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Retraction

Retracted: Topological Aspects of Certain Covalent Organic Frameworks and Metal Organic Frameworks

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Manipulated or compromised peer review

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] G. Zhang, M. Azeem, A. Aslam, S. Yousaf, and S. Kanwal, "Topological Aspects of Certain Covalent Organic Frameworks and Metal Organic Frameworks," *Journal of Function Spaces*, vol. 2022, Article ID 5426037, 9 pages, 2022.

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Research Article

Topological Aspects of Certain Covalent Organic Frameworks and Metal Organic Frameworks

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Topological indices are numerical numbers assigned to molecular graphs and are expected to predict certain of its physical or chemical properties. Metal-organic frameworks (MOFs) are inorganic/organic porous crystalline materials with a regular array of positively charged metal ions which surrounds organic linkers. Covalent organic frameworks (COFs) are a class of organic polymers with highly ordered structure and permanent porosity. In this work, we have computed some degree-based topological indices of naphthalene metal-organic frameworks and thiophene-based covalent triazine framework.

1. Introduction

Metal-organic frameworks (MOFs) are inorganic/organic porous crystalline materials with regular array of positively charged metal ions which surrounds organic linkers. The arm of linkers joins the metal ions to form a repeating cage like structure. In 1959, Kinoshita et al. [1] reported the first MOF. After that, many researchers synthesize different MOFs with potential applications. MOFs have large internal surface area due to their hollow structure. The applications of MOFs are in drug delivery [2–4], gas catalysis [5–7], separation [8, 9], and absorption [10–14].

Covalent organic frameworks (COFs) are a class of organic polymers with highly ordered structure and permanent porosity. An important property of COFs is that they are synthetically controllable, structurally predesignable, and functionally manageable. The COFs were introduced by Cote et al. [15] as the new type of crystalline porous organic polymers. The COFs' ability of self-heating and thermodynamically controlled covalent bonding are helpful in forming long range ordered crystalline structures. An important property of COFs is that they exhibit excellent chemical stability in organic solvents. The high stability of COFs is due to metal-free structures and pure covalently bonding of COFs. As compared to other inorganic zoelites and porous silicas, COFs have large pores. This property of COFs is helpful in catalysis where large pores increase the speed of desorption of product and diffusion of reactant, thereby enhancing selectivity and product yield [16].

In mathematical chemistry, a molecular graph is a representation of structural formula of a chemical compound. The atoms of molecule are represented by atom and the bonds represent the edges between the atoms. Let $G=(V, E)$ be a graph, where V denotes the vertex set and E denotes the edge set. Any two vertices $x, y \in V(G)$ are adjacent if there is an edge between x and y. The set of neighbors N_x

of $x \in V(G)$ is defined as $N_x = \{y \in V(G): xy \in E(G)\}$. The degree of $x \in V(G)$ is the cardinality of N_x and is denoted by d_x. The sum of degrees of the neighbor of $x \in V(G)$ is denoted by S_x and is defined as $S_x = \{\sum d_y : y \in N_x\}$. For basic terminologies related to graph theory, see [17].

Molecular descriptors are useful in finding suitable predictive models. These descriptors are categorized as local and global in accordance to the characterization of molecular structure. Molecular descriptors characterize a particular aspect of a molecule [18]. Among molecular descriptors, the topological indices (TIs) are most useful [19–23]. TIs are numerical numbers assigned to a chemical structure used to correlate chemical structure with its physical/chemical properties [18]. Weiner was the first to introduce a topological index, namely, Weiner index [24], while he was working on the boiling point of Praffin. After the introduction of connectivity indices and their applications, these descriptors were widely studied [18]. Randic [25] introduced the first degree-based topological index denoted by $R_{(-1)/2}(G)$ and is defined as

$$R_{-1/2}(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d_x d_y}}. \quad (1)$$

It has been observed by Randic that this index has a very good correlation with certain properties of alkanes: enthalpies of formation, boiling points, surface areas, chromatographic retention times, and parameters in the Antoine equation for vapor pressure. This index was later generalized by Bollobas and Erdos [26] by replacing −1/2 with any real number α. The generalized Randic index is defined as

$$R_\alpha(G) = \sum_{xy \in E(G)} \left(d_x d_y\right)^\alpha. \quad (2)$$

In 1972. Gutman and Trinajsti [27] introduced the Zagreb indices and applied them to the branching problem. The first Zagreb index M_1 and second Zagreb index M_2 are defined as follows:

$$\begin{aligned} M_1(G) &= \sum_{xy \in E(G)} \left(d_x + d_y\right), \\ M_2(G) &= \sum_{xy \in E(G)} \left(d_x \times d_y\right). \end{aligned} \quad (3)$$

Shirdel et al. [28] raised up the hyper-Zagreb index:

$$\mathrm{HM}(G) = \sum_{xy \in E(G)} \left[d_x + d_y\right]^2. \quad (4)$$

The Zagreb indices and their variants have been used to study molecular complexity [29–33], chirality [34], ZE-isomerism [35], and heterosystems [36].

The sum connectivity index was proposed by Zhou and Trinajstic [37], and it was observed that the sum connectivity index correlate well with the π electron energy of hydrocarbons. It is denoted and defined as

$$\mathrm{SCI}(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{d_x + d_y}}. \quad (5)$$

Recently, Zhou and Trinajstic [38] extended this concept to the general sum connectivity index. The general sum connectivity index is defined as

$$\chi_\alpha(G) = \sum_{xy \in E(G)} \left(d_x + d_y\right)^\alpha. \quad (6)$$

In 1998, Estrada et al. [39] proposed the atom bond connectivity (ABC) index, defined as

$$\mathrm{ABC}(G) = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}. \quad (7)$$

The ABC index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [39, 40].

Recently, the well-known connectivity topological index is geometric-arithmatic (GA) which was introduced by Vukičević and Furtula in [41]. For a graph G, the GA index is denoted and defined as

$$\mathrm{GA}(G) = \sum_{xy \in E(G)} \frac{2\sqrt{d_x d_y}}{d_x + d_y}. \quad (8)$$

It has been demonstrated, on the example of octane isomers, that GA index is well-correlated with a variety of physicochemical properties.

The fourth version of the atom-bond connectivity index ABC_4 was introduced by Ghorbani et al. [34] in 2010 and is defined as

$$\mathrm{ABC}_4(G) = \sum_{xy \in E(G)} \sqrt{\frac{S_x + S_y - 2}{S_x S_y}}. \quad (9)$$

The fifth version of topological index GA is proposed by Graovac et al. [42] in 2011 which is expressed as

$$GA_5(G) = \sum_{xy \in E(G)} \frac{2\sqrt{S_x S_y}}{S_x + S_y}. \quad (10)$$

The readers can see [43–49] to have more insight on computation of topological indices.

2. Topological Aspects of 2D Structure of TBCTF Covalent Organic Frameworks

Covalent organic frameworks (COFs) are a class of organic polymers with highly ordered structure and permanent porosity. An important property of COFs is that they are synthetically controllable, structurally predesignable, and functionally manageable. COFs are usually composed of

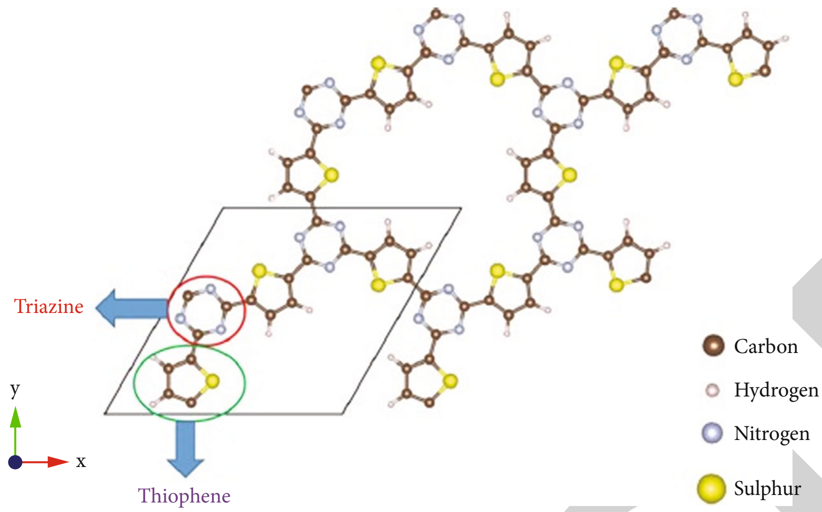

Figure 1: The geometric structure of $\mathscr{L}_1(2,2)$. The box represents a unit cell.

lightweight elements, such as B, C, N, H, O, and Si, resulting in low mass density. Huang et al. [50] reported a thiophene-based covalent triazine framework (TBCTF) for visible-light promoted selective oxidation of alcohols into corresponding aldehydes and ketones. The 2D molecular structure of TBCTF is shown in Figure 1. We observe that the unit cell of TBCTF consists of two building blocks, namely, thiophene and triazine. Constitutional isomers of TBCTF are used with the aim of band gap engineering. Let $\mathscr{L}_1(p,q)$ denotes the molecular graph of TBCTF, where p is the number of unit cells in each row and q is the number of unit cell in each column. The graph $\mathscr{L}_1(2,2)$ is shown in Figure 1. Observe that there are $33pq$ vertices and $39pq-p-q$ edges in $\mathscr{L}_1(p,q)$. In the next theorem, we compute the general sum connectivity index and general Randic connectivity index of $\mathscr{L}_1(p,q)$.

Theorem 1. *The values of general sum connectivity index and Randic index of graph $\mathscr{L}_1(p,q)$ are*

$$\chi_\alpha(\mathscr{L}_1(p,q)) = (6pq)(4)^\alpha + (3p+3q)(4)^\alpha + (18pq-2p-2q)(5)^\alpha + (15pq-2p-2q)(6)^\alpha,$$

$$R_\alpha(\mathscr{L}_1(p,q)) = (6pq)(3)^\alpha + (3p+3q)(4)^\alpha + (18pq-2p-2q)(6)^\alpha + (15pq-2p-2q)(9)^\alpha. \tag{11}$$

Proof. The sum connectivity index and Randic index of $\mathscr{L}_1(p,q)$ can be computed by finding its partition of edge set depending on the degree of end vertices of each edge. Table 1 depicts such an edge partition of $\mathscr{L}_1(p,q)$. Now, using Table 1 and the definition of the indices, we get the required result as follows:

Table 1: The edge partition of $\mathscr{L}_1(p,q)$ depending on degrees of end vertices of each edge.

(d_x, d_y) where $xy \in E(\mathscr{L}_1(p,q))$	Number of edges
(1, 3)	$6pq$
(2, 2)	$3p+3q$
(2, 3)	$18pq-2p-2q$
(3, 3)	$15pq-2p-2q$

$$\begin{aligned}\chi_\alpha(\mathscr{L}_1(p,q)) &= \sum_{xy\in\mathscr{E}_{(1,3)}(\mathscr{L}_1(p,q))}(d_x+d_y)^\alpha + \sum_{xy\in\mathscr{E}_{(2,2)}(\mathscr{L}_1(p,q))}(d_x+d_y)^\alpha \\ &+ \sum_{xy\in\mathscr{E}_{(2,3)}(\mathscr{L}_1(p,q))}(d_x+d_y)^\alpha + \sum_{xy\in\mathscr{E}_{(3,3)}(\mathscr{L}_1(p,q))}(d_x+d_y)^\alpha \\ &= (6pq)(4)^\alpha + (3p+3q)(4)^\alpha + (18pq-2p-2q)(5)^\alpha \\ &+ (15pq-2p-2q)(6)^\alpha. \\ R_\alpha(\mathscr{L}_1(p,q)) &= \sum_{xy\in\mathscr{E}_{(1,3)}(\mathscr{L}_1(p,q))}(d_xd_y)^\alpha + \sum_{xy\in\mathscr{E}_{(2,2)}(\mathscr{L}_1(p,q))}(d_xd_y)^\alpha \\ &+ \sum_{xy\in\mathscr{E}_{(2,3)}(\mathscr{L}_1(p,q))}(d_xd_y)^\alpha + \sum_{xy\in\mathscr{E}_{(3,3)}(\mathscr{L}_1(p,q))}(d_xd_y)^\alpha \\ &= (6pq)(3)^\alpha + (3p+3q)(4)^\alpha + (18pq-2p-2q)(6)^\alpha \\ &+ (15pq-2p-2q)(9)^\alpha.\end{aligned} \tag{12}$$

□

Corollary 2. *The values of Randic index, sum connectivity index, first Zagreb index, second Zagreb index, and hyper-Zagreb index of graph $\mathscr{L}_1(p,q)$ are as follows:*

$$R_{-1/2}(\mathscr{L}_1(p,q)) = \left(2\sqrt{3}+3\sqrt{6}+5\right)pq + \left(\frac{5}{6}-\frac{\sqrt{6}}{3}\right)p + \left(\frac{5}{6}-\frac{\sqrt{6}}{3}\right)q,$$

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$$M_1(\mathscr{L}_1(p,q)) = 204pq - 10p - 10q,$$

$$M_2(\mathscr{L}_1(p,q)) = 261pq - 18p - 18q,$$

$$SCI(\mathscr{L}_1(p,q)) = \left(\frac{18\sqrt{5}}{5} + \frac{5\sqrt{6}}{2} + 3\right)pq + \left(\frac{3}{2} - \frac{\sqrt{6}}{3} - \frac{2\sqrt{5}}{5}\right)p + \left(\frac{3}{2} - \frac{\sqrt{6}}{3} - \frac{2\sqrt{5}}{5}\right)q,$$

$$HM(\mathscr{L}_1(p,q)) = 1086pq - 74p - 74q. \quad (13)$$

Proof. The values of the indices can be computed by taking $\alpha = -1/2, 1, -1$ in Theorem 1. □

In the next theorem, we compute the values of the ABC index and GA index of $\mathscr{L}_1(p,q)$.

Theorem 3. *The value of ABC index and GA index of graph $\mathscr{L}_1(p,q)$ are*

$$ABC(\mathscr{L}_1(p,q)) = \left(2\sqrt{6} + 9\sqrt{2} + 10\right)pq + \left(\frac{\sqrt{2}}{2} - \frac{4}{3}\right)p + \left(\frac{\sqrt{2}}{2} - \frac{4}{3}\right)q,$$

$$GA(\mathscr{L}_1(p,q)) = \left(3\sqrt{3} + \frac{36\sqrt{6}}{5} + 15\right)pq + \left(1 - \frac{4\sqrt{6}}{5}\right)p + \left(1 - \frac{4\sqrt{6}}{5}\right)q. \quad (14)$$

Proof. Using Table 1 and the definition of the ABC index, we get

$$\begin{aligned} ABC(\mathscr{L}_1(p,q)) &= (6pq)\left(\frac{\sqrt{6}}{3}\right) + (3p+3q)\left(\frac{\sqrt{2}}{2}\right) + (18pq - 2p - 2q) \cdot \left(\frac{\sqrt{2}}{2}\right) + (15pq - 2p - 2q)\left(\frac{2}{3}\right) \\ &= \left(2\sqrt{6} + 9\sqrt{2} + 10\right)pq + \left(\frac{\sqrt{2}}{2} - \frac{4}{3}\right)p + \left(\frac{\sqrt{2}}{2} - \frac{4}{3}\right)q. \end{aligned} \quad (15)$$

Similarly, GA index can be calculated as

$$\begin{aligned} GA(\mathscr{L}_1(p,q)) &= (6pq)\left(\frac{\sqrt{3}}{2}\right) + (3p+3q)(1) + (18pq - 2p - 2q) \cdot \left(\frac{2\sqrt{6}}{5}\right) + (15pq - 2p - 2q)(1) \\ &= \left(3\sqrt{3} + \frac{36\sqrt{6}}{5} + 15\right)pq + \left(1 - \frac{4\sqrt{6}}{5}\right)p + \left(1 - \frac{4\sqrt{6}}{5}\right)q. \end{aligned} \quad (16)$$

□

In the next theorem, we calculate the expressions of the ABC_4 index and GA_5 index.

Theorem 4. *The values ABC_4 index and GA_5 index of $\mathscr{L}_1(p,q)$ are*

$$\begin{aligned} ABC_4(\mathscr{L}_1(p,q)) &= \left(\frac{4\sqrt{42}}{7} + \frac{3\sqrt{182}}{7} + \frac{2\sqrt{462}}{7} + \frac{6\sqrt{3}}{7} + 3\right)pq \\ &+ \left(\frac{19\sqrt{14}}{42} + \frac{\sqrt{35}}{5} + \frac{\sqrt{30}}{10} + \frac{\sqrt{110}}{20} - \frac{2\sqrt{42}}{21} - \frac{\sqrt{182}}{14} - \frac{\sqrt{462}}{14} + \frac{2\sqrt{2}}{5} - \frac{2\sqrt{3}}{7} - 1\right)p \\ &+ \left(\frac{19\sqrt{14}}{42} + \frac{\sqrt{35}}{5} + \frac{\sqrt{30}}{10} + \frac{\sqrt{110}}{20} - \frac{2\sqrt{42}}{21} - \frac{\sqrt{182}}{14} - \frac{\sqrt{462}}{14} + \frac{2\sqrt{2}}{5} - \frac{2\sqrt{3}}{7} - 1\right)q, \\ GA_5(\mathscr{L}_1(p,q)) &= \left(\frac{24\sqrt{3}}{7} + \frac{16\sqrt{14}}{5} + \frac{6\sqrt{21}}{5} + \frac{24\sqrt{42}}{13} + 3\right)pq \\ &+ \left(\frac{2\sqrt{2}}{3} - \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{4\sqrt{10}}{13} - \frac{8\sqrt{14}}{15} - \frac{\sqrt{21}}{5} + \frac{2\sqrt{30}}{11} + \frac{\sqrt{35}}{3} - \frac{6\sqrt{42}}{13}\right)p \\ &+ \left(\frac{2\sqrt{2}}{3} - \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{4\sqrt{10}}{13} - \frac{8\sqrt{14}}{15} - \frac{\sqrt{21}}{5} + \frac{2\sqrt{30}}{11} + \frac{\sqrt{35}}{3} - \frac{6\sqrt{42}}{13}\right)q. \end{aligned} \quad (17)$$

Proof. The ABC_4 index and GA_5 index of $\mathscr{L}_1(p,q)$ can be computed by finding its partition of edge set depending on the sum of degree of neighbors of end vertices of each edge. Table 2 depicts such an edge partition of $\mathscr{L}_1(p,q)$. Now, using Table 2 and the definition of the indices, we get the required result as follows:

$$\begin{aligned} ABC_4(\mathscr{L}_1(p,q)) &= (p+q)\left(\frac{\sqrt{14}}{6}\right) + (6pq - p - q)\left(\frac{2\sqrt{42}}{21}\right) + (2p+2q) \cdot \left(\frac{\sqrt{35}}{10}\right) + (p+q)\left(\frac{2\sqrt{2}}{5}\right) + (p+q)\left(\frac{\sqrt{30}}{10}\right) \\ &+ (2p+2q)\left(\frac{\sqrt{14}}{7}\right) + (p+q)\left(\frac{\sqrt{110}}{20}\right) + (12pq - 3p - 3q)\left(\frac{\sqrt{462}}{42}\right) + (6pq - 2p - 2q)\left(\frac{1}{2}\right) \\ &+ (3pq - p - q)\left(\frac{2\sqrt{3}}{7}\right) + (12pq - 2p - 2q)\left(\frac{\sqrt{182}}{28}\right) \\ &= \left(\frac{4\sqrt{42}}{7} + \frac{3\sqrt{182}}{7} + \frac{2\sqrt{462}}{7} + \frac{6\sqrt{3}}{7} + 3\right)pq \\ &+ \left(\frac{19\sqrt{14}}{42} + \frac{\sqrt{35}}{5} + \frac{\sqrt{30}}{10} + \frac{\sqrt{110}}{20} - \frac{2\sqrt{42}}{21} - \frac{\sqrt{182}}{14} - \frac{\sqrt{462}}{14} + \frac{2\sqrt{2}}{5} - \frac{2\sqrt{3}}{7} - 1\right)p \\ &+ \left(\frac{19\sqrt{14}}{42} + \frac{\sqrt{35}}{5} + \frac{\sqrt{30}}{10} + \frac{\sqrt{110}}{20} - \frac{2\sqrt{42}}{21} - \frac{\sqrt{182}}{14} - \frac{\sqrt{462}}{14} + \frac{2\sqrt{2}}{5} - \frac{2\sqrt{3}}{7} - 1\right)q. \end{aligned} \quad (18)$$

TABLE 2: The edge partition of $\mathscr{L}_1(p, q)$ based on the sum of degree of neighbors.

(S_x, S_y) where $xy \in E(\mathscr{L}_1(p, q))$	Number of edges
$(3, 6)$	$p + q$
$(3, 7)$	$6pq - p - q$
$(4, 5)$	$2p + 2q$
$(5, 5)$	$p + q$
$(5, 6)$	$p + q$
$(5, 7)$	$2p + 2q$
$(5, 8)$	$p + q$
$(6, 7)$	$12pq - 3p - 3q$
$(6, 8)$	$6pq - 2p - 2q$
$(7, 7)$	$3pq - p - q$
$(7, 8)$	$12pq - 2p - 2q$

Similarly, the value of GA_5 index can be calculated as

$$\begin{aligned}
\mathrm{GA}_5(\mathscr{L}_1(p, q)) &= (p+q)\left(\frac{2\sqrt{2}}{3}\right) + (6pq - p - q)\left(\frac{\sqrt{21}}{5}\right) + (2p+2q) \\
&\cdot \left(\frac{4\sqrt{5}}{9}\right) + (p+q)(1) + (p+q)\left(\frac{2\sqrt{30}}{11}\right) + (2p+2q) \\
&\cdot \left(\frac{\sqrt{35}}{6}\right) + (p+q)\left(\frac{4\sqrt{10}}{13}\right) + (12pq - 3p - 3q) \\
&\cdot \left(\frac{2\sqrt{42}}{13}\right) + (6pq - 2p - 2q)\left(\frac{4\sqrt{3}}{7}\right) + (3pq - p - q)(1) \\
&+ (12pq - 2p - 2q)\left(\frac{4\sqrt{14}}{15}\right) = \left(\frac{24\sqrt{3}}{7} + \frac{16\sqrt{14}}{5} + \frac{6\sqrt{21}}{5}\right. \\
&\left. + \frac{24\sqrt{42}}{13} + 3\right)pq + \left(\frac{2\sqrt{2}}{3} - \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9} + \frac{4\sqrt{10}}{13} - \frac{8\sqrt{14}}{15}\right. \\
&\left. - \frac{\sqrt{21}}{5} + \frac{2\sqrt{30}}{11} + \frac{\sqrt{35}}{3} - \frac{6\sqrt{42}}{13}\right)p + \left(\frac{2\sqrt{2}}{3} - \frac{8\sqrt{3}}{7} + \frac{8\sqrt{5}}{9}\right. \\
&\left. + \frac{4\sqrt{10}}{13} - \frac{8\sqrt{14}}{15} - \frac{\sqrt{21}}{5} + \frac{2\sqrt{30}}{11} + \frac{\sqrt{35}}{3} - \frac{6\sqrt{42}}{13}\right)q.
\end{aligned} \tag{19}$$

□

3. Topological Aspects of 2D Naphthalene Lattice

In recent years, 2D materials have attracted researchers due to their unique chemical and physical properties. A 2D metal-organic superlattice consist of naphthalene molecule functionalized by transition metals and eight amine groups which are surrounded by four -NH moieties, creating a square planar geometry (see Figure 2). A unit cell is depicted in a rectangular box where cyan, white, brown, and blue color spheres, respectively, are carbon, hydrogen, transition metal, and nitrogen. The molecular structure of 2D naphthalene lattice is shown in Figure 2. The rectangular lattices consist of a naphthalene skeleton, whose all hydrogen atoms are replaced by amine groups and two transition metal atoms, which are bridged between adjacent unit cells to create an infinite 2D sheet. We use the notation $\mathscr{L}_2(p, q)$ to denote the graph of 2D metal-organic superlattice, where p and q represent the number of unit cell in each row and column, respectively. The graph $\mathscr{L}_2(2, 2)$ is shown in Figure 2. Observe that there are $28pq$ vertices and $35pq - 2p - 2q$ edges in $\mathscr{L}_2(p, q)$. In the next theorem, we compute the general sum connectivity index and general Randic connectivity index of $\mathscr{L}_2(p, q)$.

Theorem 5. *The values of general sum connectivity index and Randic index of graph $\mathscr{L}_2(p, q)$ are*

$$\begin{aligned}
\chi_\alpha(\mathscr{L}_2(p, q)) &= (2p + 2q)(3)^\alpha + (8pq - 2p - 2q)(4)^\alpha + (4p + 4q)(5)^\alpha \\
&+ (19pq - 2p - 2q)(6)^\alpha + (8pq - 4p - 4q)(7)^\alpha, \\
R_\alpha(\mathscr{L}_2(p, q)) &= (2p + 2q)(2)^\alpha + (8pq - 2p - 2q)(3)^\alpha + (4p + 4q)(6)^\alpha \\
&+ (19pq - 2p - 2q)(9)^\alpha + (8pq - 4p - 4q)(12)^\alpha.
\end{aligned} \tag{20}$$

Proof. The sum connectivity index and Randic index of $\mathscr{L}_2(p, q)$ can be computed by finding its partition of edge set depending on the degree of end vertices of each edge. Table 3 depicts such an edge partition of $\mathscr{L}_2(p, q)$. Now, using Table 3 and the definition of the indices, we get the required result as follows:

$$\begin{aligned}
R_\alpha(\mathscr{L}_2(p, q)) &= \sum_{xy \in \mathscr{E}_{(1,2)}(\mathscr{L}_2(p,q))} (d_x d_y)^\alpha + \sum_{xy \in \mathscr{E}_{(1,3)}(\mathscr{L}_2(p,q))} (d_x d_y)^\alpha \\
&+ \sum_{xy \in \mathscr{E}_{(2,3)}(\mathscr{L}_2(p,q))} (d_x d_y)^\alpha + \sum_{xy \in \mathscr{E}_{(3,3)}(\mathscr{L}_2(p,q))} (d_x d_y)^\alpha \\
&+ \sum_{xy \in \mathscr{E}_{(3,4)}(\mathscr{L}_2(p,q))} (d_x d_y)^\alpha = (2p + 2q)(2)^\alpha \\
&+ (8pq - 2p - 2q)(3)^\alpha + (4p + 4q)(6)^\alpha \\
&+ (19pq - 2p - 2q)(9)^\alpha + (8pq - 4p - 4q)(12)^\alpha, \\
\chi_\alpha(\mathscr{L}_2(p, q)) &= \sum_{xy \in \mathscr{E}_{(1,2)}(\mathscr{L}_2(p,q))} (d_x + d_y)^\alpha + \sum_{xy \in \mathscr{E}_{(1,3)}(\mathscr{L}_2(p,q))} (d_x + d_y)^\alpha \\
&+ \sum_{xy \in \mathscr{E}_{(2,3)}(\mathscr{L}_2(p,q))} (d_x + d_y)^\alpha + \sum_{xy \in \mathscr{E}_{(3,3)}(\mathscr{L}_2(p,q))} (d_x + d_y)^\alpha \\
&+ \sum_{xy \in \mathscr{E}_{(3,4)}(\mathscr{L}_2(p,q))} (d_x + d_y)^\alpha = (2p + 2q)(3)^\alpha \\
&+ (8pq - 2p - 2q)(4)^\alpha + (4p + 4q)(5)^\alpha \\
&+ (19pq - 2p - 2q)(6)^\alpha + (8pq - 4p - 4q)(7)^\alpha.
\end{aligned} \tag{21}$$

□

Corollary 6. *The values of Randic index, sum connectivity index, first Zagreb index, second Zagreb index, and hyper-*

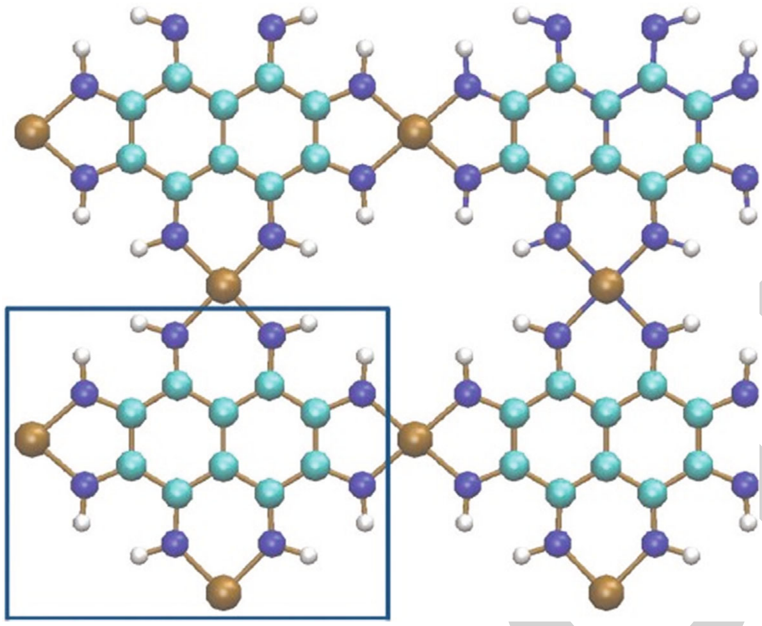

Figure 2: Top view of the 2D metal-organic superlattice.

Table 3: The edge partition of $\mathscr{L}_2(p,q)$ depending on degrees of end vertices of each edge.

(d_x, d_y) where $xy \in E(\mathscr{L}_2(p,q))$	Number of edges
$(1, 2)$	$2p + 2q$
$(1, 3)$	$8pq - 2p - 2q$
$(2, 3)$	$4p + 4q$
$(3, 3)$	$19pq - 2p - 2q$
$(3, 4)$	$8pq - 4p - 4q$

Zagreb index of graph $\mathscr{L}_2(p,q)$ are as follows:

$$R_{-1/2}(\mathscr{L}_2(p,q)) = \left(4\sqrt{3} + \frac{19}{3}\right)pq + \left(\sqrt{2} - \frac{4\sqrt{3}}{3} + \frac{2\sqrt{6}}{3} - \frac{2}{3}\right)p + \left(\sqrt{2} - \frac{4\sqrt{3}}{3} + \frac{2\sqrt{6}}{3} - \frac{2}{3}\right)q,$$

$$M_1(\mathscr{L}_2(p,q)) = 202pq - 22p - 22q,$$

$$M_2(\mathscr{L}_2(p,q)) = 291pq - 44p - 44q,$$

$$SCI(\mathscr{L}_2(p,q)) = \left(\frac{19\sqrt{6}}{6} + \frac{8\sqrt{7}}{7} + 4\right)pq + \left(\frac{2\sqrt{3}}{3} + \frac{4\sqrt{5}}{5} - \frac{\sqrt{6}}{3} - \frac{4\sqrt{7}}{7} - 1\right)p + \left(\frac{2\sqrt{3}}{3} + \frac{4\sqrt{5}}{5} - \frac{\sqrt{6}}{3} - \frac{4\sqrt{7}}{7} - 1\right)q,$$

$$HM(\mathscr{L}_2(p,q)) = 1204pq - 182p - 182q. \quad (22)$$

Proof. The values of the indices can be computed by taking $\alpha = -1/2, 1, -1$ in Theorem 5. □

In the next theorem, we compute the values of the ABC index and GA index of $\mathscr{L}_2(p,q)$.

Theorem 7. *The value of the ABC index and GA index of graph $\mathscr{L}_2(p,q)$ are as follows:*

$$ABC(\mathscr{L}_2(p,q)) = \left(\frac{8\sqrt{6}}{3} + \frac{4\sqrt{15}}{3} + \frac{38}{3}\right)pq + \left(3\sqrt{2} - \frac{2\sqrt{15}}{3} - \frac{\sqrt{6}}{3} - \frac{4}{3}\right)p + \left(3\sqrt{2} - \frac{2\sqrt{15}}{3} - \frac{\sqrt{6}}{3} - \frac{4}{3}\right)q,$$

$$GA(\mathscr{L}_2(p,q)) = \left(\frac{60\sqrt{3}}{7} + 19\right)pq + \left(\frac{4\sqrt{2}}{3} - \frac{23\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} - 2\right)p + \left(\frac{4\sqrt{2}}{3} - \frac{23\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} - 2\right)q. \quad (23)$$

Proof. Using Table 3 and the definition of the ABC index, we get

$$\begin{aligned}\mathrm{ABC}(\mathscr{L}_2(p,q)) &= (2p+2q)\left(\frac{\sqrt{2}}{2}\right) + (8pq-2p-2q)\left(\frac{\sqrt{6}}{3}\right) + (4p+4q) \\ &\cdot \left(\frac{\sqrt{2}}{2}\right) + (19pq-2p-2q)\left(\frac{2}{3}\right) + (8pq-4p-4q) \\ &\cdot \left(\frac{\sqrt{15}}{6}\right) = \left(\frac{8\sqrt{6}}{3} + \frac{4\sqrt{15}}{3} + \frac{38}{3}\right)pq \\ &+ \left(3\sqrt{2} - \frac{2\sqrt{15}}{3} - \frac{\sqrt{6}}{3} - \frac{4}{3}\right)p \\ &+ \left(3\sqrt{2} - \frac{2\sqrt{15}}{3} - \frac{\sqrt{6}}{3} - \frac{4}{3}\right)q. \end{aligned} \tag{24}$$

Similarly, the GA index can be calculated as

$$\begin{aligned}\mathrm{GA}(\mathscr{L}_2(p,q)) &= (2p+2q)\left(\frac{2\sqrt{2}}{3}\right) + (8pq-2p-2q)\left(\frac{\sqrt{3}}{2}\right) \\ &+ (4p+4q)\left(\frac{2\sqrt{6}}{5}\right) + (19pq-2p-2q)(1) \\ &+ (8pq-4p-4q)\left(\frac{4\sqrt{3}}{7}\right) = \left(\frac{60\sqrt{3}}{7} + 19\right)pq \\ &+ \left(\frac{4\sqrt{2}}{3} - \frac{23\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} - 2\right)p \\ &+ \left(\frac{4\sqrt{2}}{3} - \frac{23\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} - 2\right)q. \end{aligned} \tag{25}$$

□

In the next theorem, we calculate the expressions of ABC_4 index and GA_5 index of $\mathscr{L}_2(p,q)$.

Theorem 8. *The values ABC_4 index and GA_5 index of $\mathscr{L}_2(p,q)$ are*

$$\begin{aligned}ABC_4(\mathscr{L}_2(p,q)) &= \left(2\sqrt{6} + \frac{2\sqrt{30}}{3} + 2\sqrt{3} + \frac{44}{9}\right)pq \\ &+ \left(\frac{\sqrt{10}}{3} - \sqrt{6} + \frac{\sqrt{14}}{3} + \frac{\sqrt{78}}{9} + \sqrt{2}\right. \\ &\left. - \sqrt{3} + \frac{\sqrt{5}}{2} - \frac{16}{9}\right)p + \left(\frac{\sqrt{10}}{3} - \sqrt{6}\right. \\ &+ \frac{11\sqrt{14}}{24} - \frac{\sqrt{30}}{6} + \frac{\sqrt{78}}{9} + \sqrt{2} - \sqrt{3} \\ &\left. + \frac{\sqrt{5}}{2} - \frac{4}{3}\right)q + \frac{\sqrt{14}}{8} - \frac{\sqrt{30}}{6} + \frac{4}{9}, \end{aligned}$$

Table 4: The edge partition of $\mathscr{L}_2(p,q)$ based on the sum of degree of neighbors.

(S_x, S_y) where $xy \in E(\mathscr{L}_2(p,q))$	Number of edges
(2, 4)	$2p+2q$
(3, 6)	$2p+2q$
(3, 8)	$8pq-4p-4q$
(4, 8)	$2p+2q$
(6, 6)	$2p+2q$
(6, 9)	$2p+2q$
(8, 8)	$q+1$
(8, 9)	$8pq-2q-2$
(8, 12)	$8pq-4p-4q$
(9, 9)	$11pq-4p-3q+1$

$$\begin{aligned}GA_5(\mathscr{L}_2(p,q)) &= \left(\frac{96\sqrt{2}}{17} + \frac{336\sqrt{6}}{55} + 11\right)pq \\ &+ \left(4\sqrt{2} - \frac{124\sqrt{6}}{55} - 2\right)p \\ &+ \left(\frac{44\sqrt{2}}{17} - \frac{124\sqrt{6}}{55}\right)q + 2 - \frac{24\sqrt{24}}{17}. \end{aligned} \tag{26}$$

Proof. The ABC_4 index and GA_5 index of $\mathscr{L}_2(p,q)$ can be computed by finding its partition of edge set depending on the sum of degree of neighbors of end vertices of each edge. Table 4 depicts such an edge partition of $\mathscr{L}_2(p,q)$. Now, using Table 4 and the definition of the indices, we get the required result as follows:

$$\begin{aligned}ABC_4(\mathscr{L}_2(p,q)) &= (2p+2q)\left(\frac{\sqrt{2}}{2}\right) + (2p+2q)\left(\frac{\sqrt{14}}{6}\right) + (8pq-4p-4q) \\ &\cdot \left(\frac{\sqrt{6}}{4}\right) + (2p+2q)\left(\frac{\sqrt{5}}{4}\right) + (2p+2q)\left(\frac{\sqrt{10}}{6}\right) \\ &+ (2p+2q)\left(\frac{\sqrt{78}}{18}\right) + (q+1)\left(\frac{\sqrt{14}}{8}\right) + (8pq-2q-2) \\ &\cdot \left(\frac{\sqrt{30}}{12}\right) + (8pq-4p-4q)\left(\frac{\sqrt{3}}{4}\right) + (11pq-4p-3q+1) \\ &\cdot \left(\frac{4}{9}\right) = \left(2\sqrt{6} + \frac{2\sqrt{30}}{3} + 2\sqrt{3} + \frac{44}{9}\right)pq \\ &+ \left(\frac{\sqrt{10}}{3} - \sqrt{6} + \frac{\sqrt{14}}{3} + \frac{\sqrt{78}}{9} + \sqrt{2} - \sqrt{3} + \frac{\sqrt{5}}{2} - \frac{16}{9}\right)p \\ &+ \left(\frac{\sqrt{10}}{3} - \sqrt{6} + \frac{11\sqrt{14}}{24} - \frac{\sqrt{30}}{6} + \frac{\sqrt{78}}{9} + \sqrt{2} - \sqrt{3}\right. \\ &\left. + \frac{\sqrt{5}}{2} - \frac{4}{3}\right)q + \frac{\sqrt{14}}{8} - \frac{\sqrt{30}}{6} + \frac{4}{9}. \end{aligned} \tag{27}$$

Similarly, the value of GA_5 index can be calculated as

$$\begin{aligned}
\mathrm{GA}_5(\mathscr{L}_2(p,q)) &= (2p+2q)\left(\frac{2\sqrt{2}}{3}\right) + (2p+2q)\left(\frac{2\sqrt{2}}{3}\right) \\
&\quad + (8pq-4p-4q)\left(\frac{4\sqrt{6}}{11}\right) + (2p+2q)\left(\frac{2\sqrt{2}}{3}\right) \\
&\quad + (2p+2q)(1) + (2p+2q)\left(\frac{2\sqrt{6}}{5}\right) + (q+1)(1) \\
&\quad + (8pq-2q-2)\left(\frac{12\sqrt{2}}{17}\right) + (8pq-4p-4q) \\
&\quad \cdot \left(\frac{2\sqrt{6}}{5}\right) + (11pq-4p-3q+1)(1) \\
&= \left(\frac{96\sqrt{2}}{17} + \frac{336\sqrt{6}}{55} + 11\right)pq + \left(4\sqrt{2} - \frac{124\sqrt{6}}{55} - 2\right)p \\
&\quad + \left(\frac{44\sqrt{2}}{17} - \frac{124\sqrt{6}}{55}\right)q + 2 - \frac{24\sqrt{24}}{17}.
\end{aligned} \tag{28}$$

□

4. Conclusion

In this work, we have studied two organic frameworks, namely, naphthalene metal-organic frameworks and thiophene-based covalent triazine framework via topological indices. We have computed some important degree-based indices of these structures that may be helpful to study some physical/chemical properties of these organic frameworks. One can study eccentricity-based topological descriptors for the frameworks.

Data Availability

No data is required to support the study.

Disclosure

This work is carried out as a part of employment of authors.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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