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Topological Characterization of Hexagonal Network and Non-Kekulean Benzenoid Hydrocarbon

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Abstract. Graph theory has great deal of application in disciplines like biology, computer science, informatics, engineering, mathematics, social science, linguistics and medicine. Topological indices are created by labeling the chemical structure through numerical parameters. These notations link chemical compounds physicochemical features such as boiling temperature, stability, strain energy etc, to its molecular structure. Different topological features of chemical structure have been explored. One of the molecular graphs topological indices are the connection indices defined on the number of connection between vertices of distance two. In this work, we compute the first Zagreb connection index, second Zagreb connection index, and modified first Zagreb connection index for hexagonal network and non kekulean benzenoid hydrocarbon.

2020 Mathematics Subject Classifications: 0508, 05C92, 92E10

Key Words and Phrases: Topological Indices, Connection Index, Hexagonal Network, Non-Kekulean Benzenoid Hydrocarbon

1. Introduction

Graph theory has been recognized as a separate branch of mathematics which has given chemists several useful tips, like topological indices and graph energy. The structural formula of a chemical compound is represented by a molecular graph. Topological indices are most important part of graph theory we use these indices for the understanding and

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representation of chemical properties of different structures. In this branch of mathematics we study the behavior of molecular structure, by using numerical.
Graph can indicate local relationship between interacting pieces of a system in statistical physics. The hexagon unit cell is distinguished by the presence of a single line, known as a six-fold symmetrical axis, along which cells can be turned by 60Â° or 120Â° without changing their shape. Hexagon is a worldwide part of digital reality systems that combine sensor, software, and self-driving technology. The Zhou et al. defined the basis of a novel connection index, sum connectivity index and topological indices [30, 31]. Vukicevik, and Furtula computed topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges in [28]. Naji and Soner worked on first leap Zagreb indices of some graph operations [26]. Based on vertex degrees, the idea of Randic (R), atom-bond connectivity (ABC), and geometric-arithmetic (GA) topological indices was formed in chemical graph theory. This theory is related to quantitative analysis, statistics, topology, and complex mathematics [27, 29]. In addition to graph models, such dynamic systems can be modeled using multi-agent systems, Markov chain and/or petri-nets, [4, 5, 11, 18]. Among other aspects of mathematics this theory has been widely applied in subjects like computer science, economics, physics and chemistry. It is used to debate molecules in chemistry and physics, in condensed matter physics, 3D structure of advanced simulated crystal structures can be investigated quantitatively by gathering data on curve properties related to the atom's topology.
In chemistry, a graph is a natural representation of a molecule, with vertices representing atoms and edges signifying bonds. For certain nanostructures their ABC and GA indices for this critical class of networks are studied in [10, 23, 24]. One can also see the literature related to structural invariants of graphs in [3, 6, 12, 13, 16, 17, 21, 25, 32]. Iqbal et al. defined degree based indices and eccentricity based topological indices of some graphs in [19, 20]. Ducoffe et al. computed first three maximal modified first Zagreb connection indices, [7]. Farahani, et al. computed first Zagreb index, second Zagreb index, atomic bond connectivity index, redefined first Zagreb connection index, second Zagreb connection index and third Zagreb connection index in [8, 9].
Graph is a mathematical rendition of a system and define connection between vertices and edges. A connected graph is a graph that has connection in sense of a topological space there is a path from one point to any other point in the graph. Zagreb indices are one of the oldest and most studied indices. Zagreb connection indices provide better correlation coefficient then the classical Zagreb indices. Based on vertex and edge data, the topological indices of connection number are define in [15]. The first Zagreb connection index is stated as,

$$ZC_1(G) = \sum_{\overline{a} \in V(G)} (\tau_G(\overline{a}))^2. \tag{1}$$

The second Zagreb connection index is stated as,

$$ZC_2(G) = \sum_{\breve{a}\overline{a} \in E(G)} (\tau_G(\breve{a}) \times \tau_G(\overline{a})). \tag{2}$$

The modified first Zagreb connection index is stated as,

$$ZC^*1(G) = \sum_{\breve{a}\overline{a}\in E(G)} (\tau_G(\breve{a}) + \tau_G(\overline{a})). \tag{3}$$

Where, τ_G represents the connection number(vertex count at distance two).

2. Hexagonal Network

The world of information technology has been witnessing the evolvement of computer networks to serve many different real-life applications. The hexagonal system is one of the major structural categories that may be thoroughly understood crystal pieces are defined in this system using four axes, three separate axes positioned at 120Â° with one another, and a fourth plane perpendicular to the axes of the other three. The lattice will define the margins of an orderly stack of blocks, or unit cells, the atoms or molecular groups of the solid are represented by locations and the points are linked by lines.

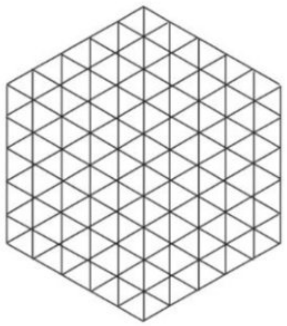

Figure 1: Hexagonal Network.

2.1. Related Theorems and Results

The total number of vertices and edge in hexagonal network are 3n(n-1)+1 and (9n-15)+6 respectively, where n$\geqslant$ 3, n represent the number of molecules. Now we define the vertices partition and edges partition by labelling the vertices with their respective connection number in Table 1 and 2. Further we calculate the indices. We also computed some numerical value of these indices in Table 3, to show their trend in the Figure 2 for this structure.

Theorem 1. *Consider a hexagonal network, then its first Zagreb connection index is,*

$$ZC_1(Q) = 2700n^2 - 9150n + 9126.$$

Proof. Let Q be a graph of a hexagonal network, now by using the information in Table 1 and the Equation 1 we have,

$$ZC_1(Q) = \sum_{\bar{a}\in V(Q)} (\tau_Q(\bar{a}))^2,$$

Table 1: Vertices Partition of Hexagonal Network Based on Connection Number.

Vertices Partition	*Count*
11	6
14	$6n-12$
23	$6n-12$
30	$3n^2-15n+19$

Table 2: Edges Partition of Hexagonal Network Based on Connection Number.

Edges Partition	*Count*
$(11,14)$	12
$(11,23)$	6
$(14,14)$	$6n-18$
$(14,23)$	$12n-24$
$(23,23)$	$6n-12$
$(23,30)$	$12n-30$
$(30,30)$	$9n^2-51n+72$

$$\begin{aligned} &= (6)(11)^2+(6n-12)(14)^2+(6n-12)(23)^2+(3n^2-15n+19)(30)^2, \\ ZC_1(Q) &= 2700n^2-9150n+9126. \end{aligned}$$

Theorem 2. *Consider a hexagonal network, then its second Zagreb connection index is,*

$$ZC_2(Q) = 8100n^2-29406n+29862.$$

Proof. Let Q graph be a hexagonal network, now by using the information in Table 2 and the Equation 2 we have,

$$\begin{aligned} ZC_2(Q) &= \sum_{\check{a}\bar{a}\in E(Q)} (\tau_Q(\check{a})\times\tau_Q(\bar{a})), \\ ZC_2(Q) &= (12)(11\times14)+(6)(11\times23)+(6n-18)(14\times14) \\ &\quad +(12n-24)(14\times23)+(6n-12)(23\times23) \\ &\quad +(12n-30)(23\times30)+(9n^2-51+72)(30\times30), \\ &= 8100n^2-29406n+29862. \end{aligned}$$

Theorem 3. *Consider a hexagonal network, then its modified first Zagreb connection index is,*

$$ZC_1^*(Q) = 540n^2-1536n+1290.$$

Proof. Let Q be a graph of hexagonal network, now by using the information in Table 2 and the Equation 3 we have,

$$\begin{aligned} ZC_1^*(Q) &= \sum_{\check{a}\bar{a}\in E(Q)} (\tau_Q(\check{a}) + \tau_Q(\bar{a})), \\ &= (12)(11+14) + (6)(11+23) + (6n-18)(14+14) \\ &\quad +(12n-24)(14+23) + (6n-12)(23+23) \\ &\quad +(12n-30)(23+30) + (9n^2-15n+72)(30+30), \\ ZC_1^*(Q) &= 540n^2 - 1536n + 1290. \end{aligned}$$

Table 3: Numerical Behaviour of $ZC_1(Q)$, $ZC_2(Q)$, $ZC_1^*(Q)$, for Hexagonal Network .

n	$ZC_1(Q)$	$ZC_2(Q)$	$ZC_1^*(Q)$
4	15726	41838	3786
5	30876	85332	7110
6	51426	145026	11514
7	77376	220920	16998
8	108726	313014	23562
9	145476	421308	31206
10	187626	545802	39930

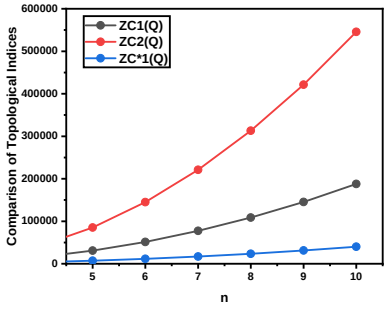

Figure 2: $ZC_1(Q)$, $ZC_2(Q)$, and $ZC_1^*(Q)$.

3. Non-Kekulean Benzenoid Hydrocarbon

These numerical parameters assist us to recognize physical features, chemical reactivity and biological activities of chemical structures. The interesting fact is that they are structure invariant. The results can also play key role in the identification of the significance of non-kekulean benzenoid hydrocarbon in the chemical and pharmaceutical industries.

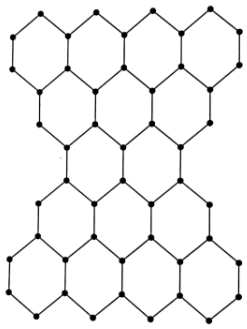

Figure 3: Non-Kekulean Benzenoid Hydrocarbon.

3.1. Related Theorems and Results

The total number of vertices and edge in non-kekulean benzenoid hydrocorban are 12n+14 and 17n+14 respectively, where n⩾3, n represent the number of molecules. Now we define the vertices partition and edges partition by labelling the vertices with their respective connection number in Table 4 and 5. Further we calculate the indices. We also computed some numerical value of these indices in Table 6, to show their trend in the Figure 4 for this structure.

Table 4: Vertices Partition of Non-Kekulean Benzenoid Hydrocarbon Based on Connection Number.

Vertices Partition	*Count*
2	4
3	8
4	$4n+6$
5	4
6	$8n-8$

Table 5: Edges Partition of Non-Kekulean Benzenoid Hydrocarbon Based on Connection Number.

Edges Partition	*Count*
$(2,3)$	8
$(3,4)$	8
$(4,4)$	$4n$
$(4,5)$	4
$(4,6)$	$2n+4$
$(5,5)$	2
$(6,5)$	4
$(6,6)$	$11n-16$

Theorem 4. *Consider a non-Kekulean benzenoid hydrocarbon network then its first Zagreb*

connection index is,

$$ZC_1(K) = 352n - 4.$$

Proof. Let K be a graph of non-kekulean benzenoid hydrocarbon, now by using the information in Table 4 and the Equation 1 we have,

$$\begin{aligned} ZC_1(K) &= \sum_{\bar{a}\in V(K)} (\tau_K(\bar{a}))^2, \\ &= (4)(2)^2 + (8)(3)^2 + (4n+6)(4)^2 + (4)(5)^2 + (8n-8)(6)^2, \\ &= 352n - 4. \end{aligned}$$

Theorem 5. *Consider a non-Kekulean benzenoid hydrocarbon network, then its second Zagreb connection index is,*

$$ZC_2(K) = 508n - 86.$$

Proof. Let K be a non-Kekulean benzenoid hydrocarbon network, now by using the information in Table 5 and the Equation 2 we have,

$$\begin{aligned} ZC_2(K) &= \sum_{\check{a}\bar{a}\in E(K)} (\tau_K(\check{a}) \times \tau_K(\bar{a})), \\ &= (8)(2\times 3) + (8)(3\times 4) + (4n)(4\times 4) + (4)(4\times 5) \\ &\quad +(2n+4)(4\times 6) + (2)(5\times 5) + (4)(6\times 5) \\ &\quad +(11n-16)(6\times 6), \\ &= 508n - 86. \end{aligned}$$

Theorem 6. *Consider a non-Kekulean benzenoid hydrocarbon network, then its modified first Zagreb connection index is,*

$$ZC_1^*(K) = 184n + 44.$$

Proof. Let K be a graph of non-Kekulean benzenoid hydrocarbon network, now by using the information in Table 5 and the Equation 3 we have,

$$\begin{aligned} ZC_1^*(K) &= \sum_{\check{a}\bar{a}\in E(K)} (\tau_K(\check{a}) + \tau_K(\bar{a})), \\ &= (8)(2+3) + (8)(3+4) + (4n)(4+4) + (4)(4+5) \\ &\quad +(2n+4)(4+6) + (2)(5+5) + (4)(6+5) \\ &\quad +(11n-16)(4+6), \\ &= 184n + 44. \end{aligned}$$

Table 6: Numerical Behaviour of $ZC_1(Q)$, $ZC_2(Q)$, $ZC_1^*(Q)$, for Non-Kekulean Benzenoid Hydrocarbon.

n	$ZC_1(Q)$	$ZC_2(Q)$	$ZC_1^*(Q)$
3	1052	1438	596
4	1404	1946	780
5	1756	2454	964
6	2108	2962	1148
7	2460	3470	1332
8	2812	3978	1516
9	3164	4486	1700
10	3516	4994	1884

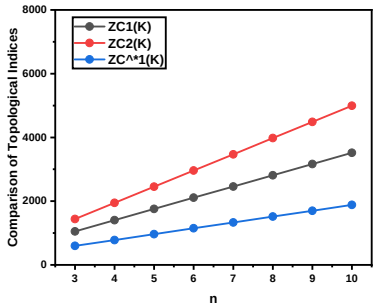

Figure 4: $ZC_1(Q)$, $ZC_2(Q)$, and $ZC_1^*(Q)$.

4. Applications and Statement of Novelty

Topological indices are massively employed as structural descriptors for Quantitative Structure Activity Relationships, Quantitative Structure Property Relationships, Quantitative Structure Toxicity Relationships. These models are widely used in pharmaceutical and agricultural industry for chemical screening. Once a correlation between physicochemical properties and molecular structure is developed it is achievable to forecast the certain properties of chemical networks for any molecular size, [4, 14]. Over the decades numerous structural topological descriptors have been defined, keeping in view the importance and applications of these structures we have defined Zagreb connection indices for hexagonal network and non-kekulean benzenoid hydrocarbon.

5. Conclusions

In mathematics, graph theory [1, 2, 22] is defined as the study of graphs which are mathematical structures employed to model pairwise relation between objects. In this paper, we calculated the connection number based indices for hexagonal network and non kekulean benzenoid hydrocarbon. We defined the first Zagreb connection index, the second Zagreb connection index and modified first Zagreb connection index based on vertices and edges. Further we have computed some numerical values of these indices with different n,

and provided their graphical representation. The graphs show an increasing trend of the indices. In future one can study different types of topological indices of these networks. It will be fascinating to debate the distance-based important parameters of these structure because topological indices are widely used in chemistry, it may be interesting to discover new chemical characteristics and explore their mathematical features.

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