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Degree-Edge Based Topological Indices Of Chain Graphs

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Abstract

Zagreb indices are degree-based indices. If degree and edge of a molecular graph is combined it defines the degree-edge based topological index. The first K-Banhatti index is defined as:
$B_1(G) = \sum_{ue}(d_u + d_e)$,where ue means that the vertex u and edge e are incident in G.
In this paper K-Banhatti indices of Penta chain and graphene chain with t = 1 row and S-benzene rings in a row are investigated.

Keywords: Degree, edge, F-index, graphene, K-Banhatti indices, molecular graph, penta chain, Zagreb indices.

1. Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Let G = (V, E) be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it are represented by V = V(G) and E = E(G), respectively [1-5].Topological indices describe the structure of molecules numerically and are used in the development of qualitative structure activity relationships (QSARs) [6].In the QSPR/QSAR study, physicochemical properties and topological indices such as Szeged index, Weiner index, Randic index, Zagreb index, ABC index are used to predict bioactivity of the chemical compounds [7].In analyzing the structure dependency of Π-electron energy the first and second Zagreb indices are defined as: $M_1(G) = \sum_{uv\in E(G)}(d_u+d_v)$ and $M_2(G) = \sum_{uv\in E(G)}(d_u * d_v)$ which are degree based topological indices. The number of edges incident on vertex v is called degree d_v of a vertex [8]. According to the above Zagreb indices, the first and second Zagreb polynomials have been defined as: $M_1(G,x) = \sum_{uv\in E(G)} x^{(d_u+d_v)}$ and

$M_2(G,x) = \sum_{uv \in E(G)} x^{(d_u d_v)}$ [9-11]. Degree based topological indices of Nicotine are studied in [12].Topological indices of graphene are studied in [13].The multiplicative Zagreb indices of nanostructures and chains are studied by W.Gao [14].Redefined Zagreb, Randic, Harmonic and GA indices of graphene are studied by R.Pradeep Kumar [15]. K-Banhatti and hyper K-Banhatti indices of circulant graphs are studied by A.Asghar [16]. K-Banhatti indices of Hexagonal, Honeycomb and derived networks are studied in [17]. ABC K-Banhatti and Augmented K-Banhatti indices of Chemical networks are studied in [18]. K-Banhatti indices of molecular graphs are studied in [19-20].

The first K-Banhatti index $B_1(G)$ and the second K-Banhatti $B_2(G)$ of a graph G are defined as:

$B_1(G) = \sum_{ue}(d_u + d_e)$ and $B_2(G) = \sum_{ue}(d_u\, d_e)$, where ue means that the vertex u and edge e are incident in G [21].

The first and second multiplicative K-Banhatti indices are defined as:

$PB_1(G) = \prod_{ue}(d_u + d_e)$ and $PB_2(G) = \prod_{ue}(d_u d_e)$.

Albertson index A(G) to determine the irregularity of a graph [22] is defined as:

$A(G) = \sum_{uv} |d_u - d_v|$ and by analogy with this topological index, Albertson K-Banhatti index can be introduced as: $AB(G) = \sum_{ue} |d_u - d_e|$.

And reformulated K Banhatti index is defined as: $RB(G) = \sum_{uv}[d_u + d_e - 2]^2$.

The first and second hyper K-Banhatti indices are

$HB_1(G) = \sum_{uv}[d_u + d_e]^2$ and $HB_2(G) = \sum_{uv}[d_u\ d_e]^2$.

We introduce for Randic index, reciprocal Randic index, the K-Banhatti Randic index and K-Banhatti reciprocal Randic index as [8],

K-Banhatti Randic index,

$BR(G) = \sum_{ue} \frac{1}{\sqrt{d_u\, d_e}}$ and K-Banhatti reciprocal Randic index = $BRR(G) = \sum_{uv} \sqrt{d_u\, d_e}$.

Where ue means that the vertex u and edge e are incident in G and d_u is degree of vertex u in G.

The Forgotten index is defined as [23-25]:

$F = F(G) = \sum_{uv \in E(G)} d_u^{\,3} = \sum_{uv \in (G)}[d_u^{\,2} + d_v^{\,2}]$.

We introduce by combining degree and edge of G the Forgotten K-Banhatti index as:

$FB(G) = \sum_{ue} (d_u^{\,2} + d_e^{\,2})$.

The notations used in this paper are standard and mainly taken from books [26-30]. In this paper K-Banhatti indices of Penta chain and graphene chain with t = 1 row, S-benzene rings in a row is investigated.

2. Results and discussion

The molecular graphs considered in this paper are finite, connected, loop less and without multiple edges. Let G= (V, E) be a graph with n vertices and m edges. The first K-Banhatti index is defined as: $B_1(G) = \sum_{us}(d_u + d_s)$,where uv denotes the edge of the graph G connecting the vertices u and v and d_u denotes the degree of the vertex u and $d_e= d_u+ d_v-2$. By combining degree and edge the K-Banhatti indices can be defined for molecular graphs. For formulas of degree-edge based K-Banhatti indices of molecular graph refer to [16-21]. The first and multiple K-Banhatti index, Albertson K-Banhatti index, reformulated K-Banhatti index, first and second hyper K-Banhatti indices, K-Banhatti Randic index, K-Banhatti reciprocal Randic index and Forgotten K-Banhatti index are computed for penta chain and graphene chain. The K-Banhatti indices for penta chain and graphene chain are computed as:

2.1 K-Banhatti indices for penta chain

The 2-dimensional graph for double row penta chain $G(n,S_2)$ is shown in figure (1). It is observed from figure (1) there are four edges as: E_{22}, E_{23}, E_{34} and E_{44}.The number of edges with frequency are represented in table 1.

The first hyper K-Banhatti index is computed as:

$HB_1(G) = \sum_{us}(d_u+ d_s)^2$

$= 4[(2+2)+(2+2)]^2 +(4n)[(2+3)+(3+3)]^2+(2n)[(3+5)+(4+5)]^2+(n-2)[(4+6)+(4+6)]^2$

$= 1062n-144$

The second hyper K-Banhatti index is computed as:

$HB_2(G) = \sum_{us}(d_u\, d_s)^2$

$=6[(2*2)*(2*2)]^2 +(4n)[(2*3)*(3*3)]^2+(2n)[(3*5)*(4*5)]^2+(n-2)[(4*6)*(4*6)]^2.$

$=523440n-662528.$

2.2 K-Banhatti indices for graphene chain

Graphene is a two-dimensional layer of pure carbon. It is one atom-thick and single tightly packed layer of carbon atoms that are bonded together in a repeating pattern of hexagon, with each carbon atom covalently bonded to three other carbon atoms. In this section we compute K-Banhatti indices for graphene chain with t = 1 and S benzene rings in this row. The 2-dimensional graph of graphene with t = 1 row and S benzene rings is shown in figure (2). The first and second hyper K-Banhatti indices for graphene are computed as:

First and second hyper K-Banhatti indices for graphene

It is observed from figure (2),the graphene chain with t=1 and S benzene rings in this row has three edges:E_{22},E_{23} and E_{33} with.| $d_{2,2}$|= 6,|$d_{2,3}$|= (4S-4) and |$d_{3,3}$| = (S-1) (table 2).

The first hyper K-Banhatti index is computed as:

$HB_1(G) = \sum_{us}(d_u+d_s)^2$

$= 6[(2+2)+(2+2)]^2 +(4S-4)[(2+3)+(3+3)]^2+(S-1)[(3+4)+(3+4)]^2$

$= 680S-296.$

The second hyper K-Banhatti index is computed as:

$HB_2(G) = \sum_{us}(d_u\, d_s)^2$

$=6[(2*2)*(2*2)]^2 +(4S-4)[(2*3)*(3*3)]^2+(S-1)[(3*4)*(3*4)]^2 = 644972544(4S-4)(S-1).$

First and second multiple K-Banhatti indices, AK-Banhatti index, Reformulated K-Banhatti index, First and second hyper K-Banhatti indices, K-Banhatti Randic index, K-Banhatti reciprocal Randic index and Forgotten K-Banhatti index are computed for penta chain and graphene chain and are represented in table number (3).

Figure no.1: 2-dimensional graph for double row penta chain G(n,S_2).

Figure no. 2: dimensional graph for graphene t =1row, S-benzene rings.

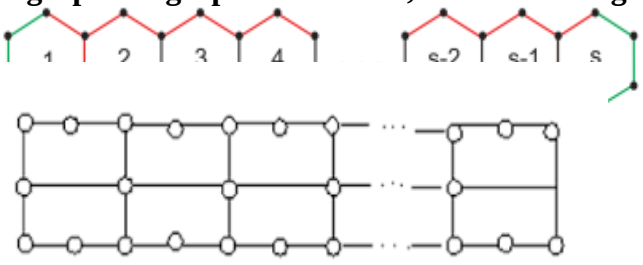

Figure: 1

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Table no. (1): The degree-edge partition for double row penta chain G(n,S_2).

$d_G(u)$, $d_G(v)$\e= u v ∈ E(G)	(2,2)	(2,3)	(3,4)	(4,4)
$d_G(e)$	2	3	5	6
Number of edges	4	4n	2n	n-2

Table no. (2): The degree-edge partition for graphene t =1 row, S-benzene rings.

$d_G(u)$, $d_G(v)$\e= u v ∈ E(G)	(2,2)	(2,3)	(3,3)
$d_G(e)$	2	3	4
Number of edges	6	(4S-4)	(S-1)

Table no. (3): K-Banhatti indices for Penta chain and Graphene chain.

Serial Number	Topological indices	Penta chain	Graphene chain
1.	First multiple K-Banhatti index	$975440(n-2)n^2$	7392(4S-4)(S-1)
2.	Second multiple K-Banhatti index	$4777574400(n-2)n^2$	746496(4S-4)(S-1)
3.	Albertson K-Banhatti index	14n-8	2S-2
4.	Reformulated K-Banhatti index	1098n-504	468S-252
5.	First hyper K-Banhatti index	1062n-144	680S-296
6.	Second hyper K-Banhatti index	523440n-662528	644972544(4S-4)(S-1)
7.	K-Banhatti Randic index	0.982n+0.9002	0.6281S+1.4538
8.	K-Banhatti reciprocal Randic index	61.589n-32	41.394S-17.394
9.	Forgotten K-Banhatti index	918n-272	522S-330

3. Conclusion

The degree-edge based K-Banhatti indices are studied for penta chain and graphene chain. To compute degree-based topological indices for molecular graph degree of each vertex and edge are important. The first and second multiple K-Banhatti indices, AK-Banhatti index, reformulated K-Banhatti index, first and second hyper K-Banhatti indices, K-Banhatti Randic index, K-Banhatti, reciprocal Randic index and Forgotten K-Banhatti index are computed for penta chain and graphene chain. The degree-edge based K-Banhatti of molecular graphs may be used in QSPR and QSAR studies.

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