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Molecular Topological Properties of Spider's Web Graph and their Possible applications

Ahmed Ayache[a], Abdu Alameri[b,*]

[a]Department of Mathematics, Faculty of Science, University of Bahrain

[b]Department of Biomedical Engineering, Faculty of Engineering, University of Science and Technology, Yemen

Abstract

Topological indices are real numbers related to graphs, They have many applications as tools for modeling chemical and other properties of molecules. In this paper, we study new graphs called Spider's web graph. Wiener index, Hyper-Wiener index, Wiener polarity and the Schultz indices of Spider's web graph have been computed. Furthermore, we found the correlation between these topological indices of Spider's web graph by some statistical parameters.

Keywords: Spider's Web Graph, Wiener index, Wiener dimension, Hyper-Wiener index, Wiener polarity, Schultz index

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1. Introduction

Chemical graph theory which is a fascinating branch of graph theory has many applications related to chemistry. A topological index which is a numerical quantity derived from the chemical graph of a molecule is used to modelling chemical and physical properties of molecules in quantitative Structure-Property-Relationships (QSPR) and quantitative structure-activity relationships (QSAR) researches [1, 2, 7, 10]. Throughout this paper, we consider simple connected graphs (without loops and multiple edges). The vertex and the edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree of a vertex a of G is denoted by $\delta(a)$. The distance between any two vertices a and b of G is denoted by $d_G(a, b)$, and it is defined as the number of edges in a shortest path connecting the vertices a and b. The greatest distance between any two vertices of G is called diameter of G and denoted $d(G)$. Chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. The basic idea of chemical graph theory is that physicochemical properties of molecules can be studied using the information. In the contemporary mathematico-chemical literature, there are exist several dozens of vertex degree-based molecular structure descriptors. Zagreb coindices are a generalization of classical Zagreb indices of chemical graph theory. A topological index is a real number related to a graph that must be a structural invariant. Several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules [3, 4, 5, 6].

*Corresponding author

Email addresses: aaayache@yahoo.com (Ahmed Ayache), a.alameri2222@gmail.com (Abdu Alameri)

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The usage of topological indices in chemistry began in 1947 when a chemist Harold Wiener developed the Wiener index and used it to determine physical properties of types of alkane known as paraffin [9]. In a graph theoretical language, the *Wiener index* $W(G)$ of a graph G is equal to the count of all shortest distances in a graph; that is

$$W(G) = \sum_{a,b \in V(G)} d(a,b)$$

The Wiener polynomial is defined as follows [13, 15]:

$$W(G;x) = \sum_{a,b \in V(G)} x^{d(a,b)}$$

It is well known that, the first derivative of the Wiener polynomial evaluated at $x = 1$ equals the Wiener index. Subsequently, other topological indices were introduced for a graph G. *The Wiener polarity index* is defined as [12]: $W_p(G) = d(G,3)$; that is the number of unordered pairs of vertices $\{a,b\}$ of G such that $d_G(a,b) = 3$. *The Hyper-Wiener index* [14, 16] of acyclic graphs was introduced by Milan Randic in 1993. Then Klein et al, generalized Randic's definition for all connected graphs, as a generalization of the Wiener index.

It is defined as follows:

$$WW(G) = \frac{1}{2} \sum_{a,b \in V(G)} d^2(a,b) + d(a,b)$$

The First and Second Hyper-Zagreb indices are defined respectively as [8]:

$$M_1(G) = \sum_{ab \in E(G)} (\delta_G(a) + \delta_G(b)), \quad M_2(G) = \sum_{ab \in E(G)} \delta_G(a)\,\delta_G(b)$$

The Schultz and modified Schultz indices and their *polynomials* are defined respectively as [8]:

$$W_+(G) = \sum_{a,b \in V(G)} (\delta_G(a) + \delta_G(b))d(a,b), \quad W_*(G) = \sum_{a,b \in V(G)} \delta_G(a)\,\delta_G(b)\,d(a,b)$$

$$W_+(G;x) = \sum_{a,b \in V(G)} (\delta_G(a) + \delta_G(b))x^{d(a,b)}, \quad W_*(G;x) = \sum_{a,b \in V(G)} \delta_G(a)\,\delta_G(b)\,x^{d(a,b)}$$

Its clear that

$$W'_+(G;0) = M_1(G), \qquad W'_*(G;0) = M_2(G),$$
$$W'_+(G;1) = W_+(G), \qquad W'_*(G;1) = W_*(G).$$

In 2012, Essalih, El-Marraki and Al-hagri [11] obtained the Wiener index of Spider's web graph but this paper, introduced several topological indices of Spider's web graph, such as: Wiener index, Hyper-Wiener index, Wiener polarity and Schultz indices by introducing a useful polynomials. Moreover, a strong correlations between these topological indices of Spider's web graph have been Appeared.

Define a Spider's web graph $S_n(m)-$*graph* $S = S_n(m), (n \geqslant 3, m \geqslant 2)$ as the union of m cycles together with n paths where;

$$C_n^1 = \{u_1^1, u_2^1, \cdots, u_n^1\}, C_n^2 = \{u_1^2, u_2^2, \cdots, u_n^2\}, \cdots, C_n^m = \{u_1^m, u_2^m, \cdots, u_n^m\},$$

$$P_1^m = \{u_1^1, u_1^2, \cdots, u_1^m\}, P_2^m = \{u_2^1, u_2^2, \cdots, u_2^m\}, \cdots, P_n^m = \{u_n^1, u_n^2, \cdots, u_n^m\}.$$

For instance a Spider's web graph are illustrated below in Figures 1,2.

Figure 1: Spider's web

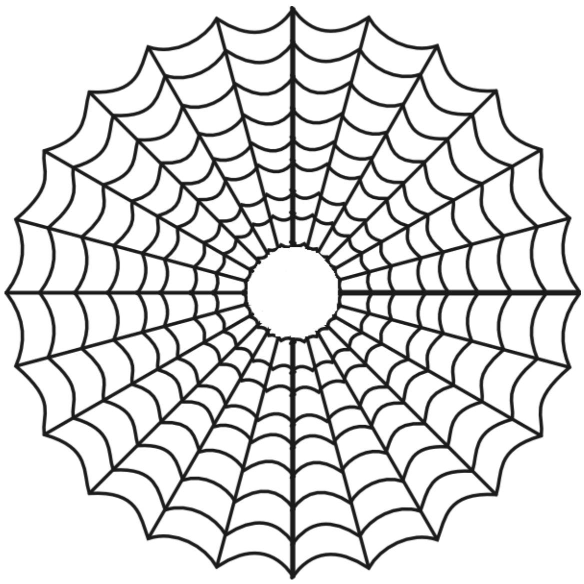

Figure 2: $S_{24}(9)$

It is simple matter to verify that $|V(S)| = mn$ and $|E(S)| = n(2m-1)$. Note that the case $n = 2$ is omitted because $S_2(m)$ has parallel edges, whereas the case $m = 1$ is trivial since $S_n(1) = C_n$.

This paper is devoted to the computation of the preceding topological indices concerning the $S_n(m)-$graph. After evaluating the diameter and the Wiener dimension $S = S_n(m)$ in the second paragraph, we begin our second paragraph by introducing a useful polynomial

$$F(x) = \sum_{\{u,v\} \subseteq V(S_n(m))} F(u) * F(v) x^{d_S(u,v)}.$$

By considering different definitions of the star operation $*$, the polynomial $F(x)$ enables us to derive simultaneously all the previous topological indices for the graph $S_n(m)$. Finally, an example of application is exhibited to illustrate our study.

2. Diameter and Wiener Dimension of Spider's web graph

We start by some preliminary statements concerning two arbitrary vertices u_i^h and u_j^k of $S = S_n(m)$. For $i, j \in \{1, 2, \cdots, n\}$ and $h, k \in \{1, 2, \cdots, m\}$:

(i) $d_S(u_i^h, u_i^k) = |h - k|$.

(ii) $$d_S(u_i^h, u_j^h) = \begin{cases} |i-j| \quad , & \text{if} \quad |i-j| \leqslant d(C_n) \\ n - |i-j|, & \text{if} \quad |i-j| > d(C_n) \end{cases}$$

(iii) $$d_S(u_i^h, u_j^k) = \begin{cases} |h-k| + |i-j| \quad , & \text{if} \quad |i-j| \leqslant d(C_n) \\ |h-k| + n - |i-j|, & \text{if} \quad |i-j| > d(C_n) \end{cases}$$

where $d(C_n) = n/2$ when n is even and $d(C_n) = (n-1)/2$ when n is odd.

Proposition 2.1: $d(S_n(m)) = m - 1 + d(C_n)$.

Proof. Set $d := d(C_n)$. Let u_i^h, u_j^k be two arbitrary vertices of $S = S_n(m)$.

If $|i-j| \leqslant d$, then $d_s(u_i^h, u_j^k) = |h-k| + |i-j| \leqslant m - 1 + d$. Let us assume that $|i-j| \geqslant d + 1$. Then $d_s(u_i^h, u_j^k) = |h-k| + n - |i-j|$.

As $d = \frac{n}{2}$ when n is even and $d = \frac{n-1}{2}$ when n is odd, then $n - d - 1 = d$ or $d - 1$. Thus

$$\begin{aligned} d_s(u_i^h, u_j^k) &\leqslant m - 1 + n - |i-j| \\ &\leqslant m - 1 + n - d - 1 \\ &\leqslant m - 1 + d \end{aligned}$$

Therefore,

$$d(S_n(m)) \leqslant m - 1 + d$$

Now, let u_k^m be the vertex of C_n^m that satisfies $d = d_s(u_1^m, u_k^m)$. Then

$$d_s(u_1^1, u_k^m) = d_s(u_1^1, u_1^m) + d_s(u_1^m, u_k^m) = m - 1 + d.$$

Hence,

$$d(S_n(m)) = m - 1 + d. \square$$

Our next result concerns the Wiener dimension of $S_n(m)$. Recall that *the Wiener dimension* [1] of a graph G, denoted $\dim_W G$, is the number of different distances of its vertices. But before embarking in this direction, notice that the Wiener dimension of a cycle C_n is 1. Indeed, since all the vertices $u \in C_n$ have a common distance, namely

$$d_{C_n}(u) = \begin{cases} \frac{n^2}{4} & , n \quad \textit{even.} \\ \frac{n^2-1}{4} & , n \quad \text{odd.} \end{cases}$$

Proposition 2.2: $\dim_W(S_n(m)) = \begin{cases} \frac{m}{2} & , m \quad even. \\ \\ \frac{m+1}{2} , m & \text{odd}. \end{cases}$

Proof. For convenience, we set $S := S_n(m)$. Since $d_S(u_i^k) = d_S(u_1^k)$, then the possible different distances of vertices of S are among

$$\{d_S(u_1^1), d_S(u_1^2), \cdots, d_S(u_1^m)\}.$$

We will evaluate $d_S(u_1^k)$ for each $k \in \{1, 2, \cdots, m\}$.

$$\begin{aligned} d_S(u_1^k) &= \sum{}_{h=1}^{m} \sum{}_{u \in C_n^h} d_S(u_1^k, u) \\ &= \sum{}_{h=1}^{m} \sum{}_{u \in C_n^h} d_S(u_1^k, u_1^h) + d_S(u_1^h, u) \\ &= \sum{}_{h=1}^{m} (\sum{}_{u \in C_n^h} |h-k| + \sum{}_{u \in C_n^h} d_S(u_1^h, u)) \\ &= \sum{}_{h=1}^{m} (n|h-k| + d_{C_n^h}(u_1^h)) \\ &= n[(1+2+\cdots+(k-1)) + (1+2+\cdots+(m-k))] + m d_{C_n}(u_1^1) \\ &= \tfrac{n}{2}[(m-k)^2 + (k-1)^2 + m - 1] + m d_{C_n}(u_1^1) \end{aligned}$$

Note that

$$d_S(u_1^k) - d_S(u_1^h) = n(k-h)(k+h-m-1)$$

for $h, k \in \{1, 2, \cdots, m\}$. So $d_S(u_1^k) = d_S(u_1^h)$ when $h = k$ or $h + k = m + 1$. It follows that

$$\{d_S(u_1^1), d_S(u_1^2), \cdots, d_S(u_1^{\frac{m}{2}})\}$$

is the set of different distances when m is even, and

$$\{d_S(u_1^1), d_S(u_1^2), \cdots, d_S(u_1^{\frac{m-1}{2}}), d_S(u_1^{\frac{m+1}{2}})\}$$

is the set of different distances when m is odd.

3. Topological indices of Spider's web graph

We continue to set $S := S_n(m)$. To compute different indices simultaneously, we introduce the following function which will play a prominent role: Let $F : S \to \mathcal{N}$ be the function defined by

$$F(u) = \begin{cases} a \ , \ u \in V(C_n^1 \bigcup C_n^m) \\ \\ b \ , \ u \in \bigcup_{h=2}^{m-1} V(C_n^h) \end{cases}$$

Let $*$ be an operation defined on $\{a, b\}$ by the table

$*$	a	b
a	α	β
b	β	γ

and consider the polynomial

$$F(x) = \sum_{\{u,v\}\subseteq V(S_n(m))} F(u) * F(v) x^{d_S(u,v)}.$$

We will evaluate $F(x)$ in terms of α, β, γ. To this end, we introduce two polynomials $T_s(x)$ and $R_s(x)$ defined by

$T_0(x) = 0\ ,\ T_s(x) = sx + (s-1)x^2 + \cdots + 2x^{s-1} + x^s,\ s \geqslant 1$

$R_0(x) = 0\ ,\ R_s(x) = x + x^2 + \cdots + x^s,\ s \geqslant 1$

It is easy to show that

$$T_s(x) + R_{s+1}(x) = T_{s+1}(x)$$

Lemma 3.1: For $s \geqslant 1, T_s(x) = \sum_{1\leqslant h<k\leqslant s+1} x^{k-h}$.

Proof: For each $t \in \{1, 2, \cdots, s\}$, define

$$B_t = \{(h,k) \in \{1,2,\cdots,s+1\}^2 : k-h = t\}.$$

It is easy to show that $|B_t| = s+1-t$. Therefore,

$$\sum_{1\leqslant h<k\leqslant s+1} x^{k-h} = \sum_{t=1}^{s} \sum_{(h,k)\in B_t} x^t = \sum_{t=1}^{s} (s+1-t)x^t = T_S(x). \quad \square$$

Proposition 3.2 :

$$F(x) = [\alpha x^{m-1} + (2\beta-\gamma)R_{m-2} + \gamma T_{m-2}](n + 2W(C_n, x))$$
$$+(2\alpha + \gamma(m-2))W(C_n, x).$$

Proof: We have $F(x) = A + B + C$, where A, B, C are evaluated separately below:

$A = \sum_{1\leqslant h<k\leqslant m, i\in\{1,2,\cdots,n\}} f(u_i^h) * f(u_i^k) x^{d_S(u_i^h, u_i^k)}$

$= n\sum_{2\leqslant h<k\leqslant m-1} \gamma x^{k-h} + n\sum_{k=2}^{m-1} \beta x^{k-1} + n\sum_{h=2}^{m-1} \beta x^{m-h} + \alpha n x^{m-1}$

$= n\gamma \sum_{2\leqslant h<k\leqslant m-1} x^{k-h} + 2n\beta \sum_{k=2}^{m-1} x^{k-1} + \alpha n x^{m-1}$

$= n\gamma(T_{m-2} - R_{m-2}) + 2n\beta R_{m-2} + \alpha n x^{m-1}$

$= \alpha n x^{m-1} + n(2\beta-\gamma)R_{m-2} + n\gamma T_{m-2}$

$= n(\alpha x^{m-1} + (2\beta-\gamma)R_{m-2} + \gamma T_{m-2})$

$B = \sum_{h\in\{1,2,\cdots,m\},1\leqslant i<j\leqslant n} f(u_i^h) * f(u_j^h) x^{d_s(u_i^h,u_j^h)}$

$= \alpha \sum_{1\leqslant i<j\leqslant n} x^{d_s(u_i^1,u_j^1)} + \sum_{h=2}^{m-1} \gamma \sum_{1\leqslant i<j\leqslant n} x^{d_s(u_i^h,u_j^h)} + \alpha \sum_{1\leqslant i<j\leqslant n} x^{d_s(u_i^m,u_j^m)}$

$= 2\alpha W(C_n,x) + \gamma(m-2)W(C_n,x) = (2\alpha+\gamma(m-2))W(C_n,x)$

$C = \sum_{1\leqslant h<k\leqslant m, i\neq j\in\{1,2,\cdots,m\}} f(u_i^h) * f(u_j^k) x^{d_s(u_i^h,u_j^k)}$

$= 2\sum_{1\leqslant h<k\leqslant m, 1\leqslant i<j\leqslant n} f(u_i^h) * f(u_j^k) x^{d_s(u_i^h,u_j^k)}$

Since

$$(d_S(u_i^h,u_j^k) = d_S(u_i^h,u_i^k) + d_S(u_i^k,u_j^k) = k-h+d_S(u_i^k,u_j^k))$$

$= 2\sum_{1\leqslant h<k\leqslant m} f(u_i^h) * f(u_j^k) x^{k-h} \sum_{1\leqslant i<j\leqslant n} x^{d_s(u_i^k,u_j^k)}$

$= 2\frac{A}{n} W(C_n,x).$

Thus, $F(x)$ can be deduced by adding A, B and C. □

Theorem 3.3: $W(S_n(m),x) = T_{m-1}(n+2W(C_n,x)) + mW(C_n,x)$.

Proof: Consider $F : S = S_n(m) \to \mathcal{N}$ defined by $F(u) = 1$ for all $u \in V(S)$, and let $*$ be the usual multiplication. Then

$$\alpha = \beta = \gamma = 1.$$

In this case, we have

$F(x) = W(S,x) = (x^{m-1} + R_{m-2} + T_{m-2})(n+2W(C_n,x)) + mW(C_n,x)$

$= T_{m-1}(n+2W(C_n,x)) + mW(C_n,x).$ □

By differentiating $W(S_n(m),x)$, we derive the values of $W(S_n(m))$ and $WW(S_n(m))$.

Corollary 3.4:

1) $W(S_n(m)) = m^2W(C_n) + \frac{n^2}{6}m(m^2-1)$.

2) $WW(S_n(m)) = m^2WW(C_n) + \frac{1}{3}m(m^2-1)W(C_n) + \frac{n^2}{24}m(m^2-1)(m+2)$.

3) $W_p(S_n(m)) = 3n(2m-3)$.

Theorem 3.5:

$W_+(S_n(m),x) = (6T_{m-1} + 2T_{m-2})(n+2W(C_n,x)) + (8m-4)W(C_n,x)$

Proof: Consider $F : S = S_n(m) \to \mathcal{N}$ the function defined by $F(u) = \delta(u)$, and let $*$ be the usual addition. Then

$$\alpha = 6, \beta = 7, \gamma = 8.$$

In this case, we have

$$W_{+}(S,x) = (6x^{m-1} + 6R_{m-2} + 8T_{m-2})(n + 2W(C_n,x)) + (8m-4)W(C_n,x)$$
$$= (6T_{m-1} + 2T_{m-2})(n + 2W(C_n,x)) + (8m-4)W(C_n,x). \quad \square$$

By differentiating $W_{+}(S_n(m),x)$, we obtain the values of $M_1(S_n(m))$ and $W_{+}(S_n(m))$.

Corollary 3.6:

1) $W_{+}(S_n(m)) = m(2m-1)W_{+}(C_n) + \frac{n^2}{3}m(m-1)(4m+1)$

2) $M_1(S_n(m)) = 2n(8m-7)$

Theorem 3.7:

$W_{*}(S_n(m),x) = (x^{m-1} + 8T_{m-1} + 8T_{m-2})(n + 2W(C_n,x)) + (16m-14)W(C_n,x)$

Proof: Consider the function $F : S = S_n(m) \to \mathcal{N}$ defined by $F(u) = \delta(u)$, and let $*$ be the usual multiplication. Then

$$\alpha = 9, \beta = 12, \gamma = 16.$$

In this case, we have

$$W_{*}(S,x) = (9x^{m-1} + 8R_{m-2} + 16T_{m-2})(n + 2W(C_n,x)) + (16m-14)W(C_n,x)$$
$$= (x^{m-1} + 8T_{m-1} + 8T_{m-2})(n + 2W(C_n,x)) + (16m-14)W(C_n,x). \quad \square$$

By differentiating $W_{*}(S,x)$, we get the values of $M_2(S)$ and $W_{*}(S)$.

Corollary 3.8:

1) $W_{*}(S) = (2m-1)^2 W_{*}(C_n) + \frac{n^2}{3}(m-1)(8m^2-4m+3)$

2) $M_2(S) = 2n(16m-19)$

We end this work by an example of application.

Example 3.9: Let $S := S_4(4)$. Then

1. $d(S) = 5 \quad , \quad dim_W(S) = 2.$
2. $W(S:x) = 28x + 40x^2 + 32x^3 + 16x^4 + 4x^5.$
3. $W_{+}(S:x) = 200x + 280x^2 + 224x^3 + 104x^4 + 24x^5.$
4. $W_{*}(S:x) = 360x + 516x^2 + 388x^3 + 168x^4 + 36x^5.$
5. $W(S) = 288 \quad , \quad WW(S) = 560 \quad , \quad W_p(S) = 60.$
6. $W_{+}(S) = 1984 \quad , \quad M_1(S) = 200.$
7. $W_{*}(S) = 3408 \quad , \quad M_2(S) = 360.$

Table 1: Topological indices of Spider's web graph

(n, m)	M_1	M_2	W	WW	W_+	W_*
(3 , 3)	102	174	63	96	177	1278
(3 , 4)	150	270	138	243	418	2799
(3 , 5)	198	366	255	510	810	5112
(3 , 6)	246	462	423	948	1389	8361
(4 , 3)	136	232	136	234	896	2496
(4 , 4)	200	360	288	560	1984	6192
(4 , 5)	264	488	520	1130	3680	12576
(4 , 6)	328	616	848	2040	6112	22416
(5 , 3)	170	290	235	425	625	5130
(5 , 4)	250	450	490	995	1410	10545
(5 , 5)	330	610	875	1975	2650	18240
(5 , 6)	410	770	1415	3520	4445	28455

Table 2: Correlation between topological indices of Spider's web graph

r	M_1	M_2	W	WW	W_+	W_*
M_1	1.000000	0.999185	0.972662	0.962192	0.830710	0.973015
M_2	0.999185	1.000000	0.969683	0.960472	0.834101	0.971030
W	0.972662	0.969683	1.000000	0.998185	0.804334	0.984969
WW	0.962192	0.960472	0.998185	1.000000	0.805326	0.982561
W_+	0.830710	0.834101	0.804334	0.805326	1.000000	0.886309
W_*	0.973015	0.971030	0.984969	0.982561	0.886309	1.000000

4. Possible applications of Spider's web graph

In combinatorial chemistry, so-called topological indices are used for the description of the structural properties of molecular graphs. If we consider each vertex in Spider's web graph to be a carbon atom (the valence of carbon atom is equal four), possible this a graph is chemical graph, since it is a connected, planar and the degree (valence) of every vertex (atom) in this graph is not more than four. In other side, by above definition of a Spider's web graph, it is an union of paths (alkanes) together with cycles (cycloalkanes) that is mean we can study the properties of Spider's web graph from its initial compounds (alkanes and cycloalkanes). By general, there is no theoretical result on the correlation between the different indices yet, thus should be natural to study some strong correlation between them, since they all reflect the structural properties of graphs in some way [17]. This section tries to fill this gap a little by proposing measures for the correlation of two indices and discussing them. Then we choose the best topological index to use for the description of the structural properties of Spider's web graph. Table 1 shows some topological indices (first Zagreb index, second Zagreb index, Wiener index, Hyper Wiener index, Schultz index and Gutman index) of the spider diagram resulting from the union of alkanes P_3, P_4, P_5 with cycloalkanes C_3, C_4, C_5, C_6. Note: In general, it is possible to calculate the topological indices for the spider web from any group of alkanes with a group of cycloalkanes using the program in the appendix (where we designed it using the MATLAB program). According to Table 2, all topological indices considered are a strong correlated where $0.80 \leqslant r \leqslant 1$. Therefore, we can use these indices to properties of Spider's web graph that result from two chemical groups alkanes with cycloalkanes. Also, we conclude among the topological indices we considered, the three best correlation coefficients between first Zagreb index, second Zagreb index ($r = 0.999185$), and then between Wiener index, Hyper Wiener index ($r = 0.998185$), and then between Wiener index, Gutman index ($r = 0.984969$).

5. Concluding Remarks

Several articles are concerned the calculations of topological indices for different types of graphs. Some of them have found applications, but others were devoted to the mathematical side in order to throw more light on the relationship between these various concepts. In this paper, we computed some topological indices of new graphs called Spider's web. Moreover, we found a strong correlation between these indices of Spider's web graph. this paper open a wide window for other researches on Spider's web graph such as some other topological indices or their coindices.

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