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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

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C35

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

$$^{m}M_1(G)=\sum_{u\in V(G)}\frac{1}{d_G(u)^2}, \qquad ^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d_G(u)d_G(v)}.$$

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

$$^{m}B_1(G)=\sum_{ue}\frac{1}{d_G(u)+d_G(e)}, \qquad ^{m}B_2(G)=\sum_{ue}\frac{1}{d_G(u)d_G(e)}.$$

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

The harmonic index of a graph G is defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)}.$$

This index was studied by Favaron et.al. [5] and Zhong [6].

Motivated by the definition of the harmonic index and by previous research on topological indices, we now introduce the harmonic *K*-Banhatti index of a graph as follows:

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

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

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

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

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

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:

$E_3 = \{e = uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_3| = 2$.

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

(1) To compute ${}^mB_1(P_n)$, we see that

$$ {}^mB_1(G) = \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E_3} \left(\frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right) $$
$$ + \sum_{uv \in E_4} \left(\frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right) $$
$$ = \left(\frac{1}{1+1} + \frac{1}{2+1} \right) 2 + \left(\frac{1}{2+2} + \frac{1}{2+2} \right)(n-3) = \frac{1}{2}n + \frac{1}{6}. $$

(2) To compute ${}^mB_2(P_n)$, we see that

$$ {}^mB_2(G) = \sum_{ue} \frac{1}{d_G(u) d_G(e)} $$
$$ = \sum_{uv \in E_3} \left(\frac{1}{d_G(u) d_G(e)} + \frac{1}{d_G(v) d_G(e)} \right) + \sum_{uv \in E_4} \left(\frac{1}{d_G(u) d_G(e)} + \frac{1}{d_G(v) d_G(e)} \right) $$
$$ = \left(\frac{1}{1\times 1} + \frac{1}{2\times 1} \right) 2 + \left(\frac{1}{2\times 2} + \frac{1}{2\times 2} \right)(n-3) = \frac{1}{2}n + \frac{3}{2}. $$

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

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

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

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

(2) To compute ${}^mB_2(K_n)$, we see that

$$ {}^mB_2(G) = \sum_{ue} \frac{1}{d_G(u) d_G(e)} = \sum_{uv \in E(G)} \left(\frac{1}{d_G(u) d_G(e)} + \frac{1}{d_G(v) d_G(e)} \right) $$
$$ = \left(\frac{1}{(n-1)(2n-4)} + \frac{1}{(n-1)(2n-4)} \right) \frac{n(n-1)}{2} = \frac{n}{2(n-2)}. $$

(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 $1 \le r \le s$ and $s \ge 2$. Then

(1) $^{m}B_1(K_{r,s})=\left(\frac{1}{r+2s-2}+\frac{1}{2r+s-2}\right)rs$ (2) $^{m}B_2(K_{r,s})=\frac{r+s}{r+s-2}$

(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 $|V_1| = r \ge 1$, $|V_2| = s \ge 2$ $r \le s$, $V(K_{r,s}) = V_1 \cup V_2$. Every vertex of V_1 is incident with s edges and every vertex of V_2 is incident with r edges.

(1) To compute $^{m}B_1(K_{r,s})$, we see that

$$^{m}B_1(G)=\sum_{ue}\frac{1}{d_G(u)+d_G(e)}=\sum_{uv\in E(G)}\left(\frac{1}{d_G(u)+d_G(e)}+\frac{1}{d_G(v)+d_G(e)}\right)$$

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

(2) To compute $^{m}B_1(K_{r,s})$, we see that

$$^{m}B_2(G)=\sum_{ue}\frac{1}{d_G(u)d_G(e)}=\sum_{uv\in E(G)}\left(\frac{1}{d_G(u)d_G(e)}+\frac{1}{d_G(v)d_G(e)}\right)$$

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

(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 $1 \le r \le s$ and $s \ge 2$. Then

(1) $^{m}B_1(K_{r,s})=\frac{2r^2}{3r-2}$, if $s = r$,

$=\frac{3s-1}{2s-1}$, if $r = 1$.

(2) $^{m}B_2(K_{r,s})=\frac{r}{r-1}$, if $s = r$,

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

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

$$= \frac{2(3s-1)}{2s-1}, \qquad \text{if } r = 1.$$

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

(1) ${}^{m}B_1(G) = \frac{nr}{3r-2}$ (2) ${}^{m}B_2(G) = \frac{n}{2(r-1)}$ (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 ${}^{m}B_1(G)$, we see that

$$ {}^{m}B_1(G) = \sum_{ue} \frac{1}{d_G(u) + d_G(e)} = \sum_{uv \in E(G)} \left(\frac{1}{d_G(u) + d_G(e)} + \frac{1}{d_G(v) + d_G(e)} \right) $$

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

(2) To compute ${}^{m}B_2(G)$, we see that

$$ {}^{m}B_2(G) = \sum_{ue} \frac{1}{d_G(u) d_G(e)} = \sum_{uv \in E(G)} \left(\frac{1}{d_G(u) d_G(e)} + \frac{1}{d_G(v) d_G(e)} \right) $$

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

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

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

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.

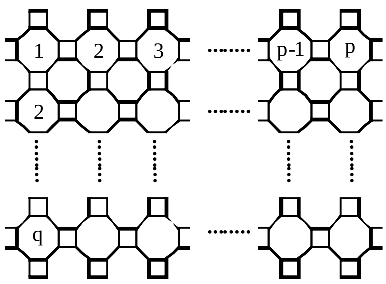

Figure1: The graph of 2-*D* lattice of $TUC_4C_8[p, q]$

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

$$^{m}B_1(G) = \frac{24}{7}pq + \frac{199}{105}p.$$

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.

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(2, 2)	(2, 3)	(3,3)
$d_G(e)$	2	3	4
Number of edges	$2p$	$4p$	$12pq - 2p$

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

To determine $^{m}B_1(G)$, we see that

$$^{m}B_1(G) = \sum_{ue} \frac{1}{d_G(u)+d_G(e)} = \sum_{uv\in E_4}\left(\frac{1}{d_G(u)+d_G(e)} + \frac{1}{d_G(v)+d_G(e)}\right)$$
$$+ \sum_{uv\in E_5}\left(\frac{1}{d_G(u)+d_G(e)} + \frac{1}{d_G(v)+d_G(e)}\right) + \sum_{uv\in E_6}\left(\frac{1}{d_G(u)+d_G(e)} + \frac{1}{d_G(v)+d_G(e)}\right)$$
$$= \left(\frac{1}{2+2}+\frac{1}{2+2}\right)2p + \left(\frac{1}{2+3}+\frac{1}{3+3}\right)4p + \left(\frac{1}{3+4}+\frac{1}{3+4}\right)(12pq - 2p)$$
$$= \frac{24}{7}pq + \frac{199}{105}p.$$

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

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

$$^{m}B_2(G) = 2pq + \frac{16}{9}p.$$

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

$$^{m}B_2(G) = \sum_{ue} \frac{1}{d_G(u)d_G(e)} = \sum_{uv\in E_4}\left(\frac{1}{d_G(u)d_G(e)} + \frac{1}{d_G(v)d_G(e)}\right)$$

$$+\sum_{uv\in E_5}\left(\frac{1}{d_G(u)d_G(e)}+\frac{1}{d_G(v)d_G(e)}\right)+\sum_{uv\in E_6}\left(\frac{1}{d_G(u)d_G(e)}+\frac{1}{d_G(v)d_G(e)}\right)$$
$$=\left(\frac{1}{2\times 2}+\frac{1}{2\times 2}\right)2p+\left(\frac{1}{2\times 3}+\frac{1}{3\times 3}\right)4p+\left(\frac{1}{3\times 4}+\frac{1}{3\times 4}\right)(12pq-2p)$$
$$=2pq+\frac{16}{9}p.$$

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
$$H_b(G)=\sum_{ue}\frac{2}{d_G(u)+d_G(e)}=2\sum_{ue}\frac{1}{d_G(u)+d_G(e)}=\frac{48}{7}pq+\frac{298}{105}p\,.$$

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_4 in the first row and q is the number of cycles C_4 is the first column as depicted in Figure 2.

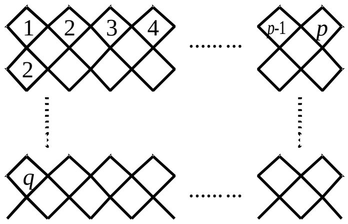

Figure 2: 2-*D* graph of $G = TUC_4[p, q]$

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:

$E_6 = \{e = uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_6|=4p$.

$E_8 = \{e = uv \in E(G) \mid d_G(u) = d_G(v) = 4\}$, $|E_8|=4pq - 2p$.

Further the edge degree partition of the nanotube $TUC_4[p, q]$ is given in Table 2.

$d_G(u)$ $d_G(v)\backslash e = uv\in E(G)$	(2, 4)	(4, 4)
$d_G(e)$	4	6
Number of edges	$4p$	$4pq - 2p$

Table 2: Edge degree partition of $TUC_4[p, q]$

To compute ${}^mB_1(G)$, we see that

$$ {}^mB_1(G) = \sum_{ue} \frac{1}{d_G(u)+d_G(e)} $$
$$ = \sum_{uv\in E_6}\left(\frac{1}{d_G(u)+d_G(e)}+\frac{1}{d_G(v)+d_G(e)}\right)+\sum_{uv\in E_8}\left(\frac{1}{d_G(u)+d_G(e)}+\frac{1}{d_G(v)+d_G(e)}\right) $$
$$ = \left(\frac{1}{2+4}+\frac{1}{4+4}\right)4p+\left(\frac{1}{4+6}+\frac{1}{4+6}\right)(4pq-2p) = \frac{4}{5}pq+\frac{23}{30}p. $$

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

Theorem 10. Let $G = TUC_4[p, q]$ be the nanotubes. Then

$$ {}^mB_2(G) = \frac{1}{3}pq+\frac{7}{12}p. $$

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

$$ {}^mB_2(G) = \sum_{ue} \frac{1}{d_G(u)d_G(e)} $$
$$ = \sum_{uv\in E_6}\left(\frac{1}{d_G(u)d_G(e)}+\frac{1}{d_G(v)d_G(e)}\right)+\sum_{uv\in E_8}\left(\frac{1}{d_G(u)d_G(e)}+\frac{1}{d_G(v)d_G(e)}\right) $$
$$ = \left(\frac{1}{2\times 4}+\frac{1}{4\times 4}\right)4p+\left(\frac{1}{4\times 6}+\frac{1}{4\times 6}\right)(4pq-2p) = \frac{1}{3}pq+\frac{7}{12}p. $$

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

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

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