





Research Article

Topological Descriptors for the Metal Organic Network and Its Structural Properties

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Metal organic structures and networks are extensively studied in modern chemistry. These networks are extremely adaptable and useful in a variety of fields. Metal organic networks are thought to be the home of gases, and this structure is also engaged in gas purification and separation. The fact that they have so much utility and applicability stems from that they have so many distinct properties, such as exchanging ions and altering organic ligands. This structure's chemical and physical properties are considered. There are extensive, time-consuming, and costly experiments available to investigate these physical and chemical properties. To avoid these complex experiments and tests, a mathematical study provides approximate details of these chemical and physical behaviors of a structure, which is known as topological descriptors. In this work, we discussed the metal organic network's line graph and studied the structural properties of the resulted network with the help of topological descriptors.

1. Introduction

In the chemical graph theory, the atoms and the bond between atoms are represented as vertices and edges, respectively. When a network or a complex structure is transformed into a graph and that makes the study understandable, it reduces the cost of complexity of working on networks and it also become easy to visualize [1–3]. A topological descriptor is a tool to analyze structural properties of a network in terms of graph aspects. A topological descriptor is a tool in terms of functions. The function's domain is the pattern either in degree or distance of vertices in the networks and ranging in numerical quantity. The resulted numerical quantity is used to study structural properties of a particular structure.

Topological descriptors are mainly focused for the chemical structures or networks. There is an enormous study discussed in the literature and few are cited here. For example,

the structural properties of silicon carbide with different topologies can be found in [4, 5]. The edge dividing method for finding the topological descriptors are available in [6, 7]. A particular type of topological descriptor named as atom bond connectivity index for the molecular graph is found in [8]. Some nanotubes are discussed in terms of different topological descriptors in [9]. Nanotubes can be capped with different type of materials, some capped and capped like structures can be found in [10, 11], in which they introduced a new type of chemical structure and discussed their structural properties. Certain chemical structures which are transformed are discussed in [12]. Zagreb-based topological and structural properties of nanostar dendrimers are available in [13]. Some recent literature is available at [14–16].

The 3D networks/structures can be embedded in 2D structures, one of such types of structure is studied in [17, 18], in which structural and topological properties are discussed. The recent study of sodium chloride and its topological descriptors

are available in [19]. The graphene and honeycomb network and its structural properties are available in [20]. Topological descriptors are not limited to chemical structures only; others field networks and structures are also studied with the novel method of topological descriptors. Such a hypercube network is studied in [21], optical transpose interconnection systems or OTIS networks are studied in [22, 23], the hexagon star networks are discussed in [24], and the nanotube structure of titanium dioxide which is a single-walled structure is available in [25]. There are some recent topics related to this study that are discussed in [26–30]. Relevant studies on the topic of mathematical chemistry, structures, and their topologies are available in [31–33].

In Reference [34], authors investigated the first and second Zagreb indices of the Cartesian, composition, join, disjunction, and symmetric difference graph operations. The author of [35] computed the forgotten topological index of different corona products of graphs, and the authors of [36] gave the exact expressions of Zagreb indices of the generalized hierarchical product of graphs. For more discussion and results, we refer to [37, 38].

Let G be a graph and $L(G)$ is an associated line graph of G . The vertex set of G is usually denoted as $V(G)$ and $E(G)$ for the edge set of a graph. The $E(G)$ becomes a vertex set of line graph of G , simply $V(L(G)) = E(G)$ and the edge relation only follows the detail from original graph. It means that if two edges are adjacent in the original graph, then, in the line graph, the vertices will share the edges or become adjacent, (original graph's edges becomes line graphs vertices). One can find an easy and descriptive study on the line graph of chemical structures in the literature and we refer [39, 40]. The number of edges attached with vertex a is known as the degree of a vertex. In this work, we denote this concept with the notation ζ_a . The edge partition is denoted as (ζ_a, ζ_b) for an edge ab , with ζ_a and ζ_b are degrees of vertices a and b , respectively.

Following are the methodologies or the topological descriptors which are used in this study to discuss some structural properties of a line graph of the metal organic network.

Definition 1. The topological descriptor known as $SDI(G)$ for a graph G is introduced by the authors of [41] in 2010, by the name of symmetric division index.

$$SDI(G) = \sum_{ab \in E(G)} \frac{\zeta_a^2 + \zeta_b^2}{\zeta_a \times \zeta_b}. \quad (1)$$

Definition 2. The topological descriptors $RRR(G)$ and $RM_2(G)$ for a spectral graph G is introduced by the authors of [42] in 2014 and named them as the reduced reciprocal Randić and reduced second Zagreb index, respectively.

$$RRR(G) = \sum_{ab \in E(G)} \sqrt{(\zeta_a - 1)(\zeta_b - 1)}. \quad (2)$$

$$RM_2(G) = \sum_{ab \in E(G)} (\zeta_a - 1)(\zeta_b - 1). \quad (3)$$

Definition 3. The topological descriptor $A(G)$ is very famous for the distance-based study of graphs. It is the advance version of imbalance of an edge parameter. While for the study of Ramsey graphs, the Albertson index was introduced by the authors of [43].

$$A(G) = \sum_{ab \in E(G)} |\zeta_a - \zeta_b|. \quad (4)$$

Definition 4. The topological descriptor $A^*(G)$ is the refined version of the Albertson index and was named the modified Albertson index by the authors of [44].

$$A^*(G) = \sum_{ab \in E(G)} |\zeta_a^2 - \zeta_b^2|. \quad (5)$$

Definition 5. The topological descriptor $R'(G)$ is known as the variation of Randić index and was introduced by the authors of [45].

$$R'(G) = \sum_{ab \in E(G)} \frac{1}{\max\{\zeta_a, \zeta_b\}}. \quad (6)$$

Definition 6. The topological descriptors SK , SK_1 , and SK_2 index for a molecular graph G is defined by the authors of [46] and formulated as follows, respectively:

$$SK(G) = \sum_{ab \in E(G)} \frac{\zeta_a + \zeta_b}{2}, \quad (7)$$

$$SK_1(G) = \sum_{ab \in E(G)} \frac{\zeta_a \times \zeta_b}{2}, \quad (8)$$

$$SK_2(G) = \sum_{ab \in E(G)} \left(\frac{\zeta_a + \zeta_b}{2} \right)^2. \quad (9)$$

2. Results of Topological Descriptors of the Line Graph of a Metal Organic Network

The fundamental metal organic network and the important network to build its subsequent topologies, which are presented in Figure 1, are shown in Figure 2. These two networks, as well as their connected networks, may be found in [47,48]. The line graph of a metal organic network, which we termed $L(MON(n))$, is shown in Figure 3. The order, size, and the edge of the graph is given in Table 1. In addition, the number of vertices and edges, which are referred to as order and size, respectively, are shown in Table 1.

Throughout the results, we will consider G is a line graph of the metal organic network $MON(n)$, or simply $L(MON(n))$.

Theorem 1. *If $n \geq 2$ in $G \cong L(MON(n))$, then the symmetric division index is as follows:*

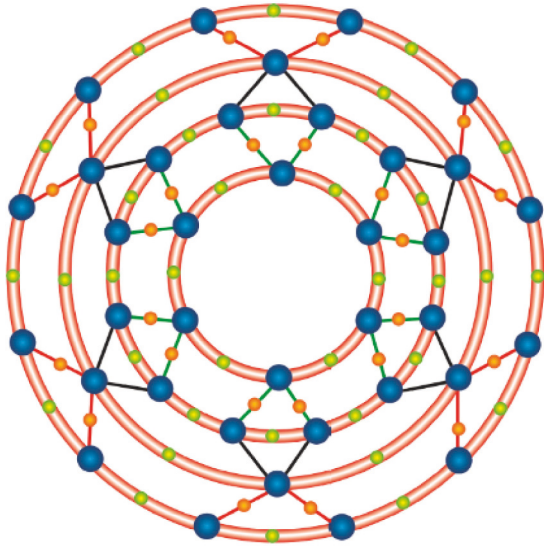


FIGURE 1: Metal organic network with 2 layers or MON(2) [47,48].

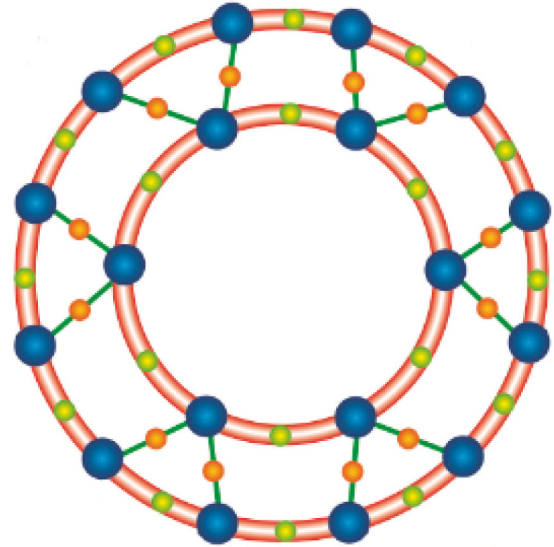


FIGURE 2: Basic metal organic network [47].

$$SDI(G) = 880n - 349. \tag{10}$$

Proof. The edge partition defined in the Table 1, using these edge partitions into the Equation (1), which is formulated in the Definition 1. Then, the final result for the symmetric division index is as follows:

$$\begin{aligned}
 SDI(G) &= \sum_{ab \in E(G)} \frac{\zeta_a^2 + \zeta_b^2}{\zeta_a \times \zeta_b} \\
 &= +36(n-1) \left(\frac{4^2 + 8^2}{4 \times 8} \right) + 60(n-1) \left(\frac{6^2 + 6^2}{6 \times 6} \right) \\
 &\quad + 48(n-1) \left(\frac{6^2 + 8^2}{6 \times 8} \right) \\
 &\quad + 48 \left(\frac{3^2 + 3^2}{3 \times 3} \right) + 12(n-1) \left(\frac{3^2 + 6^2}{3 \times 6} \right) \\
 &\quad + (50 + 30(n-1)) \left(\frac{4^2 + 4^2}{4 \times 4} \right) \\
 &\quad + 60(n-1) \left(\frac{8^2 + 8^2}{8 \times 8} \right) = 880n - 349.
 \end{aligned} \tag{11}$$

□

Theorem 2. If $n \geq 2$ in $G \cong L(MON(n))$, then the reduced reciprocal Randić index is as follows:

$$RRR(G) = 1296.891887n - 1050.891887. \tag{12}$$

Proof. Using the edge partition from Table 1, in equation (2), defined in Definition 2. Then, the final result for the reduced reciprocal Randić index is as follows:

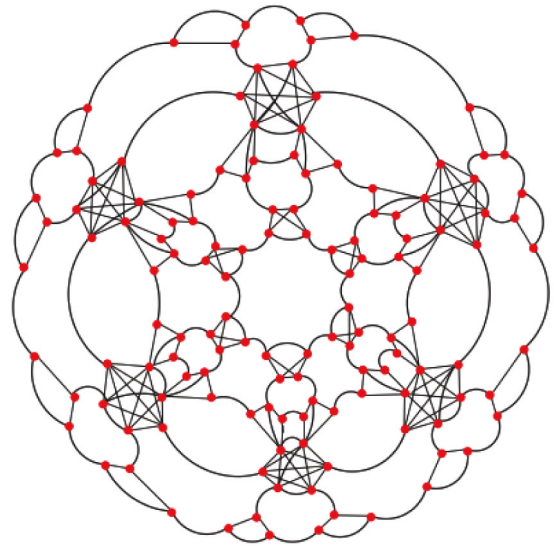


FIGURE 3: Line graph of the metal organic network with 2 layers or $L(MON(2))$ [48].

TABLE 1: Edge partition of $L(MON(n))$.

(ζ_a, ζ_b)	Frequency	Set of edges
(3, 3)	48	E_1
(3, 6)	$12(n-1)$	E_2
(4, 4)	$50 + 30(n-1)$	E_3
(4, 8)	$36(n-1)$	E_4
(6, 6)	$60(n-1)$	E_5
(6, 8)	$48(n-1)$	E_6
(8, 8)	$60(n-1)$	E_7
Size	$192n + 98$	$ E(G) $
Order	$72n - 12$	$ V(G) $

$$\begin{aligned}
RRR(G) &= \sum_{ab \in E(G)} \sqrt{(\zeta_a - 1)(\zeta_b - 1)}, \\
&= 48\sqrt{(3-1)(3-1)} + 12(n-1)\sqrt{(3-1)(6-1)} \\
&\quad + (50 + 30(n-1))\sqrt{(4-1)(4-1)} \\
&\quad + 36(n-1)\sqrt{(4-1)(8-1)} \\
&\quad + 60(n-1)\sqrt{(6-1)(6-1)} + 48(n-1) \\
&\quad \times \sqrt{(6-1)(8-1)} + 60(n-1)\sqrt{(8-1)(8-1)} \\
&= 1296.891887n - 1050.891887. \quad \square
\end{aligned} \tag{13}$$

Theorem 3. If $n \geq 2$ in $G \cong L(MON(n))$, then the reduced second Zagreb index is as follows:

$$RM_2(G) = 7266n - 6624. \tag{14}$$

Proof. Using the edge partition from Table 1, in equation (3), defined in Definition 2. Then, the final result for the reduced second Zagreb index is as follows:

$$\begin{aligned}
RM_2(G) &= \sum_{ab \in E(G)} (\zeta_a - 1)(\zeta_b - 1), \\
&= 48(3-1)(3-1) + 12(n-1)(3-1)(6-1) \\
&\quad + (50 + 30(n-1))(4-1)(4-1) \\
&\quad + 36(n-1)(4-1)(8-1) \\
&\quad + 60(n-1)(6-1)(6-1) \\
&\quad + 48(n-1)(6-1)(8-1) \\
&\quad + 60(n-1)(8-1)(8-1) = 7266n - 6624. \\
&\quad \square
\end{aligned} \tag{15}$$

Theorem 4. If $n \geq 2$ in $G \cong L(MON(n))$, then the Albertson index is as follows:

$$A(G) = 276(n-1). \tag{16}$$

Proof. Using the edge partition from Table 1, in equation (4), defined in Definition 3. Then, the final result for the Albertson index is as follows:

$$\begin{aligned}
A(G) &= \sum_{ab \in E(G)} |\zeta_a - \zeta_b|, \\
&= 48|3-3| + 12(n-1)|3-6| \\
&\quad + (50 + 30(n-1))|4-4| + 36(n-1)|4-8| \\
&\quad + 60(n-1)|6-6| + 48(n-1)|6-8| \\
&\quad + 60(n-1)|8-8| = 276(n-1). \quad \square
\end{aligned} \tag{17}$$

Theorem 5. If $n \geq 2$ in $G \cong L(MON(n))$, then the modified Albertson index is as follows:

$$A^*(G) = 3396(n-1). \tag{18}$$

Proof. Using the edge partition from Table 1, in equation (5), defined in Definition 4. Then, the final result for the modified Albertson index is as follows:

$$\begin{aligned}
A^*(G) &= \sum_{ab \in E(G)} |\zeta_a^2 - \zeta_b^2|, \\
&= 48|3^2 - 3^2| + 12(n-1)|3^2 - 6^2| \\
&\quad + (50 + 30(n-1))|4^2 - 4^2| + 36(n-1)|4^2 - 8^2| \\
&\quad + 60(n-1)|6^2 - 6^2| + 48(n-1)|6^2 - 8^2| \\
&\quad + 60(n-1)|8^2 - 8^2| = 3396(n-1). \quad \square
\end{aligned} \tag{19}$$

Theorem 6. If $n \geq 2$ in $G \cong L(MON(n))$, then the variation of Randić index is as follows:

$$R'(G) = \frac{75n - 18}{2}. \tag{20}$$

Proof. Using the edge partition from Table 1, in equation (6), defined in Definition 5. Then, the final result for the variation of Randić index is as follows:

$$\begin{aligned}
R'(G) &= \sum_{ab \in E(G)} \frac{1}{\max\{\zeta_a, \zeta_b\}}, \\
&= 48 \frac{1}{\max\{3, 3\}} + 12(n-1) \frac{1}{\max\{3, 6\}} \\
&\quad + (50 + 30(n-1)) \frac{1}{\max\{4, 4\}} + 36(n-1) \\
&\quad \times \frac{1}{\max\{4, 8\}} + 60(n-1) \frac{1}{\max\{6, 6\}} \\
&\quad + 48(n-1) \frac{1}{\max\{6, 8\}} + 60(n-1) \frac{1}{\max\{8, 8\}}, \\
&= \frac{75n - 18}{2}. \quad \square
\end{aligned} \tag{21}$$

Theorem 7. If $n \geq 2$ in $G \cong L(MON(n))$, then the SK index is as follows:

$$SK(G) = 1566n - 1222. \tag{22}$$

Proof. Using the edge partition from Table 1, in equation (7), defined in Definition 6. Then, the final result for the SK index is as follows:

TABLE 2: Comparison of symmetric division, reduced Randić, and reduced second Zagreb.

n	SDI ($L(\text{MON}(n))$)	RRR ($L(\text{MON}(n))$)	RM_2 ($L(\text{MON}(n))$)
2	1411	1542.891887	7908
3	2291	2839.783774	15174
4	3171	4136.675661	22440
5	4051	5433.5675484	29706
6	4931	6730.459435	36972
7	5811	8027.3513224	44238
8	6691	9324.243209	515044
9	7571	10621.135096	58770
10	8451	11918.0269834	660364
11	9331	13214.91887	73302

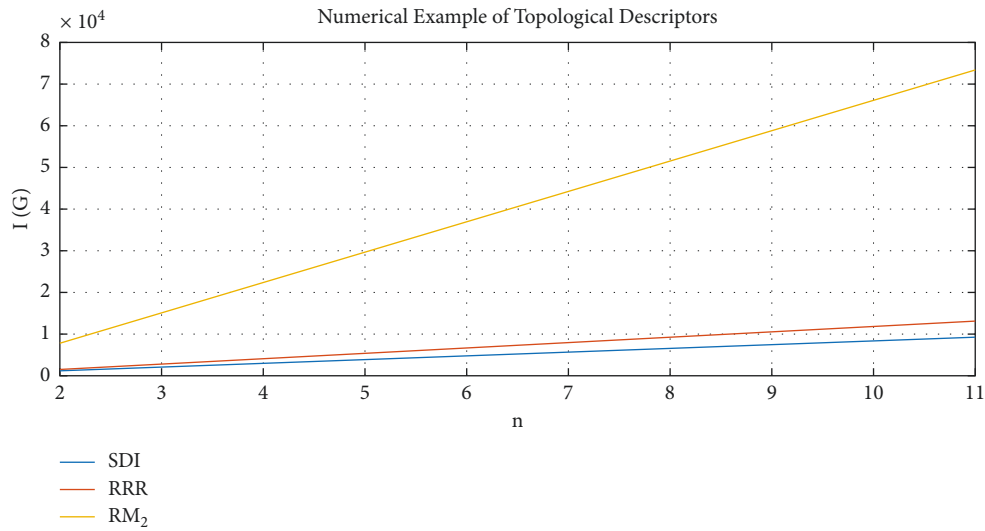


FIGURE 4: Graphical examples for SDI, RRR, and RM_2 .

$$\begin{aligned}
 \text{SK}(G) &= \sum_{ab \in E(G)} \frac{\zeta_a + \zeta_b}{2}, \\
 &= 48 \left(\frac{3+3}{2} \right) + 12(n-1) \left(\frac{3+6}{2} \right) \\
 &\quad + (50 + 30(n-1)) \left(\frac{4+4}{2} \right) + 36(n-1) \\
 &\quad \times \left(\frac{4+8}{2} \right) + 60(n-1) \left(\frac{6+6}{2} \right) \\
 &\quad + 48(n-1) \left(\frac{6+8}{2} \right) \\
 &\quad + 60(n-1) \left(\frac{8+8}{2} \right), \\
 &= 1566n - 1222.
 \end{aligned}
 \tag{23}$$

□

Theorem 8. If $n \geq 2$ in $G \cong L(\text{MON}(n))$, then the SK_1 index is as follows:

$$\text{SK}_1(G) = 5076n - 4460. \tag{24}$$

Proof. Using the edge partition from Table 1, in equation (8), defined in Definition 6. Then, the final result for the SK_1 index is as follows:

$$\begin{aligned}
 \text{SK}_1(G) &= \sum_{ab \in E(G)} \frac{\zeta_a \times \zeta_b}{2}, \\
 &= 48 \left(\frac{3 \times 3}{2} \right) + 12(n-1) \left(\frac{3 \times 6}{2} \right) \\
 &\quad + (50 + 30(n-1)) \left(\frac{4 \times 4}{2} \right) + 36(n-1) \\
 &\quad \times \left(\frac{4 \times 8}{2} \right) + 60(n-1) \left(\frac{6 \times 6}{2} \right) \\
 &\quad + 48(n-1) \left(\frac{6 \times 8}{2} \right) + 60(n-1) \left(\frac{8 \times 8}{2} \right), \\
 &= 5076n - 4460.
 \end{aligned}
 \tag{25}$$

□

TABLE 3: Comparison of the Albertson, modified Albertson, and variation of Randić indexes.

n	$A(L(MON(n)))$	$A^*(L(MON(n)))$	$R'(L(MON(n)))$
2	276	3396	66
3	552	6792	103.50
4	828	10188	141
5	1104	13584	178.50
6	1380	16980	216
7	1656	20376	253.50
8	1932	23772	291
9	2208	27168	328.50
10	2484	30564	366
11	2760	33960	403.50

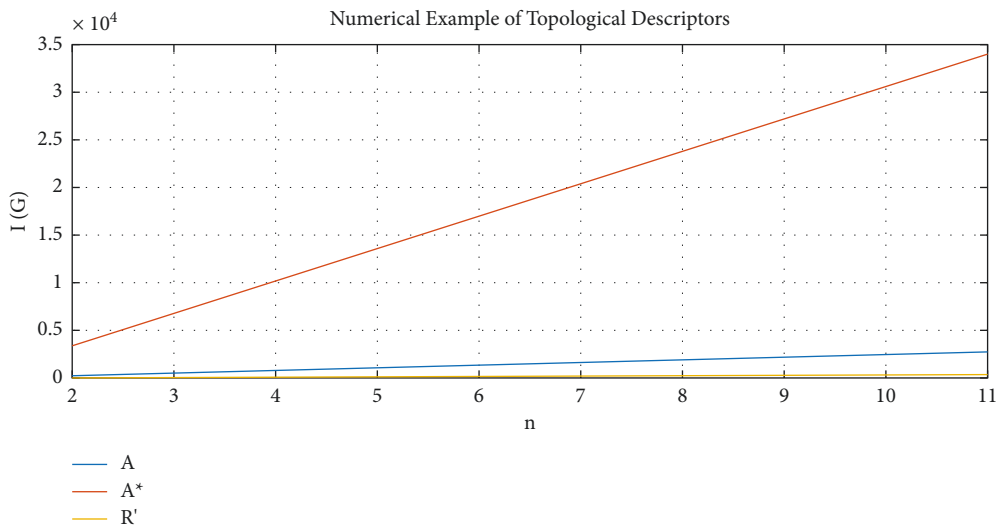


FIGURE 5: Graphical examples for AA^* and R' .

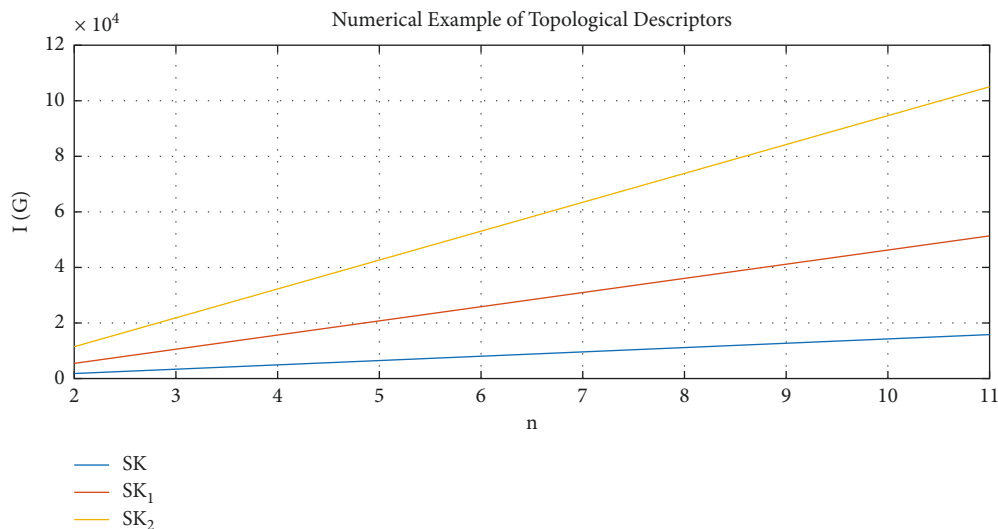
TABLE 4: Comparison of SK and its types.

n	$SK(. (n))$	$SK_1(.. (n))$	$SK_2(.. (n))$
2	1910	5692	11603
3	3476	10768	21974
4	5042	15844	32345
5	6608	20920	42716
6	8174	25996	53087
7	9740	31072	63458
8	11306	36148	73829
9	12872	41224	84200
10	14438	46300	94571
11	16004	51376	104942

Theorem 9. If $n \geq 2$ in $G \cong L(MON(n))$, then the SK_2 index is as follows:

$$SK_2(G) = 10371n - 9139. \tag{26}$$

Proof. Using the edge partition from Table 1, in equation (9), defined in Definition 6. Then, the final result for the SK_2 index is as follows:

FIGURE 6: Graphical examples for SK, SK₁, and SK₂.

$$\begin{aligned}
 SK_2(G) &= \sum_{ab \in E(G)} \left(\frac{\zeta_a + \zeta_b}{2} \right)^2, \\
 &48 \left(\frac{3+3}{2} \right)^2 + 12(n-1) \left(\frac{3+6}{2} \right)^2 \\
 &+ (50 + 30(n-1)) \left(\frac{4+4}{2} \right)^2 + 36(n-1) \\
 &\times \left(\frac{4+8}{2} \right)^2 + 60(n-1) \left(\frac{6+6}{2} \right)^2 \\
 &+ 48(n-1) \left(\frac{6+8}{2} \right)^2 + 60(n-1) \left(\frac{8+8}{2} \right)^2 \\
 &= 10371n - 9139.
 \end{aligned} \tag{27}$$

3. Conclusion and Discussion

The topological descriptors, such as symmetric division, reduced Randić, reduced second Zagreb, Albertson, modified Albertson, variation of Randić, and SK and its types which are SK₁ and SK₂ indices, are studied in this research work for the structure of line graph of the metal organic network with n -layers. All the indices defined above are known as topological descriptors and are developed to study the structural properties of chemical or molecular graphs, networks, and structures. Mostly, the topological descriptors are new and developed recently. To study new parameters, this structure helps researchers to visualize the properties of the metal organic network or its line graph in a more easy and less expensive way with less effort.

The particular examples of Theorems 1–3 are depicted here. For some particular values of running parameter n and the values of symmetric division, reduced Randić, and reduced second Zagreb indices are elaborated in Table 2. Its associated graph is shown in Figure 4. It can be seen easily

that the reduced second Zagreb index is growing rapidly compared to others.

The particular examples of Theorems 4–6 are depicted here. Some particular values of running parameter n and the values of Albertson, modified Albertson, and variation of Randić indices are elaborated in Table 3. Its associated graph is shown in Figure 5. It can be seen easily that the modified Albertson index is growing rapidly compared to others.

The particular examples of Theorems 7–9 are depicted here. Some particular values of running parameter n and the values of SK, SK₁, and SK₂ indices are elaborated in Table 4. Its associated graph is shown in Figure 6. It can be seen easily that SK₂ index is growing rapidly compared to others.

Data Availability

□ All the data supporting the results are included within the manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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