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Connectivity Banhatti indices for certain families of Benzenoid Systems

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Abstract

Chemical graph theory is a branch of Mathematical chemistry which has an important effect on the development of the chemical sciences. The study of topological indices is currently one of the most active research fields in chemical graph theory. In this paper, we compute the connectivity Banhatti indices of certain families of Benzenoid systems.

Key words: Connectivity Banhatti index, sum connectivity Banhatti index, Benzenoid system.

1. Introduction

All graphs considered in this paper are finite, connected, undirected with-out loops and multiple edges. Let $G = (V, E)$ be a connected graph with n vertices and m edges. 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 terminology and notation not given here we refer the reader to Kulli[1].

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. 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. There are numerous molecular descriptors, which are also referred to as topological indices[2-4] that have found some applications in theoretical chemistry, especially in QSPR/QSAR research. One of the best known and widely used topological index is the product-connectivity index (or Randic index, connectivity index) by Randic[5], who has shown this index to reflect molecular branching. The connectivity index of G is defined as $P(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)\, d_G(v)}}$.

Motivated by Randic's definition of the product connectivity index, the sum connectivity index was initiated by Zhou and Trinajstic[6-7], which is defined by $X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}$. For more details on degree based topological indices, see [8-10].

Recently, Kulli *et al.*,[11] introduced a closely related variant of connectivity indices of G in terms of vertex-edge incident as follows. The product connectivity (or simply, connectivity) Banhatti index of G is defined as $PB(G) = \sum_{ue} \frac{1}{\sqrt{d_G(u)\, d_G(e)}}$ and the sum connectivity Banhatti index of G is defined as $SB(G) = \sum_{ue} \frac{1}{\sqrt{d_G(u) + d_G(e)}}$, where ue means that the vertex u and edge e are incident in G.

A benzenoid system is a subset (with 1-connected interior) of a regular tiling of the plane by hexagonal tiles. To each benzenoid system we can assign a graph, taking the vertices of hexagons as the vertices, and the sides of hexagons as the edges of the graph. The resulting simple, plane and bipartite graph is called a benzenoid graph. For more details on Benzenoid System, see [12].

Now, we present some special kinds of benzenoid graphs as follows.

2. Results for Triangular Benzenoid

In this section, we consider the graph of triangular benzenoid as shown in Figure 1. We denote this graph by T_p in which p is the number of hexagons in the base graph.

Clearly, the total number of hexagons in T_p is $\frac{1}{2}\, p(p+1)$.

Figure 1. Triangular Benzenoid

Theorem 2. 1.
Let T_p be a triangular benzenoid. Then

$$(i)\quad PB(T_p) = \frac{\sqrt{3}}{2}\, p^2 + \left(2 + \sqrt{6} - \frac{\sqrt{3}}{2}\right) p + (4 - \sqrt{6}).$$

$$(ii)\quad SB(T_p) = \frac{3}{\sqrt{7}} p^2 + \left(\sqrt{6} + \frac{6}{\sqrt{5}} - \frac{3}{\sqrt{7}}\right) p + \left(6 - \sqrt{6} - \frac{6}{\sqrt{5}}\right).$$

Proof. Let T_p be a triangular benzenoid. By algebraic method, we obtain

$|V(T_p)| = p^2 + 4p + 1$ and

$|E(T_p)| = \frac{3}{2} p(p+3)$.

We obtain three partitions of the edge set of T_p as follows.

$E_4 = E_4^* = \{ e = uv \in E(T_p) : d_{T_p}(u) = d_{T_p}(v) = 2 \}$; $|E_4| = |E_4^*| = 6$

$E_5 = E_6^* = \{ e = uv \in E(T_p) : d_{T_p}(u) = 3, d_{T_p}(v) = 2 \}$; $|E_5| = |E_6^*| = 6(p-1)$, and

$E_6 = E_9^* = \{ e = uv \in E(T_p) : d_{T_p}(u) = d_{T_p}(v) = 3 \}$; $|E_6| = |E_9^*| = \frac{3}{2}\, p(p-1)$.

Let $G = T_p$ be a graph of triangular benzenoid. Then an edge degree partition of G is given in table-1.

Table 1. Edge degree partition of $=T_p$.

$d_G(u), d_G(v)$: $e = uv \in E(G)$	(2, 2)	(3, 2)	(3, 3)
$d_G(e)$	2	3	4
Number of edges	6	6(*p*–1)	$\frac{3}{2}p(p-1)$

(i) To compute $PB(T_p)$, we see that

$$PB(T_p) = \sum_{ue} \frac{1}{\sqrt{d_G(u)\, d_G(e)}}$$
$$= \sum_{e=uv\in E_4^*} \left[\frac{1}{\sqrt{d_G(u)\, d_G(e)}} + \frac{1}{\sqrt{d_G(v)\, d_G(e)}}\right]$$
$$+ \sum_{e=uv\in E_6^*} \left[\frac{1}{\sqrt{d_G(u)\, d_G(e)}} + \frac{1}{\sqrt{d_G(v)\, d_G(e)}}\right]$$
$$+ \sum_{e=uv\in E_9^*} \left[\frac{1}{\sqrt{d_G(u)\, d_G(e)}} + \frac{1}{\sqrt{d_G(v)\, d_G(e)}}\right]$$
$$= 6\left[\frac{1}{\sqrt{2\times 2}} + \frac{1}{\sqrt{2\times 2}}\right]$$
$$+ 6(p-1)\left[\frac{1}{\sqrt{3\times 3}} + \frac{1}{\sqrt{2\times 3}}\right]$$
$$+ \frac{3}{2}p(p-1)\left[\frac{1}{\sqrt{3\times 4}} + \frac{1}{\sqrt{3\times 4}}\right]$$
$$= \frac{\sqrt{3}}{2}p^2 + \left(2 + \sqrt{6} - \frac{\sqrt{3}}{2}\right)p + (4 - \sqrt{6}).$$

(ii) To compute $SB(T_p)$, we see that

$$SB(T_p) = \sum_{ue} \frac{1}{\sqrt{d_G(u) + d_G(e)}}$$
$$= \sum_{e=uv\in E_4} \left[\frac{1}{\sqrt{d_G(u) + d_G(e)}} + \frac{1}{\sqrt{d_G(v) + d_G(e)}}\right]$$
$$+ \sum_{e=uv\in E_5} \left[\frac{1}{\sqrt{d_G(u) + d_G(e)}} + \frac{1}{\sqrt{d_G(v) + d_G(e)}}\right]$$
$$+ \sum_{e=uv\in E_6} \left[\frac{1}{\sqrt{d_G(u) + d_G(e)}} + \frac{1}{\sqrt{d_G(v) + d_G(e)}}\right]$$
$$= 6\left[\frac{1}{\sqrt{2+2}} + \frac{1}{\sqrt{2+2}}\right]$$
$$+ 6(p-1)\left[\frac{1}{\sqrt{3+3}} + \frac{1}{\sqrt{2+3}}\right]$$
$$+ \frac{3}{2}p(p-1)\left[\frac{1}{\sqrt{3+4}} + \frac{1}{\sqrt{3+4}}\right]$$
$$= \frac{3}{\sqrt{7}}p^2 + \left(\sqrt{6} + \frac{6}{\sqrt{5}} - \frac{3}{\sqrt{7}}\right)p$$
$$+ \left(6 - \sqrt{6} - \frac{6}{\sqrt{5}}\right).$$

3. Results for Benzenoid Rhombus

In this section, we consider the graph of benzenoid rhombus as shown in Figure-2. We denote this graph by R_p which is obtained from two copies of a triangular benzenoid T_p by identifying hexagons in one of their base rows that is shown in Figure-2.

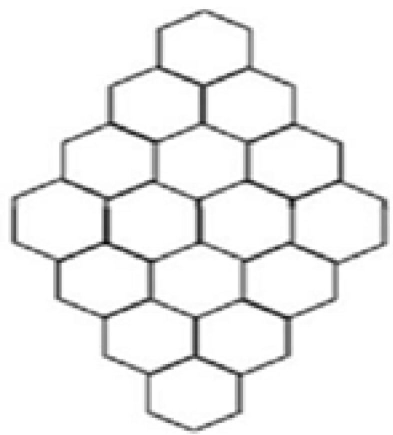

Figure-2. Benzenoid Rhombus R_4.

Theorem 3.1.

Let R_p be a benzenoid rhombus. then

$$(i)\quad PB(R_p) = \sqrt{3}\,p^2 + \left(\frac{8}{3} + \frac{8}{\sqrt{6}} - \frac{4}{\sqrt{3}}\right)p$$
$$+ \left(\frac{10}{3} - \frac{8}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right)$$

$$(ii)\ SB(R_p) = \frac{6}{\sqrt{7}}p^2 + \left(\frac{8}{\sqrt{6}} + \frac{8}{\sqrt{5}} - \frac{8}{\sqrt{7}}\right)p + \left(6 - \frac{8}{\sqrt{6}} - \frac{8}{\sqrt{5}} - \frac{2}{\sqrt{7}}\right).$$

Proof. Let R_p be a benzenoid rhombus. By algebraic method, we obtain $|V(R_p)| = 2p(p+2)$ and $|E(R_p)| = 3p^2 + 4p - 1$. We obtain three partitions of the edge set of R_p as follows.

$E_4 = E_4^* = \{e = uv \in E(R_p): d_{R_p}(u) = d_{R_p}(v) = 2\}$; $|E_4| = |E_4^*| = 6$

$E_5 = E_6^* = \{e = uv \in E(R_p): d_{R_p}(u) = 3, d_{R_p}(v) = 2\}$; $|E_5| = |E_6^*| = 8(p-1)$, and

$E_6 = E_9^* = \{e = uv \in E(R_p): d_{R_p}(u) = d_{R_p}(v) = 3\}$; $|E_6| = |E_9^*| = 3p^2 - 4p + 1$.

Let $G = R_p$ be a graph of benzenoid rhombus. Then an edge degree partition of G is given in table-2.

Table 2. Edge degree partition of $G = R_p$

$d_G(u), d_G(v)$: $e = uvE(G)$	(2, 2)	(3, 2)	(3, 3)
$d_G(e)$	2	3	4
Number of edges	6	$8(p-1)$	$3p^2 - 4p + 1$

(i) To compute $PB(R_p)$, we see that

$$PB(R_p) = \sum_{ue} \frac{1}{\sqrt{d_G(u)\, d_G(e)}}$$
$$= 6\left[\frac{1}{\sqrt{2\times2}} + \frac{1}{\sqrt{2\times2}}\right] + 8(p-1)\left[\frac{1}{\sqrt{3\times3}} + \frac{1}{\sqrt{2\times3}}\right] + (3p^2 - 4p + 1)\left[\frac{1}{\sqrt{3\times4}} + \frac{1}{\sqrt{3\times4}}\right]$$
$$= \sqrt{3}\,p^2 + \left(\frac{8}{3} + \frac{8}{\sqrt{6}} - \frac{4}{\sqrt{3}}\right)p + \left(\frac{10}{3} - \frac{8}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right).$$

(ii) To compute $SB(R_p)$, we see that

$$SB(R_p) = \sum_{ue} \frac{1}{\sqrt{d_G(u) + d_G(e)}}$$
$$= 6\left[\frac{1}{\sqrt{2+2}} + \frac{1}{\sqrt{2+2}}\right] + 8(p-1)\left[\frac{1}{\sqrt{3+3}} + \frac{1}{\sqrt{2+3}}\right] + (3p^2 - 4p + 1)\left[\frac{1}{\sqrt{3+4}} + \frac{1}{\sqrt{3+4}}\right]$$
$$= \frac{6}{\sqrt{7}}p^2 + \left(\frac{8}{\sqrt{6}} + \frac{8}{\sqrt{5}} - \frac{8}{\sqrt{7}}\right)p + \left(6 - \frac{8}{\sqrt{6}} - \frac{8}{\sqrt{5}} - \frac{2}{\sqrt{7}}\right).$$

4. Results for Benzenoid Hourglass

In this section, we consider the graph of benzenoid hourglass as shown in Figure-3. We denote this graph by X_p which is obtained from two copies of a triangular benzenoid T_p by overlapping their external hexagons.

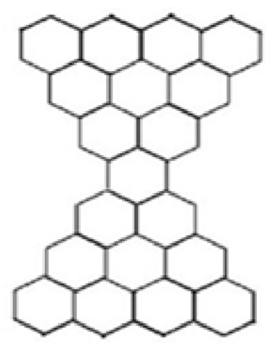

Figure-3. Benzenoid Hourglass .

Theorem 4.1.

Let X_p be a benzenoid hourglass. Then

$$(i)\ PB(X_p) = \sqrt{3}\,p^2 + (4 - \sqrt{3} + 2\sqrt{6})p + \left(\frac{8}{3} - \frac{16}{\sqrt{6}} + \frac{4}{\sqrt{3}}\right)$$

$$(ii)\ SB(X_p) = \frac{6}{\sqrt{7}}p^2 + \left(2\sqrt{6} + \frac{12}{\sqrt{5}} - \frac{6}{\sqrt{7}}\right)p + \left(8 - \frac{16}{\sqrt{6}} - \frac{16}{\sqrt{5}} + \frac{8}{\sqrt{7}}\right).$$

Proof. Let X_p be a benzenoid hourglass. By algebraic method, we obtain

$|V(X_p)| = 2(p^2 + 4p - 2)$ and

$|E(X_p)| = 3p^2 + 9p - 4$.

We also obtain three partitions of the edge set of benzenoid hourglass X_p as follows.

$E_4 = E_4^* = \{e = uv \in E(X_p): d_{X_p}(u) = d_{X_p}(v) = 2\}$; $|E_4| = |E_4^*| = 8$

$E_5 = E_6^* = \{e = uv \in E(X_p): d_{X_p}(u) = 3, d_{X_p}(v) = 2\}$; $|E_5| = |E_6^*| = 4(3p - 4)$,

and

$E_6 = E_9^* = \{e = uv \in E(X_p): d_{X_p}(u) = d_{X_p}(v) = 3\}$; $|E_6| = |E_9^*| = 3p^2 - 3p + 4$.

Let $G = X_p$ be a graph of benzenoid hourglass. Then an edge degree partition of G is given in table-3.

Table- 3. Edge degree partition of $G = X_p$.

$d_G(u), d_G(v)$: $e = uv \in E(G)$	(2, 2)	(3, 2)	(3, 3)
$d_G(e)$	2	3	4
Number of edges	8	$4(3p-4)$	$3p^2 - 3p + 4$

(i) To compute $PB(X_p)$, we see that

$$PB(X_p) = \sum_{ue} \frac{1}{\sqrt{d_G(u)\, d_G(e)}}$$
$$= 8\left[\frac{1}{\sqrt{2\times 2}} + \frac{1}{\sqrt{2\times 2}}\right]$$
$$+ \quad 4(3p-4)\left[\frac{1}{\sqrt{3\times 3}} + \frac{1}{\sqrt{2\times 3}}\right]$$
$$+ (3p^2 - 3p + 4)\left[\frac{1}{\sqrt{3\times 4}} + \frac{1}{\sqrt{3\times 4}}\right]$$
$$= \sqrt{3}\, p^2 + (4 - \sqrt{3} + 2\sqrt{6})p$$
$$+ \left(\frac{8}{3} - \frac{16}{\sqrt{6}} + \frac{4}{\sqrt{3}}\right).$$

(ii) To compute $SB(X_p)$, we see that

$$SB(X_p) = \sum_{ue} \frac{1}{\sqrt{d_G(u) + d_G(e)}}$$
$$= 8\left[\frac{1}{\sqrt{2+2}} + \frac{1}{\sqrt{2+2}}\right]$$
$$+ \ 4(3p-4)\left[\frac{1}{\sqrt{3+3}} + \frac{1}{\sqrt{2+3}}\right]$$
$$+ (3p^2 - 3p + 4)\left[\frac{1}{\sqrt{3+4}} + \frac{1}{\sqrt{3+4}}\right]$$
$$= \frac{6}{\sqrt{7}} p^2 + \left(2\sqrt{6} + \frac{12}{\sqrt{5}} - \frac{6}{\sqrt{7}}\right)p$$
$$+ \left(8 - \frac{16}{\sqrt{6}} - \frac{16}{\sqrt{5}} + \frac{8}{\sqrt{7}}\right).$$

5. Results for Benzenoid Jagged-Rectangle

In this section, we focus on the structure of a type of Benzenoid System called jagged-rectangle $B_{p,q}$ for all p, $q \in N-1$, see Figure - 4 and compute the connectivity Banhatti index and sum connectivity Banhatti index of a Benzenoid System jagged-rectangle $B_{p,q}$.

A Benzenoid jagged-rectangle forms a rectangle and the number of benzenoid (benzene or hexagon C_6) called in each chain alternate p and $p - 1$.

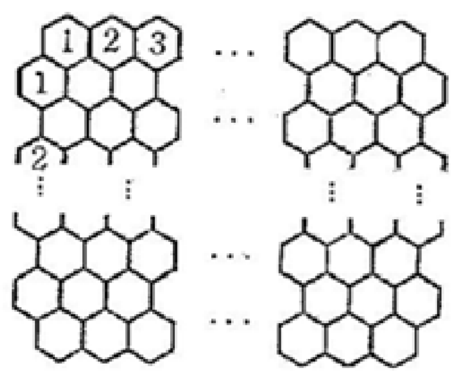

Figure- 4. Benzenoid jagged-rectangle $B_{p,q}$

Theorem 5.1.

Let $B_{p,q}$ be a benzenoid system jagged − rectangle with $p, q \in N - 1$. Then

$(i)\ PB(B_{p,q}) = 2\sqrt{3}\,pq + \left(\frac{4}{3} + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right)p + \left(\frac{10}{3} + \frac{4}{\sqrt{6}} - \frac{5}{\sqrt{3}}\right)q + \left(\frac{8}{3} - \frac{4}{\sqrt{6}} - \frac{4}{\sqrt{3}}\right)$

$(ii)\ SB(B_{p,q}) = \frac{12}{\sqrt{7}}pq + \left(\frac{4}{\sqrt{6}} + \frac{4}{\sqrt{5}} + \frac{2}{\sqrt{7}}\right)p + \left(2 + \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{5}} - \frac{10}{\sqrt{7}}\right)q + \left(4 - \frac{4}{\sqrt{6}} - \frac{4}{\sqrt{5}} - \frac{8}{\sqrt{7}}\right).$

Proof. Let $B_{p,q}$ be a benzenoid system jagged-rectangle with $p, q \in N$–1. By algebraic method, we obtain

$$|V(B_{p,q})| = 2q(2p-1) + 2(2p-1) = 4pq + 4p + 2q - 2\,.$$

From Figure -4, we see that there are two partitions of the vertex set

$V_2 = \{ v \in V(B_{p,q}) : d_{B_{p,q}}(v) = 2\}$; $|V_2| = 2p + 4q + 2$, and

$V_3 = \{ v \in V(B_{p,q}) : d_{B_{p,q}}(v) = 3\}$; $|V_3| = 4pq + 2p - 2q - 4$. Therefore

$$|E(B_{p,q})| = \frac{1}{2}[2(2p + 4q + 2) + 3(4pq + 2p - 2q - 4)] = 6pq + 5p + q - 4.$$

We also obtain three partitions of the edge set of benzenoid system jagged - rectangle $B_{p,q}$ as follows.

$E_4 = E_4^* = \{ e = uv \in E(B_{p,q}) : d_{B_{p,q}}(u) = d_{B_{p,q}}(v) = 2\}$; $|E_4| = |E_4^*| = 2q + 4$,

$E_5 = E_6^* = \{ e = uv \in E(B_{p,q}) : d_{B_{p,q}}(u) = 3,\ d_{B_{p,q}}(v) = 2\}$; $|E_5| = |E_6^*| = 4p + 4q - 4)$, and

$E_6 = E_9^* = \{ e = uv \in E(B_{p,q}) : d_{B_{p,q}}(u) = d_{B_{p,q}}(v) = 3\}$; $|E_6| = |E_9^*| = 6pq + p - 5q - 4$.

Let $B_{p,q}$ be a benzenoid system jagged-rectangle with $p, q \in N$–1. Then an edge degree partition of G is given in table-4.

Table - 4. Edge degree partition of $G = B_{p,q}$.

$d_G(u), d_G(v)$: $e = uv \in E(G)$	(2, 2)	(3, 2)	(3, 3)
$d_G(e)$	2	3	4
Number of edges	$2q + 4$	$4p$+ $4q$–4	$4pq$+q –$4q$–4

(i) To compute $PB(B_{p,q})$, we see that

$$PB(B_{p,q}) = \sum_{ue} \frac{1}{\sqrt{d_G(u)\,d_G(e)}}$$

$$= (2q+4)\left[\frac{1}{\sqrt{2\times 2}} + \frac{1}{\sqrt{2\times 2}}\right] + (4p + 4q - 4)\left[\frac{1}{\sqrt{3\times 3}} + \frac{1}{\sqrt{2\times 3}}\right] + (6pq + p - 5q - 4)\left[\frac{1}{\sqrt{3\times 4}} + \frac{1}{\sqrt{3\times 4}}\right]$$

$$= 2\sqrt{3}\,pq + \left(\frac{4}{3} + \frac{4}{\sqrt{6}} + \frac{1}{\sqrt{3}}\right)p + \left(\frac{10}{3} + \frac{4}{\sqrt{6}} - \frac{5}{\sqrt{3}}\right)q + \left(\frac{8}{3} - \frac{4}{\sqrt{6}} - \frac{4}{\sqrt{3}}\right).$$

(ii) To compute $SB(B_{p,q})$, we see that

$$SB(B_{p,q}) = \sum_{ue} \frac{1}{\sqrt{d_G(u) + d_G(e)}}$$

$$= (2q+4)\left[\frac{1}{\sqrt{2+2}} + \frac{1}{\sqrt{2+2}}\right] + (4p + 4q - 4)\left[\frac{1}{\sqrt{3+3}} + \frac{1}{\sqrt{2+3}}\right] + (6pq + p - 5q - 4)\left[\frac{1}{\sqrt{3+4}} + \frac{1}{\sqrt{3+4}}\right]$$

$$= \frac{12}{\sqrt{7}}pq + \left(\frac{4}{\sqrt{6}} + \frac{4}{\sqrt{5}} + \frac{2}{\sqrt{7}}\right)p + \left(2 + \frac{4}{\sqrt{6}} + \frac{4}{\sqrt{5}} - \frac{10}{\sqrt{7}}\right)q + \left(4 - \frac{4}{\sqrt{6}} - \frac{4}{\sqrt{5}} - \frac{8}{\sqrt{7}}\right).$$

6. Conclusion

Chemical graph theory is an important tool for studying molecular structures and has an important effect on the development of chemical sciences. The study of topological indices is currently one of the most active research fields in chemical graph theory. We have established in this paper some theoretical results on "Connectivity Banhatti indices for certain families of Benzenoid Systems". These formulae make it possible to correlate the chemical structure of nanostructures with a large amount of information about their physical features.

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