УДК 519.17

О МНОГОЧЛЕНЕ ХОСОЯ ЦЕПНОЙ ШЕСТНАДЦАТЕРИЧНОЙ СЕТИ ТРЕТЬЕГО ТИПА

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Топологический индекс играет важную роль в характеристике различных физических свойств, биологической и химической активности молекулярного графа. Полином Хосоя используется для оценки основанных на расстоянии топологических индексов, таких как индекс Винера, индекс гипер-Винера, индекс Харари и индекс Тратча – Станкевича – Зефирова. В настоящем исследовании определяется замкнутая форма многочлена Хосоя для третьего типа цепной шестнадцатеричной производной сети размерности n и выводятся основанные на расстоянии топологические индексы сети с помощью их прямых формул, а также с помощью полученного многочлена Хосоя. Графически представлены вычисленные топологические индексы на основе расстояния и полином Хосоя базовой сети, чтобы понять их геометрическую структуру. Настоящее исследование полинома Хосоя и соответствующих индексов может заложить основу для дальнейшего изучения цепных шестнадцатеричных сетей и их свойств.

Ключевые слова: графические индексы; топологический индекс; шестнадцатеричная сеть третьего типа; топологические индексы на основе расстояний; полином Хосоя; полином графа.

ON THE HOSOYA POLYNOMIAL OF THE THIRD TYPE OF THE CHAIN HEX-DERIVED NETWORK

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A topological index plays an important role in characterising various physical properties, biological activities, and chemical reactivities of a molecular graph. The Hosoya polynomial is used to evaluate the distance-based topological indices such as the Wiener index, hyper-Wiener index, Harary index, and Tratch – Stankevitch – Zefirov index. In the present study, we determine a closed form of the Hosoya polynomial for the third type of the chain hex-derived network of dimension n and derive the distance-based topological indices of the network with the help of their direct formulas and alternatively via using the obtained Hosoya polynomial. Finally, we graphically represent the computed distance-based topological indices and the Hosoya polynomial of the underlying network to comprehend their geometrical pattern. This study of the Hosoya polynomial and the corresponding indices can set the basis for more exploration into chain hex-derived networks and their properties.

Keywords: graphical indices; topological index; third type of chain hex-derived network; distance-based topological indices; Hosoya polynomial; graph polynomial.

Образец цитирования:
Дас Ш, Рай Ш. О многочлене Хосоя цепной шестнадцатеричной сети третьего типа. *Журнал Белорусского государственного университета. Математика. Информатика.* 2022;3:67–78 (на англ.).
https://doi.org/10.33581/2520-6508-2022-3-67-78

For citation:
Das S, Rai S. On the Hosoya polynomial of the third type of the chain hex-derived network. *Journal of the Belarusian State University. Mathematics and Informatics.* 2022; 3:67–78.
https://doi.org/10.33581/2520-6508-2022-3-67-78

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Introduction

Let $G = (V, E)$ be a simple connected undirected graph, where the vertex set and the edge set are denoted by $V = V(G)$ and $E = E(G)$, respectively. The degree of a vertex $p \in V(G)$ in a graph G is the number of edges that are incident on p and we denote it as $d(p)$. The distance $d(p, q)$ between two vertices p and q of a graph G is the minimum number of edges in a path connecting them and the diameter $d(G)$ of a graph G is the longest distance among the distances of all pairs of vertices of G [1].

In chemical graph theory, a given chemical compound is represented by a graph where the vertices correspond to the atoms of that molecule and the edges correspond to the chemical bonds between them. The interconnection between graph theory and chemistry and their various chemical applications are discussed in references [2; 3]. In the field of chemical graph theory, the topological indices are graph invariants that predict the biological, physico-chemical and other properties of a molecule when calculated for a molecular graph. In general, it is a numeric quantity that has various applications in the studies of quantitative structure – property relationships and quantitative structure – activity relationships.

There are several classes of topological indices such as distance-based topological indices [4], degree-based topological indices [5], degree and distance-based topological indices [6], and counting related topological indices [7], etc. All these classes of topological indices are helpful in predicting and modelling the physical, chemical, biological, and other properties of a chemical structure. Usually, we adopt the basic definitions of the topological indices to calculate their respective numerical values. Instead, the concept of a polynomial is introduced in the graph theory to calculate different topological indices of a particular class [8]. The reason behind introducing the polynomial in graph theory is that by deriving a single closed polynomial expression, one can calculate several topological indices by differentiating or integrating (or a combination of both) it (the polynomial). We often use these graphic polynomials for the chemical applications of graph theory.

Hosoya polynomial. In the literature, numerous polynomials have been defined – the matching polynomial [9], the Hosoya polynomial [10], the Tutte polynomial [11], the Clar covering polynomial (also known as the Zhang – Zhang polynomial) [12], the Schultz polynomial [13], the *M*-polynomial [14; 15], to name but a few. Amid all of these polynomials, the Hosoya polynomial is used to calculate the distance-based topological indices.

In 1988, H. Hosoya introduced a counting polynomial and named it Wiener polynomial (commonly known as Hosoya polynomial) [10]. Generally, it sums up the number of distances of paths of different lengths in the graph. One of the most important applications of the Hosoya polynomial is to determine almost all the distance-based topological indices which are used to predict the chemical, physical, and other properties of chemical compounds. There are many articles in the literature in which the Hosoya polynomial has been obtained for the graphs of several classes (see [16–24]).

Definition 1 [10]. The Hosoya polynomial of a graph G in a variable x is denoted by $H(G, x)$ and is defined as

$$H(G, x) = \sum_{\{p, q\} \subseteq V(G)} x^{d(p, q)} = \sum_{r=1}^{d(G)} d(G, r) x^r,$$

where $d(G, r)$ denotes the number of pairs of vertices of G which are at a distance r from each other.

Allied distance-based topological indices. This section deals with the distance-based topological indices which are derived from the Hosoya polynomial of a given network. In order to determine the boiling point of paraffins, H. Wiener [25] introduced a Wiener index (also known as Wiener number) in 1947. Theoretically, the Wiener index of a graph G is the sum of the lengths of the shortest path between all (unordered) pairs of vertices and it is denoted as $W(G)$. Mathematically,

$$W(G) = \sum_{\{p, q\} \subseteq V(G)} d(p, q).$$

In 1993, M. Randić introduced the hyper-Wiener index which predicts the physico-chemical properties of organic compounds [26]. It is denoted as $WW(G)$ and defined as

$$WW(G) = \sum_{\{p, q\} \subseteq V(G)} \left[\frac{1}{2} d(p, q)^2 + \frac{1}{2} d(p, q)\right] =$$

$$= \frac{1}{2}\left[\sum_{\{p, q\} \subseteq V(G)} d(p, q)^2 + \sum_{\{p, q\} \subseteq V(G)} d(p, q)\right] = \frac{1}{2}\left[\sum_{\{p, q\} \subseteq V(G)} d(p, q)^2 + W(G)\right].$$

In 1990, Tratch et al. [27] further expanded the Wiener index which is known as Tratch – Stankevitch – Zefirov index, denoted as $TSZ(G)$ and mathematically represented as

$$TSZ(G)=\sum_{\{p,q\}\subseteq V(G)}\left[\frac{1}{6}d(p,q)^3+\frac{1}{2}d(p,q)^2+\frac{1}{3}d(p,q)\right]=$$

$$=\left[\frac{1}{6}\sum_{\{p,q\}\subseteq V(G)}d(p,q)^3+\frac{1}{2}\sum_{\{p,q\}\subseteq V(G)}d(p,q)^2+\frac{1}{3}\sum_{\{p,q\}\subseteq V(G)}d(p,q)\right].$$

Plavšić et al. [28], in 1993, introduced a more pragmatic approach to design a distance index that is slightly different from the Wiener index and named Harary index in admiration of professor F. Harary. The Harary index of a graph G is denoted as $Har(G)$ and defined as

$$Har(G)=\sum_{\{p,q\}\subseteq V(G)}\frac{1}{d(p,q)}.$$

The relational formulas [29] associated with the Hosoya polynomial and the distance-based topological indices are mentioned in table 1.

Table 1

**Relationship formulas
between distance-based topological indices and Hosoya polynomial**

No.	Topological index	Notation	Derivation from $H(G, x)$
(i)	Wiener index [25]	$W(G)$	$\frac{d}{dx}H(G,x)\Big\vert_{x=1}$
(ii)	Hyper-Wiener index [26]	$WW(G)$	$\frac{1}{2}\frac{d^2}{dx^2}\left[xH(G,x)\right]\Big\vert_{x=1}$
(iii)	Tratch – Stankevitch – Zefirov index [27]	$TSZ(G)$	$\frac{1}{3!}\frac{d^3}{dx^3}\left[x^2H(G,x)\right]\Big\vert_{x=1}$
(iv)	Harary index [28]	$Har(G)$	$\int_0^1\frac{H(G,x)}{x}dx$

Chain hex-derived network of the third type of dimension *n*. Nocetti et al. [30] introduced the n-dimensional hexagonal network in 2002 and also discussed its properties. During 2008, the n-dimensional hex-derived network of the first type (*HDN*1) and the hex-derived network of the second type (*HDN*2) are derived by using the hexagonal network [31]. Hex-derived networks have a wide range of applications in electronics, pharmaceutical sciences, and communication networks. Besides this, Raj et al. [32] designed some new chemical networks from the hexagonal network of dimension n in 2017, called hex-derived networks of the third type. Taking into account the chain silicate network [33] and the third type of the hex-derived network [32], a chain hex-derived network of the third type of dimension[1] n (*CHDN*3[n]) has been constructed (for a detailed drawing algorithm of the *CHDN*3[n] network, please refer to [34]). An example of the third type of chain hex-derived network of dimension 5 (i. e., *CHDN*3[5]) is shown in fig. 1.

In reference [35], various degree-based topological indices of the *CHDN*3[n] network are calculated with the help of their direct formulas. Whereas, very recently in reference [34], the same was derived by using the M-polynomial of the *CHDN*3[n] network and one also plotted the topological indices and the M-polynomial to understand their mathematical characteristics. Also, in reference [36], the structure of the subdivided hex-derived network of the third type of dimension n (*SHDN*3[n]) was designed and its M-polynomial and corresponding topological indices were estimated.

An outline of our work. In this paper, we will compute the distance-based topological indices of the *CHDN*3[n] network in two different ways. In the first place, we will use the direct mathematical formulas to calculate the indices of the *CHDN*3[n] network in section «Direct computation of distance-based topological indices of the *CHDN*3[n] network». Secondly, in section «Finding the Hosoya polynomial for the *CHDN*3[n]

[1]Dimension n indicates the number of edges in a row line for the third type of chain hex-derived network of dimension n.

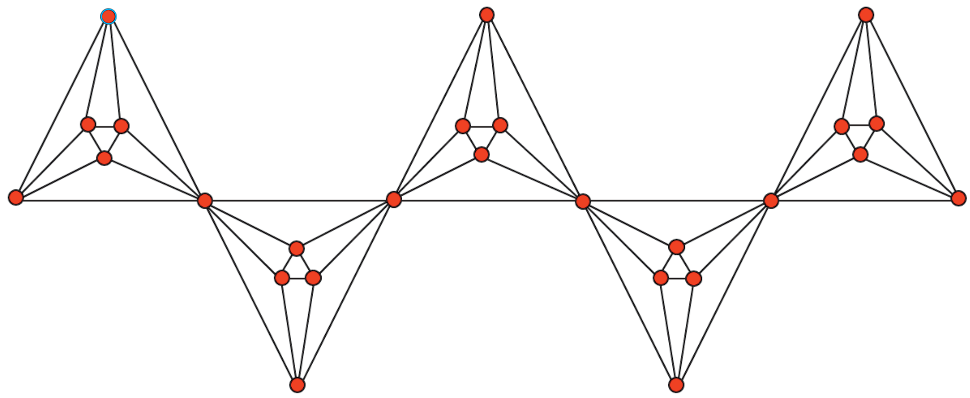

Fig. 1. The third type of chain hex-derived network of dimension 5 (*CHDN*3[5])

network», we obtain an exact expression of a Hosoya polynomial for the *CHDN*3[*n*] network and thereafter derive the related distance-based topological indices of the network by using the Hosoya polynomial. Additionally, we will sketch the Hosoya polynomial and correlated distance-based topological indices of the network for different dimensions in section «Graphical illustrations of our obtained results» to understand their geometrical behaviours.

Direct computation of distance-based topological indices of the *CHDN*3[*n*] network

Let us now estimate the distance-based topological indices of the chain hex-derived network of the third type of dimension n directly by using their respective topological formulas mentioned in the previous section.

Theorem 1. *Consider the third type of the chain hex-derived network of dimension n (CHDN*3[*n*]*), where $n \geq 5$, then we have the following results:*

$(i)\ W(CHDN3[n]) = \frac{25}{6}n^3 + \frac{35}{2}n^2 - \frac{11}{3}n;$

$(ii)\ WW(CHDN3[n]) = \frac{25}{24}n^4 + \frac{95}{12}n^3 + \frac{527}{24}n^2 - \frac{119}{12}n;$

$(iii)\ TSZ(CHDN3[n]) = \frac{5}{24}n^5 + \frac{5}{2}n^4 + \frac{93}{8}n^3 + \frac{53}{2}n^2 - \frac{101}{6}n;$

$(iv)\ Har(CHDN3[n]) = \frac{46n^2 + 126n + 70}{n(n+1)(n+2)} + 5\sum_{r=4}^{n-1}\frac{1}{r}(5n - 5r + 7) + \frac{59}{2}n - \frac{64}{3}.$

P r o o f. Let us first assume that p and q are two arbitrary vertices of *CHDN*3[*n*] and $d(p, q) = r$. For different pairs of vertices, the following cases arise which are shown in table 2.

Table 2

Different cases of counting of pairs of vertices which are at distance *r* from each other

Different cases	Distances	Pairs of degree			Total number of such pairs
		$d(p)=4$, $d(q)=4$	$d(p)=4$, $d(q)=8$	$d(p)=8$, $d(q)=8$	
Case 1	$d(p, q)=1$	$5n+6$	$6n-4$	$n-2$	$12n$
Case 2	$d(p, q)=2$	$10n-1$	$8n-12$	$n-3$	$19n-16$
Case 3	$d(p, q)=3$	$15n-16$	$8n-20$	$n-4$	$24n-40$
Case 4	$d(p, q)=r$, $4 \leq r \leq n-1$	$16(n-r+2)$	$4(2n-2r+1)$	$n-r-1$	$5(5n-5r+7)$
Case 5	$d(p, q)=n$	33	2	0	35

Ending table 2

Different cases	Distances	Pairs of degree			Total number of such pairs
		$d(p)=4,$ $d(q)=4$	$d(p)=4,$ $d(q)=8$	$d(p)=8,$ $d(q)=8$	
Case 6	$d(p,q)=n+1$	10	0	0	10
Case 7	$d(p,q)=n+2$	1	0	0	1

Hence, we have
(i) Wiener index:

$$W(CHDN3[n]) = \sum_{\{p,q\}\subseteq V(G)} d(p,q) =$$

$$= \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=1}} d(p,q) + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=2}} d(p,q) + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=3}} d(p,q) +$$

$$+ \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=r,\ r\in\{4,\dots,n-1\}}} d(p,q) + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=n}} d(p,q) =$$

$$= 12n\cdot 1 + (19n-16)\cdot 2 + (24n-40)\cdot 3 + \sum_{r=4}^{n-1} 5(5n-5r+7)\cdot r + 35\cdot n +$$

$$+10\cdot(n+1) + 1\cdot(n+2) = 168n - 140 + 5\sum_{r=4}^{n-1} r(5n-5r+7) = \frac{25}{6}n^3 + \frac{35}{2}n^2 - \frac{11}{3}n;$$

(ii) Hyper-Wiener index:

$$WW(CHDN3[n]) = \frac{1}{2}\sum_{\{p,q\}\subseteq V(G)} d(p,q)^2 + \frac{1}{2}W(G) =$$

$$= \frac{1}{2}\Bigg[\sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=1}} d(p,q)^2 + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=2}} d(p,q)^2 + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=3}} d(p,q)^2 +$$

$$+ \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=r,\ r\in\{4,\dots,n-1\}}} d(p,q)^2 + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=n}} d(p,q)^2 +$$

$$+ \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=n+1}} d(p,q)^2 + \sum_{\substack{\{p,q\}\subseteq V(G),\\ d(p,q)=n+2}} d(p,q)^2\Bigg] + \frac{1}{2}\left[\frac{25}{6}n^3 + \frac{35}{2}n^2 - \frac{11}{3}n\right] =$$

$$= \frac{1}{2}\Bigg[12n\cdot 1^2 + (19n-16)\cdot 2^2 + (24n-40)\cdot 3^2 + \sum_{r=4}^{n-1} 5(5n-5r+7)\cdot r^2 + 35\cdot n^2 +$$

$$+10\cdot(n+1)^2 + 1\cdot(n+2)^2\Bigg] + \frac{1}{2}\left[\frac{25}{6}n^3 + \frac{35}{2}n^2 - \frac{11}{3}n\right] =$$

$$= \frac{1}{2}\left[46n^2 + 328n - 410 + 5\sum_{r=4}^{n-1} r^2(5n-5r+7)\right] + \frac{1}{2}\left[\frac{25}{6}n^3 + \frac{35}{2}n^2 - \frac{11}{3}n\right] =$$

$$=\frac{1}{2}\left[\frac{25}{12}n^4+\frac{35}{3}n^3+\frac{317}{12}n^2-\frac{97}{6}n\right]+\frac{1}{2}\left[\frac{25}{6}n^3+\frac{35}{2}n^2-\frac{11}{3}n\right]=$$

$$=\frac{25}{24}n^4+\frac{95}{12}n^3+\frac{527}{24}n^2-\frac{119}{12}n;$$

(iii) Tratch – Stankevitch – Zefirov index:

$$TSZ(CHDN3[n])=\sum_{\{p,\,q\}\subseteq V(G)}\left[\frac{1}{6}d(p,\,q)^3+\frac{1}{2}d(p,\,q)^2+\frac{1}{3}d(p,\,q)\right]=$$

$$=\frac{1}{6}\left[\sum_{\{p,\,q\}\subseteq V(G)}d(p,\,q)^3\right]+\frac{1}{2}\left[\sum_{\{p,\,q\}\subseteq V(G)}d(p,\,q)^2\right]+\frac{1}{3}\left[\sum_{\{p,\,q\}\subseteq V(G)}d(p,\,q)\right]=$$

$$=\frac{1}{6}\left[\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=1}}d(p,\,q)^3+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=2}}d(p,\,q)^3+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=3}}d(p,\,q)^3+\right.$$

$$+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=r,\,r\in\{4,\,\ldots,\,n-1\}}}d(p,\,q)^3+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=n}}d(p,\,q)^3+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=n+1}}d(p,\,q)^3+$$

$$\left.+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=n+2}}d(p,\,q)^3\right]+\frac{1}{2}\left[\frac{25}{12}n^4+\frac{35}{3}n^3+\frac{317}{12}n^2-\frac{97}{6}n\right]+\frac{1}{3}\left[\frac{25}{6}n^3+\frac{35}{2}n^2-\frac{11}{3}n\right]=$$

$$=\frac{1}{6}\left[12n\cdot 1^3+(19n-16)\cdot 2^3+(24n-40)\cdot 3^3+\sum_{r=4}^{n-1}5(5n-5r+7)\cdot r^3+35\cdot n^3+10\cdot(n+1)^3+\right.$$

$$\left.+1\cdot(n+2)^3\right]+\frac{1}{2}\left[\frac{25}{12}n^4+\frac{35}{3}n^3+\frac{317}{12}n^2-\frac{97}{6}n\right]+\frac{1}{3}\left[\frac{25}{6}n^3+\frac{35}{2}n^2-\frac{11}{3}n\right]=$$

$$=\frac{1}{6}\left[46n^3+36n^2+854n-1190+5\sum_{r=4}^{n-1}r^3(5n-5r+7)\right]+\frac{1}{2}\left[\frac{25}{12}n^4+\frac{35}{3}n^3+\frac{317}{12}n^2-\frac{97}{6}n\right]+$$

$$+\frac{1}{3}\left[\frac{25}{6}n^3+\frac{35}{2}n^2-\frac{11}{3}n\right]=\frac{1}{6}\left[\frac{5}{4}n^5+\frac{35}{4}n^4+\frac{317}{12}n^3+\frac{179}{4}n^2-\frac{271}{6}n\right]+$$

$$+\frac{1}{2}\left[\frac{25}{12}n^4+\frac{35}{3}n^3+\frac{317}{12}n^2-\frac{97}{6}n\right]+\frac{1}{3}\left[\frac{25}{6}n^3+\frac{35}{2}n^2-\frac{11}{3}n\right]=\frac{5}{24}n^5+\frac{5}{2}n^4+\frac{279}{24}n^3+\frac{53}{2}n^2-\frac{101}{6}n;$$

(iv) Harary index:

$$Har(CHDN3[n])=\sum_{\{p,\,q\}\subseteq V(G)}\frac{1}{d(p,\,q)}=$$

$$=\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=1}}\frac{1}{d(p,\,q)}+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=2}}\frac{1}{d(p,\,q)}+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=3}}\frac{1}{d(p,\,q)}+$$

$$+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=r,\,r\in\{4,\,\ldots,\,n-1\}}}\frac{1}{d(p,\,q)}+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=n}}\frac{1}{d(p,\,q)}+$$

$$+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=n+1}}\frac{1}{d(p,\,q)}+\sum_{\substack{\{p,\,q\}\subseteq V(G),\\ d(p,\,q)=n+2}}\frac{1}{d(p,\,q)}=$$

$$=\frac{12n}{1}+\frac{19n-16}{2}+\frac{24n-40}{3}+\sum_{r=4}^{n-1}\frac{5(5n-5r+7)}{r}+\frac{35}{n}+\frac{10}{n+1}+\frac{1}{n+2}=$$

$$=\frac{46n^2+126n+70}{n(n+1)(n+2)}+5\sum_{r=4}^{n-1}\frac{1}{r}(5n-5r+7)+\frac{35}{n}+\frac{59}{2}n-\frac{64}{3}.$$

Finding the Hosoya polynomial for the *CHDN*3[*n*] network

Here we compute an exact expression of the Hosoya polynomial for the third type of the chain hex-derived network of dimension n to derive the related distance-based topological indices which are calculated in the previous section.

Theorem 2. *The Hosoya polynomial of the third type of the chain hex-derived network of dimension n* $(CHDN3[n])$*, where n ≥ 5, is*

$$H(CHDN3[n],\,x)=12nx+(19n-16)x^2+(24n-40)x^3+$$
$$+\sum_{r=4}^{n-1}5(5n-5r+7)x^r+35x^n+10x^{n+1}+x^{n+2}.$$

P r o o f. Let p and q be two arbitrary vertices of the third type of the chain hex-derived network of dimension n. Note that the longest distance among distances of all pairs of vertices (i. e., diameter) of the $CHDN3[n]$ network is $n + 2$. Here, we use the data tabulated in table 2, which gives the counting of the number of pairs of vertices of the $CHDN3[n]$ network which are at a distance r from each other, where $1 \le r \le n + 2$. Therefore, from definition 1 of the Hosoya polynomial, we have

$$H(CHDN3[n],\,x)=\sum_{\{p,\,q\}\subseteq V(CHDN3[n])}x^{d(p,\,q)}=\sum_{r=1}^{n+2}d(CHDN3[n],\,r)x^r=$$

$$=d(CHDN3[n],\,1)\,x^1+d(CHDN3[n],\,2)\,x^2+d(CHDN3[n],\,3)x^3+\sum_{r=4}^{n-1}d(CHDN3[n],\,r)\,x^r+$$

$$+\,d(CHDN3[n],\,n)\,x^n+d(CHDN3[n],\,n+1)\,x^{n+1}+d(CHDN3[n],\,n+2)\,x^{n+2}=$$

$$=12nx+(19n-16)x^2+(24n-40)x^3+\sum_{r=4}^{n-1}5(5n-5r+7)x^r+35x^n+10x^{n+1}+x^{n+2}.$$

Underneath we derive the distance-based topological indices of the $CHDN3[n]$ network by using the above single closed expression of the Hosoya polynomial and the relational formulas outlined in table 1.

Theorem 3. *Let CHDN*3[*n*] *be the third type of the chain hex-derived network of dimension n (n ≥ 5). Then form the Hosoya polynomial* $H(CHDN3[n],\,x)$:

(i) $W(CHDN3[n])=\frac{25}{6}n^3+\frac{35}{2}n^2-\frac{11}{3}n;$

(ii) $WW(CHDN3[n])=\frac{25}{24}n^4+\frac{95}{12}n^3+\frac{527}{24}n^2-\frac{119}{12}n;$

(iii) $TSZ(CHDN3[n])=\frac{5}{24}n^5+\frac{5}{2}n^4+\frac{93}{8}n^3+\frac{53}{2}n^2-\frac{101}{6}n;$

(iv) $Har(CHDN3[n])=\frac{46n^2+126n+70}{n(n+1)(n+2)}+5\sum_{r=4}^{n-1}\frac{1}{r}(5n-5r+7)+\frac{59}{2}n-\frac{64}{3}.$

P r o o f. The Hosoya polynomial for the $CHDN3[n]$ network, as obtained in theorem 2, is

$$H(CHDN3[n],\,x)=12nx+(19n-16)x^2+(24n-40)x^3+$$
$$+\sum_{r=4}^{n-1}5(5n-5r+7)x^r+35x^n+10x^{n+1}+x^{n+2}.$$

By applying the relational formulas (listed in table 1) over the Hosoya polynomial $H(CHDN3[n], x)$, we derive the distance-based topological indices as follows.

(i) The Wiener index and the Hosoya polynomial are related by

$$W(CHDN3[n]) = \frac{d}{dx} H(CHDN3[n], x)\Big|_{x=1} =$$

$$= \frac{d}{dx}\Bigg[12nx + (19n-16)x^2 + (24n-40)x^3 +$$

$$+ \sum_{r=4}^{n-1} 5(5n-5r+7)x^r + 35x^n + 10x^{n+1} + x^{n+2}\Bigg]\Bigg|_{x=1} = \frac{25}{6}n^3 + \frac{35}{2}n^2 - \frac{11}{3}n.$$

(ii) The relation between the hyper-Wiener index and the Hosoya polynomial is

$$W(CHDN3[n]) = \frac{1}{2}\frac{d^2}{dx^2}\big[x \cdot H(CHDN3[n], x)\big]\Big|_{x=1} =$$

$$= \frac{1}{2}\frac{d^2}{dx^2}\Big[12nx^2 + (19n-16)x^3 + (24n-40)x^4 +$$

$$+ \sum_{r=4}^{n-1} 5(5n-5r+7)x^{r+1} + 35x^{n+1} + 10x^{n+2} + x^{n+3}\Big]\Big|_{x=1} =$$

$$= \frac{1}{2}\Bigg[24n + 6(19n-16) + 12(24n-40) + \sum_{r=4}^{n-1} 5r(r+1)(5n-5r+7) +$$

$$+ 35n(n+1) + 10(n+1)(n+2) + (n+2)(n+3)\Bigg] =$$

$$= 23n^2 + 248n - 275 + \frac{5}{2}\sum_{r=4}^{n-1} r(r+1)(5n-5r+7) =$$

$$= \frac{25}{24}n^4 + \frac{95}{12}n^3 + \frac{527}{24}n^2 - \frac{119}{12}n.$$

(iii) The Tratch – Stankevitch – Zefirov index and the Hosoya polynomial are connected by

$$TSZ(CHDN3[n]) = \frac{1}{3!}\frac{d^3}{dx^3}\big[x^2 \cdot H(CHDN3[n], x)\big]\Big|_{x=1} =$$

$$= \frac{1}{6}\frac{d^3}{dx^3}\Bigg[12nx^3 + (19n-16)x^4 + (24n-40)x^5 + \sum_{r=4}^{n-1} 5(5n-5r+7)x^{r+2} +$$

$$+ 35x^{n+2} + 10x^{n+3} + x^{n+4}\Bigg]\Bigg|_{x=1} = \frac{5}{24}n^5 + \frac{5}{2}n^4 + \frac{93}{8}n^3 + \frac{53}{2}n^2 - \frac{101}{6}n.$$

(iv) The relation between the Harary index and the Hosoya polynomial is

$$Har(CHDN3[n]) = \int_0^1 \frac{H(G, x)}{x}dx =$$

$$= \int_0^1 \Bigg[12n + (19n-16)x + (24n-40)x^2 + \sum_{r=4}^{n-1} 5(5n-5r+7)x^{r-1} + 35x^{n-1} +$$

$$+ 10x^n + x^{n+1}\Bigg] = \frac{46n^2 + 126n + 70}{n(n+1)(n+2)} + 5\sum_{r=4}^{n-1}\frac{1}{r}(5n-5r+7) + \frac{59}{2}n - \frac{64}{3}.$$

Hence, the results of theorem 1 are verified. Moreover, we can see that finding the Wiener index, hyper-Wiener index, Tratch – Stankevitch – Zefirov index, and Harary index via the Hosoya polynomial of the *CHDN*3[*n*] network is more easy, feasible, and compact than computing (as shown in section «Direct computation of distance-based topological indices of the *CHDN*3[*n*] network») these indices of the network directly by their respective definitions.

Graphical illustrations of our obtained results

A graphical model of the chain hex-derived network of the third type of dimension n is discussed in subsection «Chain hex-derived network of the third type of dimension n». By using this model, the expression of the Hosoya polynomial and the corelated distance-based topological indices have been derived which are functions of n and x (table 3). To understand the geometrical behaviours of these expressions of the *CHDN*3[*n*] network, we draw the Hosoya polynomial for the third type of the chain hex-derived network of dimension $n = 5$ in the domain $0 \le x \le 2$ in fig. 2 and the corresponding distance-based topological indices of the network for different dimension[2] n ($5 \le n \le 10$ is considered here) in fig. 3, with the help of *Maple-13* software. From fig. 3, it can be observed that as the dimension increases, the values of each of the topological indices are also increasing.

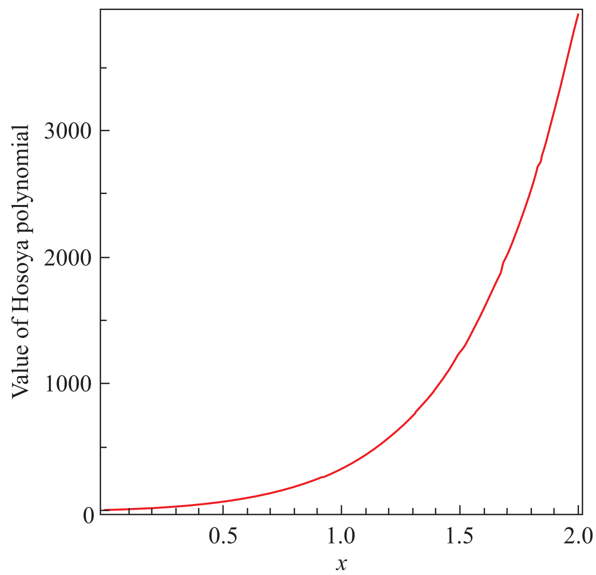

Fig. 2. The plot of the Hosoya polynomial of the *CHDN*3[5] for $0 \le x \le 2$

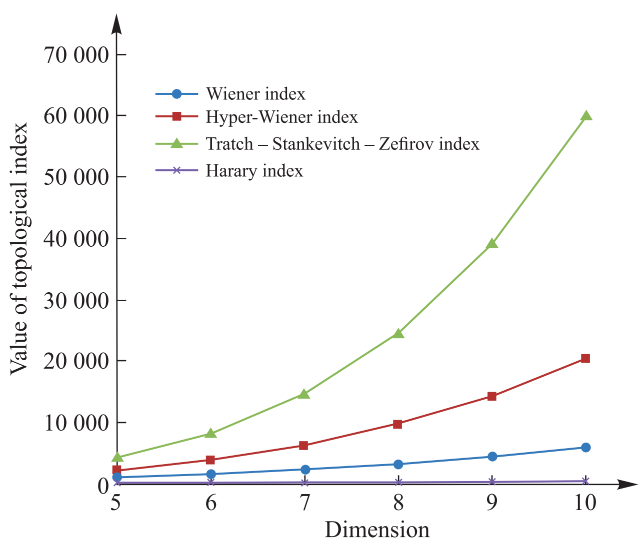

Fig. 3. The plot of the Wiener, hyper-Wiener, Tratch – Stankevitch – Zefirov, and Harary indices of the *CHDN*3[*n*] network for different values of n ($5 \le n \le 10$)

[2]Note that, the upper bound of the dimension n of the network has no limit.

Table 3

Hosoya polynomials and the respective distance-based topological indices of the *CHDN*3[*n*] network at different values of *n*

No.	Topological index	Dimension					
		$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$	$n = 10$
		Hosoya polynomial					
		$60x + 79x^2 + 80x^3 + 60x^4 + 35x^5 + 10x^6 + x^7$	$72x + 98x^2 + 104x^3 + 85x^4 + 60x^5 + 35x^6 + 10x^7 + x^8$	$84x + 117x^2 + 128x^3 + 110x^4 + 85x^5 + 60x^6 + 35x^7 + 10x^8 + x^9$	$96x + 136x^2 + 152x^3 + 135x^4 + 110x^5 + 85x^6 + 60x^7 + 35x^8 + 10x^9 + x^{10}$	$108x + 155x^2 + 176x^3 + 160x^4 + 135x^5 + 110x^6 + 85x^7 + 60x^8 + 35x^9 + 10x^{10} + x^{11}$	$120x + 174x^2 + 200x^3 + 185x^4 + 160x^5 + 135x^6 + 110x^7 + 85x^8 + 60x^9 + 35x^{10} + 10x^{11} + x^{12}$
(i)	Wiener index	940	1508	2261	3224	4422	5880
(ii)	Hyper-Wiener index	2140	3791	6223	9646	14 295	20 430
(iii)	Tratch – Stankevitch – Zefirov index	4245	8224	14 672	24 580	39 174	59 940
(iv)	Harary index	149.9762	196.3036	246.0278	298.7408	354.1226	411.9150

Conclusions

In the current study, a chemical network named as the third type of the chain hex-derived network of dimension n ($CHDN3[n]$) has been considered to investigate the analytical expression of some of its distance-based topological descriptors. Initially, we used the distance-dependent mathematical formulas to evaluate the distance-based topological indices, namely, Wiener, hyper-Wiener, Tratch – Stankevitch – Zefirov, and Harary indices of the $CHDN3[n]$ network. Afterwards, we derived the same indices by using our proposed closed form of the Hosoya polynomial of the $CHDN3[n]$ network. And hence, we concluded that calculating these indices via the Hosoya polynomial is more simple, shorter, compact, and more practical, instead of computing them directly by using their mathematical formulas. Moreover, we graphically represented the Hosoya polynomial and the distance-based topological indices of the underlying structure to realise their geometrical behaviour. The obtained results may play a key role in amplifying our understanding of the behaviour and nature of chain hex-derived networks further.

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Received 16.07.2022 / revised 10.11.2022 / accepted 10.11.2022.