$ and $MON_2(p)$ in the following two sections.

2.1. Irregularity Indices for Metal-Organic Network $MON_1(p)$. This section is about irregularity indices of the metal-organic network $MON_1(p)$. The molecular graph of the metal-organic network $MON_1(p)$ for $p = 2$ is given in Figure 2. We can observe from Figure 2 that there are four types of vertices present in the molecular graph of $MON_1(p)$, i.e., $2, 3, 4,$ and $6$. The cardinality of vertices $2, 3, 4,$ and $6$ is $30p, 12, 12p - 6,$ and $6p - 6$, respectively. The cardinality of the vertex set of $MON_1(p)$ is $48p$, i.e., $\vert V(MON_1(p)) \vert = 48p$. There are four different types of edges present in the molecular graph of $MON_1(p)$, i.e., $\{2, 3\}, \{2, 4\}, \{2, 6\},$ and $\{4, 6\}$. Their cardinalities are $36, 36p - 12, 24p - 24,$ and $12p - 12,$ respectively. The cardinality of the edge set of $MON_1(p)$ is $72p - 12$, i.e., $\vert E(MON_1(p)) \vert = 72p - 12$.

The edge partition of the metal-organic network $MON_1(p)$ is given in Table 2.

![Figure 1: Basic metal-organic network.](image)

Table 1: Definitions of irregularity indices.

| Irregularity index | Mathematical form |
|--------------------|-------------------|
| VAR                | $\sum_{uv \in E(G)} (d_u - 2mn)^2 = (M_1(G)/n - 2mn)^2$ |
| AL                 | $\sum_{uv \in E(G)} |d_u - d_v| = M_1(G) - 2LM$ |
| IR1                | $\sqrt{\sum_{uv \in E(G)} |d_u - d_v|^2} = F(G) - M_1(G)$ |
| IR2                | $\sum_{uv \in E(G)} (d_u - d_v)^2 = F(G) - 2M_1(G)$ |
| IRFW               | IRC |
| IRA                | $\sum_{uv \in E(G)} |d_u - d_v| = M_1(G) - 2LM$ |
| IRB                | $(\sum_{uv \in E(G)} |d_u - d_v|^2) = (M_1(G))/M_1(G)$ |
| IRC                | $\sum_{uv \in E(G)} |d_u - d_v| = (M_1(G))/M_1(G)$ |
| IRDIF              | $\sum_{uv \in E(G)} |d_u - d_v| = (M_1(G))/M_1(G)$ |
| IRL                | $\sum_{uv \in E(G)} |d_u - d_v| = (M_1(G))/M_1(G)$ |
| IRDU               | $\sum_{uv \in E(G)} |d_u - d_v| = (M_1(G))/M_1(G)$ |
| IRLA               | $\sum_{uv \in E(G)} |d_u - d_v| = (M_1(G))/M_1(G)$ |
| IRGA               | $\sum_{uv \in E(G)} ((d_u + d_v)/2 - (d_u - d_v)/2) = \sum_{uv \in E(G)} (i + j)(i + j)$ |

Proof. Using definitions of irregularity indices given in Table 1 and edge partition given in Table 2, we have

(8) $IRB(G) = 528p - 204 - (2(24\sqrt{6} + 72\sqrt{2} + 48\sqrt{3}))p - 24\sqrt{6} + 48\sqrt{2} + 96\sqrt{3}$

(9) $IRC(G) = (4\sqrt{6} p^2 + 2\sqrt{6} p + 12\sqrt{2} p^2 + 8\sqrt{3} p^2 - 4\sqrt{2} p - 8\sqrt{3} p - 36p^2 - 12p - 1)/2p (6p - 1)$

(10) $IRDIF(G) = 127.9980p - 61.9992$

(11) $IRL(G) = 56.1840p - 24.9516$

(12) $IRLU(G) = 90p - 48$

(13) $IRLF(G) = 58.0668p - 26.4012$

(14) $IRLA(G) = 52.7976p - 22.3992$

(15) $IRDI(G) = 131.0064p - 42.4776$

(16) $IRGA(G) = 8.0172p - 5.8716$
\[
\begin{align*}
\text{VAR}(G) &= \sum_{u \in V} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \left( \frac{2m}{n} \right)^2 \\
&= \left( \frac{528p - 204}{48p} \right) - \left( \frac{2(72p - 12)}{48p} \right)^2 \\
&= \frac{(8p^2 - 5p - 1)}{4p^2}
\end{align*}
\]

\[
\begin{align*}
\text{AL}(G) &= \sum_{uv \in E(G)} |d_u - d_v| \\
&= |2 - 3|(36) + |2 - 4|(36p - 12) + |2 - 6|(24p - 1) + |4 - 6|(12p - 1) \\
&= 192p - 108,
\end{align*}
\]

\[
\begin{align*}
\text{IR1}(G) &= \sum_{u \in V} d_u^2 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(G) - \left( \frac{2m}{n} \right)M_1(G) \\
&= (2304p - 1356) - \frac{2(72p - 12)}{48p} (528p - 204) \\
&= \frac{6(120p^2 - 80p - 17)}{p}
\end{align*}
\]

\[
\begin{align*}
\text{IR2}(G) &= \sqrt{\text{IRF}(G)} \\
&= \frac{\sum_{uv \in E(G)} d_u d_v}{m} - \frac{2m}{n} = \sqrt{\frac{M_2(G)}{m} - \frac{2m}{n}} \\
&= \frac{864p - 456}{72p - 12} - \left( \frac{2(72p - 12)}{48p} \right) \\
&= \sqrt{\frac{864p - 456}{48p} - \frac{72p - 12}{24p}}
\end{align*}
\]

\[
\begin{align*}
\text{IRF}(G) &= \sum_{uv \in E(G)} (d_u - d_v)^2 \\
&= (2 - 3)^2(36) + (2 - 4)^2(36p - 12) + (2 - 6)^2(24p - 1) + (4 - 6)^2(12p - 1) \\
&= 576p - 444,
\end{align*}
\]

\[
\begin{align*}
\text{IRFW}(G) &= \frac{\text{IRF}(G)}{M_2(G)} \\
&= \frac{48p - 37}{2(36p - 19)}
\end{align*}
\]

\[
\begin{align*}
\text{IRA}(G) &= \sum_{uv \in E(G)} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(G) \\
&= (48p) - 2((9 \sqrt{2} + \sqrt{3} + \sqrt{6})p - (3 \sqrt{2} + 4 \sqrt{3} - 5 \sqrt{6})) \\
&= 48p - 2(\sqrt{6} + 9 \sqrt{2} + 4 \sqrt{3}))p - 10 \sqrt{6} + 6 \sqrt{2} + 8 \sqrt{3},
\end{align*}
\]

\[
\begin{align*}
\text{IRB}(G) &= \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2 = M_1(D_n P_n) - 2RR(G) \\
&= (528p - 204) - 2((72 \sqrt{2} + 48 \sqrt{3} + 24 \sqrt{6})p - (24 \sqrt{2} + 48 \sqrt{3} - 12 \sqrt{6}))
\end{align*}
\]
$= 528p - 204 - (2(24\sqrt{6} + 72\sqrt{2} + 48\sqrt{3}))p - 24\sqrt{6} + 48\sqrt{2} + 96\sqrt{3}$,

\[\text{IRC}(G) = \sum_{uv \in E(G)} \frac{d_u - d_v}{\min(d_u, d_v)} \]

\[= \frac{2}{3} (36) + \frac{2}{2} (36p - 12) + \frac{2}{6} (24p - 1) + \frac{4}{6} (12p - 1)
\]

\[= 58,0668p - 26,4012,
\]

\[\text{IRLF}(G) = \sum_{uv \in E(G)} \frac{|d_u - d_v|}{\sqrt{d_u d_v}}
\]

\[= 2 \frac{|2 - 3|}{5} (36) + 2 \frac{|2 - 4|}{6} (36p - 12) + 2 \frac{|2 - 6|}{8} (24p - 1) + 2 \frac{|4 - 6|}{10} (12p - 1)
\]

\[= 52,7976p - 22,3992,
\]

\[\text{IRD1}(G) = \sum_{uv \in E(G)} \ln|1 + |d_u - d_v||
\]

\[= \ln[1 + |2 - 3|] (36) + \ln[1 + |2 - 4|] (36p - 12) + \ln[1 + |2 - 6|] (24p - 1) + \ln[1 + |4 - 6|] (12p - 1)
\]

\[= 131,0064p - 42,4776,
\]

\[\text{IRGA}(G) = \sum_{uv \in E(G)} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right)
\]

\[= \ln\left(\frac{2 + 3}{2}\sqrt{2} \times 3\right) (36) + \ln\left(\frac{2 + 4}{2\sqrt{2} \times 4}\right) (36p - 1) + \ln\left(\frac{2 + 6}{2\sqrt{4} \times 6}\right) (24p - 1) + \ln\left(\frac{4 + 6}{2\sqrt{4} \times 6}\right) (12p - 1)
\]

\[= 8.0172p - 5.8716.
\]

2.2. Irregularity Indices for Metal-Organic Network $\text{MON}_2(p)$. In this section, we will compute irregularity indices for the metal-organic network $\text{MON}_2(p)$. The molecular graph of the metal-organic network $\text{MON}_2(p)$ for $p = 2$ is given in Figure 3. It is clear from Figure 3 that there are three types of vertices in the molecular graph of
MON$_2$(p), i.e., 2, 3, and 4. The cardinality of vertices 2, 3, and 4 is 12$p + 18$, 24$p − 12$, and 12$p − 6$, respectively. The cardinality of the vertex set of MON$_2$(p) is 48$p$, i.e., |V (MON$_2$(p))| = 48$p$. There are five different types of edges present in the molecular graph of MON$_2$(p), i.e., {2, 3}, {2, 4}, {3, 3}, {3, 4}, and {4, 4}. Their cardinalities are 12$p + 24$, 12$p + 12$, 24$p − 24$, 12$p − 12$, and 12$p − 12$, respectively. The cardinality of the edge set of MON$_2$(p) is 72$p − 12$, i.e., |E(MON$_1$(p))| = 72$p − 12$.

The edge partition of the metal-organic network MON$_2$(p) is given in Table 3.

### Table 2: Partition of E(MON$_1$(p)).

| (d$_u$, d$_v$) | Frequency |
|--------------|-----------|
| (2, 3)       | 36        |
| (2, 4)       | 12 (3$p − 1$) |
| (2, 6)       | 24 (p − 1)  |
| (4, 6)       | 12 (p − 1)  |

### Table 3: Partition of E(MON$_2$(p)).

| (d$_u$, d$_v$) | Frequency |
|--------------|-----------|
| (2, 3)       | 12 (p + 2) |
| (2, 4)       | 12 (p + 1) |
| (3, 3)       | 24 (p − 1) |
| (3, 4)       | 12 (p − 1) |
| (4, 4)       | 12 (p − 1) |

#### Theorem 2. E(MON$_2$(p)) Let G be the metal-organic network MON$_2$(p). The irregularity indices are

1. VAR(G) = (2$p^2 + p − 1$)/4$p^2$
2. AL(G) = 48$p + 36$
3. IRI$_1$(G) = 6(24$p^2 + 10p − 11$)/$p$
4. IRI$_2$(G) = $\sqrt{(720p^2 − 312)/48p − ((72p − 12)/24p}$
5. IRI$_F$(G) = 72$p + 60$
6. IRIFW(G) = (72$p + 60$)/(720$p − 312$)
7. IRA(G) = 32$p + 16 + 2(2\sqrt{6} + 4\sqrt{3} + 3\sqrt{2})p − 8\sqrt{6} − 6\sqrt{2} + 8\sqrt{3}$
8. IRIB(G) = 216$p + 108 − (2(12\sqrt{6} + 24\sqrt{2} + 24\sqrt{3}))p − 48\sqrt{6} − 48\sqrt{2} + 48\sqrt{3}$
9. IRC(G) = $(2\sqrt{6} p^2 + 4\sqrt{6} p + 4\sqrt{3} p^2 + 4\sqrt{2} p^2 − 4\sqrt{3} p + 4\sqrt{2} p − 16p^2 − 8p − 1)/2p (6p − 1)$
10. IRDIF(G) = 34.9992$p + 30.9996$
11. IRL(G) = 16.8660$p + 14.3664$
12. IRLU(G) = 21.9996$p + 20.0004$
13. IRLF(G) = 16.8468$p + 14.8188$
14. IRLA(G) = 16.2276$p + 14.1708$
15. IRDL(G) = 29.8176$p + 21.5004$
16. IRGA(G) = 1.0740$p + 1.0716$

**Proof.** Using definitions of irregularity indices given in Table 1 and edge partition given in Table 3, we have
$$\text{VAR}(G) = \sum_{uv \in E(G)} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(G)}{n} - \left( \frac{2m}{n} \right)^2$$

$$= \left( \frac{456p - 132}{48p} \right) - \left( \frac{2(72p - 12)}{48p} \right)^2$$

$$= \left( \frac{2p^2 + p - 1}{4p^2} \right)$$

$$\text{AL}(G) = \sum_{uv \in E(G)} | d_u - d_v |$$

$$= |2 - 3|(12p + 24) + |2 - 4|(12p + 12) + |3 - 3|(24p - 24) + |3 - 4|(12p - 12) + |4 - 4|(12p - 12)$$

$$= 48p + 36,$$

$$\text{IR1}(G) = \sum_{uv \in E(G)} d_u^2 - \frac{2m}{n} \sum_{uv \in E(G)} d_u = F(G) - \left( \frac{2m}{n} \right) M_1(G)$$

$$= (1512p - 564) - \frac{2(72p - 12)}{48p} (456p - 132)$$

$$= \frac{6(24p^2 + 10p - 11)}{p},$$

$$\text{IR2}(G) = \sqrt{\sum_{uv \in E(G)} d_u d_v} - \frac{2m}{n} = \sqrt{\frac{M_1(G)}{m}} - \frac{2m}{n}$$

$$= \frac{720p - 312}{72p - 12} - \left( \frac{272p - 12}{48p} \right)$$

$$= \frac{720p - 312}{48p} - \frac{72p - 12}{24p}$$

$$\text{IRF}(G) = \sum_{uv \in E(G)} \left( d_u - d_v \right)^2$$

$$= (2 - 3)^2(12p + 24) + (2 - 4)^2(12p + 12) + (3 - 3)^2(24p - 24) + (3 - 4)^2(12p - 12) + (4 - 4)^2(12p - 12)$$

$$= 72p + 60,$$

$$\text{IRFW}(G) = \frac{\text{IRF}(G)}{M_1(G)}$$

$$= \frac{72p + 60}{720p - 312}$$

$$\text{IRA}(G) = \sum_{uv \in E(G)} \left( d_u^{1/2} - d_v^{1/2} \right)^2 = n - 2R(G) = (48p) - 2(8p - 8 + (3 \sqrt{2} + 4 \sqrt{3} + 2 \sqrt{6})p + (3 \sqrt{2} - 4 \sqrt{3} + 4 \sqrt{6}))$$

$$= 32p + 16 - 2(2 \sqrt{6} + 4 \sqrt{3} + 3 \sqrt{2})p - 8 \sqrt{6} - 6 \sqrt{2} + 8 \sqrt{3},$$

$$\text{IRB}(G) = \sum_{uv \in E(G)} \left( d_u^{1/2} - d_v^{1/2} \right)^2 = M_1(G) - 2RR(G)$$

$$= (456p - 132) - 2(120p - 120 + (24 \sqrt{2} + 24 \sqrt{3} + 12 \sqrt{6})p + (24 \sqrt{6} - 24 \sqrt{3} + 24 \sqrt{2}))$$

$$= 216p + 108 - (2(12 \sqrt{6} + 24 \sqrt{3} + 24 \sqrt{3}))p - 48 \sqrt{6} - 48 \sqrt{2} + 48 \sqrt{3},$$
\[ IRC(G) = \sum_{\text{ave}(G)} \sqrt{d_u d_v} - \frac{2m}{n} \quad \text{RR}(G) = \frac{2m}{n} \]
\[ = \frac{120p - 120 + (24\sqrt{2} + 24\sqrt{3} + 12\sqrt{6})p + (24\sqrt{6} - 24\sqrt{3} + 24\sqrt{2})}{2(72p - 12)} \]
\[ = \frac{2\sqrt{6}p^2 + 4\sqrt{6}p + 4\sqrt{3}p^2 + 4\sqrt{2}p^2 - 4\sqrt{3}p + 4\sqrt{2}p - 16p^2 - 8p - 1}{2p(6p - 1)} , \]

\[ \text{IRDIF}(G) = \sum_{\text{ave}(G)} \left| \frac{d_u - d_v}{d_u d_v} \right| \]
\[ = \left| \frac{2 - 3}{2} \right| (12p + 24) + \left| \frac{2 - 4}{2} \right| (12p + 12) + \left| \frac{3 - 3}{3} \right| (24p - 24) + \left| \frac{3 - 4}{4} \right| (12p - 12) + \left| \frac{4 - 4}{4} \right| (12p - 12) , \]
\[ = 34.9992p + 30.9996 , \]

\[ \text{IRL}(G) = \sum_{\text{ave}(G)} \left| \ln d_u - \ln d_v \right| \]
\[ = \ln 2 - \ln 3 | (12p + 24) + \ln 2 - \ln 4 | (12p + 12) + \ln 3 - \ln 3 | (24p - 24) + \ln 3 - \ln 4 | (12p - 12) \]
\[ + \ln 4 - \ln 4 | (12p - 12) \]
\[ = 16.8660p + 14.3664 , \]

\[ \text{IRLU}(G) = \sum_{\text{ave}(G)} \left| \frac{d_u - d_v}{\min(d_u,d_v)} \right| \]
\[ = \left| \frac{2 - 3}{2} \right| (12p + 24) + \left| \frac{2 - 4}{2} \right| (12p + 24) + \left| \frac{3 - 3}{3} \right| (24p - 24) + \left| \frac{3 - 4}{4} \right| (12p - 12) + \left| \frac{4 - 4}{4} \right| (12p - 12) , \]
\[ = 21.9996p + 20.0004 , \]

\[ \text{IRLF}(G) = \sum_{\text{ave}(E(G))} \left| \frac{d_u - d_v}{\sqrt{d_u d_v}} \right| \]
\[ = \left| \frac{2 - 3}{2} \right| (12p + 24) + \left| \frac{2 - 4}{2} \right| (12p + 12) + \left| \frac{3 - 3}{3} \right| (24p - 24) + \left| \frac{3 - 4}{4} \right| (12p - 12) + \left| \frac{4 - 4}{4} \right| (12p - 12) , \]
\[ = 16.8468p + 14.8188 , \]

\[ \text{IRLA}(G) = \sum_{\text{ave}(E(G))} \left| \frac{d_u - d_v}{d_u + d_v} \right| \]
\[ = 2 \left| \frac{2 - 3}{5} \right| (12p + 24) + 2 \left| \frac{2 - 4}{6} \right| (12p + 12) + 2 \left| \frac{3 - 3}{6} \right| (24p - 24) + 2 \left| \frac{3 - 4}{7} \right| (12p - 12) + 2 \left| \frac{4 - 4}{8} \right| (12p - 12) , \]
\[ = 16.2276p + 14.1708 , \]

\[ \text{IRI}(G) = \sum_{\text{ave}(E(G))} \ln \left[ 1 + \left| d_u - d_v \right| \right] \]
\[ = \ln \left[ 1 + \left| 2 - 3 \right| \right] (12p + 24) + \ln \left[ 1 + \left| 2 - 4 \right| \right] (12p + 12) + \ln \left[ 1 + \left| 3 - 3 \right| \right] (24p - 24) + \ln \left[ 1 + \left| 3 - 4 \right| \right] (12p - 12) \]
\[ + \ln \left[ 1 + \left| 4 - 4 \right| \right] (12p - 12) \]
\[ = 29.8176p + 21.5004 , \]

\[ \text{IRGA}(G) = \sum_{\text{ave}(E(G))} \ln \left( \frac{d_u + d_v}{2\sqrt{d_u d_v}} \right) \]
\[ = \ln \left( \frac{2 + 3}{2\sqrt{2} \times 3} \right) (12p + 24) + \ln \left( \frac{2 + 4}{2\sqrt{2} \times 4} \right) (12p + 12) + \ln \left( \frac{3 + 3}{2\sqrt{3} \times 3} \right) (24p - 24) + \ln \left( \frac{3 + 4}{2\sqrt{3} \times 4} \right) (12p - 12) \]
\[ + \ln \left( \frac{4 + 4}{2\sqrt{4} \times 4} \right) (12p - 12) \]
\[ = 1.0740p + 1.0716 . \]
Figure 4: Continued.
Figure 4: Continued.
3. Graphical Comparison

In this section, we give the graphical comparison of results of the metal-organic networks $\text{MON}_1(p)$ and $\text{MON}_2(p)$. In Figure 4, the red color is fixed for $\text{MON}_1(p)$ and the green color is fixed for $\text{MON}_2(p)$.

4. Conclusion

Topological indices associate a single number with a chemical structure. In quantitative structure activity relationship, knowledge of topological indices plays an important role. In this article, we computed sixteen irregularity indices for metal-organic networks $\text{MON}_1(p)$ and $\text{MON}_2(p)$. Most of the calculated topological indices depend on degree-based indices. In the field of chemical graph theory, molecular topology, and mathematical chemistry, a degree-based index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used, for example, in the development of quantitative structure activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. Our results are helpful in drug delivery and computer engineering.

Data Availability

All data required for this research are included within this paper.

Conflicts of Interest

The authors do not have any conflicts of interest.

Authors’ Contributions

All authors contributed equally in this paper.

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