Annual Methodological Archive Research Review
http://amresearchreview.com/index.php/Journal/about
Volume 4, Issue 4 (2026)

Online ISSN 3007-3197
Print ISSN 3007-3189

http://amresearchreview.com/index.php/Journal/about

Harary and Hosoya Polynomials of Some Chain Networks

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ABSTRACT

Chemical graph theory is a branch of mathematics that computes topological indices-molecular descriptors derived from the graph representation of a chemical compound. In 1988, Hosoya introduced the Hosoya polynomial of a graph, which has the distinctive ability to sum the number of paths of varying distances within the graph. To better understand the geometric patterns underlying the computed distance-based topological indices and the Hosoya polynomial of the network, we present graphical illustrations. This analysis of the Hosoya polynomial and its associated indices lays the groundwork for further investigations into chain hex-derived networks and their properties. In this article, we derive the closed-form expressions for the Wiener, hyper-Wiener, and Harary indices, as well as the general form of the Hosoya polynomial, for three specific network types: the Chain Oxide, Chain Silicate, and Chain Hex-Derived Network of Type 3.

Keywords: Topological Indices, Hosoya Polynomials, Harary Polynomials, Wiener Index, Chain Oxide Network, Chain Silicate Network, Chain Hex Derived Network

Introduction

The mathematical modelling of chemical phenomena is done using graph theory in the

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Volume 4, Issue 4 (2026)

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topology section of mathematical chemistry known as chemical graph theory. For chemists, one of the most useful techniques that graph theory has provided are topological indices. A representation of a molecule's molecular formula is called a molecular graph in the basics of graph theory [1], its edges reflect its chemical bonds, while its vertices represent its atoms [2]. A popular discipline that combines chemistry, mathematics, and data science is called cheminformatics. A topological index is a quantity that can be directly calculated from a molecule's structural graph. Being a graph structural invariant, it is independent of how a graph is labelled or illustrated. In general, different topological indices indicate molecular size and structure. Topological indices [3], which graph theory provides, are an essential tool. Chemistry and graph theory might be combined to create the chemical graph theory. The fields of information science, mathematics, and chemistry are combined in the modern academic field known as cheminformatics. It looks at the connections between two methods used to predict biological activity and chemical compound attributes [4], known as (QSAR) and (QSPR). The inventor of TIs, Wiener, came up with this notion in 1947 while researching the boiling points of paraffins. It was first introduced by Wiener, who initially used the term path number (1947). It is the fundamental topological index based on distance [5, 6].

Topological indices can transform the chemical structure into numerical values, making them useful in (QSAR) and (QSPR) investigations [7]. To determine the relationship between the atoms, more than 100 topological characteristics were assessed.Chemical graph theory is credited to Balaban, Graovac, Gutman, Hosoya, Milan Randic', and Trinajstic' as its creators (also Harry Wiener and others). Several hundred researchers were apparently engaged in this field in 1988, and they turned out 500 articles annually. There have been many monographs written in the field, such as the two-volume comprehensive text Chemical Graph Theory by Trinajstic', which gave an overview of the topic up to the mid-1980s. A connectivity index, also referred to as a topological index, is a term used to define the topology of a chemical compound's molecular graph [8]. The degree, distance, and spectrum of various topological indices [9]are used to categorise them. The most basic topological indices merely distinguish between the related undirected molecular graph, disregarding hydrogen atoms and double bonds.Additionally useful application for polynomials can be found in science; For example, A graph's Hosoya Polynomial generates a function for distributing distances, introduced by *Hosoya* (1988) [10] and for Ω', a connecting graph, is defined as

$$H(\Omega', y) = \frac{1}{2}\sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} y^{d(u,w)},$$

where d(u,w) indicate the distance between vertices u and w. There are numerous chemical applications for the Hosoya polynomial [11], especially, It is possible to compute practically all distance-based topological indices using this polynomial [12, 13].

A connected graph's Wiener index, indicated by $W(\Omega')$, is the sum of the distances between every pair of its vertices in Ω'; i.e., it may be written as

$$W(\Omega') = \frac{1}{2}\sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} d(u,w).$$

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Harold Wiener initially developed the Wiener index in 1947 to investigate the paraffin melting points [14]. The problems with the so-called inverted structure-property connections depend on it greatly [15]. Please review the article series and references therein for additional information regarding this topological polynomial and index [16-24]. Note that the Hosoya polynomial's first derivative and the Wiener index are the same at y=1:

$$W(\Omega') = \frac{\partial H(\Omega')}{\partial y}|_{y=1}$$

The connected graph's Modified Wiener index is represented by the symbol $W\alpha(\Omega')$ and is described as the sum of every pair of vertices' α power distances, where $\alpha \in \mathbb{N}$;i.e., it can be written as

$$W_\alpha(\Omega') = \frac{1}{2}\sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} d(u,w)^\alpha.$$

Another distance-based graph invariant is the hyper Wiener index, used to forecast physiochemical characteristics of organic compounds [25]. Randic [26] was introduced the hyper Wiener index as

$$WW(\Omega') = \frac{1}{2}\sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} (d(u,w) + d(u,w)^2).$$

A connected graph's Modified Hyper Wiener index, indicated by the symbol $WW\alpha(\Omega')$, is defined as

$$WW_\alpha(\Omega') = \frac{1}{2}\sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} (d(u,w)^\alpha + d(u,w)^{2\alpha}).$$

A connected graph's Harary polynomial, indicated by the symbol h(Ω'), is defined as

$$h(\Omega') = \sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} \frac{1}{d(u,w)} y^{d(u,w)}.$$

Using the symbol $h_t(\Omega')$, For a connected graph Ω', the Generalized Harary index is defined as

$$h_t(\Omega') = \sum_{u\in V(\Omega')} \sum_{w\in V(\Omega')} \frac{1}{d(u,w)+t},$$

where $t \in \mathbb{N}$. A connected graph's Multiplicative Wiener index, indicated by the symbol $\Pi(\Omega')$, is defined as

$$\Pi(\Omega') = \prod_{u,w\subseteq V(\Omega')} d(u,w).$$

In this study, the topological indices of COX(n), CSL(n), and $CHDN_3(n)$ were calculated. We refer to [27-34] to learn more about topological indices and their applications.

Methodology

A simple graph $\Omega'=(V,E)$ consists of an ordered set of pairs of various vertices of Ω' known as edges and a finite nonempty collection of objects known as vertices. The quantity of vertices pairs at distances of 1,2,3, ... , $d(\Omega')$ must be determined to be able

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to calculate the Hosoya polynomial of a graph K, where $d(\Omega') = maxd(u,w); u,w \in V(\Omega')$. For this object, we use mathematical induction. Hosoya polynomial is viewed generally as follows:

$$H(\Omega'; y) = |c_0(n)|y^0 + |c_1(n)|y^1 + |c_2(n)|y^2 + \cdots + |c_d(n)|y^d,$$

where $|c_i(n)|$=number of pairs of vertices at 'i' distance. Basic calculus is applicable to calculate the Wiener index and hyper Wiener index.

Computational Results

We demonstrate our computational findings in this section.

Chain Oxide Network COX(n)

In order to fully understand silicate networks, oxide networks are essential. An oxide network OX(n) results from the removal of silicate network's silicon vertices.COX(n) stands for a Chain Oxide Network. Figure 1 illustrates the oxide network COX(n).

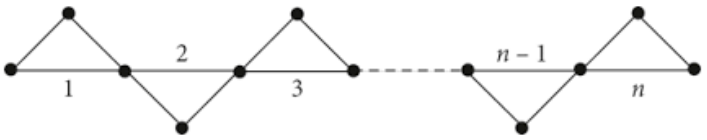

Figure 1: Chain Oxide Network COX(n)

Lemma 1. The Chain Oxide Network has 3n edges and 2n+1 vertices.

Theorem 3.1.1. For the Chain Oxide Network COX(n) for $n \geq 2$, where n is length of Chain Oxide Network, we have

$$H(COX(n); y) = (2n+1) + (3n)y + \sum_{r=2}^{n} 4(n-r+1)y^r.$$

Proof: In order to verify this theorem, we must calculate $|c_r(n)|$, where $r = 2,3,4, \ldots, n$. Obviously, from Lemma 1 we have

$$|c_0(n)| = |V| = 2n+1$$
$$|c_1(n)| = |E| = 3n$$

Following is the remaining proof.

$$|c_2(2)| = 4(1)$$
$$|c_2(3)| = 4(2)$$
$$|c_2(4)| = 4(3)$$
$$|c_2(5)| = 4(4)$$
$$|c_2(6)| = 4(5)$$
$$|c_2(7)| = 4(6)$$

Now, one can draw the conclusion that

$$|c_2(n)| = 4(n-1)$$

Now for $|c_3(n)$

$$|c_3(3)| = 4(1)$$
$$|c_3(4)| = 4(2)$$
$$|c_3(5)| = 4(3)$$
$$|c_3(6)| = 4(4)$$

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$$|c_3(7)| = 4(5)$$
$$|c_3(8)| = 4(6)$$

Now, one can draw the conclusion that

$$|c_3(n)| = 4(n-2)$$

Now for $|c_4(n)|$

$$|c_4(4)| = 4(1)$$
$$|c_4(5)| = 4(2)$$
$$|c_4(6)| = 4(3)$$
$$|c_4(7)| = 4(4)$$
$$|c_4(8)| = 4(5)$$
$$|c_4(9)| = 4(6)$$

Now, one can draw the conclusion that

$$|c_4(n)| = 4(n-3)$$

We can generalize from the above-mentioned method

$$|c_2(n)| = 4(n-1)$$
$$|c_3(n)| = 4(n-2)$$
$$|c_4(n)| = 4(n-3)$$
$$|c_5(n)| = 4(n-4)$$
$$|c_6(n)| = 4(n-5)$$

Now, one can draw the conclusion that

$$|c_r(n)| = 4(n-r+1)y^r$$

Using the information provided above, The Hosoya polynomial of the Chain Oxide Network COX(n) can be computed as follows:

$$H(COX(n;y) = (2n+1) + (3n)y + \sum_{r=2}^{n} 4(n-r+1)y^r.$$

Theorem 3.1.2. The Harary Polynomial of the Chain Oxide Network COX(n) is

$$h(COX(n);y) = \sum_{r=2}^{n} 4\frac{1}{r}(n-r+1)y^r$$

Proof: Theorem 3.1.1's calculation yields the following results:

$$h(\Omega';y) = \sum_{u\in V(COX(n))} \sum_{w\in V(COX(n))} \frac{1}{d(u,w)} y^{d(u,w)},$$
$$= \sum_{u\in V(COX(n))} \sum_{w\in V(COX(n))} \frac{1}{r} y^r$$
$$= \sum_{r=2}^{n} 4\frac{1}{r}(n-r+1)y^r$$

Theorem 3.1.3. For the Chain Oxide Network COX(n), we have

$$(1) W_\alpha(COX(n)) = 3n + \sum_{r=2}^{n} 4(n-r+1)r^\alpha$$
$$(2) WW_\alpha(COX(n)) = 3n + \sum_{r=2}^{n} 4(n-r+1)(r^\alpha + r^{2\alpha})$$
$$(3) H_t(COX(n)) = 3n + \sum_{r=2}^{n} \frac{4(n-r+1)}{r+t}$$
$$(4) \prod(COX(n)) = \prod_{r=2}^{n} 1^{(3n)} \times \prod_{r=2}^{n} r^{4(n-r+1)}$$

Proof: Theorem 3.1.2's calculation yields the following results:

(1) The Modified Wiener Index (MWI) is

$$W_\alpha(COX(n)) = \frac{1}{2}\sum_{u\in V(COX(n))} \sum_{w\in V(COX(n))} d(u,w)^\alpha$$
$$= \frac{1}{2}\sum_{u\in V(COX(n))} \sum_{w\in V(COX(n))} (1)^\alpha +$$

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Volume 4, Issue 4(2026)

Online ISSN 3007-3197
Print ISSN 3007-3189
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$$\frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} r^{\alpha} = 3n + \sum_{r=2}^{n} 4(n-r+1)r^{\alpha}$$

$\frac{\alpha}{n}$	2	3	4	5	6
1	14	37	76	135	218
2	22	77	196	415	778
3	38	181	580	1479	3242
4	70	461	1876	5791	14890
5	134	1237	6436	24135	72938
6	262	3437	22996	105055	373738

Table 1: MWI of COX.

For various values of n and α, where $n \geq 2$, Table 1 shows the values of the Modified Wiener index of COX.

(2) The Modified Hyper Wiener Index (MHWI) is

$$\begin{aligned} WW_{\alpha}(COX(n)) &= \frac{1}{2}\left(\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} d(u,w)^{\alpha}\right. \\ &\left.+\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} d(u,w)^{2\alpha}\right) \\ &= W_{\alpha}(COX(n)) + \frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} d(u,w)^{2\alpha} \\ &= W_{\alpha}(COX(n)) + \frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} (1)^{2\alpha} \\ &+\frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} (r)^{2\alpha} \\ &= \frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} (1^{\alpha} \\ &+1^{2\alpha}) + \frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))} (r^{\alpha}+r^{2\alpha}) \\ &= 3n(1^{\alpha}+1^{2\alpha}) + \sum_{r=2}^{n} 4(n-r+1)(r^{\alpha}+r^{2\alpha}) \end{aligned}$$

$\frac{\alpha}{n}$	2	3	4	5	6
1	36	114	272	550	996
2	92	538	2072	6206	15668
3	300	3618	23576	106534	376980
4	1100	28762	319592	2175422	10754900
5	4236	245634	4685432	48200230	333610836
6	16652	2161978	71432552	1117328126	10870539668

Table 2: MHWI of COX.

Table 2 provides values for the Modified hyper Wiener index of COX for various values of n and α, where $n \geq 2$.

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Volume 4, Issue 4 (2026)

Online ISSN 3007-3197
Print ISSN 3007-3189
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(3) The Generalized Harary Index (GHI) is

$$h_t(COX(n)) = \frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))}\frac{1}{d(u,w)+t}$$
$$= \frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))}\frac{1}{1+t}$$
$$+\frac{1}{2}\sum_{u\in V(COX(n))}\sum_{w\in V(COX(n))}\frac{1}{r+t}$$
$$= \frac{3n}{1+t}+\sum_{r=2}^{n}\frac{4(n-r+1)}{r+t}$$

$\frac{t}{n}$	2	3	4	5	6
0	8	43/3	65/3	149/5	193/5
1	13/3	49/6	64/5	181/10	839/35
2	3	29/5	139/15	1397/105	1249/70
3	23/10	271/60	767/105	1483/140	1805/126
4	28/15	389/105	423/70	556/63	1513/126
5	11/7	22/7	325/63	2386/315	11959/1155

Table 3: GHI of COX.

The values of Generalized Harary index of COX are shown in Table 3 for various values of n and α, where $n \geq 2$.

(4) The Multiplicative Wiener Index (MWI) is

$$\prod(K) = \prod_{u,w\subseteq V(COX(n))} d(u,w)$$
$$= \prod_{u,w\subseteq V(COX(n))} (1) \times \prod_{u,w\subseteq V(COX(n))} (r)$$
$$= \prod_{r=2}^{n} 1^{(3n)} \times \prod_{r=2}^{n} r^{4(n-r+1)}$$

Chain Silicate Network CSL(n)

The chain silicate networks, a separate class of silicate networks, are next presented, and their distinct indices topologically based on degrees are computed. Here, we are presenting chain silicate networks CSL(n), where n is the dimension:

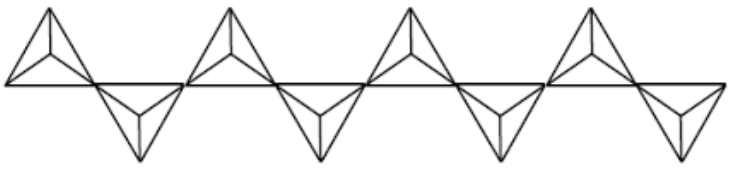

Figure 2: Chain Silicate Network CSL

Lemma 2. The Chain Silicate network has 6n edges and 3n+1 vertices.

Theorem 3.2.1. For the Chain Silicate network CSL(n) for $n \geq 2$, where Chain silicate network's length is n, we have

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Volume 4, Issue 4(2026)

Online ISSN 3007-3197
Print ISSN 3007-3189
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$$H(CSL(n); y) = (3n + 1) + (6n)y + \sum_{r=2}^{n} 9(n - r + 1)y^r$$

Proof: In order to validate this theorem, we must calculate $|c_r(n)|$, where $r = 2,3,4, \ldots, n$. Obviously, Lemma 2 gives us

$$|c_0(n)| = |V| = 3n + 1$$
$$|c_1(n)| = |E| = 6n$$

Following is the remaining proof.

$$|c_2(2)| = 9(1)$$
$$|c_2(3)| = 9(2)$$
$$|c_2(4)| = 9(3)$$
$$|c_2(5)| = 9(4)$$
$$|c_2(6)| = 9(5)$$
$$|c_2(7)| = 9(6)$$

Now, one can draw the conclusion that

$$|c_2(n)| = 9(n - 1)$$

Now for $|c_3(n)$

$$|c_3(3)| = 9(1)$$
$$|c_3(4)| = 9(2)$$
$$|c_3(5)| = 9(3)$$
$$|c_3(6)| = 9(4)$$
$$|c_3(7)| = 9(5)$$
$$|c_3(8)| = 9(6)$$

Now, one can draw the conclusion that

$$|c_3(n)| = 9(n - 2)$$

Now for $|c_4(n)|$

$$|c_4(4)| = 9(1)$$
$$|c_4(5)| = 9(2)$$
$$|c_4(6)| = 9(3)$$
$$|c_4(7)| = 9(4)$$
$$|c_4(8)| = 9(5)$$
$$|c_4(9)| = 9(6)$$

Now, one can draw the conclusion that

$$|c_4(n)| = 9(n - 3)$$

We can generalize from the above-mentioned method

$$|c_2(n)| = 9(n - 1)$$
$$|c_3(n)| = 9(n - 2)$$
$$|c_4(n)| = 9(n - 3)$$
$$|c_5(n)| = 9(n - 4)$$
$$|c_6(n)| = 9(n - 5)$$

Now, one can draw the conclusion that

$$|c_r(n)| = 9(n - r + 1)y^r$$

The Chain Silicate Network's Hosoya polynomial calculations can be made using the information given above.

$$H(CSL(n; y) = (3n + 1) + (6n)y + \sum_{r=2}^{n} 9(n - r + 1)y^r.$$

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Theorem 3.2.2. The Harary Polynomial is the following for the Chain Silicate network:

$$h(CSL(n); y) = \sum_{r=2}^{n} 9\frac{1}{r}(n-r+1)y^r$$

Proof: Theorem 3.2.1's calculation yields the following results:

$$h(\Omega'; y) = \sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} \frac{1}{d(u,w)} y^{d(u,w)}$$
$$= \sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} \frac{1}{r} y^r$$
$$= \sum_{r=2}^{n} 9\frac{1}{m}(n-r+1)y^r$$

Theorem 3.2.3. For Chain Silicate network CSL(n), we have

$$(1) W_\alpha(CSL(n)) = 6n + \sum_{r=2}^{n} 9(n-r+1)r^\alpha$$
$$(2) WW_\alpha(CSL(n)) = 6n + \sum_{r=2}^{n} 9(n-r+1)(r^\alpha + r^{2\alpha})$$
$$(3) H_t(CSL(n)) = 6n + \sum_{r=2}^{n} \frac{9(n-r+1)}{r+t}$$
$$(4) \prod (CSL(n)) = \prod_{r=2}^{n} 1^{(6n)} \times \prod_{r=2}^{n} r^{9(n-r+1)}$$

Proof: Theorem 3.2.2's calculations yields the following results

(1) The Modified Wiener Index (MWI) is

$$W_\alpha(CSL(n) = \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} d(u,w)^\alpha$$
$$= \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} (1)^\alpha + \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} r^\alpha$$
$$= 6n + \sum_{r=2}^{n} 9(n-r+1)r^\alpha$$

$\frac{\alpha}{n}$	2	3	4	5	6
1	30	81	168	300	486
2	48	171	438	930	1746
3	84	405	1302	3324	7290
4	156	1035	4218	13026	33498
5	300	2781	14478	54300	164106
6	588	7731	51738	236370	840906

Table 4: MWI of CSL.

For various values of n and α, where $n \geq 2$, Table 4 shows the values of the Modified Wiener index of CSL.

(2) The Modified Hyper Wiener Index (MHWI) is

$$WW_\alpha(CSL(n)) = \frac{1}{2}(\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} d(u,w)^\alpha$$
$$+ \sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} d(u,w)^{2\alpha})$$
$$= W_\alpha(CSL(n)) + \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} d(u,w)^{2\alpha}$$
$$= W_\alpha(CSL(n)) + \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} (1)^{2\alpha}$$
$$+ \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} (r)^{2\alpha}$$
$$= \frac{1}{2}\sum_{u\in V(CSL(n))} \sum_{w\in V(CSL(n))} (1^\alpha + 1^{2\alpha})$$

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$$+\frac{1}{2}\sum_{u\in V(CSL(n))}\sum_{w\in V(CSL(n))}(r^{\alpha}+r^{2\alpha})$$
$$=6n(1^{\alpha}+1^{2\alpha})+\sum_{r=2}^{n}9(n-r+1)(r^{\alpha}+r^{2\alpha})$$

$\frac{\alpha}{n}$	2	3	4	5	6
1	78	252	606	1230	2232
2	204	1206	4656	13956	35244
3	672	8130	53040	239694	848196
4	2472	64704	719076	489692	24198516
5	9528	552672	10542216	108450510	750624372
6	37464	4864440	160723236	2513988276	24458714244

Table 5: MHWI of CSL

For various values of n and α, where $n \geq 2$, Table 5 shows the values of the Modified Hyper Wiener index of CSL.

(3) The Generalized Harary Index (GHI) is

$$h_t(CSL(n))=\frac{1}{2}\sum_{u\in V(CSL(n))}\sum_{w\in V(CSL(n))}\frac{1}{d(u,w)+t}$$
$$=\frac{1}{2}\sum_{u\in V(CSL(n))}\sum_{w\in V(CSL(n))}\frac{1}{1+t}+\frac{1}{2}\sum_{u\in V(CSL(n))}\sum_{w\in V(CSL(n))}\frac{1}{r+t}$$
$$=\frac{6n}{1+t}+\sum_{r=2}^{n}\frac{9(n-r+1)}{r+t}$$

$\frac{\alpha}{n}$	2	3	4	5	6
0	33/2	30	183/4	633/10	1647/20
1	9	69/4	273/10	777/20	1809/35
2	25/5	123/10	397/20	1004/35	10821/280
3	25/4	48/5	549/32	6411/280	871/28
4	39/10	276/35	3639/280	535/28	7313/280
5	23/7	375/56	311/28	4597/280	17361/770

Table 6: GHI of CSL.

The Generalized Harary index of CSL values are presented in Table 6, for different values of n and α, where $n \geq 2$.

(4) The Multiplicative Wiener Index is

$$\prod(K)=\prod_{u,w\subseteq V(CSL(n))}d(u,w)$$
$$=\prod_{u,w\subseteq V(CSL(n))}(m)$$
$$=\prod_{m=2}^{n}1^{(6n)}\times\prod_{m=2}^{n}m^{9(n-m+1)}$$

Chain Hex Derive Network $CHDN_3$

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Online ISSN 3007-3197
Print ISSN 3007-3189
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The Chain Hex Derived network family of silicate networks is presented, and its distinct indices topologically based on degrees are calculated. Here, we are presenting Chain Silicate networks of dimension *n*, $CHDN_3(n)$.

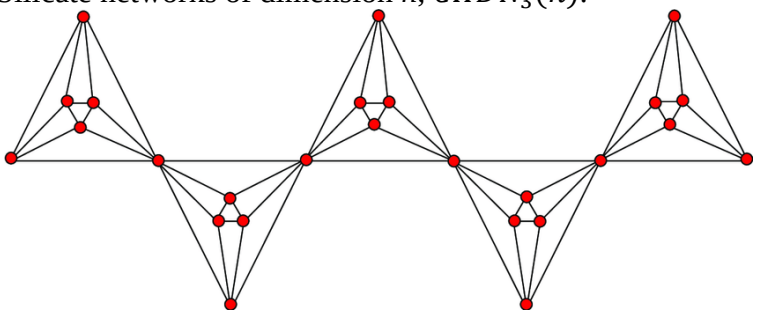

Figure 3: Chain Hex Derived Network $CHDN_3$

Lemma 3. The Chain Hex Derived network has *12n* edges and *5n+1* vertices.

Theorem 3.3.1. For Chain Hex Derived network $CHDN_3$ for $n \geq 4$, where the Chain Hex Derived network's length is *n*, we have

$$H(CHDN_3; y) = (5n + 1) + (12n)y + \sum_{r=4}^{n} 9(n - r + 1)y^r$$

Proof: In order to validate this theorem, we need to calculate $|c_r(n)|$, where $r = 2,3,4, \ldots, n$. Obviously, from Lemma 3 we have

$$|c_0(n)| = |V| = 5n + 1$$
$$|c_1(n)| = |E| = 12n$$

Following is the remaining proof.

$$|c_2(2)| = 22$$
$$|c_2(3)| = 41$$
$$|c_2(4)| = 60$$
$$|c_2(5)| = 79$$
$$|c_2(6)| = 98$$

Now, one can draw the conclusion that

$|c_2(n)| = 19n - 16$

Now for $|c_3(n)$

$$|c_3(3)| = 32$$
$$|c_3(4)| = 56$$
$$|c_3(5)| = 80$$
$$|c_3(6)| = 104$$
$$|c_3(7)| = 128$$

Now, one can draw the conclusion that

$|c_3(n)| = 25n - 65$

Now for $|c_4(n)|$

$$|c_4(4)| = 35$$
$$|c_4(5)| = 60$$
$$|c_4(6)| = 85$$
$$|c_4(7)| = 110$$
$$|c_4(8)| = 135$$

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Now, one can draw the conclusion that
$|c_4(n)| = 25n - 65$
We can generalize from the above-mentioned method

$$|c_2(n)| = 19n - 16$$
$$|c_3(n)| = 24n - 40$$
$$|c_4(n)| = 25n - 65$$
$$|c_5(n)| = 25n - 90$$
$$|c_6(n)| = 25n - 115$$

Now, one can draw the conclusion that
$|c_r(n)| = (25(n + r) - 35)y^r$

Using the information provided above, for Hosoya polynomial of Chain hex derived network $CHDN_3$ we can perform the calculations below.

$H(CHDN_3(n; y) = (5n + 1) + (12n)y + (19n - 16)y^2 + (24n - 40)y^3 + \sum_{r=4}^{n} (25(n + r) - 35)y^r$.

Theorem 3.3.2. For Chain Hex Derived network $CHDN_3(n)$, the Harary Polynomial is
$h(CHDN_3(n); y) = (12n)y + (19n - 16)y^2 + (24n - 40)y^3 + \sum_{r=4}^{n} \frac{1}{r}(25(n + r) - 35)y^r$
Proof: Theorem 3.1.1's calculation yields the following conclusions:

$$h(\Omega'; y) = \frac{1}{2}\sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{d(u,w)} y^{d(u,w)}.$$
$$= \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{1}y^1 + \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{2}y^2 + \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{3}y^3 + \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{r}y^r$$
$$= (12n)y + \frac{(19n-16)}{2}y^2 + \frac{24n-40}{3}y^3 + \sum_{r=4}^{n} 9\frac{1}{r}(25(n + r) - 35)y^r$$

Theorem 3.3.3. For Chain Hex Derived network $CHDN_3$(n), we have the following

$$(1)W_\alpha(CHDN_3(n)) = (12n)1^\alpha + (19n - 16)2^\alpha + (24n - 40)3^\alpha + \sum_{r=4}^{n} (25(n + r) - 35)r^\alpha$$
$$(2)WW_\alpha(CHDN_3(n)) = (12n)(1^\alpha + 1^{2\alpha}) + (19n - 16)(2^\alpha + 2^{2\alpha}) + (24n - 40)(3^\alpha + 3^{3\alpha}) + \sum_{r=4}^{n} (25(n + r) - 35)(r^\alpha + r^{2\alpha})$$
$$(3)H_t(CHDN_3(n)) = \frac{12n}{1+t} + \frac{19n-16}{2+t} + \frac{24n-40}{3+t} + \sum_{r=4}^{n} \frac{(25(n+r)-35)}{r+t}$$
$$(4)\prod (CHDN_3(n)) = 1^{(12n)} \times 2^{(19n-16)} \times 3^{(24n-40)} \times \prod_{r=4}^{n} r^{(25(n+r)-35)}$$

Proof: Theorem 3.3.2's calculation yields the following results:
(1) The Modified Wiener Index (MWI) is

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$$W_\alpha(CHDN_3(n) = \frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} d(u,w)^\alpha$$
$$= \frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (1)^\alpha$$
$$+\frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3)(n)} (2)^\alpha$$
$$+\frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (3)^\alpha$$
$$+\frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} r^\alpha$$
$$= 12n + (19n-16)2^\alpha + (24n-40)3^\alpha + \sum_{r=4}^{n}(25(n+r)-35)r^\alpha$$

$\frac{\alpha}{n}$	4	5	6	7	8
1	996	2293	4230	6932	10524
2	3432	9511	20380	38044	64858
3	12600	41887	104664	223646	430038
4	47784	190819	558544	1371544	2983294
5	184536	888463	3059280	8658062	21343134
6	720552	4201051	17076640	55814224	156116158

Table 7: MWI of $CHDN_3$.

For various values of n and α, where $n \geq 4$, Table 7 shows the values of Modified Wiener index of $CHDN_3$.

(2) The Modified Hyper Wiener Index (MHWI) is

$$WW_\alpha(CHDN_3(n)) = \frac{1}{2}(\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} d(u,w)^\alpha$$
$$+\sum_{u\in V(CHDN(n))}\sum_{w\in V(CHDN_3(n))} d(u,w)^{2\alpha})$$
$$= W_\alpha(CHDN_3(n)) + \frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} d(u,w)^{2\alpha}$$
$$= W_\alpha(CHDN_3(n)) + \frac{1}{2}(\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (1)^{2\alpha}$$
$$+\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (2)^{2\alpha}$$
$$+\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (3)^{2\alpha})$$
$$+\frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (r)^{2\alpha}$$
$$= \frac{1}{2}(\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (1^\alpha + 1^{2\alpha})$$
$$+\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (2^\alpha + 2^{2\alpha})$$
$$+\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (3^\alpha + 3^{2\alpha}))$$
$$+\frac{1}{2}\sum_{u\in V(CHDN_3(n))}\sum_{w\in V(CHDN_3(n))} (r^\alpha + r^{2\alpha})$$
$$= 12n(1^\alpha + 1^{2\alpha}) + (19n-16)(2^\alpha + 2^{2\alpha}) + (24n-40)(3^\alpha + 3^{2\alpha})$$
$$+\sum_{r=4}^{n}(25(n+r)-35)(r^\alpha + r^{2\alpha})$$

$\frac{\alpha}{n}$	2	3	4	5	6
1	4428	11804	24610	44976	75382
2	51216	200330	578924	1409588	3048152
3	733152	4242938	17181304	56037870	156546196

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4	11244048	97172198	554204528	2424486608	8747458988
5	176567808	2304532154	18602031280	109370779566	510144557692
6	2798967696	55724945390	639120198464	5060120461208	30549817288652

Table 8: MHWI of $CHDN_3$.

The values of Modified Hyper Wiener index of $CHDN_3$ are shown in Table 8 for various values of n and α, where $n \geq 4$. (3) The Generalized Harary Index (GHI) is

$$h_t(CHDN_3(n)) = \frac{1}{2}\sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{d(u,w)+t}.$$
$$= \frac{1}{2}(\sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{1+t}$$
$$+ \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{2+t}$$
$$+ \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{3+t})$$
$$+ \sum_{u\in V(CHDN_3(n))} \sum_{w\in V(CHDN_3(n))} \frac{1}{r+t}.$$
$$= \frac{12n}{1+t} + \frac{19n-16}{2+t} + \frac{24n-40}{3+t} + \sum_{r=4}^{n} \frac{(25(n+r)-35)}{r+t}.$$

$\frac{\alpha}{n}$	2	3	4	5	6
0	1655/12	650/3	3619/12	783/2	81583/168
1	91	901/6	4526/21	48043/168	6493/18
2	697/10	9923/84	144937/840	16237/70	745033/2520
3	1195/21	82447/840	45704/315	496103/2520	1168039/4620
4	1929/40	21227/252	35177/280	1189649/6930	6147019/27720
5	880/21	9311/126	10987/99	140905/924	1783058/9009

Table 9: GHI of $CHDN_3$.

For various values of n and α, where $n \geq 4$, we provide values of the generalized Harary index of $CHDN_3$ in Table 9.

(4) The Multiplicative Wiener Index (MWI) is

$$\prod(K) = \prod_{p,q\subseteq V(CHDN_3(n))} d(u,w)$$
$$= \prod_{u,w\subseteq V(CHDN_3(n))} (1) \times \prod_{u,w\subseteq V(CHDN_3(n))} (2)$$
$$\times \prod_{u,w\subseteq V(CHDN_3(n))} (3) \times \prod_{u,w\subseteq V(CHDN_3(n))} (r)$$
$$= \prod_{r=4}^{n} 1^{(12n)} \times \prod_{m=4}^{n} 2^{(19n-16)} \times \prod_{r=4}^{n} 3^{(24n-40)}$$
$$\times \prod_{r=4}^{n} r^{(25(n+r)-35)}$$

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• We calculated the MWI, MHWI and GHI for chain type networks COX, CSL and $CHDN_3$. Their graphical structures are given below.

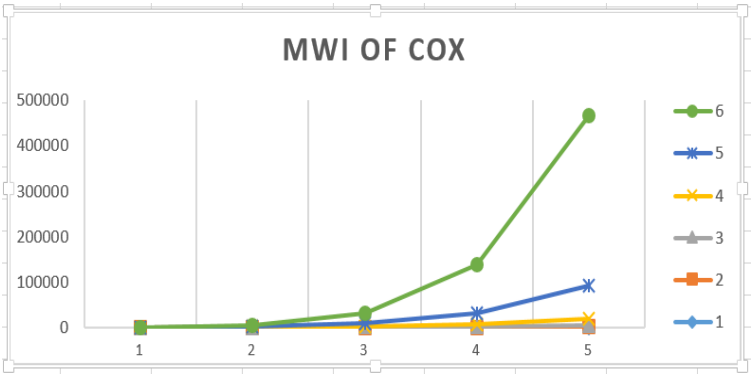

Figure 4: MWI of Chain Oxide Network COX

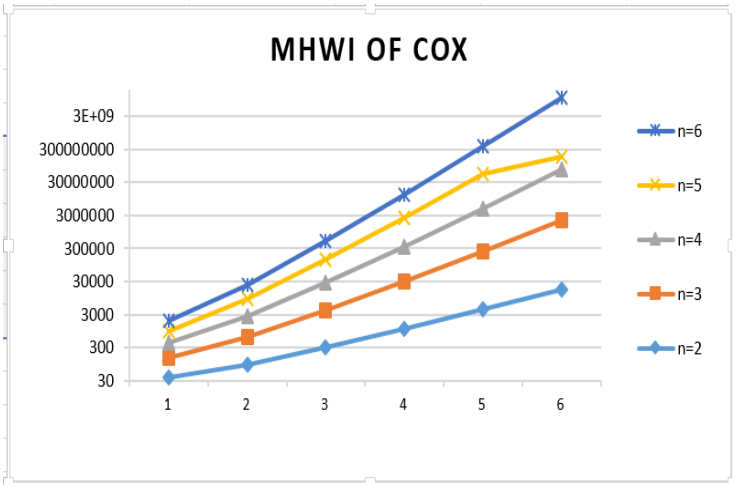

Figure 5: MHWI of Chain Oxide Network COX

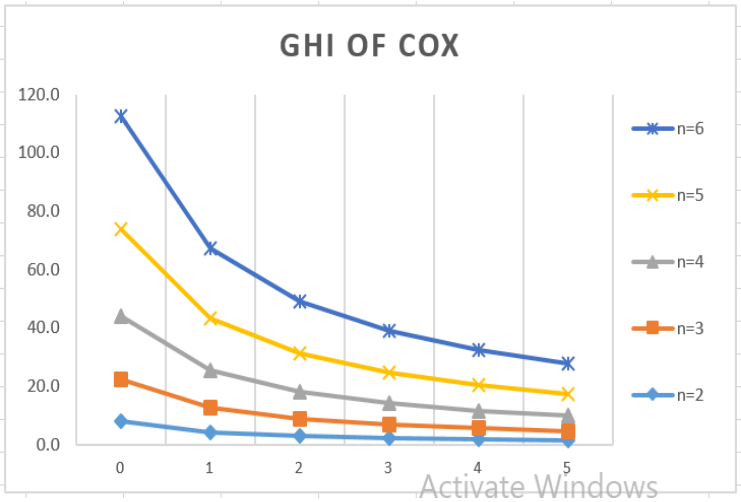

Figure 6: GHI of Chain Oxide Network COX

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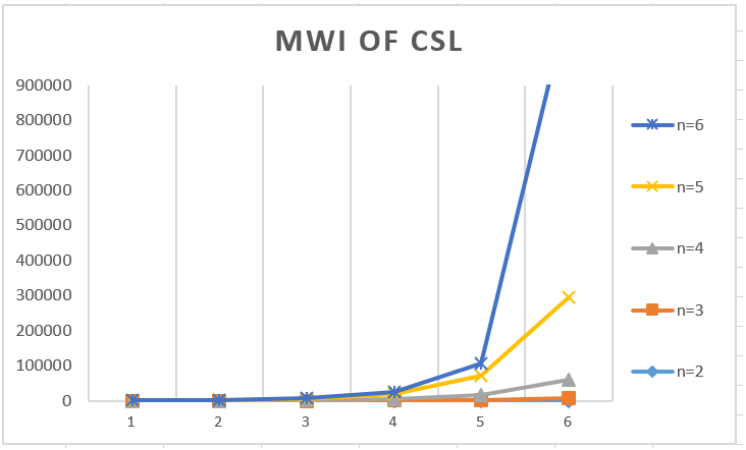

Figure 7: MWI of Chain Silicate Network CSL

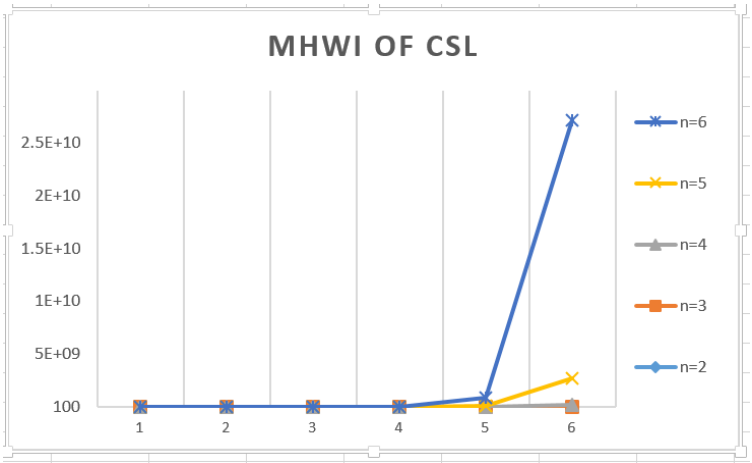

Figure 8: MHWI of Chain Silicate Network CSL

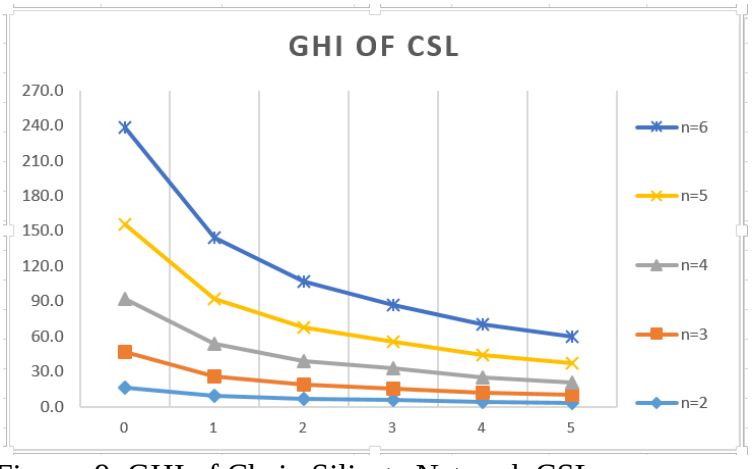

Figure 9: GHI of Chain Silicate Network CSL

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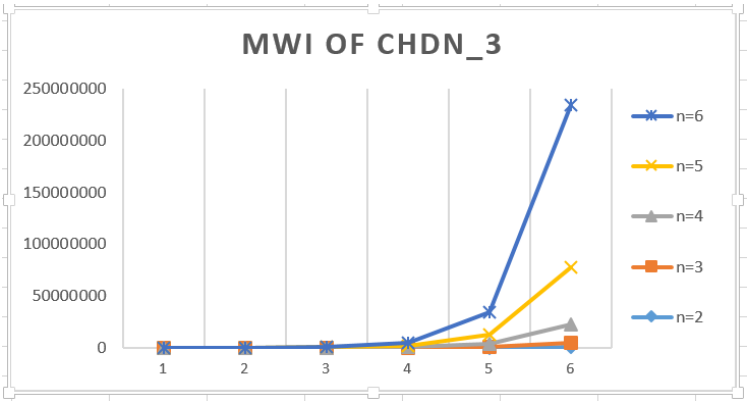

Figure 10: MWI of Chain Hex-Derived Network $CHDN_3$

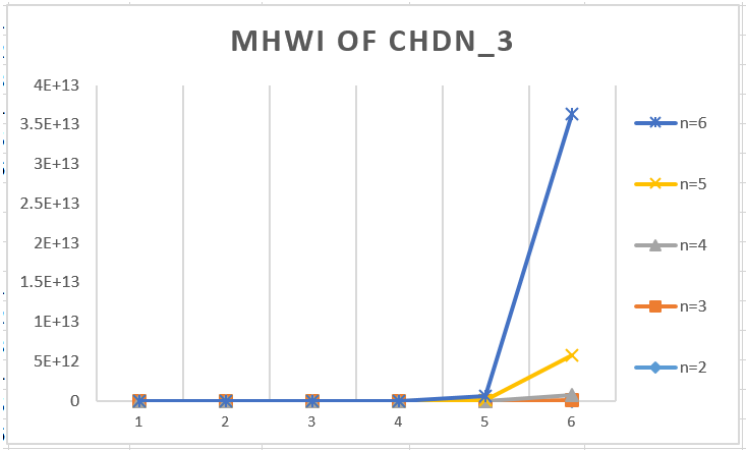

Figure 11: MHWI of Chain Hex-Derived Network $CHDN_3$

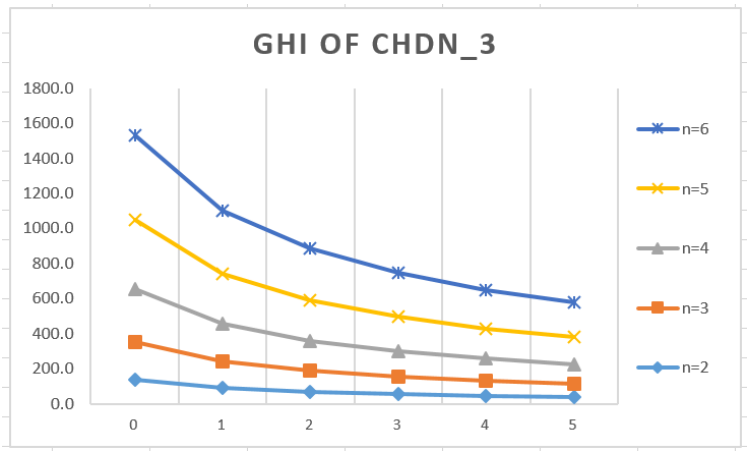

Figure 12: GHI of Chain Hex-Derived Network $CHDN_3$

Conclusion

The chain-type network of dimension n is a chemical network employed in this study to derive analytical expressions for several distance-based topological characteristics.

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Wiener demonstrated a strong correlation between the Wiener index and the boiling points of alkanes. Within the context of structure–property relationships, the Wiener index serves as a valuable topological descriptor, as it quantifies the compactness of a molecule in relation to fundamental properties such as branching and cyclicity. In this work, we compute the Hosoya polynomial, Wiener index, and hyper-Wiener index for chain-type networks. Deriving distance-based topological indices for families of graphs remains an intriguing and challenging problem.

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