Further results on computation of topological indices of certain networks

Shaohui Wang\textsuperscript{a}, Jia-Bao Liu\textsuperscript{b}, Chunxiang Wang\textsuperscript{c}, Sakander Hayat\textsuperscript{d}

\textsuperscript{a} Department of Mathematics, The University of Mississippi, University, MS 38677, USA
\textsuperscript{b} School of Mathematics and Physics, Anhui Jianzhu University, Hefei, 230601, P.R. China
\textsuperscript{c} School of Mathematics and Statistics, Central China Normal University, Wuhan, 430079, P.R. China
\textsuperscript{d} School of Mathematical Sciences, University of Science and Technology of China, Hefei, 230026, China

Abstract

There are various topological indices such as degree based topological indices, distance based topological indices and counting related topological indices etc. These topological indices correlate certain physicochemical properties such as boiling point, stability of chemical compounds. In this paper, we compute the sum-connectivity index and multiplicative Zagreb indices for certain networks of chemical importance like silicate networks, hexagonal networks, oxide networks, and honeycomb networks. Moreover, a comparative study using computer-based graphs has been made to clarify their nature for these families of networks.

Keywords: Sum-connectivity index, Multiplicative Zagreb indices, Silicate networks, Hexagonal networks, Oxide networks, Honeycomb networks.

AMS subject classification: 94C15

1 Introduction

Throughout this paper $G = (V, E)$ is a finite, simple and connected graph with vertex set $V(G)$ and edge set $E(G)$. For other undefined notations, readers may refer to [1, 23, 24]. Chemical graph theory is a branch of graph theory whose focus of interest is finding topological indices of chemical graphs which correlate well with chemical properties of the chemical molecules. A topological index is a numerical parameter mathematically derived from the graph structure.

\textsuperscript{0}This work is partially supported by National Natural Science Foundation of China (nos. 11471016, 11401004, 1157134, 11371162), Anhui Provinical Natural Science Foundation (nos. KJ2015A331, KJ2013B105, 1408085QA03), the Self-determined Research Funds of Central China Normal University from the colleges basic research and operation of MOE, and the Summer Graduate Research Assistantship Program of Graduate School at the University of Mississippi.

*Corresponding author.

E-mail addresses: S. Wang (swang4@go.olemiss.edu, shaohuiwang@yahoo.com), J.B. Liu (liujiabaoad@163.com), C. Wang (wcxiang@mailccnu.edu.cn), S. Hayat(sakander1566@gmail.com)
The topological indices have been found to be useful for establishing correlations between the structure of a molecular compound and its physicochemical properties or biological activity [3, 7, 22].

Let \(d(u), d(v)\) be the degrees of the vertices \(u\) and \(v\) respectively. One of the topological indices used in mathematical chemistry is that of the so-called degree-based topological indices, which are defined in terms of the degrees of the vertices of a graph. For instance, the first and second Zagreb indices of \(G\) are respectively defined as

\[
M_1(G) = \sum_{u \in \mathcal{V}(G)} d(u)^2, \quad M_2(G) = \sum_{uv \in \mathcal{E}(G)} d(u)d(v).
\]

The background and applications of Zagreb indices can be found in [15, 17, 19, 33].

In the 1980s, Narumi and Katayama [28] characterized the structural isomers of saturated hydrocarbons and considered the product \(NK(G) = \prod_{v \in \mathcal{V}(G)} d(v)\), which is called the NK index. Two fairly new indices with higher prediction ability [35], named the first and second multiplicative Zagreb indices [18], are respectively defined as

\[
\Pi_1,c(G) = \prod_{v \in \mathcal{V}(G)} d(v)^c, \quad \Pi_2(G) = \prod_{uv \in \mathcal{E}(G)} d(u)d(v).
\]

Obviously, the first multiplicative Zagreb index is the power of the NK index. Moreover, the second multiplicative Zagreb index can be rewritten as \(\Pi_2(G) = \prod_{u \in \mathcal{V}(G)} d(u)^{d(u)}\). The properties of \(\Pi_{1,c}(G), \Pi_2(G)\) for some chemical structures have been studied extensively in [36, 8, 16, 31].

The multiplicative version of ordinary first Zagreb index \(M_1\) is defined as

\[
\Pi^*_1(G) = \prod_{uv \in \mathcal{E}(G)} (d(u) + d(v)).
\]

The general sum-connectivity index is defined as

\[
\chi_\alpha(G) = \sum_{uv \in \mathcal{E}(G)} (d(u) + d(v))^{\alpha}, \text{where } \alpha \text{ is a real number},
\]

and given with the purpose of extending the classical sum-connectivity index, \(\chi_1\) \((G)\). The properties of \(\Pi^*_1(G), \chi_\alpha(G)\) polynomials for some chemical structures have been studied in [8, 41]. For other work on topological indices, the readers are referred to [2, 10, 11, 12, 14, 21, 25, 26, 27, 28, 31, 38, 39, 40].

Silicates are the most important elements of Earth’s crust, as well as the other terrestrial planets, rocky moons, and asteroids. Sand, Portland cement, and thousands of minerals are constituted by silicates. The tetrahedron \((SiO_4)\) is a basic unit of silicates, in which the central vertex is silicon vertex and the corner vertices are oxygen vertices, see Figure 1.

One of most interesting topics is to obtain the quantitative structure activity/property/toxicity relationships [5, 6, 20, 30, 32]. In this paper, we explore the silicate, chain silicate, hexagonal, oxide and honeycomb networks and provide exact polynomials of \(\chi_\alpha(G), \Pi^*_1(G), \Pi_{1,c}(G)\) and \(\Pi_2(G)\) for these networks. Furthermore, we use the pictures to compare the chemical indices on these silicate-related networks.
Figure 1: $SiO_4$ Tetrahedron.

Figure 2: Different sheet silicates.
2 Main results and discussion

In this section, we explore the silicate, chain silicate, hexagonal, oxide and honeycomb networks and provide exact formulas of \( \chi_\alpha(G) \), \( \prod_1^*(G) \), \( \prod_{1,c}(G) \) and \( \prod_2(G) \) for these networks. In order to compute certain topological indices of the silicate networks, we will divide the vertex set and the edge set based on degrees of end vertices of each edge of the graph. In addition, we utilized some techniques and figures (Figs. 1 - 7) in [20, 30].

We first give the general remarks how to compute the relation between the numbers of vertices and edges from the literature. In general, we follow the approaches of Gutman, Deutsch and Klažar [5, 6, 13] for which some definitions are needed first.

Lemma 2.0.1. [5, 6, 13] Given that \( G \) is a connected graph with \( n = |V(G)| \) and \( m = |E(G)| \). Let \( n_i \) be the number of vertices of degree \( i \) and \( m_{i,j} \) be the number of edges with end vertices of degree \( i \) and \( j \), \( i,j \geq 1 \). Then

\[
\begin{align*}
n_1 + n_2 + n_3 + n_4 + n_5 + n_6 &= n, \\
m_{12} + m_{13} + m_{14} + m_{15} + m_{16} &= n_1, \\
m_{21} + 2m_{22} + m_{23} + m_{24} + m_{25} + m_{26} &= 2n_2, \\
m_{31} + 2m_{31} + 2m_{33} + m_{34} + m_{35} + m_{36} &= 3n_3, \\
m_{41} + m_{42} + m_{43} + 2m_{44} + m_{45} + m_{46} &= 4n_4, \\
m_{51} + m_{52} + m_{53} + m_{54} + 2m_{55} + m_{56} &= 5n_5, \\
m_{61} + m_{62} + m_{63} + m_{64} + m_{65} + 2m_{66} &= 6n_6, \\
n_1 + 2n_2 + 3n_3 + 4n_4 + 5n_5 + 6n_6 &= 2m.
\end{align*}
\]

2.1 Silicate networks

Silicates are the largest, very interesting and most complicated minerals by far. Silicates are obtained by fusing metal oxides or metal carbonates with sand [20], see Figure 2. A silicate network of dimension \( n \) symbolizes as \( SL_n \), where \( n \) is the number of hexagons between the center and boundary of \( SL_n \). A silicate network of dimension two is shown in Figure 3. The number of vertices in \( SL_n \) are \( 15n^2 + 3n \), and the number of edges are \( 36n^2 \).

In the following theorem, the exact formulas of \( \chi_\alpha(SL_n) \), \( \prod_1^*(SL_n) \), \( \prod_{1,c}(SL_n) \) and \( \prod_2(SL_n) \) for silicate networks are computed.

Theorem 2.1.1. Consider the silicate networks \( SL_n \), then the indices of \( \chi_\alpha(SL_n) \), \( \prod_1^*(SL_n) \), \( \prod_{1,c}(SL_n) \) and \( \prod_2(SL_n) \) are equal to

\[
\begin{align*}
\prod_{1,c}(SL_n) &= 2^{9n^2c-3nc}3^{15n^2c+3nc}, \\
\prod_2(SL_n) &= 2^{54n^2-18n}3^{72n^2}, \\
\chi_\alpha(SL_n) &= n6^{\alpha+1} + 3(2^{\alpha+1}(6n^2 + 2n) + 2^{2\alpha+1+1}(3n^2 - 2n), \\
\prod_1^*(SL_n) &= 2^{36n^2-18n}3^{54n^2+6n}.
\end{align*}
\]
Figure 3: Silicate network of dimension two, the solid vertices denote the oxygen atoms whereas the plain vertices represent the silicon atoms.

**Proof.** Let $G$ be the graph of silicate network $SL_n$ with $|V(SL_n)| = 15n^2 + 3n$ and $|E(SL_n)| = 36n^2$. By the properties of $SL_n$, the vertex partition of silicate networks $SL_n$ based on the degree of vertices comprises the vertices of degrees 3 and 6. The vertices on the center of $SiO_4$ are of degree 3, the vertices on both the boundary of $SL_n$ and its $SiO_4$ are degree 3 and others are of degree 6. Table 1 provides such partition for $SL_n$ below.

| Degrees | 3   | 6               |
|---------|-----|-----------------|
| Number of vertices | $6n^2 + 6n$ | $9n^2 - 3n$ |

By Table 1, $\Pi_{1,c}(G) = \prod_{v \in V(G)} d(v)^c$ and $\Pi_2(G) = \prod_{u \in V(G)} d(u)^{d(u)}$, we have

\[ \Pi_{1,c}(SL_n) = 3^{c(6n^2 + 6n)} 6^{c(9n^2 - 3n)} = 2^{9n^2 - 3nc} 3^{15n^2 c + 3nc}, \]

\[ \Pi_2(SL_n) = 3^{3(6n^2 + 6n)} 6^{6(9n^2 - 3n)} = 2^{54n^2 - 18n^3} 3^{72n^2}. \]

From the graphic properties of a silicate network, there are three types of edges based on the degree of the vertices of each edge. By Table 1, we get

\[ n_3 = 6n^2 + 6n, \quad n_6 = 9n^2 - 3n. \]

Note that $m_{3,3} + m_{3,6} + m_{6,6} = 36n^2 = |E(SL_n)|$. In addition, by Lemma 2.0.1, one can obtain

\[ 2m_{3,3} + m_{3,6} = 3n_3, \quad m_{3,6} + 2m_{6,6} = 6n_6. \]

Consequently,

\[ m_{3,3} = 6n, \quad m_{3,6} = 18n^2 + 6n, \quad m_{6,6} = 18n^2 - 12n. \]
Table 2: Edge partition of $SL_n$ based on degrees of end vertices of each edge.

| $(d(u), d(v))$ where $u, v \in E(G)$ | (3, 3)   | (3, 6)   | (6, 6)   |
|--------------------------------------|----------|----------|----------|
| Number of edges                     | $6n$     | $18n^2 + 6n$ | $18n^2 - 12n$ |

The following table gives the three types and the number of edges in each type for $SL_n$.

By Table 2, $\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha$ and $\prod_1^\alpha(G) = \prod_{uv \in E(G)} (d(u) + d(v))$, we obtain

$$\chi_\alpha(SL_n) = 6^\alpha \cdot 6n + 9^\alpha(18n^2 + 6n) + 12^\alpha(18n^2 - 12n)$$

$$= n6^{\alpha+1} + 32^{\alpha+1}(6n^2 + 2n) + 22^{\alpha+1}3^{\alpha+1}(3n^2 - 2n),$$

$$\prod_1^\alpha(SL_n) = 2^{36n^2 - 18n2^54n^2 + 6n}.$$

This completes the proof. □

2.2 Chain silicate networks

Next, we provide another family of silicate networks named as chain silicate networks and then compute its certain degree based topological indices. Here we provide chain silicate networks $CS_n$ of dimension $n$ as follows: A chain silicate network of dimension $n$ symbolizes as $CS_n$ is obtained by arranging $n$ tetrahedra linearly, see Figure 4. The number of vertices in $CS_n$ are $3n + 1$ and number of edges are $6n$.

Figure 4: Ortho, Pyro and chain silicates.

Theorem 2.2.1. Consider the chain silicate networks $CS_n$, then the indices of $\chi_\alpha(CS_n)$,
\( \Pi_1^*(CS_n), \Pi_{1,c}(CS_n) \) and \( \Pi_2(CS_n) \) are equal to

\[
\begin{align*}
\Pi_{1,c}(CS_n) &= 2^{nc-c}3^{3nc+c}, \\
\Pi_2(CS_n) &= 2^{6n-6}3^{12n}, \\
\chi_\alpha(CS_n) &= \begin{cases} \\
6^{\alpha+1}, & \text{if } n = 1, \\
2^{\alpha}3^{\alpha}(n+4) + 3^{2\alpha}(4n-2) + 2^{2\alpha}3^{\alpha}(n-2), & \text{if } n \geq 2,
\end{cases} \\
\Pi_1^*(CS_n) &= \begin{cases} \\
46656, & \text{if } n = 1, \\
2^{3n}3^{10n-2}, & \text{if } n \geq 2.
\end{cases}
\end{align*}
\]

**Proof.** Let \( G \) be the graph of chain silicate network \( CS_n \) with \( |V(CS_n)| = 3n + 1 \) and \( |E(CS_n)| = 6n \). Based on the graphic properties with the degree of vertices, the vertex partition of silicate networks \( CS_n \) are vertices of degree 3 and that of 6. Table 3 explains such partition for \( CS_n \).

| Degrees | 3 | 6 |
|---------|---|---|
| Number of vertices | \( 2n + 2 \) | \( n - 1 \) |

By Table 3, \( \Pi_{1,c}(G) = \prod_{v \in V(G)} d(v)^c \) and \( \Pi_2(G) = \prod_{u \in V(G)} d(u)^d(u) \), we have

\[
\begin{align*}
\Pi_{1,c}(CS_n) &= 3^{c(2n+2)}6^{c(n-1)} = 2^{nc-c}3^{3nc+c}, \\
\Pi_2(CS_n) &= 3^{3(2n+2)}6^{6(n-1)} = 2^{6n-6}3^{12n}.
\end{align*}
\]

The edge partition of silicate networks \( CS_n \) can be obtained by the degree sum of vertices for each edge of the graph. Note that \( m_{3,3} + m_{3,6} + m_{6,6} = n + 4 + 4n - 2 + n - 2 = 6n = |E(CS_n)| \). In addition, by Lemma 2.0.1, one can obtain

\[
2m_{3,3} + m_{3,6} = 3n_3, \quad m_{3,6} + 2m_{6,6} = 6n_6.
\]

Combining with \( n_3 = 2n + 2, \quad n_4 = n - 1 \), we arrive to

\[
m_{3,3} = n + 4, \quad m_{3,6} = 4n - 2, \quad m_{6,6} = n - 2.
\]

Table 4 gives such edges partition for \( CS_n \).

| \( d(u), d(v) \) where \( u, v \in E(G) \) | (3, 3) | (3, 6) | (6, 6) |
|--------------------------|-------|-------|-------|
| Number of edges \( n = 1 \) | 6     | 0     | 0     |
| \( n \geq 2 \)            | \( n + 4 \) | \( 4n - 2 \) | \( n - 2 \) |
By Table 4, \( \chi \alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha \) and \( \prod_1^\ast(G) = \prod_{uv \in E(G)} (d(u) + d(v)) \), we have

\[
\begin{align*}
\chi \alpha(CS_n) &= \begin{cases} 
6^{\alpha+1}, & \text{if } n = 1, \\
2^{\alpha}3^\alpha(n + 4) + 3^{2\alpha}(4n - 2) + 2^{2\alpha}3^\alpha(n - 2), & \text{if } n \geq 2,
\end{cases} \\
\prod_1^\ast(CS_n) &= \begin{cases} 
46656, & \text{if } n = 1, \\
2^{3n}3^{10n-2}, & \text{if } n \geq 2.
\end{cases}
\end{align*}
\]

This completes the proof. \( \square \)

2.3 Hexagonal networks

It is known that there exist three regular plane tilings with composition of same kind of regular polygons such as triangular, hexagonal and square. In the construction of hexagonal networks, triangular tiling is used. A hexagonal network of dimension \( n \) is usually denoted as \( HX_n \), where \( n \) is the number of vertices on each side of hexagon. The number of vertices in hexagonal networks \( HX_n \) are \( 3n^2 - 3n + 1 \) and number of edges are \( 9n^2 - 15n + 6 \).

Here, we compute the exact formulas of \( \chi \alpha(HX_n), \prod_1^\ast(HX_n), \prod_{1,c}(HX_n) \) and \( \prod_2(HX_n) \) for hexagonal networks.

**Theorem 2.3.1.** Consider the hexagonal networks \( HX_n \), then the indices of \( \chi \alpha(HX_n), \prod_1^\ast(HX_n), \prod_{1,c}(HX_n) \) and \( \prod_2(HX_n) \) are equal to

\[
\begin{align*}
\prod_{1,c}(HX_n) &= 2^{3n^2c+3nc-17c}3^{3n^2c-9nc+13c}, \\
\prod_2(HX_n) &= 2^{18n^2-6n-563}18n^2-54n+60, \\
\chi \alpha(HX_n) &= 2^{3n+1}3(n - 3) + 2^{8+2\alpha+1}(n - 2) - 2^{2\alpha}3^{\alpha+1}(3n^2 - 11n + 10) + 7^n12 + 3^{2\alpha}6, \\
\prod_1^\ast(HX_n) &= 2^{18n^2-46n-18}3^{9n^2-33n+42}5^{12n-24}7^{12}.
\end{align*}
\]

Figure 5: Hexagonal network of dimension 6.
Proof. Let $G$ be the graph of hexagonal network $HX_n$ with $|V(HX_n)| = 3n^2 - 3n + 1$ and $|E(CS_n)| = 9n^2 - 15n + 6$. In a hexagonal network $HX_n$, there are three types of degree of vertices. The vertices on the corners are of degree 3, the vertices on the boundary except the corners, are of degree 4 and others are of degree 6. By Table 5, we get

$$n_3 = 6, \ n_4 = 6n - 12, \ n_6 = 3n^2 - 9n + 7.$$ 

Note that $m_{3,6} = 6, m_{3,4} + m_{3,6} + m_{4,4} + m_{4,6} + m_{6,6} = 9n^2 - 15n + 6 = |E(HX_n)|$. In addition, by Lemma 2.0.1, one can obtain

$$m_{3,4} + m_{3,6} = 3n_3,$$
$$m_{3,4} + 2m_{4,4} + m_{4,6} = 4n_4,$$
$$m_{3,6} + m_{4,6} + 2m_{6,6} = 6n_6.$$ 

Consequently,

$$m_{3,4} = 12,$$
$$m_{3,6} = 6,$$
$$m_{4,4} = 6n - 18,$$
$$m_{4,6} = 12n - 24,$$
$$m_{6,6} = 9n^2 - 33n + 30.$$ 

Table 5 provides the vertex partition of hexagonal networks $HX_n$.

| Degrees | 3     | 4     | 6     |
|---------|-------|-------|-------|
| Number of vertices | 6     | $6n - 12$ | $3n^2 - 9n + 7$ |

By Table 5, $\prod_{1,c}(G) = \prod_{v \in V(G)} d(v)^c$ and $\prod_2(G) = \prod_{u \in V(G)} d(u)^{d(u)}$, we have

$$\prod_{1,c}(HX_n) = 2^{3n^2 + 3nc - 17c^3} 3^{3n^2 c - 9nc + 13c},$$
$$\prod_2(HX_n) = 2^{18n^2 - 6n - 56} 3^{18n^2 - 54n + 60}.$$ 

In a hexagonal network $HX_n$, there are five types of edges based on the degree of the vertices of each edge. The graphic properties on the degree sum of vertices for each edge imply the edge partition of silicate networks $HX_n$. By Lemma 2.0.1., Table 6 explains such partition.

| $(d(u), d(v))$ where $u, v \in E(G)$ | (3,4) | (3,6) | (4,4) | (4,6) | (6,6) |
|-----------------------------------|-------|-------|-------|-------|-------|
| Number of edges                   | 12    | 6     | $6n - 18$ | $12n - 24$ | $9n^2 - 33n + 30$ |
By Table 6, $\chi_\alpha(G) = \sum_{uv \in E(G)}(d(u) + d(v))^\alpha$ and $\prod_1^\infty(G) = \prod_{uv \in E(G)}(d(u) + d(v))$, we have
\[
\chi_\alpha(HX_n) = 2^{3\alpha + 1}(n - 3) + 2^{\alpha + 2}3^{\alpha + 1}(n - 2) - 2^{2\alpha}3^{\alpha + 1}(3n^2 - 11n + 10) + 7^{\alpha}12 + 3^{2\alpha}6,
\]
\[
\prod_1^\infty(HX_n) = 2^{18n^2 - 46n + 3n^2 - 33n + 42512n - 2472}.
\]

This completes the proof. \hfill \square

### 2.4 Oxide networks

Oxide networks are of vital importance in the study of silicate networks. If we delete silicon vertices from a silicate network, we obtain an oxide network. An $n$-dimensional oxide network is denoted as $OX_n$. The number of vertices is $9n^2 + 3n$ and the edge set cardinality is $18n^2$.

The exact formulas of $\chi_\alpha(OX_n)$, $\prod_1^\infty(OX_n)$, $\prod_{1,c}(OX_n)$ and $\prod_2(OX_n)$ for oxide networks are computed below.

![Figure 6: Oxide network of dimension 5.](image)

**Theorem 2.4.1.** Consider the oxide networks $OX_n$, then the indices of $\chi_\alpha(OX_n)$, $\prod_1^\infty(OX_n)$, $\prod_{1,c}(OX_n)$ and $\prod_2(OX_n)$ are equal to

- $\prod_{1,c}(OX_n) = 2^{18n^2}$,
- $\prod_2(OX_n) = 2^{72n^2 - 12n}$,
- $\chi_\alpha(OX_n) = n2^{\alpha + 2}3^{\alpha + 1} + 3n(3n - 2)2^{3\alpha + 1}$,
- $\prod_1^\infty(OX_n) = 2^{54n^2 - 24n}3^{12n}$.

**Proof.** Let $G$ be the graph of oxide network $OX_n$ with $|V(OX_n)| = 9n^2 + 3n$ and $|E(OX_n)| = 18n^2$. Because of the graphic properties on the degree of vertices, we have the vertex partition of hexagonal networks $OX_n$. Table 7 explains such partition for $OX_n$.

By Table 7, $\prod_{1,c}(G) = \prod_{v \in V(G)}d(v)^c$ and $\prod_2(G) = \prod_{u \in V(G)}d(u)^d(u)$, we have
Table 7: Vertex partition of $O X_n$ based on degrees of vertices.

| Degrees | 2    | 4    |
|---------|------|------|
| Number of vertices | $6n$ | $9n^2 - 3n$ |

$$\Pi_{1,c}(O X_n) = 2^{6cn}4^{(9n^2-3n)} = 218n^2c,$$
$$\Pi_2(O X_n) = 2^{12n}4^{(9n^2-3n)} = 272n^2-12n.$$  

Based on the graphic properties and Table 7, we get

$$n_2 = 6n, \quad n_4 = 9n^2 - 3n.$$  

Note that $m_{2,4} + m_{4,4} = 18n^2 = |E(O X_n)|$. In addition, by Lemma 2.0.1, one can obtain

$$m_{2,4} = 2n_2, \quad m_{2,4} + 2m_{4,4} = 4n_4.$$  

Consequently,

$$m_{2,4} = 12n, \quad m_{4,4} = 18n^2 - 12n.$$  

By the above calculation, the edge partition of silicate networks $O X_n$ are obtained in Table 8.

Table 8: Edge partition of $O X_n$ based on degrees of end vertices of each edge.

| $(d(u), d(v))$ where $u, v \in E(G)$ | (2,4) | (4,4) |
|--------------------------------|------|------|
| Number of edges | $12n$ | $18n^2 - 12n$ |

By Table 8, $\chi_\alpha(G) = \sum_{u,v \in E(G)}(d(u) + d(v))^\alpha$ and $\Pi_{1,1}(G) = \prod_{u,v \in E(G)}(d(u) + d(v))$, we have

$$\chi_\alpha(OX_n) = 12n6^\alpha + (18n^2 - 12n)8^\alpha = n2^{\alpha+2}3^{\alpha+1} + 3n(3n - 2)2^{3\alpha+1},$$
$$\Pi_{1,1}(OX_n) = 6^{12n}8^{18n^2-12n} = 2^{54n^2-24n^3}3^{12n}.$$  

This completes the proof.

2.5 Honeycomb networks

Honeycomb networks are very useful in computer graphics, cellular phone base stations, image processing and as a representation of benzenoid hydrocarbons in chemistry. If we recursively use hexagonal tiling in a particular pattern, honeycomb networks are formed. An $n$-dimensional honeycomb network is denoted as $H C_n$, where $n$ is the number of hexagons between central and boundary hexagon. Honeycomb network $H C_n$ is constructed from $H C_{n-1}$ by adding a layer of hexagons around boundary of $H C_{n-1}$. The number of vertices are $6n^2$ and the number of edges are $9n^2 - 3n$.


In the following result, the exact formulas of \( \chi_\alpha(HC_n) \), \( \Pi_1^*(HC_n) \), \( \Pi_{1,c}(HC_n) \) and \( \Pi_2(HC_n) \) for honeycomb networks are calculated.

**Theorem 2.5.1.** Consider the honeycomb networks \( HC_n \), then the indices of \( \chi_\alpha(HC_n) \), \( \Pi_1^*(HC_n) \), \( \Pi_{1,c}(HC_n) \) and \( \Pi_2(HC_n) \) are equal to

\[
\begin{align*}
\Pi_{1,c}(HC_n) &= 2^{6nc}3^{6n^2c-6nc}, \\
\Pi_2(HC_n) &= 2^{12n3^{18n^2-18n}}, \\
\chi_\alpha(HC_n) &= 3 \cdot 2^{2\alpha+1} + 12(n-1)5^\alpha + 2^{\alpha}3^{\alpha+1}(3n^2 - 5n + 2), \\
\Pi_1^*(HC_n) &= 2^{9n^2-15n+18}9^{9n^2-15n+65}12(n-1).
\end{align*}
\]

**Proof.** Let \( G \) be the graph of honeycomb network \( HC_n \) with \( |V(HC_n)| = 6n^2 \) and \( |E(HC_n)| = 9n^2 - 3n \). The vertex partition of honeycomb networks \( HC_n \) based on the degree of vertices are vertices of degree 2 and 3. The vertices of the boundary in one hexagon are either of degree 2 and others are of degree 3. Table 9 shows such partition for \( HC_n \) below.

| Degrees | 2            | 3            |
|---------|--------------|--------------|
| Number of vertices | \( 6n \)      | \( 6n^2 - 6n \) |

By Table 9, \( \Pi_{1,c}(G) = \prod_{v \in V(G)} d(v)^c \) and \( \Pi_2(G) = \prod_{u \in V(G)} d(u)^d(u) \), we have

\[
\begin{align*}
\Pi_{1,c}(HC_n) &= 2^{6nc}3^{6n^2c-6nc}, \\
\Pi_2(HC_n) &= 2^{12n3^{18n^2-18n}}.
\end{align*}
\]

In a honeycomb network \( HC_n \), there are three types of edges based on the degree of the vertices of each edge. There are three types of edges of honeycomb network \( HC_n \) based on
degrees of vertices. Based on the graphic properties and Table 9, we get
\[ n_2 = 6n, \quad n_3 = 6n^2 - 6n. \]

Note that \( m_{2,2} + m_{2,3} + m_{3,3} = 9n^2 - 3n = |E(HC_n)| \). In addition, by Lemma 2.0.1, one can obtain
\[ 2m_{2,2} + m_{2,3} = 2n_2, \quad m_{2,3} + 2m_{3,3} = 3n_3. \]

Consequently,
\[ m_{2,2} = 6, \quad m_{2,3} = 12n - 12, \quad m_{3,3} = 9n^2 - 15n + 6. \]

By the above calculation, Table 10 shows them with corresponding partite set cardinalities.

| \((d(u), d(v))\) where \(u, v \in E(G)\) | (2,2) | (2,3) | (3,3) |
|-----------------|--------|--------|--------|
| Number of edges | 6      | 12n - 12 | 9n^2 - 15n + 6 |

By Table 10, \( \chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha \) and \( \prod_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v)) \), we have
\[
\begin{align*}
\chi_\alpha(HC_n) &= 3 \cdot 2^{2\alpha+1} + 12(n - 1)5^\alpha + 2^\alpha3^\alpha+1(3n^2 - 5n + 2), \\
\prod_1^*(HC_n) &= 4^65^{12(n-1)}6^{9n^2-15n+6} = 2^{9n^2-15n+18}3^{9n^2-15n+6}5^{12(n-1)}. 
\end{align*}
\]

This completes the proof. \( \square \)

3 Conclusion

This paper is devoted to the study of certain degree based topological indices of certain chemical networks having both chemical and structural significance. More precisely, we have considered the silicate networks, hexagonal networks, honeycomb networks and oxide networks for their structural study. We determined the sum-connectivity index \( \chi_\alpha(G) \), the multiplicative version of ordinary first Zagreb index \( \prod_1(G) \), the first multiplicative Zagreb indices \( \prod_{1,c}(G) \) and the second multiplicative Zagreb indices \( \prod_2(G) \) for these chemical networks.

Furthermore, we provide the direct relation of \( \chi_\alpha(G), \prod_1(G), \prod_{1,c}(G) \) and \( \prod_2(G) \) under considered networks. It will be quite helpful to understand their underlying topologies. For the sake of refinement of the image, we fix \( \alpha \) and \( c \) equal to 2, \( n \geq 2 \). In the figures 8-11, the comparisons of these networks with all those indices are given.

4 Acknowledgment

The authors would like to express their sincere gratitude to Dr. Emeric Deutsch and his insightful suggestions, which led to a number of improvements.
Figure 8: The computer-based comparative graphs of the first multiplicative Zagreb index for all network families.

Figure 9: The comparative graphs of the second multiplicative Zagreb index for all the families of networks.
Figure 10: The comparisons for the sum-connectivity index for all network families.

Figure 11: The graphical representations of multiplicative version of ordinary first Zagreb index for all network families.
References

[1] J. A. Bondy, U. S. R. Murty, Graph Theory, Springer, New York, 2008.

[2] L. Berrocal, A. Olivieri, J. Rada, Extremal values of vertex-degree-based topological indices over hexagonal systems with fixed number of vertices, Appl. Math. Comput. 243 (2014) 176-183.

[3] H. Chen, R. Wu, H. Deng, The extremal values of some topological indices in bipartite graphs with a given matching number, Appl. Math. Comput. 280 (2016) 103-109.

[4] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, Discrete Math. 285 (2004) 57-66.

[5] E. Deutsch, S. Klavžar, Computing the Hosoya Polynomial of Graphs from Primary Subgraphs, MATCH Commun. Math. Comput. Chem. 70 (2013) 627-644.

[6] E. Deutsch, S. Klavžar, M-polynomial and degree-based topological indices, Iranian J. Math. Chem, 6 (2015) 93-102.

[7] H. Deng, G. Huang, X. Jiang, A unified linear programming modeling of some topological indices, J. Comb. Optim. 30(3) (2015) 826-837.

[8] M. Eliasi, A. Iranmanesh, I. Gutman, Multiplicative version of first Zagreb index, MATCH Commun. Math. Comput. Chem. 68 (2012) 217-230.

[9] J. Estes, B. Wei, Sharp bounds of the Zagreb indices of k-trees, J. Comb. Optim. 27(2014) 271-291.

[10] M.R. Farahani, First and Second Zagreb polynomials of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes, Int. Letters of Chemistry, Physics and Astronomy 12 (2014) 56-62.

[11] M.R. Farahani, Zagreb Indices and Zagreb Polynomials of Pent-Heptagon Nanotube $VAC_5C_7(S)$, Chemical Physics Research Journal 6(1) (2013) 35-40.

[12] M.R. Farahani, Zagreb Indices and Zagreb Polynomials of Polycyclic Aromatic Hydrocarbons PAHs, Journal of Chemica Acta. 2 (2013) 70-72.

[13] I. Gutman, Molecular graphs with minimal and maximal Randić indices, Croatica Chem. Acta 75 (2002) 357-369.

[14] I. Gutman, R. Cruz, J. Rada, Wiener index of Eulerian graphs, Discrete Appl. Math. 162 (2014) 247-250.

[15] I. Gutman, B. Rušičić, N. Trinajstić, C.F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, J. Chem. Phys. 62 (1975) 3399-3405.
[16] I. Gutman, B. Furtula, Z.K. Vukicevic, G. Popivoda, On Zagreb Indices and Coincides, MATCH Commun. Math. Comput. Chem. 74 (1) (2015) 5-16.

[17] I. Gutman, B. Furtula, Ž Kovijanić Vuković, G. Popivoda, Zagreb indices and coincides, MATCH Commun. Math. Comput. Chem. 74 (2015) 5-16.

[18] I. Gutman, Multiplicative Zagreb indices of trees, Bull. Soc. Math. Banja Luka 18 (2011) 17-23.

[19] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi$-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972) 535-538.

[20] S. Hayat, M. Imran, Computation of topological indices of certain networks, Appl. Math. Comput., 240 (2014) 213-228.

[21] R. Kazemi, Note on the multiplicative Zagreb indices, Discrete Appl. Math. 198 (2016) 147-154.

[22] P. V. Khadikar, On a Novel Structural Descriptor PI, Nat. Acad. Sci. Lett. 23(2000) 113-118.

[23] J. B. Liu, X. F. Pan, Asymptotic incidence energy of lattices, Physica A 422 (2015) 193-202.

[24] J. B. Liu, X. F. Pan, F. T. Hu, F. F. Hu, Asymptotic Laplacian-energy-like invariant of lattices, Appl. Math. Comput. 253 (2015) 205-214.

[25] J. B. Liu, X.F. Pan, L. Yu, D. Li, Complete characterization of bicyclic graphs with minimal Kirchhoff index, Discrete Appl. Math. 200 (2016) 95-107.

[26] J. B. Liu, W.R. Wang, X.F. Pan, Y.M. Zhang, On degree resistance distance of cacti, Discrete Appl. Math. 203 (2016) 217-225.

[27] S. Li, Q. Zhao, Sharp upper bounds on Zagreb indices of bicyclic graphs with a given matching number. Math. and Comp. Model. 54 (2011) 2869-2879.

[28] H. Narumi, M. Katayama, Simple topological index. A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons, Mem. Fac. Engin. Hokkaido Univ. 16 (1984) 209-214.

[29] S. Nikolić, G. Kovačević, A. Milic'cević, N. Trinajstić, The Zagreb indices 30 years after. Croat. Chem. Acta 76 (2003), 113-124.

[30] B. Rajan, A. William, C. Grigorious, S. Stephen, On Certain Topological Indices of Silicate, Honeycomb and Hexagonal Networks, J. Comp. & Math. Sci., 3 (2012) 530-535.
[31] Y. Shi, Note on two generalizations of the Randic index, Appl. Math. Comput. 265 (2015) 1019-1025.

[32] M. K. Siddiquia, M. Imranb, A. Ahmadc, On Zagreb indices, Zagreb polynomials of some nanostar dendrimers Appl. Math. Comput. 280 (2016) 132-139.

[33] M. K. Siddiqui, M. Imran, A. Ahmad, On Zagreb indices, Zagreb polynomials of some nanostar dendrimers, Appl. Math. Comput. 280 (2016) 132-139.

[34] R. M. Tache, On degree-based topological indices for bicyclic graphs, MATCH Commun. Math. Comput. Chem. 76 (2016) 99-116.

[35] R. Todeschini, V. Consoni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees, MATCH Commun. Math. Comput. Chem. 64 (2010) 359-372.

[36] S. Wang, B. Wei, Multiplicative Zagreb indices of k-trees, Discrete Appl. Math. 180 (2015) 168-175.

[37] S. Wang, B. Wei, Multiplicative Zagreb indices of cacti, Discrete Math. Algorithm. Appl., DOI: 10.1142/S1793830916500403.

[38] C. Wang, S. Wang, B. Wei, Cacti with extremal PI index, Transactions on Combinatorics, in press.

[39] K. Xu, H. Hua, A unified approach to extremal multiplicative Zagreb indices for trees, unicyclic and bicyclic graphs, MATCH Commun. Math. Comput. Chem. 68 (2012) 241-256.

[40] Q. Zhao, S. Li, On the maximum Zagreb index of graphs with $k$ cut vertices. Acta Appl. Math. 111 (2010), 93-106.

[41] B. Zhou, N. Trinajstić, On general sum-connectivity index, J. Math. Chem. 47 (2010) 210-218.