Research Article

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The measure of irregularities of nanosheets

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Abstract: Nanosheets are two-dimensional polymeric materials, which are among the most active areas of investigation of chemistry and physics. Many diverse physicochemical properties of compounds are closely related to their underlying molecular topological descriptors. Thus, topological indices are fascinating beginning points to any statistical approach for attaining quantitative structure–activity (QSAR) and quantitative structure–property (QSPR) relationship studies. Irregularity measures are generally used for quantitative characterization of the topological structure of non-regular graphs. In various applications and problems in material engineering and chemistry, it is valuable to be well-informed of the irregularity of a molecular structure. Furthermore, the estimation of the irregularity of graphs is helpful for not only QSAR/QSPR studies but also different physical and chemical properties, including boiling and melting points, enthalpy of vaporization, entropy, toxicity, and resistance. In this article, we compute the irregularity measures of graphene nanosheet, *H*-naphthalenic nanosheet, SiO₂ nanosheet, and the nanosheet covered by C₃ and C₆.

Keywords: molecular graph, irregularity indices, nanosheets

1 Introduction

Nanotechnology is a fast-flourishing field that needs the production, design, and exploitation of structures at the

nanoscale. A nano-object with all three external dimensions in the nanoscale is described as a nanoparticle. One of the most outstanding applications of nanotechnology is in the field of medicine [15]. Nanomedicine plays an appreciable role in cancer treatment, drug delivery, and so on. Nanostructures, which have the scale less than 100 nm, include nanosheets, nanoparticles, and nanotubes. Nanosheets have a sharp edge and a large surface; due to these factors, they perform a prominent role in many applications such as optoelectronics [54], bioelectronics [35], energy storage [26,50,55], and catalysis [11]. Generally, nanosheets are inorganic materials, which can be formed from bulk crystalline layered materials that have excellent electrochemical performance, fascinating properties, high potential for separation applications, and functionalities because of their unusual molecular properties [57].

A modern trend in computational and mathematical chemistry is the use of topological approaches to characterize a molecular structure. These descriptors also have useful applications in quantitative structure–activity/quantitative structure–property (QSAR/QSPR) studies convenient for unknown drug discovery, molecular design, and hazard assessment of chemicals. Mathematical characterization of molecular graphs can be successfully obtained by the graph invariants [25,51]. For isomorphic graphs, the graph invariants of both graphs are either identical or have the same value. A topological index is a numeric measure that linked with a graph and characterizes its topology [28]. These graph invariants are sensitive to such structural aspects of molecules as symmetry, shape, size, the degree of complexity of atomic neighbourhoods, the content of heteroatoms, and bonding pattern. Topological descriptors have gained respectable significance in the last few years due to the ease of generation and the speed with which these calculations can be accomplished. These molecular descriptors are an appreciable part of the chemical graph theory. There are a lot of graph-related numerical descriptors, which are vitally important in nanotechnology and theoretical chemistry. Therefore, computation of these numerical descriptors is one of the attractive areas of research. Some prominent categories of numerical descriptors of graphs are distance-based, degree-based, and counting-related. Among degree-based descriptors, irregularity measures may play a prominent role in chemistry, particularly in the QSPR/QSAR studies [22,47] as well as in the network theory [9,12,48].

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For a comprehensive study of different types of topological indices, see [17–20,24,31,33,36,58,59] and references therein. Throughout this article, all graphs are finite, undirected, and simple. In the chemical graph theory, a graph in which every vertex has the degree less than 5 is called as a molecular graph. Molecular graphs of fullerenes, cycloalkanes, and annulenes are examples of regular molecular graphs. A large majority of molecular graphs is non-regular; some are more non-regular than the others. Let $M = (v(M), \mathcal{E}(M))$ be such a graph with vertex set $v(M)$ and edge set $\mathcal{E}(M)$. The order M is the number of elements in its vertex set and size is the number of edges in its edge set. The vertices of M correspond to atoms, and an edge is associated with the chemical bond between two vertices. Let us denote the degree of any vertex x of a graph M by $\omega_M(x)$ and is defined as the number of edges incident with x . For the detailed discussions about these graph invariants, we refer to [2–5,21,39,40,45,46,49,60]. Although plenty of studies have been executed on the distance-based and degree-based indices of molecular graphs, the analyses of irregularity measures for chemical structures still need attention. In [4,16,22,32], the irregularity measures of various chemical structures were investigated.

2 Irregularity indices of graphene

In this section, we find the irregularity indices of graphene. First, we describe the significance of graphene. It is constructed by carbon atoms. It is one of the most eye-catching nanomaterials due to its remarkable properties. It is used in a wide spectrum of implementations ranging from electronics to optics, biodevices, and sensors. Furthermore, it is the most efficient material for electromagnetic interference shielding [41,42,56]. Nowadays, graphene is attracting the interest of a lot of scientists, researchers, and industries worldwide due to its wide range of potential applications in different areas. Some topological aspects and applications of this structure are discussed in [6,34,43,44]. We denote graphene nanosheet by $M_1(a, c)$ with c rows of benzene rings and a benzene rings in each row (Figure 1).

Theorem 2.1. For $c = 1$ and $a \geq 1$, the irregularity indices of graphene $M_1(a, c)$ are as follows:

- (a) $\text{IRDIF}(M_1(a, c)) = \frac{10a - 10}{3}$,
- (b) $\text{AL}(M_1(a, c)) = 4a - 4$,
- (c) $\text{IRL}(M_1(a, c)) = (4a - 4) \left| \frac{\ln 2}{\ln 3} \right|$,
- (d) $\text{IRLU}(M_1(a, c)) = 2a - 2$,

Figure 1: 2D structure of graphene $M_1(a, c)$ with c rows and a benzene rings in each row.

- (e) $\text{IRLF}(M_1(a, c)) = \frac{4a - 4}{\sqrt{6}}$,
- (f) $\text{IRF}(M_1(a, c)) = 4a - 4$,
- (g) $\text{IRLA}(M_1(a, c)) = \frac{8a - 8}{5}$,
- (h) $\text{IRDI}(M_1(a, c)) = (4a - 4) \ln 2$,
- (i) $\text{IRA}(M_1(a, c)) = \frac{(10 - 4\sqrt{2}\sqrt{3})a - 10 + 4\sqrt{2}\sqrt{3}}{3}$,
- (j) $\text{IRGA}(M_1(a, c)) = (4a - 4) \ln \left(\frac{5\sqrt{6}}{12} \right)$,
- (k) $\text{IRB}(M_1(a, c)) = (-8\sqrt{2}\sqrt{3} + 20)a + 8\sqrt{2}\sqrt{3} - 20$, and
- (l) $\text{IRR}_t(M_1(a, c)) = 2a - 2$.

Proof. For $c = 1$ and $a \geq 1$, let us consider that the subset $\mathcal{E}_{kl} \subset \mathcal{E}(M_1(a, c))$ contains the edges having end vertices of degrees k and l . We divide $\mathcal{E}(M_1(a, c))$ into subsets on the basis of the degrees of end vertices of edges. The cardinalities of these subsets are $|\mathcal{E}_{22}| = 6$, $|\mathcal{E}_{23}| = 4a - 4$, and $|\mathcal{E}_{33}| = a - 1$. With the help of these data and the representations of irregularity indices shown in Table 1, the precise values of these indices can be computed in the following way:

$$\begin{aligned}
 & \text{IRDIF}(M_1(a, c)) \\
 &= \sum_{de \in \mathcal{E}(M_1(a, c))} \left| \frac{\omega_{M_1(a, c)}(d)}{\omega_{M_1(a, c)}(e)} - \frac{\omega_{M_1(a, c)}(e)}{\omega_{M_1(a, c)}(d)} \right| \\
 &= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) \left| \frac{\omega_{M_1(a, c)}(d)}{\omega_{M_1(a, c)}(e)} - \frac{\omega_{M_1(a, c)}(e)}{\omega_{M_1(a, c)}(d)} \right| \\
 &= 6 \left| \frac{2}{2} - \frac{2}{2} \right| + (4a - 4) \left| \frac{2}{3} - \frac{3}{2} \right| + (a - 1) \left| \frac{3}{3} - \frac{3}{3} \right| \\
 &= \frac{10a - 10}{3}.
 \end{aligned}$$

Table 1: Irregularity indices

Irregularity indices	Mathematical form
IRDIF index [47]	$\text{IRDIF}(M) = \sum_{de \in \mathcal{E}(M)} \left \frac{\omega_M(d)}{\omega_M(e)} - \frac{\omega_M(e)}{\omega_M(d)} \right $
AL index [7]	$\text{AL}(M) = \sum_{de \in \mathcal{E}(M)} \omega_M(d) - \omega_M(e) $
IRL index [53]	$\text{IRL}(M) = \sum_{de \in \mathcal{E}(M)} \ln(\omega_M(d)) - \ln(\omega_M(e)) $
IRLU index [53]	$\text{IRLU}(M) = \sum_{de \in \mathcal{E}(M)} \frac{ \omega_M(d) - \omega_M(e) }{\min(\omega_M(d), \omega_M(e))}$
IRLF index [47]	$\text{IRLF}(M) = \sum_{de \in \mathcal{E}(M)} \frac{ \omega_M(d) - \omega_M(e) }{\sqrt{(\omega_M(d) \omega_M(e))}}$
IRF index [14,23]	$\text{IRF}(M) = \sum_{de \in \mathcal{E}(M)} (\omega_M(d) - \omega_M(e))^2$
IRLA index [47]	$\text{IRLA}(M) = 2 \sum_{de \in \mathcal{E}(M)} \frac{ \omega_M(d) - \omega_M(e) }{(\omega_M(d) + \omega_M(e))}$
IRDI index [47]	$\text{IRDI}(M) = \sum_{de \in \mathcal{E}(M)} \ln \{1 + \omega_M(d) - \omega_M(e) \}$
IRA index [47]	$\text{IRA}(M) = \sum_{de \in \mathcal{E}(M)} \left(\frac{1}{\sqrt{\omega_M(d)}} - \frac{1}{\sqrt{\omega_M(e)}} \right)^2$
IRGA index [47]	$\text{IRGA}(M) = \sum_{de \in \mathcal{E}(M)} \ln \left(\frac{\omega_M(d) + \omega_M(e)}{2\sqrt{\omega_M(d)\omega_M(e)}} \right)$
IRB index [47]	$\text{IRB}(M) = \sum_{de \in \mathcal{E}(M)} (\sqrt{\omega_M(d)} - \sqrt{\omega_M(e)})^2$
IR R_t index [1]	$\text{IRR}_t(M) = \frac{1}{2} \sum_{de \in \mathcal{E}(M)} \omega_M(d) - \omega_M(e) $

$$\begin{aligned}
\text{AL}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= 6|2 - 2| + (a - 1)|3 - 3| + (4a - 4)|2 - 3| \\
&= 4a - 4.
\end{aligned}$$

$$\begin{aligned}
\text{IRL}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} |\ln(\omega_{M_1(a, c)}(d)) - \ln(\omega_{M_1(a, c)}(e))| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) |\ln(\omega_{M_1(a, c)}(d)) - \ln(\omega_{M_1(a, c)}(e))| \\
&= 6|\ln 2 - \ln 2| + (a - 1)|\ln 3 - \ln 3| \\
&\quad + (4a - 4)|\ln 2 - \ln 3| \\
&= (4a - 4) \left| \frac{\ln 2}{\ln 3} \right|.
\end{aligned}$$

$$\begin{aligned}
\text{IRLU}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\min(\omega_{M_1(a, c)}(d), \omega_{M_1(a, c)}(e))} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\min(\omega_{M_1(a, c)}(d), \omega_{M_1(a, c)}(e))} \\
&= 6 \frac{|2 - 2|}{\min(2, 2)} + (a - 1) \frac{|3 - 3|}{\min(3, 3)} + (4a - 4) \frac{|2 - 3|}{\min(2, 3)} \\
&= 2a - 2.
\end{aligned}$$

$$\begin{aligned}
\text{IRLF}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\sqrt{(\omega_{M_1(a, c)}(d) \omega_{M_1(a, c)}(e))}} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\sqrt{(\omega_{M_1(a, c)}(d) \omega_{M_1(a, c)}(e))}} \\
&= 6 \frac{|2 - 2|}{\sqrt{2 \times 2}} + (a - 1) \frac{|3 - 3|}{\sqrt{3 \times 3}} + (4a - 4) \frac{|2 - 3|}{\sqrt{2 \times 3}} \\
&= \frac{4a - 4}{\sqrt{6}}.
\end{aligned}$$

$$\begin{aligned}
\text{IRF}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} (\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e))^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) (\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e))^2 \\
&= 6(2 - 2)^2 + (a - 1)(3 - 3)^2 + (4a - 4)(2 - 3)^2 \\
&= 4a - 4.
\end{aligned}$$

$$\begin{aligned}
\text{IRLA}(M_1(a, c)) &= 2 \sum_{de \in \mathcal{E}(M_1(a, c))} \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{(\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e))} \\
&= 2 \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{(\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e))} \\
&= 2 \left(6 \frac{|2 - 2|}{2 + 2} + (a - 1) \frac{|3 - 3|}{3 + 3} + (4a - 4) \frac{|2 - 3|}{2 + 3} \right) \\
&= \frac{8a - 8}{5}.
\end{aligned}$$

$$\begin{aligned}
\text{IRDI}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} \ln \{1 + |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|\} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \ln \{1 + |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|\} \\
&= 6 \ln \{1 + |2 - 2|\} + (a - 1) \ln \{1 + |3 - 3|\} \\
&\quad + (4a - 4) \ln \{1 + |2 - 3|\} \\
&= (4a - 4) \ln 2.
\end{aligned}$$

$$\begin{aligned}
\text{IRA}(M_1(a, c)) &= \sum_{de \in \mathcal{E}(M_1(a, c))} \left(\frac{1}{\sqrt{\omega_{M_1(a, c)}(d)}} - \frac{1}{\sqrt{\omega_{M_1(a, c)}(e)}} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \left(\frac{1}{\sqrt{\omega_{M_1(a, c)}(d)}} - \frac{1}{\sqrt{\omega_{M_1(a, c)}(e)}} \right)^2 \\
&= 6 \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 + (a - 1) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \\
&\quad + (4a - 4) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 \\
&= \frac{(10 - 4\sqrt{2}\sqrt{3})a - 10 + 4\sqrt{2}\sqrt{3}}{3}.
\end{aligned}$$

$$\begin{aligned}
& \text{IRGA}(M_1(a, c)) \\
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \ln \left(\frac{\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e)}{2\sqrt{\omega_{M_1(a, c)}(d)\omega_{M_1(a, c)}(e)}} \right) \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \times \ln \left(\frac{\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e)}{2\sqrt{\omega_{M_1(a, c)}(d)\omega_{M_1(a, c)}(e)}} \right) \\
&= 6 \ln \left(\frac{2+2}{2\sqrt{2 \times 2}} \right) + (a-1) \ln \left(\frac{3+3}{2\sqrt{3 \times 3}} \right) \\
&\quad + (4a-4) \ln \left(\frac{2+3}{2\sqrt{2 \times 3}} \right) \\
&= (4a-4) \ln \left(\frac{5\sqrt{6}}{12} \right).
\end{aligned}$$

$$\begin{aligned}
& \text{IRB}(M_1(a, c)) \\
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \left(\sqrt{\omega_{M_1(a, c)}(d)} - \sqrt{\omega_{M_1(a, c)}(e)} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \left(\sqrt{\omega_{M_1(a, c)}(d)} - \sqrt{\omega_{M_1(a, c)}(e)} \right)^2 \\
&= 6(\sqrt{2} - \sqrt{2})^2 + (a-1)(\sqrt{3} - \sqrt{3})^2 \\
&\quad + (4a-4)(\sqrt{2} - \sqrt{3})^2 \\
&= (-8\sqrt{2}\sqrt{3} + 20)a + 8\sqrt{2}\sqrt{3} - 20.
\end{aligned}$$

$$\begin{aligned}
& \text{IRR}_t(M_1(a, c)) \\
&= \frac{1}{2} \sum_{de \in \mathcal{E}(M_1(a, c))} |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= \frac{1}{2} \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= \frac{1}{2} (6|2-2| + (a-1)|3-3| + (4a-4)|2-3|) \\
&= 2a - 2. \quad \square
\end{aligned}$$

Theorem 2.2. For $c \geq 2$ and $a \geq 1$, the irregularity indices of graphene $M_1(a, c)$ are as follows:

- (a) $\text{IRDIF}(M_1(a, c)) = \frac{10a + 5c - 10}{3}$,
- (b) $\text{AL}(M_1(a, c)) = 4a + 2c - 4$,
- (c) $\text{IRL}(M_1(a, c)) = (4a + 2c - 4) \left| \frac{\ln 2}{\ln 3} \right|$,
- (d) $\text{IRLU}(M_1(a, c)) = 2a + c - 2$,
- (e) $\text{IRLF}(M_1(a, c)) = \frac{\sqrt{6}(4a + 2c - 4)}{6}$,
- (f) $\text{IRF}(M_1(a, c)) = 4a + 2c - 4$,
- (g) $\text{IRLA}(M_1(a, c)) = \frac{2(4a + 2c - 4)}{5}$,
- (h) $\text{IRDI}(M_1(a, c)) = (4a + 2c - 4) \ln 2$,
- (i) $\text{IRA}(M_1(a, c)) = \frac{(5 - 2\sqrt{2}\sqrt{3})c + (10 - 4\sqrt{2}\sqrt{3})a - 10 + 4\sqrt{2}\sqrt{3}}{3}$,

$$(j) \text{IRGA}(M_1(a, c)) = (4a + 2c - 4) \ln \left(\frac{5\sqrt{6}}{12} \right),$$

$$(k) \text{IRB}(M_1(a, c)) = (-4\sqrt{2}\sqrt{3} + 10)c + (-8\sqrt{2}\sqrt{3} + 20)a + 8\sqrt{2}\sqrt{3} - 20, \text{ and}$$

$$(l) \text{IRR}_t(M_1(a, c)) = 2a + c - 2.$$

Proof. For $c \geq 2$ and $a \geq 1$, let us consider that the subset $\mathcal{E}_{kl} \subset \mathcal{E}(M_1(a, c))$ contains the edges having end vertices of degrees k and l . We divide $\mathcal{E}(M_1(a, c))$ into subsets on the basis of the degrees of end vertices of edges. The cardinalities of these subsets are $|\mathcal{E}_{22}| = c + 4$, $|\mathcal{E}_{23}| = 4a + 2c - 4$, and $|\mathcal{E}_{33}| = 3ac - 2a - c - 1$. With the help of these data and the representations of irregularity indices shown in Table 1, the precise values of these indices can be computed in the following way:

$$\begin{aligned}
& \text{IRDIF}(M_1(a, c)) \\
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \left| \frac{\omega_{M_1(a, c)}(d)}{\omega_{M_1(a, c)}(e)} - \frac{\omega_{M_1(a, c)}(e)}{\omega_{M_1(a, c)}(d)} \right| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) \left| \frac{\omega_{M_1(a, c)}(d)}{\omega_{M_1(a, c)}(e)} - \frac{\omega_{M_1(a, c)}(e)}{\omega_{M_1(a, c)}(d)} \right| \\
&= (c+4) \left| \frac{2}{2} - \frac{2}{2} \right| + (3ac - 2a - c - 1) \left| \frac{3}{3} - \frac{3}{3} \right| \\
&\quad + (4a + 2c - 4) \left| \frac{2}{3} - \frac{3}{2} \right| \\
&= \frac{10a + 5c - 10}{3}.
\end{aligned}$$

$$\begin{aligned}
& \text{AL}(M_1(a, c)) \\
&= \sum_{de \in \mathcal{E}(M_1(a, c))} |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= (c+4)|2-2| + (3ac - 2a - c - 1)|3-3| \\
&\quad + (4a + 2c - 4)|2-3| \\
&= 4a + 2c - 4.
\end{aligned}$$

$$\begin{aligned}
& \text{IRL}(M_1(a, c)) \\
&= \sum_{de \in \mathcal{E}(M_1(a, c))} |\ln(\omega_{M_1(a, c)}(d)) - \ln(\omega_{M_1(a, c)}(e))| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) |\ln(\omega_{M_1(a, c)}(d)) - \ln(\omega_{M_1(a, c)}(e))| \\
&= (c+4)|\ln 2 - \ln 2| \\
&\quad + (4a + 2c - 4)|\ln 2 - \ln 3| \\
&\quad + (3ac - 2a - c - 1)|\ln 3 - \ln 3| \\
&= (4a + 2c - 4) \left| \frac{\ln 2}{\ln 3} \right|.
\end{aligned}$$

IRLU($M_1(a, c)$)

$$\begin{aligned}
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\min(\omega_{M_1(a, c)}(d), \omega_{M_1(a, c)}(e))} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\min(\omega_{M_1(a, c)}(d), \omega_{M_1(a, c)}(e))} \\
&= (c+4) \frac{|2-2|}{\min(2, 2)} + (4a+2c-4) \frac{|2-3|}{\min(2, 3)} \\
&\quad + (3ac-2a-c-1) \frac{|3-3|}{\min(3, 3)} \\
&= 2a + c - 2.
\end{aligned}$$

IRLF($M_1(a, c)$)

$$\begin{aligned}
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\sqrt{(\omega_{M_1(a, c)}(d) \omega_{M_1(a, c)}(e))}} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{\sqrt{(\omega_{M_1(a, c)}(d) \omega_{M_1(a, c)}(e))}} \\
&= (c+4) \frac{|2-2|}{\sqrt{2 \times 2}} + (3ac-2a-c-1) \frac{|3-3|}{\sqrt{3 \times 3}} \\
&\quad + (4a+2c-4) \frac{|2-3|}{\sqrt{2 \times 3}} \\
&= \frac{\sqrt{6}(4a+2c-4)}{6}.
\end{aligned}$$

IRF($M_1(a, c)$)

$$\begin{aligned}
&= \sum_{de \in \mathcal{E}(M_1(a, c))} (\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e))^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) (\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e))^2 \\
&= (c+4)(2-2)^2 + (3ac-2a-c-1)(3-3)^2 \\
&\quad + (4a+2c-4)(2-3)^2 \\
&= 4a + 2c - 4.
\end{aligned}$$

IRLA($M_1(a, c)$)

$$\begin{aligned}
&= 2 \sum_{de \in \mathcal{E}(M_1(a, c))} \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{(\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e))} \\
&= 2 \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|}{(\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e))} \\
&= 2 \left((c+4) \frac{|2-2|}{2+2} + (3ac-2a-c-1) \frac{|3-3|}{3+3} \right. \\
&\quad \left. + (4a+2c-4) \frac{|2-3|}{2+3} \right) \\
&= \frac{2(4a+2c-4)}{5}.
\end{aligned}$$

IRDI($M_1(a, c)$)

$$\begin{aligned}
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \ln \{1 + |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|\} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \ln \{1 + |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)|\} \\
&= (c+4) \ln \{1 + |2-2|\} + (4a+2c-4) \ln \{1 + |2-3|\} \\
&\quad + (3ac-2a-c-1) \ln \{1 + |3-3|\} \\
&= (4a+2c-4) \ln 2.
\end{aligned}$$

IRA($M_1(a, c)$)

$$\begin{aligned}
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \left(\frac{1}{\sqrt{\omega_{M_1(a, c)}(d)}} - \frac{1}{\sqrt{\omega_{M_1(a, c)}(e)}} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \left(\frac{1}{\sqrt{\omega_{M_1(a, c)}(d)}} - \frac{1}{\sqrt{\omega_{M_1(a, c)}(e)}} \right)^2 \\
&= (c+4) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 + (3ac-2a-c-1) \\
&\quad \times \left(\frac{1}{\sqrt{\omega_{M_1(a, c)}(d)}} - \frac{1}{\sqrt{\omega_{M_1(a, c)}(e)}} \right)^2 \\
&= (c+4) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 + (4a+2c-4) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 \\
&= \frac{(5-2\sqrt{2}\sqrt{3})c + (10-4\sqrt{2}\sqrt{3})a - 10 + 4\sqrt{2}\sqrt{3}}{3}.
\end{aligned}$$

IRGA($M_1(a, c)$)

$$\begin{aligned}
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \ln \left(\frac{\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e)}{2\sqrt{\omega_{M_1(a, c)}(d) \omega_{M_1(a, c)}(e)}} \right) \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \ln \left(\frac{\omega_{M_1(a, c)}(d) + \omega_{M_1(a, c)}(e)}{2\sqrt{\omega_{M_1(a, c)}(d) \omega_{M_1(a, c)}(e)}} \right) \\
&= (c+4) \ln \left(\frac{2+2}{2\sqrt{2 \times 2}} \right) \\
&\quad + (3ac-2a-c-1) \ln \left(\frac{3+3}{2\sqrt{3 \times 3}} \right) \\
&\quad + (4a+2c-4) \ln \left(\frac{2+3}{2\sqrt{2 \times 3}} \right) \\
&= (4a+2c-4) \ln \left(\frac{5\sqrt{6}}{12} \right).
\end{aligned}$$

$$\begin{aligned}
& \text{IRB}(M_1(a, c)) \\
&= \sum_{de \in \mathcal{E}(M_1(a, c))} \left(\sqrt{\omega_{M_1(a, c)}(d)} - \sqrt{\omega_{M_1(a, c)}(e)} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) \\
&\quad \times \left(\sqrt{\omega_{M_1(a, c)}(d)} - \sqrt{\omega_{M_1(a, c)}(e)} \right)^2 \\
&= (c+4)(\sqrt{2}-\sqrt{2})^2 + (3ac-2a-c-1)(\sqrt{3}-\sqrt{3})^2 \\
&\quad + (4a+2c-4)(\sqrt{2}-\sqrt{3})^2 \\
&= (-4\sqrt{2}\sqrt{3}+10)c + (-8\sqrt{2}\sqrt{3}+20)a \\
&\quad + 8\sqrt{2}\sqrt{3}-20.
\end{aligned}$$

$$\begin{aligned}
& \text{IRR}_t(M_1(a, c)) \\
&= \frac{1}{2} \sum_{de \in \mathcal{E}(M_1(a, c))} |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= \frac{1}{2} \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) |\omega_{M_1(a, c)}(d) - \omega_{M_1(a, c)}(e)| \\
&= \frac{1}{2} ((c+4)|2-2| \\
&\quad + (3ac-2a-c-1)|3-3| \\
&\quad + (4a+2c-4)|2-3|) \\
&= 2a+c-2.
\end{aligned}$$

□

3 Irregularity indices of H -naphtalenic nanosheet

A carbon nanotube is made by a layer of carbon atoms, which are bonded together in a hexagonal mesh. These were discovered in [37]. A H -naphtalenic nanosheet $H(r, t)$ is formed by alternating squares C_4 , octagons C_8 , and hexagons C_6 , as shown in Figure 2. The vertex set $V(H(r, t))$ has the cardinality $10rt$, where r stands for the number of paired hexagons in each alternant row with C_4 cycle and t represents the number of rows consisting of C_4 . Some topological aspects of this structure are discussed in [30,29].

Theorem 3.1. *The irregularity indices of H -Naphtalenic nanosheet $H(r, t)$ are as follows:*

- (a) $\text{IRDIF}(H(r, t)) = \frac{20r+10t-20}{3},$
- (b) $\text{AL}(H(r, t)) = 8r+4t-8,$
- (c) $\text{IRL}(H(r, t)) = (8r+4t-8) \left| \frac{\ln 2}{\ln 3} \right|,$
- (d) $\text{IRLU}(H(r, t)) = 4r+2t-4,$
- (e) $\text{IRLF}(H(r, t)) = \frac{3\sqrt{2}+4\sqrt{3}+(6r+8t-9)\sqrt{6}}{6},$
- (f) $\text{IRF}(H(r, t)) = 8r+4t-8,$

- (g) $\text{IRLA}(H(r, t)) = \frac{16r+8t-16}{5},$
- (h) $\text{IRDI}(H(r, t)) = \ln 2(8r+4t-8),$
- (i) $\text{IRA}(H(r, t)) = \left(\frac{10}{3} - \frac{4\sqrt{2}\sqrt{3}}{3} \right)t + \left(\frac{20}{3} - \frac{8\sqrt{2}\sqrt{3}}{3} \right)r - \frac{20}{3} + \frac{8\sqrt{2}\sqrt{3}}{3},$
- (j) $\text{IRGA}(H(r, t)) = 4 \ln \left(\frac{5\sqrt{6}}{12} \right)t + 8 \ln \left(\frac{5\sqrt{6}}{12} \right)r - 8 \ln \left(\frac{5\sqrt{6}}{12} \right),$
- (k) $\text{IRB}(H(r, t)) = (-8\sqrt{2}\sqrt{3}+20)t + (-16\sqrt{2}\sqrt{3}+40)r + 16\sqrt{2}\sqrt{3}-40, \text{ and}$
- (l) $\text{IRR}_t(H(r, t)) = 3r+4t-3.$

Proof. Let us consider that the subset $\mathcal{E}_{kl} \subset \mathcal{E}(H(r, t))$ contains the edges having end vertices of degrees k and l . We divide $\mathcal{E}(H(r, t))$ into subsets on the basis of the degrees of end vertices of edges. The cardinalities of these subsets are $|\mathcal{E}_{22}| = 2t+4$, $|\mathcal{E}_{23}| = 4(2r+t-2)$, and $|\mathcal{E}_{33}| = r(15t-14)-4(t-1)$. With the help of these data and the representations of irregularity indices shown in Table 1, the precise values of these indices can be computed in the following way:

$$\begin{aligned}
& \text{IRDIF}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \left| \frac{\omega_{H(r, t)}(d)}{\omega_{H(r, t)}(e)} - \frac{\omega_{H(r, t)}(e)}{\omega_{H(r, t)}(d)} \right| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{23}} + \sum_{de \in \mathcal{E}_{33}} \right) \left| \frac{\omega_{H(r, t)}(d)}{\omega_{H(r, t)}(e)} - \frac{\omega_{H(r, t)}(e)}{\omega_{H(r, t)}(d)} \right| \\
&= (2t+4) \left| \frac{2}{2} - \frac{2}{2} \right| + (4(2r+t-2)) \left| \frac{2}{3} - \frac{3}{2} \right| \\
&\quad + (r(15t-14)-4(t-1)) \left| \frac{3}{3} - \frac{3}{3} \right| \\
&= \frac{20r+10t-20}{3}.
\end{aligned}$$

Figure 2: H -Naphtalenic nanosheet $H[r, t]$.

$$\begin{aligned}
& \text{AL}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} |\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) |\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)| \\
&= (2t + 4)|2 - 2| \\
&\quad + (r(15t - 14) - 4(t - 1))|3 - 3| \\
&\quad + (4(2r + t - 2))|2 - 3| \\
&= 8r + 4t - 8.
\end{aligned}$$

$$\begin{aligned}
& \text{IRL}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} |\ln(\omega_{H(r, t)}(d)) - \ln(\omega_{H(r, t)}(e))| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) |\ln(\omega_{H(r, t)}(d)) \\
&\quad - \ln(\omega_{H(r, t)}(e))| \\
&= (r(15t - 14) - 4(t - 1))|\ln 3 - \ln 3| \\
&\quad + (4(2r + t - 2))|\ln 2 - \ln 3| \\
&\quad + (2t + 4)|\ln 2 - \ln 2| \\
&= (8r + 4t - 8) \left| \frac{\ln 2}{\ln 3} \right|.
\end{aligned}$$

$$\begin{aligned}
& \text{IRLU}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \frac{|\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|}{\min(\omega_{H(r, t)}(d), \omega_{H(r, t)}(e))} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|}{\min(\omega_{H(r, t)}(d), \omega_{H(r, t)}(e))} \\
&= (2t + 4) \frac{|2 - 2|}{\min(2, 2)} \\
&\quad + (r(15t - 14) - 4(t - 1)) \frac{|3 - 3|}{\min(3, 3)} \\
&\quad + (4(2r + t - 2)) \frac{|2 - 3|}{\min(2, 3)} \\
&= 4r + 2t - 4.
\end{aligned}$$

$$\begin{aligned}
& \text{IRLF}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \frac{|\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|}{\sqrt{(\omega_{H(r, t)}(d) \omega_{H(r, t)}(e))}} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|}{\sqrt{(\omega_{H(r, t)}(d) \omega_{H(r, t)}(e))}} \\
&= (r(15t - 14) - 4(t - 1)) \frac{|3 - 3|}{\sqrt{3 \times 3}} \\
&\quad + (4(2r + t - 2)) \frac{|2 - 3|}{\sqrt{2 \times 3}} + (2t + 4) \frac{|2 - 2|}{\sqrt{2 \times 2}} \\
&= \frac{3\sqrt{2} + 4\sqrt{3} + (6r + 8t - 9)\sqrt{6}}{6}.
\end{aligned}$$

$$\begin{aligned}
& \text{IRF}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} (\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e))^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) (\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e))^2 \\
&= (r(15t - 14) - 4(t - 1))(3 - 3)^2 \\
&\quad + (4(2r + t - 2))(2 - 3)^2 + (2t + 4)(2 - 2)^2 \\
&= 8r + 4t - 8.
\end{aligned}$$

$$\begin{aligned}
& \text{IRLA}(H(r, t)) \\
&= 2 \sum_{de \in \mathcal{E}(H(r, t))} \frac{|\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|}{(\omega_{H(r, t)}(d) + \omega_{H(r, t)}(e))} \\
&= 2 \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{|\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|}{(\omega_{H(r, t)}(d) + \omega_{H(r, t)}(e))} \\
&= 2 \left((2t + 4) \frac{|2 - 2|}{2 + 2} \right. \\
&\quad \left. + (r(15t - 14) - 4(t - 1)) \frac{|3 - 3|}{3 + 3} \right. \\
&\quad \left. + (4(2r + t - 2)) \frac{|2 - 3|}{2 + 3} \right) \\
&= \frac{16r + 8t - 16}{5}.
\end{aligned}$$

$$\begin{aligned}
& \text{IRDI}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \ln \{1 + |\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|\} \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \ln \{1 + |\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)|\} \\
&= (2t + 4) \ln \{1 + |2 - 2|\} \\
&\quad + (4(2r + t - 2)) \ln \{1 + |2 - 3|\} \\
&\quad + (r(15t - 14) - 4(t - 1)) \ln \{1 + |3 - 3|\} \\
&= \ln 2(8r + 4t - 8).
\end{aligned}$$

$$\begin{aligned}
& \text{IRA}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \left(\frac{1}{\sqrt{\omega_{H(r, t)}(d)}} - \frac{1}{\sqrt{\omega_{H(r, t)}(e)}} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \left(\frac{1}{\sqrt{\omega_{H(r, t)}(d)}} - \frac{1}{\sqrt{\omega_{H(r, t)}(e)}} \right)^2 \\
&= (2t + 4) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 \\
&\quad + (r(15t - 14) - 4(t - 1)) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \\
&\quad + (4(2r + t - 2)) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 \\
&= \left(\frac{10}{3} - \frac{4\sqrt{2}\sqrt{3}}{3} \right) t + \left(\frac{20}{3} - \frac{8\sqrt{2}\sqrt{3}}{3} \right) r - \frac{20}{3} + \frac{8\sqrt{2}\sqrt{3}}{3}.
\end{aligned}$$

$$\begin{aligned}
& \text{IRGA}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \ln \left(\frac{\omega_{H(r, t)}(d) + \omega_{H(r, t)}(e)}{2\sqrt{\omega_{H(r, t)}(d)\omega_{H(r, t)}(e)}} \right) \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \ln \left(\frac{\omega_{H(r, t)}(d) + \omega_{H(r, t)}(e)}{2\sqrt{\omega_{H(r, t)}(d)\omega_{H(r, t)}(e)}} \right) \\
&= (2t + 4) \ln \left(\frac{2 + 2}{2\sqrt{2 \times 2}} \right) \\
&\quad + (r(15t - 14) - 4(t - 1)) \ln \left(\frac{3 + 3}{2\sqrt{3 \times 3}} \right) \\
&\quad + (4(2r + t - 2)) \ln \left(\frac{2 + 3}{2\sqrt{2 \times 3}} \right) \\
&= 4 \ln \left(\frac{5\sqrt{6}}{12} \right) t + 8 \ln \left(\frac{5\sqrt{6}}{12} \right) r - 8 \ln \left(\frac{5\sqrt{6}}{12} \right).
\end{aligned}$$

$$\begin{aligned}
& \text{IRB}(H(r, t)) \\
&= \sum_{de \in \mathcal{E}(H(r, t))} \left(\sqrt{\omega_{H(r, t)}(d)} - \sqrt{\omega_{H(r, t)}(e)} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} \right) \left(\sqrt{\omega_{H(r, t)}(d)} - \sqrt{\omega_{H(r, t)}(e)} \right)^2 \\
&= (2t + 4)(\sqrt{2} - \sqrt{2})^2 \\
&\quad + (r(15t - 14) - 4(t - 1))(\sqrt{3} - \sqrt{3})^2 \\
&\quad + (4(2r + t - 2))(\sqrt{2} - \sqrt{3})^2 \\
&= (-8\sqrt{2}\sqrt{3} + 20)t + (-16\sqrt{2}\sqrt{3} + 40)r \\
&\quad + 16\sqrt{2}\sqrt{3} - 40.
\end{aligned}$$

$$\begin{aligned}
& \text{IRR}_t(H(r, t)) \\
&= \frac{1}{2} \sum_{de \in \mathcal{E}(H(r, t))} |\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)| \\
&= \left(\sum_{de \in \mathcal{E}_{22}} + \sum_{de \in \mathcal{E}_{33}} + \sum_{de \in \mathcal{E}_{23}} \right) \frac{1}{2} |\omega_{H(r, t)}(d) - \omega_{H(r, t)}(e)| \\
&= \frac{1}{2} ((2t + 4)|2 - 2| \\
&\quad + (r(15t - 14) - 4(t - 1))|3 - 3| \\
&\quad + (4(2r + t - 2))|2 - 3|) \\
&= 4r + 2t - 4.
\end{aligned}$$

□

4 Irregularity indices of SiO₂ nanosheet

Silicon dioxide (SiO₂) is a prominent material. It has various applications in biology and semiconductor industry. It is used in tablet-making, as an anti-caking agent, as a disintegrant, as an absorbent, and in drugs as an inactive filler. In recent years, silica-based nanomaterials have gained significant interest because of their specific surface area, tunable particle

Figure 3: $M_3(4, 6)$.

Figure 4: $M_4(5, 6)$.

size, high drug loading capability, abundant Si–OH bonds on the particle surface, chemical and thermal stability, and sustained drug release thereby enhancing the bioavailability of drugs [10,27,38,52,61]. It has a giant covalent structure in which every oxygen atom is covalently bonded to two silicon atoms, and every silicon atom is covalently bonded to four oxygen atoms. The molecular structure of silicon dioxide is an octagon structure, and these octagons construct a SiO₂ layer structure. Let $M_3(q, n)$ be the molecular graph of the SiO₂ layer structure, where the number of rows is denoted by q and the number of columns by n , and the structure in Figure 4 is of dimension (5, 6). Some topological aspects of this structure are discussed in [8,13]. We now move on to attain the precise values of irregularity indices of SiO₂ nanosheet (Figure 4).

Theorem 4.1. *The irregularity indices of $M_3(q, n)$ are as follows:*

- (a) $\text{IRDIF}(M_3(q, n)) = \frac{21q + 21n + 12qn + 30}{2},$
- (b) $\text{AL}(M_3(q, n)) = 10q + 10n + 12 + 8qn,$

- (c) $\text{IRL}(M_3(q, n)) = -2 \ln 2(2qn + 3q + 3n + 4)$,
 (d) $\text{IRLU}(M_3(q, n)) = 8q + 8n + 12 + 4qn$,
 (e) $\text{IRLF}(M_3(q, n)) = 3q + 3n + 6 + \frac{(2q + 2n + 4qn)\sqrt{2}}{2}$,
 (f) $\text{IRF}(M_3(q, n)) = 26q + 26n + 52$,
 (g) $\text{IRLA}(M_3(q, n)) = \frac{2(28q + 28n + 36 + 20qn)}{15}$,
 (h) $\text{IRDI}(M_3(q, n)) = (4 \ln 2 + 2 \ln 3)n + (4 \ln 2 + 2 \ln 3)q + 8 \ln 2 + 4qn \ln 3$,
 (i) $\text{IRA}(M_3(q, n)) = (-2\sqrt{2} + 3)qn - q\sqrt{2} - n\sqrt{2} + 2q + 2n + 1$,
 (j) $\text{IRGA}(M_3(q, n)) = \left(2 \ln \left(\frac{5}{4}\right) + 2 \ln \left(\frac{3}{4}\right)\sqrt{2}\right)n + \left(2 \ln \left(\frac{5}{4}\right) + 2 \ln \left(\left(\frac{3}{4}\right)\sqrt{2}\right)\right)q + 4 \ln \left(\frac{5}{4}\right) + 4 \ln \left(\left(\frac{3}{4}\right)\sqrt{2}\right)qn$,
 (k) $\text{IRB}(M_3(q, n)) = (-16\sqrt{2} + 24)qn + (14 - 8\sqrt{2})n + (14 - 8\sqrt{2})q + 4$, and
 (l) $\text{IRR}_t(M_3(q, n)) = 5q + 5n + 6 + 4qn$.

Proof. Let us consider that the subset $\mathcal{E}_{kl} \subset \mathcal{E}(M_3(q, n))$ contains the edges having end vertices of degrees k and l . We divide $\mathcal{E}(M_3(q, n))$ into subsets on the basis of the degrees of end vertices of edges. The cardinalities of these subsets are $|\mathcal{E}_{14}| = 2q + 2n + 4$ and $|\mathcal{E}_{24}| = 2q + 2n + 4qn$. With the help of these data and the representations of irregularity indices shown in Table 1, the precise values of these indices can be computed in the following way:

$$\begin{aligned} \text{IRDIF}(M_3(q, n)) &= \sum_{de \in \mathcal{E}(M_3(q, n))} \left| \frac{\omega_{M_3(q, n)}(d)}{\omega_{M_3(q, n)}(e)} - \frac{\omega_{M_3(q, n)}(e)}{\omega_{M_3(q, n)}(d)} \right| \\ &= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \left| \frac{\omega_{M_3(q, n)}(d)}{\omega_{M_3(q, n)}(e)} - \frac{\omega_{M_3(q, n)}(e)}{\omega_{M_3(q, n)}(d)} \right| \\ &= (2q + 2n + 4) \left| \frac{1}{4} - \frac{4}{1} \right| + (2q + 2n + 4qn) \left| \frac{2}{4} - \frac{4}{2} \right| \\ &= \frac{21q + 21n + 12qn + 30}{2}. \end{aligned}$$

$$\begin{aligned} \text{AL}(M_3(q, n)) &= \sum_{de \in \mathcal{E}(M_3(q, n))} |\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)| \\ &= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) |\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)| \\ &= (2q + 2n + 4)|1 - 4| + (2q + 2n + 4qn)|2 - 4| \\ &= 10q + 10n + 12 + 8qn. \end{aligned}$$

$$\begin{aligned} \text{IRL}(M_3(q, n)) &= \sum_{de \in \mathcal{E}(M_3(q, n))} |\ln(\omega_{M_3(q, n)}(d)) - \ln(\omega_{M_3(q, n)}(e))| \\ &= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) |\ln(\omega_{M_3(q, n)}(d)) - \ln(\omega_{M_3(q, n)}(e))| \\ &= (2q + 2n + 4)|\ln 1 - \ln 4| + (2q + 2n + 4qn)|\ln 2 - \ln 4| \\ &= -2 \ln 2(2qn + 3q + 3n + 4). \end{aligned}$$

$$\begin{aligned} \text{IRLU}(M_3(q, n)) &= \sum_{de \in \mathcal{E}(M_3(q, n))} \frac{|\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|}{\min(\omega_{M_3(q, n)}(d), \omega_{M_3(q, n)}(e))} \\ &= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \frac{|\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|}{\min(\omega_{M_3(q, n)}(d), \omega_{M_3(q, n)}(e))} \\ &= (2q + 2n + 4) \frac{|1 - 4|}{\min(1, 4)} + (2q + 2n + 4qn) \frac{|2 - 4|}{\min(2, 4)} \\ &= 8q + 8n + 12 + 4qn. \end{aligned}$$

$$\begin{aligned} \text{IRLF}(M_3(q, n)) &= \sum_{de \in \mathcal{E}(M_3(q, n))} \frac{|\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|}{\sqrt{(\omega_{M_3(q, n)}(d)\omega_{M_3(q, n)}(e))}} \\ &= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \frac{|\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|}{\sqrt{(\omega_{M_3(q, n)}(d)\omega_{M_3(q, n)}(e))}} \\ &= (2q + 2n + 4) \frac{|1 - 4|}{\sqrt{1 \times 4}} + (2q + 2n + 4qn) \frac{|2 - 4|}{\sqrt{2 \times 4}} \\ &= 3q + 3n + 6 + \frac{(2q + 2n + 4qn)\sqrt{2}}{2}. \end{aligned}$$

$$\begin{aligned} \text{IRF}(M_3(q, n)) &= \sum_{de \in \mathcal{E}(M_3(q, n))} (\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e))^2 \\ &= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) (\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e))^2 \\ &= (2q + 2n + 4)(1 - 4)^2 + (2q + 2n + 4qn)(2 - 4)^2 \\ &= 26q + 26n + 36 + 16qn. \end{aligned}$$

$$\begin{aligned} \text{IRLA}(M_3(q, n)) &= 2 \sum_{de \in \mathcal{E}(M_3(q, n))} \frac{|\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|}{(\omega_{M_3(q, n)}(d) + \omega_{M_3(q, n)}(e))} \\ &= 2 \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \frac{|\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|}{(\omega_{M_3(q, n)}(d) + \omega_{M_3(q, n)}(e))} \\ &= 2 \left((2q + 2n + 4) \frac{|1 - 4|}{1 + 4} + (2q + 2n + 4qn) \frac{|2 - 4|}{2 + 4} \right) \\ &= \frac{2(28q + 28n + 36 + 20qn)}{15}. \end{aligned}$$

$$\begin{aligned}
& \text{IRDI}(M_3(q, n)) \\
&= \sum_{de \in \mathcal{E}(M_3(q, n))} \ln \{1 + |\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|\} \\
&= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \ln \{1 + |\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)|\} \\
&= (2q + 2n + 4) \ln \{1 + |1 - 4|\} \\
&\quad + (2q + 2n + 4qn) \ln \{1 + |2 - 4|\} \\
&= (4 \ln 2 + 2 \ln 3)n + (4 \ln 2 + 2 \ln 3)q \\
&\quad + 8 \ln 2 + 4qn \ln 3.
\end{aligned}$$

$$\begin{aligned}
& \text{IRA}(M_3(q, n)) \\
&= \sum_{de \in \mathcal{E}(M_3(q, n))} \left(\frac{1}{\sqrt{\omega_{M_3(q, n)}(d)}} - \frac{1}{\sqrt{\omega_{M_3(q, n)}(e)}} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \left(\frac{1}{\sqrt{\omega_{M_3(q, n)}(d)}} - \frac{1}{\sqrt{\omega_{M_3(q, n)}(e)}} \right)^2 \\
&= (2q + 2n + 4) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}} \right)^2 \\
&\quad + (2q + 2n + 4qn) \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{4}} \right)^2 \\
&= (-2\sqrt{2} + 3)qn - q\sqrt{2} - n\sqrt{2} + 2q + 2n + 1.
\end{aligned}$$

$$\begin{aligned}
& \text{IRGA}(M_3(q, n)) \\
&= \sum_{de \in \mathcal{E}(M_3(q, n))} \ln \left(\frac{\omega_{M_3(q, n)}(d) + \omega_{M_3(q, n)}(e)}{2\sqrt{\omega_{M_3(q, n)}(d)\omega_{M_3(q, n)}(e)}} \right) \\
&= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \ln \left(\frac{\omega_{M_3(q, n)}(d) + \omega_{M_3(q, n)}(e)}{2\sqrt{\omega_{M_3(q, n)}(d)\omega_{M_3(q, n)}(e)}} \right) \\
&= (2q + 2n + 4) \ln \left(\frac{1 + 4}{2\sqrt{1 \times 4}} \right) \\
&\quad + (2q + 2n + 4qn) \ln \left(\frac{2 + 4}{2\sqrt{2 \times 4}} \right) \\
&= \left(\ln \left(\frac{5}{4} \right) + \ln \left(\frac{3}{4} \sqrt{2} \right) \right) 2n \\
&\quad + \left(\ln \left(\frac{5}{4} \right) + \ln \left(\left(\frac{3}{4} \right) \sqrt{2} \right) \right) 2q \\
&\quad + 4 \ln \left(\frac{5}{4} \right) + 4 \ln \left(\left(\frac{3}{4} \right) \sqrt{2} \right) qn.
\end{aligned}$$

$$\begin{aligned}
& \text{IRB}(M_3(q, n)) \\
&= \sum_{de \in \mathcal{E}(M_3(q, n))} \left(\sqrt{\omega_{M_3(q, n)}(d)} - \sqrt{\omega_{M_3(q, n)}(e)} \right)^2 \\
&= \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) \left(\sqrt{\omega_{M_3(q, n)}(d)} - \sqrt{\omega_{M_3(q, n)}(e)} \right)^2 \\
&= (2q + 2n + 4)(\sqrt{1} - \sqrt{4})^2 \\
&\quad + (2q + 2n + 4qn)(\sqrt{2} - \sqrt{4})^2 \\
&= (-16\sqrt{2} + 24)qn \\
&\quad + (14 - 8\sqrt{2})n + (14 - 8\sqrt{2})q + 4.
\end{aligned}$$

$$\begin{aligned}
& \text{IRR}_t(M_3(q, n)) \\
&= \frac{1}{2} \sum_{de \in \mathcal{E}(M_3(q, n))} |\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)| \\
&= \frac{1}{2} \left(\sum_{de \in \mathcal{E}_{14}} + \sum_{de \in \mathcal{E}_{24}} \right) |\omega_{M_3(q, n)}(d) - \omega_{M_3(q, n)}(e)| \\
&= \frac{1}{2} ((2q + 2n + 4)|1 - 4| \\
&\quad + (2q + 2n + 4qn)|2 - 4|) \\
&= 5q + 5n + 6 + 4qn.
\end{aligned}$$

□

5 Irregularity indices of nanosheet covered by C_3 and C_6

In this section, we compute irregularity indices of nanosheet covered by C_3 and C_6 . We represent the molecular graph of it by $M_4(p, r)$, where p stands for the number of hexagons in each row and r stands for the number of hexagons in each column. Chemical graph of this nanosheet has consecutive columns of hexagons C_6 and triangles C_3 .

Theorem 5.1. *The irregularity indices of nanosheet $M_4(p, r)$ are as follows:*

- $\text{IRDIF}(M_4(p, r)) = \frac{14p + 27r - 21}{6},$
- $\text{AL}(M_4(p, r)) = 4p + 6r - 6,$
- $\text{IRL}(M_4(p, r)) = 4r \left\lfloor \ln \left(\frac{2}{3} \right) \right\rfloor + (4p + 2r - 6) \left\lfloor \ln \left(\frac{3}{4} \right) \right\rfloor,$
- $\text{IRLU}(M_4(p, r)) = \frac{4p + 8r - 6}{3},$
- $\text{IRLF}(M_4(p, r)) = \frac{\sqrt{3}r + 2\sqrt{6}r + 2p\sqrt{3} - 3\sqrt{3}}{3},$
- $\text{IRF}(M_4(p, r)) = 4p + 6r - 6,$
- $\text{IRLA}(M_4(p, r)) = \frac{2(20p + 38r - 30)}{35},$
- $\text{IRDI}(M_4(p, r)) = \ln 2(4p + 6r - 6),$
- $\text{IRA}(M_4(p, r))$
 $= \frac{-21 + 12\sqrt{3} + (14 - 8\sqrt{3})p + (27 - 4\sqrt{3} - 8\sqrt{2}\sqrt{3})r}{6},$
- $\text{IRGA}(M_4(p, r)) = 2 \ln \left(\frac{7\sqrt{3}}{12} \right)$
 $+ 4 \ln \left(\frac{5\sqrt{6}}{12} \right) r + 4 \ln \left(\frac{5\sqrt{3}}{12} \right) p - 6 \ln \left(\frac{7\sqrt{3}}{12} \right),$
- $\text{IRB}(M_4(p, r)) = (-8\sqrt{2}\sqrt{3} - 8\sqrt{3} + 34)r$
 $+ (-16\sqrt{3} + 28)p + 24\sqrt{3} - 42, \text{ and}$
- $\text{IRR}_t(M_4(p, r)) = 2p + 3r - 3.$

Proof. Let us consider that the subset $\mathcal{E}_{jk} \subset \mathcal{E}(M_4(p, r))$ contains the edges having end vertices of degrees k and l . We divide $\mathcal{E}(M_4(p, r))$ into subsets on the basis of the

degrees of end vertices of edges. The cardinalities of these subsets are $|\mathcal{E}_{22}| = 4$, $|\mathcal{E}_{33}| = 4p - 6$, $|\mathcal{E}_{34}| = 4p + 2r - 6$, $|\mathcal{E}_{23}| = 4r$, and $|\mathcal{E}_{44}| = 6pr - 6p - 7r + 7$. With the help of these data and the representations of irregularity indices shown in Table 1, the precise values of these indices can be computed in the following way:

$$\text{IRDIF}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} \left| \frac{\omega_{M_4(p, r)}(d)}{\omega_{M_4(p, r)}(e)} - \frac{\omega_{M_4(p, r)}(e)}{\omega_{M_4(p, r)}(d)} \right| \\ &= 4 \left| \frac{2}{2} - \frac{2}{2} \right| + 4r \left| \frac{2}{3} - \frac{3}{2} \right| + (4p - 6) \left| \frac{3}{3} - \frac{3}{3} \right| \\ &\quad + (4p + 2r - 6) \left| \frac{3}{4} - \frac{4}{3} \right| \\ &\quad + (6pr - 6p - 7r + 7) \left| \frac{4}{4} - \frac{4}{4} \right| \\ &= \frac{14p + 27r - 21}{6}. \end{aligned}$$

$$\text{AL}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} |\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e)| \\ &= 4|2 - 2| + (4p - 6)|3 - 3| \\ &\quad + 4r|2 - 3| + (4p + 2r - 6)|3 - 4| \\ &\quad + (6pr - 6p - 7r + 7)|4 - 4| \\ &= 4p + 6r - 6. \end{aligned}$$

$$\text{IRL}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} |\ln(\omega_{M_4(p, r)}(d)) - \ln(\omega_{M_4(p, r)}(e))| \\ &= 4|\ln 2 - \ln 2| + (4p - 6)|\ln 3 - \ln 3| \\ &\quad + 4r|\ln 2 - \ln 3| + (4p + 2r - 6)|\ln 3 - \ln 4| \\ &\quad + (6pr - 6p - 7r + 7)|\ln 4 - \ln 4| \\ &= 4r \left| \ln \left(\frac{2}{3} \right) \right| + (4p + 2r - 6) \left| \ln \left(\frac{3}{4} \right) \right|. \end{aligned}$$

$$\text{IRLU}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} \frac{|\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e)|}{\min(\omega_{M_4(p, r)}(d), \omega_{M_4(p, r)}(e))} \\ &= 4 \frac{|2 - 2|}{\min(2, 2)} + (4p - 6) \frac{|3 - 3|}{\min(3, 3)} + 4r \frac{|2 - 3|}{\min(2, 3)} \\ &\quad + (4p + 2r - 6) \frac{|3 - 4|}{\min(3, 4)} \\ &\quad + (6pr - 6p - 7r + 7) \frac{|4 - 4|}{\min(4, 4)} \\ &= \frac{4p + 8r - 6}{3}. \end{aligned}$$

$$\text{IRLF}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} \frac{|\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e)|}{\sqrt{(\omega_{M_4(p, r)}(d) \omega_{M_4(p, r)}(e))}} \\ &= 4 \frac{|2 - 2|}{\sqrt{2 \times 2}} + (4p - 6) \frac{|3 - 3|}{\sqrt{3 \times 3}} + 4r \frac{|2 - 3|}{\sqrt{2 \times 3}} \\ &\quad + (4p + 2r - 6) \frac{|3 - 4|}{\sqrt{3 \times 4}} \\ &\quad + (6pr - 6p - 7r + 7) \frac{|4 - 4|}{\sqrt{4 \times 4}} \\ &= \frac{\sqrt{3}r + 2\sqrt{6}r + 2p\sqrt{3} - 3\sqrt{3}}{3}. \end{aligned}$$

$$\text{IRF}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} (\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e))^2 \\ &= 4(2 - 2)^2 + (4p - 6)(3 - 3)^2 + 4r(2 - 3)^2 \\ &\quad + (4p + 2r - 6)(3 - 4)^2 \\ &\quad + (6pr - 6p - 7r + 7)(4 - 4)^2 \\ &= 4p + 6r - 6. \end{aligned}$$

$$\text{IRLA}(M_4(p, r))$$

$$\begin{aligned} &= 2 \sum_{de \in \mathcal{E}(M_4(p, r))} \frac{|\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e)|}{(\omega_{M_4(p, r)}(d) + \omega_{M_4(p, r)}(e))} \\ &= 2 \left(4 \frac{|2 - 2|}{2 + 2} + (4p - 6) \frac{|3 - 3|}{3 + 3} + 4r \frac{|2 - 3|}{2 + 3} \right) \\ &\quad + 2 \left((4p + 2r - 6) \frac{|3 - 4|}{3 + 4} \right. \\ &\quad \left. + (6pr - 6p - 7r + 7) \frac{|4 - 4|}{4 + 4} \right) \\ &= \frac{2(20p + 38r - 30)}{35}. \end{aligned}$$

$$\text{IRDI}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} \ln \{1 + |\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e)|\} \\ &= 4 \ln \{1 + |2 - 2|\} + (4p - 6) \ln \{1 + |3 - 3|\} \\ &\quad + (4p + 2r - 6) \ln \{1 + |3 - 4|\} + 4r \ln \{1 + |2 - 3|\} \\ &\quad + (6pr - 6p - 7r + 7) \ln \{1 + |4 - 4|\} \\ &= \ln 2(4p + 6r - 6). \end{aligned}$$

$$\text{IRA}(M_4(p, r))$$

$$\begin{aligned} &= \sum_{de \in \mathcal{E}(M_4(p, r))} \left(\frac{1}{\sqrt{\omega_{M_4(p, r)}(d)}} - \frac{1}{\sqrt{\omega_{M_4(p, r)}(e)}} \right)^2 \\ &= 4 \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 + (4p - 6) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \\ &\quad + 4r \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 + (4p + 2r - 6) \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}} \right)^2 \\ &\quad + (6pr - 6p - 7r + 7) \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{4}} \right)^2 \\ &= \frac{-21 + 12\sqrt{3} + (14 - 8\sqrt{3})p + (27 - 4\sqrt{3} - 8\sqrt{2}\sqrt{3})r}{6}. \end{aligned}$$

$$\text{IRGA}(M_4(p, r))$$

$$= \sum_{de \in E(M_4(p, r))} \ln \left(\frac{\omega_{M_4(p, r)}(d) + \omega_{M_4(p, r)}(e)}{2\sqrt{\omega_{M_4(p, r)}(d)\omega_{M_4(p, r)}(e)}} \right)$$

$$= 4 \ln \left(\frac{2+2}{2\sqrt{2 \times 2}} \right) + (4p-6) \ln \left(\frac{3+3}{2\sqrt{3 \times 3}} \right)$$

$$+ 4r \ln \left(\frac{2+3}{2\sqrt{2 \times 3}} \right) + (4p+2r-6) \ln \left(\frac{3+4}{2\sqrt{3 \times 4}} \right)$$

$$+ (6pr-6p-7r+7) \ln \left(\frac{4+4}{2\sqrt{4 \times 4}} \right)$$

$$= 2 \ln \left(\frac{7\sqrt{3}}{12} \right) + 4 \ln \left(\frac{5\sqrt{6}}{12} \right) r$$

$$+ 4 \ln \left(\frac{5\sqrt{3}}{12} \right) p - 6 \ln \left(\frac{7\sqrt{3}}{12} \right).$$

$$\text{IRB}(M_4(p, r))$$

$$= \sum_{de \in E(M_4(p, r))} \left(\sqrt{\omega_{M_4(p, r)}(d)} - \sqrt{\omega_{M_4(p, r)}(e)} \right)^2$$

$$= 4(\sqrt{2} - \sqrt{2})^2 + (4p-6)(\sqrt{3} - \sqrt{3})^2$$

$$+ 4r(\sqrt{2} - \sqrt{3})^2 + (4p+2r-6)(\sqrt{3} - \sqrt{4})^2$$

$$+ (6pr-6p-7r+7)(\sqrt{4} - \sqrt{4})^2$$

$$= (-8\sqrt{2}\sqrt{3} - 8\sqrt{3} + 34)r$$

$$+ (-16\sqrt{3} + 28)p + 24\sqrt{3} - 42.$$

$$\text{IRR}_t(M_4(p, r))$$

$$= \frac{1}{2} \sum_{de \in E(M_4(p, r))} |\omega_{M_4(p, r)}(d) - \omega_{M_4(p, r)}(e)|$$

$$= \frac{1}{2}(4|2-2| + (4p-6)|3-3| + 4r|2-3|)$$

$$+ \frac{1}{2}((4p+2r-6)|3-4|$$

$$+ (6pr-6p-7r+7)|4-4|)$$

$$= 2p + 3r - 3.$$

□

6 Conclusion

In the past few years, the problems of computational physics on specific molecular structures have gained attention in theoretical physics. Topological indices facilitate the researchers by giving knowledge about the structure of materials that reduce their workload. Reckoning the topological indices of a compound may assist in the assessment of its medicinal behaviour. Day by day, the theory of understanding compounds through topological indices achieved great significance in the area of medicine considering that it needs no chemical-related apparatus to study. Topological indices are being widely studied for various graphs, particularly for the chemical graphs. Hence, the irregularity indices for the molecular

graphs of four types of nanosheets are manifested by using mathematical derivation approach in this article. These outcomes can also perform a valuable role in the findings on the significance of the considered structures.

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