New K-Banhatti Topological Indices

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Abstract. In this paper, we introduce the modified first and second K Banhatti indices of a graph. Also we introduce the harmonic K-Banhatti index of a graph. We initiate a study of these new invariants.

Keywords: modified first and second K-Banhatti indices, harmonic K-Banhatti index, nanotubes

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1. Introduction

Let $G$ be a finite, simple connected graph. The degree $d_G(v)$ of a vertex $v$ is the number of vertices adjacent to $v$. The edge connecting vertices $u$ and $v$ is denoted by $uv$. If $e=uv$ is an edge of $G$, then the vertex $u$ and edge $e$ are incident as are $v$ and $e$. Let $d_G(e)$ denote the degree of an edge $e$ in $G$, which is defined by $d_G(e) = d_G(u) + d_G(v) - 2$ with $e=uv$. Any undefined term here may be found in Kulli [1].

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of Mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be used to characterize some property of the graph of a molecular is called a topological index for that graph. Numerous topological descriptors have found some applications in theoretical chemistry especially in QSPR/QSAR research.

The modified first and second Zagreb indices [2] are respectively defined as

$$mM_1(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u)^2}, \quad mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u)d_G(v)}.$$

These indices were studied by Kulli in [3, 4].

Motivated by the definition of the modified first and second Zagreb indices, we introduce the modified first and second K-Banhatti indices of a graph as follows:

The modified first and second K-Banhatti indices of a graph are defined as

$$mB_1(G) = \sum_{ue \in G} \frac{1}{d_G(u) + d_G(e)}, \quad mB_2(G) = \sum_{ue \in G} \frac{1}{d_G(u)d_G(e)},$$

where $ue$ means that the vertex $u$ and edge $e$ are incident in $G$.

The harmonic index of a graph $G$ is defined as
The harmonic $K$-Banhatti index of a graph $G$ is defined as

$$H_b(G) = \sum_{ue \in E(G)} 2 \frac{d_G(u)}{d_G(u) + d_G(e)}$$

where $ue$ means that the vertex $u$ and edge $e$ are incident in $G$.

Many other topological indices were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18].

In this paper, we compute the modified first and second $K$-Banhatti indices and harmonic $K$-Banhatti index of some standard graphs, $TUC_4C_8[p, q]$ nanotubes and $TUC_4[p, q]$ nanotubes.

### 2. Computing $K$-Banhatti topological indices of some standard graphs

**Theorem 1.** Let $C_n$ be a cycle with $n \geq 3$ vertices. Then

1. $mB_1(C_n) = \frac{1}{2} n$
2. $mB_2(C_n) = \frac{1}{2} n$
3. $H_b(C_n) = n$

**Proof:** Let $G = C_n$ be a cycle with $n \geq 3$ vertices. Every vertex of a cycle $C_n$ is incident with exactly two edges and the number of edges in $C_n$ is $n$.

1. $mB_1(G) = \sum_{ue \in E(G)} \frac{1}{d_G(u) + d_G(e)} = \sum_{ue \in E(G)} \left( \frac{1}{2} + \frac{1}{2} \right) = \frac{n}{2}$.

2. $mB_2(G) = \sum_{ue \in E(G)} \frac{1}{d_G(u)} = \sum_{ue \in E(G)} \left( \frac{1}{2 \times 2} \right) = \frac{n}{2}$.

3. $H_b(G) = \sum_{ue \in E(G)} \frac{2}{d_G(u) + d_G(e)} = 2\sum_{ue \in E(G)} \frac{1}{d_G(u) + d_G(e)} = n$.

**Theorem 2.** Let $P_n$ be a path with $n \geq 3$ vertices. Then

1. $mB_1(P_n) = \frac{1}{2} n + \frac{1}{6}$
2. $mB_2(P_n) = \frac{1}{2} n + \frac{3}{2}$
3. $H_b(P_n) = n + \frac{1}{3}$.

**Proof:** Let $G = P_n$ be a path with $n \geq 3$ vertices. We obtain two partitions of the edge set of $P_n$ as follows:

$E_1 = \{e=uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_1| = 2$. 

$$E_2 = \{e=uv \in E(G) \mid d_G(u) = 2, d_G(v) = 2\}$$

$$E_3 = \{e=uv \in E(G) \mid d_G(u) = 2, d_G(v) = 1\}$$
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\[ E_4 = \{ e = uv \in E(G) \mid d_G(u) = d_G(v) = 2 \}, |E_4| = n - 3. \]

(1) To compute \( mB_1(P_n) \), we see that

\[
mB_1(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E(G)} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)
+ \sum_{uv \in E(G)} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)
= \left( \frac{1}{1+1} \right)^2 + \left( \frac{1}{1+1} \right)^2 (n-3) = \frac{1}{2} n + \frac{1}{6}.
\]

(2) To compute \( mB_2(P_n) \), we see that

\[
mB_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)}
= \sum_{uv \in E(G)} \frac{1}{2} \ \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)
+ \sum_{uv \in E(G)} \frac{1}{2} \ \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)
= \left( \frac{1}{1+1} \right)^2 + \left( \frac{1}{1+1} \right)^2 (n-3) = \frac{1}{2} n + \frac{3}{2}.
\]

(3) To compute \( H_b(P_n) \), we see that

\[
H_b(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(e)} = \frac{2}{2} \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)} = n + \frac{1}{3}.
\]

**Theorem 3.** Let \( K_n \) be a complete graph with \( n \geq 3 \) vertices. Then

(1) \( mB_1(K_n) = \frac{n(n-1)}{3n-5} \)

(2) \( mB_2(K_n) = \frac{n}{2(n-2)} \)

(3) \( H_b(K_n) = \frac{2n(n-1)}{3n-5} \)

Proof: Let \( G = K_n \) be a complete graph with \( n \geq 3 \) vertices. Every vertex of \( K_n \) is incident with exactly \( n - 1 \) edges.

(1) To compute \( mB_1(K_n) \), we see that

\[
mB_1(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E(G)} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)
= \left( \frac{1}{(n-1) + (2n-4)} + \frac{1}{(n-1) + (2n-4)} \right) \frac{n(n-1)}{2} = \frac{n(n-1)}{3n-5}.
\]

(2) To compute \( mB_2(K_n) \), we see that

\[
mB_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E(G)} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)
= \left( \frac{1}{(n-1)(2n-4)} + \frac{1}{(n-1)(2n-4)} \right) \frac{n(n-1)}{2} = \frac{n}{2(n-2)}.
\]
(3) To compute $H_b(K_n)$, we see that

$$H_b(G) = \sum_{ue} \frac{2}{d_G(u) + d_G(e)} = 2 \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \frac{2n(n-1)}{3n-5}.$$ 

**Theorem 4.** Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ and $s \geq 2$. Then

1. $mB_1(K_{r,s}) = \left(\frac{1}{r+2s-2} + \frac{1}{2r+s-2}\right)rs$
2. $mB_2(K_{r,s}) = \frac{r+s}{r+s-2}$
3. $H_b(K_{r,s}) = \left(\frac{1}{r+2s-2} + \frac{1}{2r+s-2}\right)2rs.$

**Proof:** Let $G = K_{r,s}$ be a complete bipartite graph with $r + s$ vertices and $rs$ edges such that $|V_1| = r \geq 1$, $|V_2| = s \geq 2$, $V(K_{r,s}) = V_1 \cup V_2$. Every vertex of $V_1$ is incident with $s$ edges and every vertex of $V_2$ is incident with $r$ edges.

1. To compute $mB_1(K_{r,s})$, we see that

$$mB_1(G) = \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \sum_{ue \in E(G)} \left(\frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)}\right)$$

$$= \left(\frac{1}{s+(r+s-2)} + \frac{1}{r+(r+s-2)}\right)rs = \left(\frac{1}{r+2s-2} + \frac{1}{2r+s-2}\right)rs.$$

2. To compute $mB_2(K_{r,s})$, we see that

$$mB_2(G) = \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \sum_{ue \in E(G)} \left(\frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)}\right)$$

$$= \left(\frac{1}{s(r+s-2)} + \frac{1}{r(r+s-2)}\right)rs = \frac{r+s}{r+s-2}.$$ 

3. To compute $H_b(K_{r,s})$, we see that

$$H_b(G) = \sum_{ue} \frac{2}{d_G(u) + d_G(e)} = 2 \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \left(\frac{1}{r+2s-2} + \frac{1}{2r+s-2}\right)2rs$$

**Corollary 1.** Let $K_{r,s}$ be a complete bipartite graph with $1 \leq r \leq s$ and $s \geq 2$. Then

1. $mB_1(K_{r,s}) = \frac{2r^2}{3r-2},$ if $s = r,$
   
   $$= \frac{3s-1}{2s-1},$$ if $r = 1.$

2. $mB_2(K_{r,s}) = \frac{r}{r-1},$ if $s = r,$

   $$= \frac{s+1}{s-1},$$ if $r = 1.$

3. $H_b(K_{r,s}) = \frac{4r^2}{3r-2},$ if $s = r,$

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\[ = \frac{2(3s-1)}{2s-1}, \quad \text{if } r = 1. \]

**Theorem 5.** Let $G$ be an $r$-regular graph with $n \geq 3$ vertices. Then

1. \( mB_1(G) = \frac{nr}{3r-2} \)
2. \( mB_2(G) = \frac{n}{2(r-1)} \)
3. \( H_b(G) = \frac{2nr}{3r-2} \).

**Proof:** Let $G$ be an $r$-regular graph with $n \geq 3$ vertices and \( \frac{nr}{2} \) edges. Every vertex of $G$ is incident with $r$ edges.

1. To compute $mB_1(G)$, we see that

\[
mB_1(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E(G)} \left( \frac{1}{d_G(u)} + \frac{1}{d_G(v)} \right).
\]

\[
= \left( \frac{1}{r} + \frac{1}{r+2(2r-2)} \right) \frac{nr}{2} = \frac{nr}{3r-2}.
\]

2. To compute $mB_2(G)$, we see that

\[
mB_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u)d_G(e)} = \sum_{uv \in E(G)} \left( \frac{1}{d_G(u)} \frac{1}{d_G(v)} \right).
\]

\[
= \left( \frac{1}{r(2r-2)} + \frac{1}{r+2(2r-2)} \right) \frac{nr}{2} = \frac{n}{2(r-1)}.
\]

3. To compute $H_b(G)$, we see that

\[
H_b(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(e)} = 2 \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(e)} = \frac{2nr}{3r-2}.
\]

3. **Computing $K$ Banhatti type indices of $TUC_4C_8[p,q]$ nanotubes**

We discuss $TUC_4C_8[S]$ nanotubes which are consisting of cycles $C_4$ and $C_8$. These nanotubes usually symbolized as $TUC_4C_8[p,q]$ for $p, q \in N$ in which $p$ is the number of octagons $C_8$ in the first row and $q$ is the number of octagons $C_8$ in the first column. The 2-dimensional lattice of $TUC_4C_8[p,q]$ is shown in Figure 1.

![Figure 1](image-url)
V.R. Kulli

We determine the modified first $K$ Banhatti index of $TUC_4C_8[p, q]$ nanotubes.

**Theorem 6.** Let $G = TUC_4C_8[p, q]$ be the graph of nanotubes. Then

$$mB_1(G) = \frac{24}{7}pq + \frac{199}{105}p.$$ 

**Proof:** Let $G = TUC_4C_8[p, q]$. By algebraic method, we get $|V(G)| = 8pq + 4p$ and $|E(G)| = 12pq + 4p$. From Figure 1, it is easy to see that there are three partitions of the edge set of $G$ as follows:

- $E_4 = \{e = uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_4| = 2p$.
- $E_5 = \{e = uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_5| = 4p$.
- $E_6 = \{e = uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_6| = 12pq - 2p$.

Further the edge degree partition of the nanotube $TUC_4C_8[p, q]$ is given in Table 1.

<table>
<thead>
<tr>
<th>$d_G(u), d_G(v)\mid e = uv \in E(G)$</th>
<th>$d_G(e)$</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2, 2)</td>
<td>2</td>
<td>2p</td>
</tr>
<tr>
<td>(2, 3)</td>
<td>3</td>
<td>4p</td>
</tr>
<tr>
<td>(3,3)</td>
<td>4</td>
<td>12pq - 2p</td>
</tr>
</tbody>
</table>

**Table 1:** Edge degree partition of $TUC_4C_8[p, q]$

To determine $mB_1(G)$, we see that

$$mB_1(G) = \sum_{uv} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E_4} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right) + \sum_{uv \in E_5} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right) + \sum_{uv \in E_6} \left( \frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right)$$

$$= \left( \frac{1}{2+2} + \frac{1}{2+2} \right)2p + \left( \frac{1}{2+3} + \frac{1}{3+3} \right)4p + \left( \frac{1}{3+4} + \frac{1}{3+4} \right)(12pq - 2p) + \frac{24}{7}pq + \frac{199}{105}p.$$ 

We determine the modified second $K$ Banhatti index of $TUC_4C_8[p, q]$ nanotube.

**Theorem 7.** Let $G = TUC_4C_8[p, q]$ be the graph of nanotubes. Then

$$mB_2(G) = 2pq + \frac{16}{9}p.$$ 

**Proof:** Let $G = TUC_4C_8[p, q]$ the nanotubes. By using the results from the proof of Theorem 6, we obtain

$$mB_2(G) = \sum_{uv} \frac{1}{d_G(u)d_G(e)} = \sum_{uv \in E_4} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right) + \sum_{uv \in E_5} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right) + \sum_{uv \in E_6} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right)$$

$$= \left( \frac{1}{2+2} + \frac{1}{2+2} \right)2p + \left( \frac{1}{2+3} + \frac{1}{3+3} \right)4p + \left( \frac{1}{3+4} + \frac{1}{3+4} \right)(12pq - 2p) + \sum_{uv \in E_4} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right) + \sum_{uv \in E_5} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right) + \sum_{uv \in E_6} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right)$$

$$= \left( \frac{1}{2+2} + \frac{1}{2+2} \right)2p + \left( \frac{1}{2+3} + \frac{1}{3+3} \right)4p + \left( \frac{1}{3+4} + \frac{1}{3+4} \right)(12pq - 2p) + \frac{24}{7}pq + \frac{199}{105}p.$$ 

We determine the modified second $K$ Banhatti index of $TUC_4C_8[p, q]$ nanotube.
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\[
+ \sum_{uv \in E_G} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right) + \sum_{uv \in E_G} \left( \frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)} \right) \\
= \left( \frac{1}{2 \times 2} + \frac{1}{2 \times 2} \right) 2p + \left( \frac{1}{2 \times 3} + \frac{1}{3 \times 3} \right) 4p + \left( \frac{1}{3 \times 4} + \frac{1}{3 \times 4} \right) (12pq - 2p) \\
= 2pq + \frac{16}{9} p.
\]

We compute the harmonic $K$-Banhatti index of $TUC_4C_8[p, q]$ nanotube.

**Theorem 8.** Let $G = TUC_4C_8[p, q]$ be the graph of nanotubes. Then

\[ H_b(G) = \frac{48}{7} pq + \frac{398}{105} p. \]

**Proof:** Let $G = TUC_4C_8[p, q]$ be the nanotubes. By using Theorem 6, we obtain

\[ H_b(G) = \sum_{uv \in E_G} \left( \frac{2}{d_G(u) + d_G(e)} \right) = 2 \sum_{uv \in E_G} \left( \frac{1}{d_G(u) + d_G(e)} \right) = \frac{48}{7} pq + \frac{298}{105} p. \]

4. **Computing $K$ Banhatti type indices of $TUC_4[p, q]$ nanotubes.**

In this section, we focus on the structures of a family of nanostructures and they are called $TUHRC_4[S]$ nanotubes. These nanotubes usually symbolized as $TUC_4[p, q]$ for any $p, q \in N$ in which $p$ is the number of cycles $C_u$ in the first row and $q$ is the number of cycles $C_v$ is the first column as depicted in Figure 2.

![Figure 2: 2-D graph of $G = TUC_4[p, q]$](image)

We compute the modified first $K$-Banhatti index of $TUC_4[p, q]$ nanotubes.

**Theorem 9.** Let $G$ be the $TUC_4[p, q]$ nanotubes. Then

\[ m B_1(G) = \frac{4}{5} pq + \frac{23}{30} p. \]

**Proof:** Let $G$ be the $TUC_4[p, q]$ nanotubes as depicted in Figure 2. By algebraic method, we obtain $|E(G)| = 4pq + 2p$. From Figure 2, it is easy to see that there are two partitions of the edge set of $G$ as follows:

\[ E_1 = \{ e = uv \in E(G) | d_G(u) = 2, d_G(v) = 4 \}, |E_1| = 4p. \]

\[ E_2 = \{ e = uv \in E(G) | d_G(u) = d_G(v) = 4 \}, |E_2| = 4pq - 2p. \]

Further the edge degree partition of the nanotube $TUC_4[p, q]$ is given in Table 2.
To compute $m B_2(G)$, we see that

$$m B_2(G) = \sum_{ue} \frac{1}{d_G(u) + d_G(e)}$$

$$= \sum_{ue \in E} \left( \frac{1}{d_G(u)} + \frac{1}{d_G(e)} \right) + \sum_{ue \in E} \left( \frac{1}{d_G(v)} + \frac{1}{d_G(e)} \right)$$

$$= \left( \frac{1}{2+4} + \frac{1}{4+4} \right) 4p + \left( \frac{1}{4+6} + \frac{1}{4+6} \right) (4pq - 2p) = \frac{4}{5} pq + \frac{23}{30} p.$$ 

We now compute the harmonic $K$-Banhatti index of $TUC_4[p, q]$ nanotubes.

**Theorem 11.** Let $G = TUC_4[p, q]$ be the nanotubes. Then

$$H_b(G) = \frac{8}{5} pq + \frac{23}{15} p.$$ 

**Proof:** Let $G = TUC_4[p, q]$ be the nanotubes. By using Theorem 9, we obtain

$$H_b(G) = \sum_{ue} \frac{2}{d_G(u) + d_G(e)} = \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \frac{8}{5} pq + \frac{23}{15} p.$$ 

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