

On Some Polynomials, Indices and Multiplicative Indices of Hexagonal Network of Dimension Three

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Abstract: Wiener index is the first distance - based topological index introduced by H. Wiener in 1947 [1]. In this paper some degree distance - based topological polynomials, topological indices and multiplicative indices are studied for hexagonal network of dimension three.

Keywords: Degree, distance, distance version of F - polynomial, Hosoya polynomial, Harary polynomial, multiplicative indices, topological indices, Wiener index

1. Introduction

Let $G = (V, E)$ be a graph with order $|V(G)| = n$ and size $|E(G)| = m$. The degree of a vertex, denoted by $d_G(u)$ and is defined as the number of vertices adjacent to u . The distance between two distinct vertices u and v written as $d_G(u, v)$, is the smallest length of path between them in graph. The edge connecting the vertices u and v is denoted by uv [2 - 3]. A topological index is a numerical parameter mathematically derived from the graph structure.

The k - distance degree first, second and third leap indices were introduced by A. M. Naji in 2018 [4]. New results on leap Zagreb indices were studied in [5]. The k - distance degree $d_k(v)$ of a vertex v in G is defined as the number of k - neighbors of v in G [6]. Some degree - based topological indices at distance - 2 for alkanes were investigated in [7]. The Wiener index of chemical tree by reducing the size of the distance matrix was obtained by M. Yamuna in [8]. Three methods for calculating the hyper - Wiener index of molecular graphs were discussed in [9]. The edge versions of Wiener index was introduced by A. Iranmanesh in 2009 [10 - 11].

Analytical expressions for various distance, degree - based topological indices and entropies were studied by K. Balasubramaniam [12]. Analogous to forgotten index A. Alameri et al. introduced Y - index in 2020 [13]. A representation of sodium chloride (NaCl) which is same as the cartesian product of three paths of length, is exactly like mesh network HX_3 [14]. Reduced reverse degree - based topological indices of graphyne and graphdiyne nanoribbons with applications in chemical analysis were studied in [15]. The reduced forgotten topological index is used in the analysis of drug designing which is quite helpful for pharmaceutical and medical scientists to grasp the biological and chemical characteristics of the new drugs [16].

A hexagonal network is symbolised by HX_n , where n is number of vertices on one side of hexagon and has diameter $(2n - 2)$. The n - dimensional hexagonal mesh HX_n is obtained by attaching $n - 2$ layers of triangle around HX_2 [17]. The hexagonal network of HX_3 has $9n^2 - 15n + 6$ edges and $3n^2 - 3n + 1$ vertices [18]. Wiener index was introduced by Wiener in 1947 while studying paraffin boiling points

and this index has been studied in many papers as [19 - 20]. Wiener index is the first distance - based topological index, defined as

$$\text{Wiener index} = W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u, v) \quad (1)$$

Where $d_G(u, v)$ denotes the distance between vertices u and v .

Hosoya polynomial, Schultz and modified Schultz polynomial are defined [21 - 22] as

$$\text{Hosoya polynomial} = H(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} x^{d_G(u,v)} \quad (2)$$

Schultz polynomial = $S_c(G, x) =$

$$\frac{1}{2} \sum_{u,v \in V(G)} x^{[d_G(u)+d_G(v)]d_G(u,v)} \quad (3)$$

Modified Schultz polynomial = $S_c^*(G, x) =$

$$\frac{1}{2} \sum_{u,v \in V(G)} x^{[d_G(u) \times d_G(v)]d_G(u,v)} \quad (4)$$

The Schultz and modified Schultz indices [23 - 24] are

$$\text{Schultz index} = S_c(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) + d_G(v)] d_G(u, v) \quad (5)$$

$$\text{Modified Schultz index} = S_c^*(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) \times d_G(v)] d_G(u, v) \quad (6)$$

The Harary polynomial and Harary index of a connected graph G is denoted by $h(G, x)$, $h(G)$ respectively and are defined as follows:

$$h(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)} x^{d_G(u,v)} \text{ and } h(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)} \quad (7)$$

Wiener polarity index is defined for any graph as follows:

$$\text{Wiener polarity index} = W_p(G) = \sum_{v \in V(G)} \frac{1}{2} d_3(v) \quad (8)$$

We introduce Wiener polarity polynomial as

$$W_p(G, x) = \sum_{v \in V(G)} \frac{1}{2} x^{d_3(v)} \quad (9)$$

Where $d_3(v)$ denotes the number of vertices of G that are at distance 3 from v .

Distance version of F - index appear in some papers [25 - 26] as

$$DF(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v) [d_G(u)^2 + d_G(v)^2]. \quad (10)$$

We introduce distance version of F - polynomial as

$$DF(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} x^{d_G(u,v)} [d_G(u)^2 + d_G(v)^2]. \quad (11)$$

The hyper - Wiener index was introduced by M. Randic in 1993 [27] as

$$HW(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u,v) + d_G(u,v)^2]. \quad (12)$$

The corresponding polynomial will be hyper - Wiener polynomial which can be defined as

$$HW(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} x^{[d_G(u,v) + d_G(u,v)^2]}. \quad (13)$$

The degree - distance index is defined as [28 - 29]

$$DD(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) + d_G(v)] d_G(u,v). \quad (14)$$

The Gutman index is another degree distance - based topological index [30]

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} [d_G(u) \times d_G(v)] d_G(u,v). \quad (15)$$

In [31 - 32] the reciprocal complementary Wiener index of a graph G was introduced as

$$RCW(G) = \sum_{1 \leq i \leq j \leq n} \frac{1}{1 + diam(G) - d_G(i,j)}. \quad (16)$$

The root mean square index of a graph G is

$$RMS(G) = \sqrt{\frac{1}{|V(G)|} \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)^2}. \quad (17)$$

The multiplicative Wiener index is defined [33] as

$$WII(G) = \prod_{u,v \in V(G)} d_G(u,v). \quad (18)$$

K. C. Das et al. [34 - 35] introduced the second Harary index in 2013. We introduce multiplicative second Harary index of a graph G as

$$H_1II(G) = \prod_{u,v \in V(G)} \frac{1}{d_G(u,v) + 1}. \quad (19)$$

The multiplicative versions of Gutman and degree - distance indices of some graphs were computed in [36],

$$Gut^*(G) = \frac{1}{2} \prod_{u,v \in V(G)} [d_G(u) \times d_G(v)] d_G(u,v). \quad (20)$$

$$DD^*(G) = \frac{1}{2} \prod_{u,v \in V(G)} [d_G(u) + d_G(v)] d_G(u,v). \quad (21)$$

In this paper, we compute Hosoya, Harary, Schultz, modified Schultz, Wiener polarity, distance version of F and hyper Wiener polynomials and their corresponding topological indices, and Gutman, degree - distance, reciprocal complementary index, root mean square indices along with Wiener, Gutman, degree - distance, second Harary multiplicative indices for hexagonal network of dimension three. The notations used in this paper are standard and mainly taken from books of graph theory [37 - 39].

2. Materials and Methods

A molecular graph is a simple graph related to the structure of a chemical compound. A molecular graph is constructed by representing each atom of a molecule by vertex and

bonds between atoms by edges. The molecular graph of hexagonal network of dimension three is shown in figure (1). It is easy to see that the vertices of HX_3 are of degree 3, 4 or 6. It is observed from figure that $|V(G)| = 19$, $|E(G)| = 42$ and diameter is equal to $2n - 2$, where n is number of vertices on one side of the hexagon. There are 6 vertices of degree 3, $6n - 12$ vertices of degree 4 and $3n^2 - 9n + 7$ vertices of degree 6. The distance matrix for vertices (u, v) can be constructed for all pairs. There are 42 edges for degree - distance topological polynomials and indices computation in HX_3 . The $d_3(v)$ number of vertices of G at distance 3 from v are obtained from hexagonal network of HX_3 .

3. Results and Discussion

Distance, degree - based topological polynomials and indices

Theorem 1.1: Hosoya polynomial of hexagonal network (HX_3) is $\frac{1}{2} (6x^{48} + 6x^{44} + 6x^{35} + x^{30})$.

Proof: Consider a molecular graph of hexagonal network (HX_3) as shown in figure (1). Let $d_G(u, v)$ denotes distance between the two vertices u and v . There are 19 vertices and 42 edges. From distance matrix D_{ij} and equations (1) and (2) we have Hosoya polynomial

$$H(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} x^{d_G(u,v)} \\ \frac{1}{2} [x^{48} + x^{44} + x^{35} + x^{44} + x^{48} + x^{35} + x^{30} + x^{35} + x^{48} + x^{44} + x^{35} + x^{35} + x^{44} + x^{48} + x^{44} + x^{48} + x^{44} + x^{48}] \\ = \frac{1}{2} (6x^{48} + 6x^{44} + 6x^{35} + x^{30}).$$

Wiener index = $W(G) = H'(G, x)$

$$W(G) = \left. \frac{\partial H(G, x)}{\partial x} \right|_{x=1} = \left. \frac{\partial \left(\frac{1}{2} (6x^{48} + 6x^{44} + 6x^{35} + x^{30}) \right)}{\partial x} \right|_{x=1} \\ = 396.$$

Theorem 1.2: Harary polynomial of hexagonal network (HX_3) is $\frac{1}{2} (6 \times \frac{1}{48} x^{48} + 6 \times \frac{1}{44} x^{44} + 6 \times \frac{1}{35} x^{35} + \frac{1}{30} x^{30})$.

Proof: By using equation (7) and distance matrix for hexagonal network (HX_3) we have Harary polynomial h

$$(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{1}{d_G(u,v)} x^{d_G(u,v)} \\ \frac{1}{2} \left(\frac{1}{48} x^{48} + \frac{1}{44} x^{44} + \frac{1}{35} x^{35} + \frac{1}{44} x^{44} + \frac{1}{48} x^{48} + \frac{1}{35} x^{35} + \frac{1}{30} x^{30} + \frac{1}{35} x^{35} + \frac{1}{48} x^{48} + \frac{1}{44} x^{44} + \frac{1}{48} x^{48} + \frac{1}{44} x^{44} + \frac{1}{48} x^{48} + \frac{1}{44} x^{44} + \frac{1}{48} x^{48} \right) \\ = \frac{1}{2} \left(6 \times \frac{1}{48} x^{48} + 6 \times \frac{1}{44} x^{44} + 6 \times \frac{1}{35} x^{35} + \frac{1}{30} x^{30} \right).$$

Harary index:

$$h(G) = \left. \frac{\partial h(G, x)}{\partial x} \right|_{x=1} = \left. \frac{\partial \left(\frac{1}{2} \left(6 \times \frac{1}{48} x^{48} + 6 \times \frac{1}{44} x^{44} + 6 \times \frac{1}{35} x^{35} + \frac{1}{30} x^{30} \right) \right)}{\partial x} \right|_{x=1} \\ = 9.5.$$

Theorem 1.3: Schultz polynomial of hexagonal network (HX_3) is $27x^6 + 174x^{12}$.

Proof: By using table (1) and equations (3) and (5) we have Schultz polynomial

$$S_c(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) + d_G(v)] x^{d_G(u,v)}$$

$$= \frac{1}{2} 12 \times (7) x^{12} + \frac{1}{2} 6 \times (9) x^6 + \frac{1}{2} 12 \times (10) x^{12} + \frac{1}{2} 12 \times (12) x^{12}$$

$$= 27x^6 + 174x^{12}$$

Schultz index: $S_c(G) = \frac{\partial S_c(G,x)}{\partial x} \Big|_{x=1} = \frac{\partial (27x^6 + 174x^{12})}{\partial x} \Big|_{x=1} = 2250$.

Theorem 1.4: Modified Schultz polynomial of hexagonal network (HX₃) is $432x^{12} + 54x^6$.

Proof: By using table (1) and equations (4) and (6) we have

$$S_c^*(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) \times d_G(v)] x^{d_G(u,v)}$$

$$= \frac{1}{2} 12 \times (12) x^{12} + \frac{1}{2} 6 \times (18) x^6 + \frac{1}{2} 12 \times (24) x^{12} + \frac{1}{2} 12 \times (36) x^{12}$$

$$= 432x^{12} + 54x^6$$

Modified Schultz index: $S_c^*(G) = \frac{\partial S_c^*(G,x)}{\partial x} \Big|_{x=1} = \frac{\partial (432x^{12} + 54x^6)}{\partial x} \Big|_{x=1} = 5508$.

Theorem 1.5: Wiener polarity polynomial of hexagonal network (HX₃) is $\frac{1}{2} (3x^5 + 2x^6 + 2x^4 + 2x^3 + x^2 + 4x^1)$.

Proof: The $d_3(v)$ distances are obtained for vertex v from figure (1) and using equations (9) and (8) we have Wiener polarity polynomial

$$W_p(G, x) = \frac{1}{2} \sum_{v \in V(G)} x^{d_3(v)}$$

$$= \frac{1}{2} (x^5 + x^6 + x^5 + x^6 + x^4 + x^5 + x^4 + x^3 + x^3 + x^1 + x^1 + x^2 + x^1 + x^1)$$

$$= \frac{1}{2} (3x^5 + 2x^6 + 2x^4 + 2x^3 + x^2 + 4x^1)$$

Weiner polarity index:

$W_p(G) = \frac{\partial W_p(G,x)}{\partial x} \Big|_{x=1} = \frac{\partial (\frac{1}{2} (3x^5 + 2x^6 + 2x^4 + 2x^3 + x^2 + 4x^1))}{\partial x} \Big|_{x=1} = 23.5$

Theorem 1.6: Distance version of F - polynomial of hexagonal network (HX₃) is $\frac{1}{2} (x^{300} + x^{270} + x^{624} + x^{864})$.

Proof: From equation (13) and table (1) we have distance version of F - polynomial

$$DF(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} x^{d_G(u,v)} [d_G(u)^2 + d_G(v)^2]$$

$$= \frac{1}{2} [x^{12(3^2+4^2)} + x^6(3^2+6^2) + x^{12(4^2+6^2)} + x^{12(6^2+6^2)}]$$

$$= \frac{1}{2} (x^{300} + x^{270} + x^{624} + x^{864})$$

Distance version of F - index:

$DF(G) = \frac{\partial DF(G,x)}{\partial x} \Big|_{x=1} = \frac{\partial (\frac{1}{2} (x^{300} + x^{270} + x^{624} + x^{864}))}{\partial x} \Big|_{x=1} = 1029$.

Theorem 1.7: Hyper Wiener polynomial of hexagonal network (HX₃) is $3x^{48+48^2} + 3x^{44+44^2} + 3x^{35+35^2} + \frac{1}{2} x^{30+30^2}$.

Proof: By using distance matrix for vertices (u, v) and equations (13) and (12) the Hyper Wiener polynomial is

$$HW(G, x) = \frac{1}{2} \sum_{u,v \in V(G)} x^{[d_G(u,v) + d_G(u,v)^2]}$$

$$= \frac{1}{2} [x^{(48+48^2)} + x^{(44+44^2)} + x^{(35+35^2)} + x^{(44+44^2)} + x^{(48+48^2)} + x^{(35+35^2)} + x^{(30+30^2)} + x^{(35+35^2)} + x^{(48+48^2)} + x^{(44+44^2)} + x^{(35+35^2)}]$$

$$= \frac{1}{2} (6x^{2352} + 6x^{1980} + 6x^{1260} + x^{930})$$

Hyper Wiener index:

$HW(G) = \frac{\partial HW(G,x)}{\partial x} \Big|_{x=1} = \frac{\partial (\frac{1}{2} (6x^{2352} + 6x^{1980} + 6x^{1260} + x^{930}))}{\partial x} \Big|_{x=1} = 17241$.

Distance degree - based topological indices

Theorem 2.1: Degree - distance index of hexagonal network (HX₃) is 201.

Proof: By using table (1) and equation (14) the degree distance index of hexagonal network (HX₃)

$$DD(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) + d_G(v)] d_G(u, v)$$

$$= \frac{1}{2} \times 7 \times 12 + \frac{1}{2} \times 6 \times 9 + \frac{1}{2} \times 10 \times 12 + \frac{1}{2} \times 12 \times 12 = 201$$

Theorem 2.2: Gutman index of hexagonal network (HX₃) is 486.

Proof: By table (1) and equation (15) we have Gutman index of hexagonal network (HX₃)

$$Gut(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d_G(u) \times d_G(v)] d_G(u, v)$$

$$= \frac{1}{2} \times 12 \times [3 \times 4] + \frac{1}{2} \times 6 \times [3 \times 6] + \frac{1}{2} \times 12 \times [4 \times 6] + \frac{1}{2} \times 12 \times [6 \times 6] = 486$$

Theorem 2.3: Root mean square index of hexagonal network (HX₃) is 128.5.

Proof: By using distance matrix for vertices (u, v) of hexagonal network (HX₃) and equation (17) we have root mean square index

$$RMS(G) = \sqrt{\frac{1}{2|V(G)|} \sum_{u,v \in V(G)} d_G(u, v)^2}$$

$$= \sqrt{6 \times \sqrt{\frac{1}{2} \times \frac{1}{19} (48)^2} + 6 \times \sqrt{\frac{1}{2} \times \frac{1}{19} (44)^2} + 6 \times \sqrt{\frac{1}{2} \times \frac{1}{19} (30)^2} + 6 \times \sqrt{\frac{1}{2} \times \frac{1}{19} (35)^2}}$$

$$= 128.5$$

Theorem 2.4: Reciprocal complementary Wiener index of hexagonal network (HX₃) is - 0.533.

Proof: By using equation (16), table (1) and the diameter of $G = 2n - 2$, the reciprocal complementary Wiener index of hexagonal network (HX₃)

$$RCW(G) = \sum_{u,v \in V(G)} \frac{1}{1 + \text{dia}(G) - d_G(u, v)}$$

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