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:

\[ B_1(G) = \sum_{ue} \left( d_u + d_e \right) \]

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 \( \Pi \)-electron energy the first and second Zagreb indices are defined as: 

\[ M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) \] and 
\[ M_2(G) = \sum_{uv \in E(G)} (d_u \cdot d_v) \]

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:

\[ B_1(G) = \sum_{ue} (d_u + d_e) \quad \text{and} \quad B_2(G) = \sum_{ue} (d_u d_e) \], 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:

\[ PB_1(G) = \prod_{ue} (d_u + d_e) \quad \text{and} \quad PB_2(G) = \prod_{ue} (d_u d_e) . \]

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 defined as:

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

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,

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

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]:

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

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: $B_1(G) = \sum_{uv}(d_u + d_v)$ , 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:

$$HB_1(G) = \sum_{uv}(d_u + d_v)^2$$

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

$$= 1062n - 144$$

The second hyper K-Banhatti index is computed as:

$$HB_2(G) = \sum_{uv}(d_u d_v)^2$$

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

$$= 523440n - 662528$$

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:

\[
HB_1(G) = \sum_{u\in\mathcal{G}} (d_u + d_e)^2
\]

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

\[
= 680S-296.
\]

The second hyper K-Banhatti index is computed as:

\[
HB_2(G) = \sum_{u\in\mathcal{G}} (d_u d_e)^2
\]

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

\[
= 644972544(4S-4)(S-1).
\]

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 \( t = 1 \) row, \( S \)-benzene rings.
Table no. (1): The degree-edge partition for double row penta chain $G(n,S_2)$.

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v) \in E(G)$</th>
<th>(2,2)</th>
<th>(2,3)</th>
<th>(3,4)</th>
<th>(4,4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_G(e)$</td>
<td>2</td>
<td>3</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>Number of edges</td>
<td>4</td>
<td>4$n$</td>
<td>2$n$</td>
<td>n-2</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v) \in E(G)$</th>
<th>(2,2)</th>
<th>(2,3)</th>
<th>(3,3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_G(e)$</td>
<td>2</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Number of edges</td>
<td>6</td>
<td>(4$S$-4)</td>
<td>(S-1)</td>
</tr>
</tbody>
</table>

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

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

References


