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ABC Banhatti and Augmented Banhatti Indices of Chemical Networks

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ABSTRACT

Chemical Graph Theory is a branch of Mathematical Chemistry whose focus of interest is to finding topological indices of molecular graphs which correlate well with chemical properties of the chemical molecules. In this paper, we introduce the atom bond connectivity Banhatti index and augmented Banhatti index of a molecular graph. Furthermore, we compute these indices of different chemically interesting networks like carbon nanocone networks, armchair polyhex nanotube networks, zigzag polyhex nanotube networks.

Mathematics Subject Classification: 05C05, 05C07, 05C12, 05C35

Keywords: ABC Banhatti index, augmented Banhatti index, chemical networks.

1. INTRODUCTION

A molecular graph is a graph in which the vertices correspond to the atom and the edges to the bonds of a molecule. Chemical Graph Theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. There are several topological indices that have some applications in Theoretical Chemistry, see[1].

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting the vertices u and v will be denoted by uv. Let $d_G(e)$ denote the degree of an edge $e = uv$ in G is defined by $d_G(e) = d_G(u) + d_G(v) – 2$. We refer to [1] for undefined term and notation.

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

$$B_1(G)=\sum_{ue}\left[d_G(u)+d_G(e)\right], \quad B_2(G)=\sum_{ue} r_G(u) r_G(e).$$

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

We introduce the atom bond connectivity Banhatti index and augmented Banhatti index of a molecular graph as follows:

The atom bond connectivity Banhatti index of a graph *G* is defined as

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

$$= \sum_{uv \in E(G)} \left(\sqrt{\frac{d_G(u) + d_G(e) - 2}{d_G(u)d_G(e)}} + \sum_{uv \in E(G)} \sqrt{\frac{d_G(v) + d_G(e) - 2}{d_G(v)d_G(e)}} \right) \quad (1)$$

The augmented Banhatti index of a graph *G* is defined as

$$ABI(G) = \sum_{ue} \left(\frac{d_G(u)d_G(e)}{d_G(u) + d_G(e) - 2} \right)^3$$

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

Recently, many *K* Banhatti indices were studied, for example, in[4, 5, 6, 7, 8, 9, 10, 11] and also some new topological indices were studied, for example, in[12, 13, 14,15, 16, 17, 18, 19].

In this paper, the atom bond connectivity Banhatti and augmented Banhatti indices of chemical networks are computed. For more information about chemical networks see[20].

2. RESULTS FOR CARBON NANOCONE NETWORKS

An n-dimensional one-pentagonal nanocone is symbolized by $CNC_5[n]$, where *n* is the number of hexagons layers encompassing the conical surface of the nanocone and 5 denotes that there is a pentagon on the tip called its core. A 6-dimensional one-pentagonal nanocone network is presented in Figure 1.

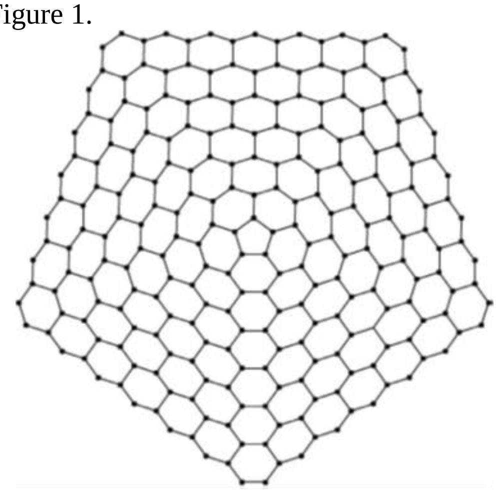

Figure 1. A 6-dimensional one-pentagonal nanocone network

Let G be the n-dimensional one-pentagoanl nanocone $CNC_5[n]$, $n\geq 2$. Then $|V(G)|=5(n+1)^2$ and $|E(G)| = \frac{15}{2}n^2 + \frac{25}{2}n + 5$.

In G, there are three types of edges based on degrees of end vertices of each edge. By calculation, the edge degree partition of G is given in Table 1.

Table 1. Edge degree partition of $G = CNC_5[n]$

$d_G(u)\, d_G(v) \backslash uv \in E(G)$	(2,2)	(2, 3)	(3, 3)
$d_G(e)$	2	3	4
Number of edges	5	$10n$	$\frac{15}{2}n^2 + \frac{5}{2}n$

In the following theorems, we compute the ABC Banhatti index and augmented Banhatti index of $CNC_5[n]$.

Theorem 1. The atom bond connectivity Banhatti index of n-dimensional one pentagonal nanocone $CNC_5[n]$, $n\geq 2$, is

$$ABCB(G) = 15\sqrt{\frac{5}{12}}n^2 + \left(\frac{1}{\sqrt{2}} + \frac{2}{3} + 5\sqrt{\frac{5}{12}}\right)n + \frac{10}{\sqrt{2}}.$$

Proof: Using equation (1) and Table 1, we deduce

$$ABCB(G) = \sum_{uv\in E(G)}\left[\sqrt{\frac{d_G(u)+d_G(e)-2}{d_G(u)d_G(e)}} + \sqrt{\frac{d_G(v)+d_G(e)-2}{d_G(v)d_G(e)}}\right].$$

$$= \left(\sqrt{\frac{2+2-2}{2\times 2}} + \sqrt{\frac{2+2-2}{2\times 2}}\right)5 + \left(\sqrt{\frac{2+3-2}{2\times 3}} + \sqrt{\frac{3+3-2}{3\times 3}}\right)10n + \left(\sqrt{\frac{3+4-2}{3\times 4}} + \sqrt{\frac{3+4-2}{3\times 4}}\right)\left(\frac{15}{2}n^2 + \frac{5}{2}n\right)$$

$$= 15\sqrt{\frac{5}{12}}n^2 + \left(\frac{1}{\sqrt{2}} + \frac{2}{3} + 5\sqrt{\frac{5}{12}}\right)10n + \frac{10}{\sqrt{2}}.$$

Theorem 2. The augmented Banhatti index of n-dimensional one-pentagonal nanocone $CNC_5[n]$, $n\geq 2$, is

$$ABI(G) = \frac{5184}{25}n^2 + \frac{5728}{25}n + 160.$$

Proof: Using equation (2) and Table 1, we obtain

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

$$= \left[\left(\frac{2\times 2}{2+2-2}\right)^3 + \left(\frac{2\times 2}{2+2-2}\right)^3\right]5 + \left[\left(\frac{2\times 3}{2+3-2}\right)^3 + \left(\frac{3\times 3}{3+3-2}\right)^3\right]10n$$

$$+\left[\left(\frac{3\times 4}{3+4-2}\right)^3+\left(\frac{3\times 4}{3+4-2}\right)^3\right]\left(\frac{15}{2}n^2+\frac{5}{2}n\right)$$
$$=\frac{5184}{25}n^2+\frac{5728}{25}n+160.$$

3. RESULTS FOR ARMCHAIR POLYHEX NANOTUBES

Carbon polyhex nanotubes are the nanotubes whose cylindrical surface is made up of entirely hexagons. These carbon nanotubes exist in nature with remarkable stability and possess very interesting electrical, thermal and mechanical properties [ ]. The armchair polyhex nanotube is symbolized by $TUAC_6[p, q]$, where p is the number of hexagons in a row whereas q is number of hexagons in a column. A 2-dimensional networks of $TUAC_6[p, q]$ is presented in Figure 2.

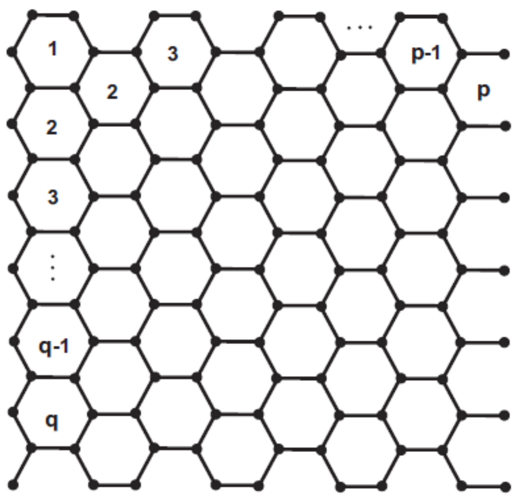

Figure 2. A 2-dimensional networks of $TUAC_6[p, q]$.

Let G be the graph of (p, q) dimensional armchair polyhex nanotube. Then G has $2p(q+1)$ vertices and $3pq+2p$ edges. In G, there are three types of edges based on degrees of end vertices of each edge. By calculation, the edge degree partition of G is given in Table 2.

Table 2. Edge degree partition of $G = TUAC_6[p, q]$

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

In the following theorems, we derive the ABC Banhatti index and augmented Banhatti index of $TUAC_6[p, q]$.

Theorem 3. The atom bond connectivity Banhatti index of a (p, q)-dimensional armchair nanotube $TUAC_6[p, q]$ is

$$ABCB(G) = \sqrt{15}\,pq + \left(\sqrt{2} + \frac{2}{3} - \sqrt{\frac{5}{12}}\right)2p.$$

Proof: Using equation (1) and Table 2, we deduce

$$ABCB(G) = \sum_{uv \in E(G)} \left[\sqrt{\frac{d_G(u)+d_G(e)-2}{d_G(u)d_G(e)}} + \sqrt{\frac{d_G(v)+d_G(e)-2}{d_G(v)d_G(e)}}\right].$$

$$= \left(\sqrt{\frac{2+2-2}{2\times 2}} + \sqrt{\frac{2+2-2}{2\times 2}}\right)p + \left(\sqrt{\frac{2+3-2}{2\times 3}} + \sqrt{\frac{3+3-2}{3\times 3}}\right)2p + \left(\sqrt{\frac{3+4-2}{3\times 4}} + \sqrt{\frac{3+4-2}{3\times 4}}\right)(3pq-p)$$

$$= \sqrt{15}\,pq + \left(\sqrt{2} + \frac{2}{3} - \sqrt{\frac{5}{12}}\right)2p.$$

Theorem 4. The augmented Banhatti index of a (p, q)-dimensional armchair polyhex nanotube $TUAC_5[p, q]$ is

$$ABI(G) = \frac{10368}{125}pq + \frac{2544}{125}p.$$

Proof: Using equation (2) and Table 2, we deduce

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

$$= \left[\left(\frac{2\times 2}{2+2-2}\right)^3 + \left(\frac{2\times 2}{2+2-2}\right)^3\right]p + \left[\left(\frac{2\times 3}{2+3-2}\right)^3 + \left(\frac{3\times 3}{3+3-2}\right)^3\right]2p$$

$$+ \left[\left(\frac{3\times 4}{3+4-2}\right)^3 + \left(\frac{3\times 4}{3+4-2}\right)^3\right](3pq-p)$$

$$= \frac{10368}{125}pq + \frac{2544}{125}p.$$

4. RESULTS FOR ZIGZAG POLYHEX NANOTUBES

The zigzag polyhex nanotube $TUZC_6[p, q]$, where p is the number of hexagons in a row whereas q is number of hexagons in a column. A 2-dimensional networks of $TUZC_6[p, q]$ is shown in Figure 3.

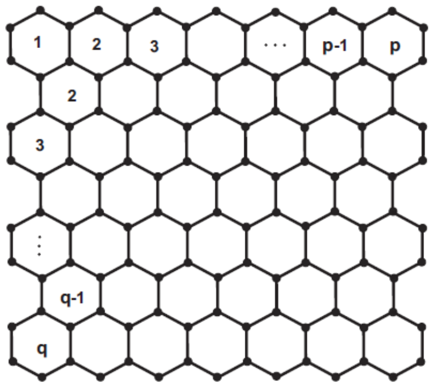

Figure 3. A 2-dimensional networks of $TUZC_6[p, q]$

Let G be the graph of a (p, q) dimensional zigzag polyhex nanotube. Then G has $2p(q+1)$ vertices and $3pq+2p$ edges. In G, there are three types of edges based on degrees of end vertices of each edge. By calculation, the edge degree partition of G is given in Table 3.

Table 3. Edge degree partition of $G = TUZC_6[p, q]$

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

In the following theorems, we compute the ABC Banhatti index and augmented Banhatti index of $TUZC_6[p, q]$.

Theorem 5. The atom bond connectivity Banhatti index of a (p, q)-dimensional zigzag polyhex nanotube $TUZC_6[p, q]$ is

$$ABCB(G) = \sqrt{15}\,pq + \left(4\sqrt{2} - 2\sqrt{\frac{5}{3}}\right)p.$$

Proof: Using equation (1) and Table 3, we deduce

$$ABCB(G) = \sum_{uv \in E(G)} \left[\sqrt{\frac{d_G(u)+d_G(e)-2}{d_G(u)d_G(e)}} + \sqrt{\frac{d_G(v)+d_G(e)-2}{d_G(v)d_G(e)}} \right].$$

$$= \left(\sqrt{\frac{2+3-2}{2\times 3}} + \sqrt{\frac{3+3-2}{3\times 3}} \right) 4p + \left(\sqrt{\frac{3+4-2}{3\times 4}} + \sqrt{\frac{3+4-2}{3\times 4}} \right) (3pq - 2p)$$

$$= \sqrt{15}\,pq + \left(4\sqrt{2} - 2\sqrt{\frac{5}{3}}\right)p.$$

Theorem 6. The augmented Banhatti index of a (*p, q*)-dimensional zigzag polyhex nanotube $TUZC_6[p, q]$ is

$$ABI(G) = \frac{10368}{125} pq + \frac{1088}{125} p.$$

Proof: Using equation (2) and Table 3, we deduce

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

$$= \left[\left(\frac{2 \times 3}{2+3-2} \right)^3 + \left(\frac{3 \times 3}{3+3-2} \right)^3 \right] 4p + \left[\left(\frac{3 \times 4}{3+4-2} \right)^3 + \left(\frac{3 \times 4}{3+4-2} \right)^3 \right] (3pq - 2p)$$

$$= \frac{10368}{125} pq + \frac{1088}{125} p.$$

REFERENCES

1. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry,* Springer, Berlin (1986).
2. V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
3. V.R. Kulli, On K Banhatti indices of graphs, *Journal of Computer and Mathematical Sciences*, 7(2016) 213-218.
4. V.R.Kulli, On *K* Banhatti indices and *K* hyper-Banhatti indices of *V*-Phenylenic nanotubes and nanotorus, *Journal of Computer and Mathematical Sciences,* 7(6), 302-307 (2016).
5. V.R. Kulli, Computing Banhatti indices of networks, *International Journal of Advances in Mathematics*, 2018(1) (2018) 31-40.
6. V.R.Kulli, Multiplicative connectivity Banhatti indices of benzenoid systems and polycyclic aromatic hydrocarbons, *Journal of Computer and Mathematical Sciences*, 9(3): 212-220, (2018).
7. V.R. Kulli, Multiplicative connectivity Banhatti indices of dendrimer nanostars, *Journal of Chemistry and Chemical Sciences*, 8(6), 964-973 (2018).
8. V.R. Kulli, A new Banhatti geometric-arithmetic index, *International Journal of Mathmatical Archive,* 8(4), 112-115 (2017).
9. V.R. Kulli, Direct and inverse sum Banhatti indices, *International Research Journal of Pure Algebra* 7(9), 823-827 (2017).
10. V.R.Kulli, B.Chaluvaraju and H.S. Baregowda, *K*-Banhatti and *K* hyper-Banhatti indices of windmill graphs, *South East Asian J. of Math. and Math. Sci*, 13(1), 11-18 (2017).
11. V.R.Kulli, B.Chaluvaraju and H.S.Boregowda, The product connectivity Banhatti index of a graph, *Discussiones Mathematicae, Graph Theory*, (2018).
12. V.R.Kulli, On K indices of graphs, *International Journal of Fuzzy Mathematical Archive*, 10(2), 105-109 (2016).

13. V.R.Kulli, On *K* coindices of graphs, *Journal of Computer and Mathematical Sciences*, 7(3), 107-112 (2016).
14. V.R.Kulli, On *K* edge index of some nanostructures, *Journal of Computer and Mathematical Sciences*, 10(2), 111-116 (2016).
15. V.R. Kulli, On *K* edge index of some nanostructures, *Journal of Computer and Mathematical Sciences*, 7(7), 373-378 (2016).
16. V.R.Kulli, Computation of some Gourava indices of titania nanotubes, *International Journal of Fuzzy Mathematical Archive*, 12(2), 75-81 (2017).
17. V.R. Kulli, Some Gourava indices and inverse sum indeg index of certain networks, *International Research Journal of Pure Algebra*, 7(7), 787-798 (2017).
18. V.R.Kulli, Revan indices and their polynomials of certain rhombus networks, *International Journal of Current Research in Life Sciences*, 7(5), 2110-2116 (2018).
19. V.R.Kulli, Some new fifth multiplicative Zagreb indices of PAMAM dendrimers, *Journal of Global Research in Mathematics*, 5(2), 82-86 (2018).
20. S. Hayat, S. Wang and J.B. Liu, Valency-based topological descriptors of chemical networks, *Applied Mathematical Modelling*, 60, 164-178 (2018).