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DIRECT AND INVERSE SUM BANHATTI INDICES

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ABSTRACT

We introduce the direct and inverse sum Banhatti indices of a molecular graph, In this paper, we compute the direct and inverse sum Banhatti indices of some standard clases of graphs. Also the direct and inverse sum Banhatti indices of certain nanotubes are determined.

Keywords: *molecular graph, direct and inverse sum Banhatti indices, nanotube.*

Mathematics Subject Classification: *05C05, 05C07.*

1. INTRODUCTION

In this paper, we consider finite simple connected graphs. Let G be a graph with vertex set $V(G)$ and and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The degree of an edge $e = uv$ in G is defined by $d_G(e) = d_G(u) + d_G(v) - 2$. For other undefined notations, readers may refer to [1].

A molecular graph or chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A single number that can be computed from the molecular graph, and used to characterize some property of the underlying molecule is said to be a topological index or molecular structure descriptor. Numerous such descriptors have been considered in theoretical chemistry, and have found some applications, especially in QSPR/QSAR research, see [2, 3, 4].

In [5] Vukičević and Gaśperov observed that many descriptors are defined simply as the sum of individual bond contributions. In order to study whether there are other possibly significant descriptors of this form, they have introduced a class of discretre Adriatic indices of a molecular graph G in [5], generally defined as

$$Adr(G) = \sum_{uv \in E(G)} f\left(g\left(p_u\right), g\left(p_v\right)\right)$$

where p_u is either the degree $d_G(u)$ of a vertex $u \in V(G)$ or the sum D_u of distance from u and all other vertices in $V(G)$, while f and g are suitably chosen functions.

The Zagreb indices were introduced as early as in 1972 [6]. The K Banhatti indices were introduced by Kulli in 2016 [7]. In [8], Gutman et al observed that these two types of indices are closely related.

Inspired by the definition of discrete Adriatic indices, and the close relationship between Banhatti and Zagreb indices, we define discrete Adriatic Banhatti indices as follows:

The discrete Adriatic Banhatti indices of a molecular graph G is defined as

$$AdrB(G) = \sum_{ue} f\left(g\left(d_G(u)\right), g\left(d_G(e)\right)\right)$$

where ue means that the vertex u and edge e are incident in G, while f and g are suitably chosen functions.

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We propose the inverse sum Banhatti index as follows:

The inverse sum Banhatti index of a molecular graph G is defined as

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

We also introduce the direct sum Banhatti index as follows:

The direct sum Banhatti index of a molecular graph G is defined as

$$DSB(G)=\sum_{ue}\left(\frac{1}{d_G(u)}+\frac{1}{d_G(e)}\right)=\sum_{ue}\frac{d_G(u)+d_G(e)}{d_G(u)d_G(e)}.$$

Recently, some topological indices were studied, for example, in [9,10,11,12,13,14,15,16,17,18].

We consider HC_5C_7 $[p, q]$ and SC_5C_7 $[p, q]$ nanotubes, see [19].

In this paper, we compute the direct and inverse sum Banhatti indices of HC_5C_7 $[p, q]$ nanotubes and SC_5C_7 $[p, q]$ nanotubes. Also we compute the direct and inverse sum Banhatti indices of some standard classes of graphs.

2. SOME STANDARD CLASSES OF GRAPHS

Proposition 1: Let C_n be a cycle with n ≥ 3 vertices. Then
(i) $DSB(C_n) = 2n$ ii) $ISB(C_n)=2n$.

Proof: Let C_n be a cycle with n≥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.

i) $DSB(C_n)=n\left(\frac{2+2}{2\times 2}+\frac{2+2}{2\times 2}\right)=2n.$ ii) $ISB(C_n)=n\left(\frac{2\times 2}{2+2}+\frac{2\times 2}{2+2}\right)=2n.$

Proposition 2: Let K_n be a complete graph with n ≥ 3 vertices. Then

i) $DSB(K_n)=\frac{n(3n-5)}{2(n-2)}$ ii) $ISB(K_n)=\frac{2n(n-1)^2(n-2)}{3n-5}.$

Proof: Let K_n be a complete graph with n≥3 vertices. Then every vertex of K_n is incident with n – 1 edges and the number of edges in K_n is $\frac{n(n-1)}{2}$.

i) $DSB(K_n)=\frac{n(n-1)}{2}\left[\frac{(n-1)+(2n-4)}{(n-1)(2n-4)}+\frac{(n-1)+(2n-4)}{(n-1)(2n-4)}\right]=\frac{n(3n-5)}{2(n-2)}.$

ii) $ISB(K_n)=\frac{n(n-1)}{2}\left[\frac{(n-1)(2n-4)}{(n-1)+(2n-4)}+\frac{(n-1)(2n-4)}{(n-1)+(2n-4)}\right]=\frac{2n(n-1)^2(n-2)}{3n-5}.$

Proposition 3: Let $K_{r,s}$ be a complete bipartite graph with $1 \le r \le s$ and $s \ge 2$ vertices. Then

i) $DSB(K_{r,s})=\frac{1}{(r+s-2)}\left[r(r+2s-2)+s(2r+s-2)\right].$

ii) $ISB(K_{r,s})=rs(r+s-2)\left[\frac{s}{r+2s-2}+\frac{r}{2r+s-2}\right].$

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

i) $$DSB(K_{r,s}) = rs\left[\frac{s+(r+s-2)}{s(r+s-2)} + \frac{r+(r+s-2)}{r(r+s-2)}\right]$$
$$= \frac{1}{r+s-2}\left[r(r+2s-2)+s(2r+s-2)\right].$$

ii) $$ISB(K_{r,s}) = rs\left[\frac{s(r+s-2)}{s+(r+s-2)} + \frac{r(r+s-2)}{r+(r+s-2)}\right]$$
$$= rs(r+s-2)\left[\frac{s}{r+2s-2} + \frac{s}{2r+s-2}\right].$$

Proposition 4: If G is an r-regular graph with n vertices and $r \geq 2$, then

i) $$DSB(G) = \frac{n(3r-2)}{2(r-1)}.$$ ii) $$ISB(G) = \frac{2nr^2(r-1)}{3r-2}.$$

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

i) $$DSB(G) = \frac{n}{2}\left[\frac{r+2r-2}{r(2r-2)} + \frac{r+2r-2}{r(2r-2)}\right] = \frac{n(3r-2)}{2(r-1)}.$$

ii) $$ISB(G) = \frac{nr}{2}\left[\frac{r(2r-2)}{r+2r-2} + \frac{r(2r-2)}{r+2r-2}\right] = \frac{2nr^2(r-1)}{3r-2}.$$

3. RESULTS FOR HC_5C_7 [p, q] NANOTUBES

We consider HC_5C_7 [p, q] nanotubes in which p is the number of heptagons in the first row and q rows of pentagones repeated alternately. The 2-dimensional lattice of nanotube HC_5C_7[8, 4] is shown in Figure 1, see [19].

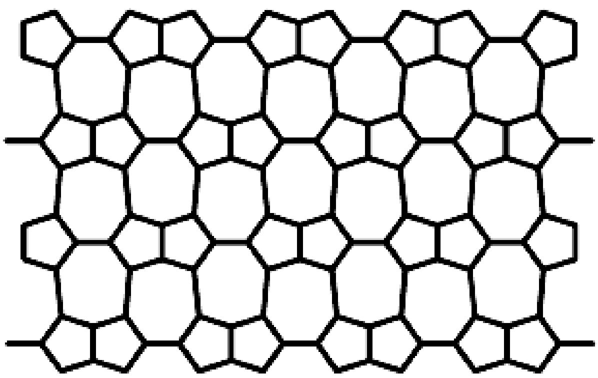

Figure-1: 2-D lattice of nanotube HC_5C_7[8, 4]

We compute the direct and inverse sum Banhatti indices of HC_5C_7 [p, q] nanotubes.

Theorem 1: Let G be the graph of HC_5C_7 [p, q] nanotube. Then
$$DSB(G) = pq + \frac{1}{6}p.$$

Proof: Let G be the graph of HC_5C_7 [p, q] nanotube. It is easy to see that the vertices of G are either of degree 2 or 3. By algebraic method, we obtain $|V(G)| = 4pq$ and $|E(G)| = 6pq - p$. In G, there are two types of edges based on the degree of end vertices of each edge. Further, by algebraic mehod, the edge degree partition of G is given in Table 1.

$d_G(u), d_G(v) \setminus e = uv \in E(G)$	(2, 3)	(3 3)
$d_G(e)$	3	4
Number of edges	$4p$	$6pq - 5p$

Table-1: Edge degree partition of G

By using the partition given in Table 1, we can apply the formula *DSB* index of G.

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

this implies that

$$DSB(G)=4p\left(\frac{2+3}{2\times 3}+\frac{3+3}{3\times 3}\right)+(6pq-5p)\left(\frac{3+4}{3\times 4}+\frac{3+4}{3\times 4}\right)=pq+\frac{1}{6}p.$$

Theorem 2: Let G be the graph of HC_5C_7 $[p, q]$ nanotube. Then

$$ISB(G)=\frac{144}{7}pq-\frac{222}{35}p.$$

Proof: By using the partition given in Table 1, we can apply the formula *ISB* index of *G*.

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

this implies that

$$ISB(G)=4p\left(\frac{2\times 3}{2+3}+\frac{3\times 3}{3+3}\right)+(6pq-5p)\left(\frac{3\times 4}{3+4}+\frac{3\times 4}{3+4}\right)=\frac{144}{7}pq-\frac{222}{35}p.$$

4. RESULTS FOR SC_5C_7 [p, q] NANOTUBES

We consider SC_5C_7 $[p, q]$ nanotubes. The 2-dimensional lattice of nanotube $SC_5C_7[8, 4]$ is shown in Figure 2.

In $SC_5C_7[p, q]$, p is the number of heptagones in the first row and q rows of vertices and edges are repeated alternately.

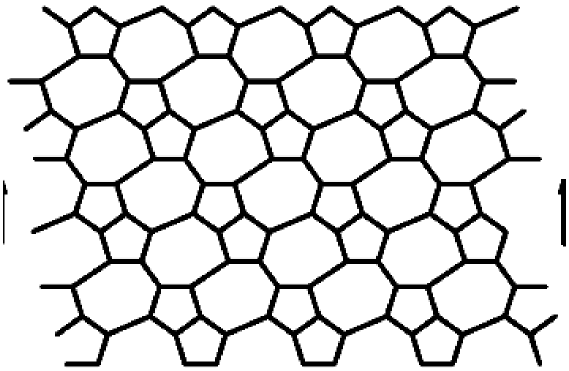

Figure-2: 2-*D* lattice of nanotube SC_5C_7 [8, 4]

In the following theorem, we compute the direct and inverse sum Banhatti indices of SC_5C_7 $[p, q]$ nanotubes.

Theorem 3: Let H be the graph of $SC_5C_7[p, q]$ nanotube. Then $DSB(H)=pq-\frac{7}{6}p+\frac{17}{6}q.$

Proof: Let H be the graph of SC_5C_7 $[p, q]$ nanotube. By algebraic metheod, we obtain that the graph H has $4pq$ vertices and $6pq-p$ edges. It is easy to see that the vertices of H are either of degree 2 or 3. In H, there are three types of edges based on the degree of end vertices of each edge. Further by algebraic method, the edge degree partition of H is given in Table 2.

$d_H(u), d_H(v)\ e=uv\in E(H)$	(2, 2)	(2, 3)	(3, 3)
$d_H(e)$	2	3	4
Number of edges	q	$6q$	$6pq-p-7q$

Table-2: Edge partition of H.

By using the partition given in Table 2, we can apply the formula *DSB* index of *H*.

Since $DSB(H)=\sum_{ue}\frac{d_H(u)+d_H(e)}{d_H(u)d_H(e)}=\sum_{uv\in E(H)}\left(\frac{d_H(u)+d_H(e)}{d_H(u)d_H(e)}+\frac{d_H(v)+d_H(e)}{d_H(v)d_H(e)}\right)$

this implies that

$$DSB(H)=q\left(\frac{2+2}{2\times 2}+\frac{2+2}{2\times 2}\right)+6q\left(\frac{2+3}{2\times 3}+\frac{3+3}{3\times 3}\right)+\left(6pq-p-7q\right)\left(\frac{3+4}{3\times 4}+\frac{3+4}{3\times 4}\right)=pq-\frac{7}{6}p+\frac{1}{6}\frac{7}{}q.$$

Theorem 4: Let H be the graph of SC_5C_7 $[p, q]$ nanotube. Then

$$ISB(H)=\frac{144}{7}pq-\frac{24}{7}p-\frac{34}{5}q.$$

Proof: By using the partition given in Table 2, we can apply the formula *ISB* index of *H*.

Since $$ISB(H)=\sum_{ue}\frac{d_H(u)d_H(e)}{d_H(u)+d_H(e)}=\sum_{uv\in E(H)}\left(\frac{d_H(u)d_H(e)}{d_H(u)+d_H(e)}+\frac{d_H(v)d_H(e)}{d_H(v)+d_H(e)}\right)$$

this implies that

$$ISB(H)=q\left(\frac{2\times 2}{2+2}+\frac{2\times 2}{2+2}\right)+6q\left(\frac{2\times 3}{2+3}+\frac{3\times 3}{3+3}\right)+\left(6pq-p-7q\right)\left(\frac{3\times 4}{3+4}+\frac{3\times 4}{3+4}\right)$$
$$=\frac{144}{7}pq-\frac{24}{7}p-\frac{34}{5}q.$$

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