

## **K BANHATTI AND K HYPER BANHATTI INDICES OF THE LINE GRAPHS OF H-PANTACENIC NANOTUBES**

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**ABSTRACT.** Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. The aim of this report is to compute the first and second K Banhatti indices of the Line Graphs of H-Pantacenic Nanotubes. We also compute the first and second K hyper Banhatti indices of the Line Graphs of H-Pantacenic Nanotubes.

*Key words :* K Banhatti index, K- hyper Banhatti index, line graph, phenylenes, H-Pantacenic nanotube

*AMS SUBJECT :* 05C12, 05C90.

### 1. INTRODUCTION

Chemical graph theory is a branch of graph theory in which a chemical compound is represented by simple graph called molecular graph in which vertices are atoms of compound and edges are the atomic bounds. A graph is connected if there is atleast one connection between its vertices. Throughout this paper we take  $G$  a connected graph. If a graph does not contain any loop or multiple edges then it is called a network. Between two vertices  $u$  and  $v$ , the distance is the shortest path between them and is denoted by  $d(u, v)$  in graph  $G$ . For

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a vertex  $v$  of  $G$  the "degree"  $d_v$  is number of vertices attached with it. The edge connecting the vertices  $u$  and  $v$  will be denoted by  $uv$ . 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  $e = uv$ . The degree and valence in chemistry are closely related with each other. We refer the book [1] for more details. Another emerging field is Cheminformatics, which helps to predict biological activities with the relationship of Structure-property and quantitative structure-activity. Topological indices and Physico-chemical properties are used in prediction of bioactivity if underlined compounds are used in these studies [2,3].

A number that describe the topology of a graph is called topological index. In 1947, the first and most studied topological index was introduced by Wiener [4]. For more details about this index can be found in [5,6]. In 1975, Milan Randić introduced the Randić index [7].

Bollobas et al. [8] and Amic et al. [9] in 1998, working independently defined the generalized Randić index. This index was studied by both mathematicians and chemists [10]. For details about topological indices, we refer [11,12]. The first and second K-Banhatti indices of  $G$  are defined as

$$B_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(e)],$$

and

$$B_2(G) = \sum_{uv \in E(G)} [d_G(u) \cdot d_G(e)],$$

respectively, where  $ue$  means that the vertex  $u$  and edge  $e$  are incident in  $G$ . The first and second K-hyper Banhatti indices of  $G$  are defined as

$$HB_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(e)]^2,$$

and

$$HB_2(G) = \sum_{uv \in E(G)} [d_G(u) \cdot d_G(e)]^2.$$

We refer [13] for details about these indices. The first and second multiplicative K Banhatti indices are defined as [14]

$$BII_1(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(e)],$$

and

$$BII_2(G) = \prod_{uv \in E(G)} [d_G(u) \cdot d_G(e)].$$

The first and second multiplicative K hyper Banhatti indices are defined as [14]

$$HBII_1(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(e)]^2,$$

and

$$HBII_2(G) = \prod_{uv \in E(G)} [d_G(u) \cdot d_G(e)]^2.$$

The line graph  $L(G)$  of a graph  $G$  is the graph each of whose vertices, represents an edge of  $G$  and two of its vertices are adjacent if their corresponding edges are adjacent in  $G$ .

**Lemma 1.** *Let  $G$  be a graph of order  $p$  and size  $q$ . Then the line graph  $L(G)$  of  $G$  is a graph of order  $p$  and size  $\frac{1}{2}M_1(G) - q$ .*

In this report we compute Banhatti indices of line graph of H-Pentacenic nanotube. The graph of H-Pentacenic nanotube is given in Figure 1 and the line graph of H-Pentacenic nanotube is given in Figure 2.

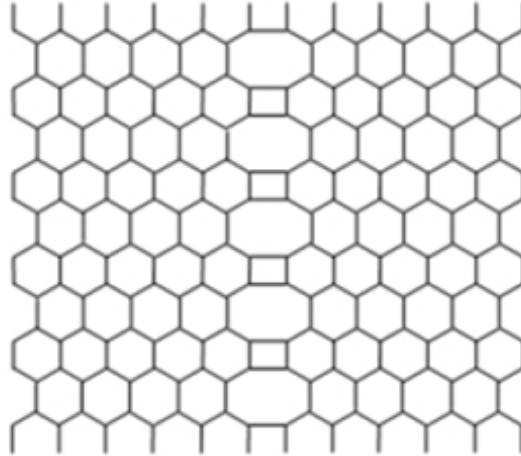


Figure 1. The H-Pentacenic nanotube  $K[p, q]$ .

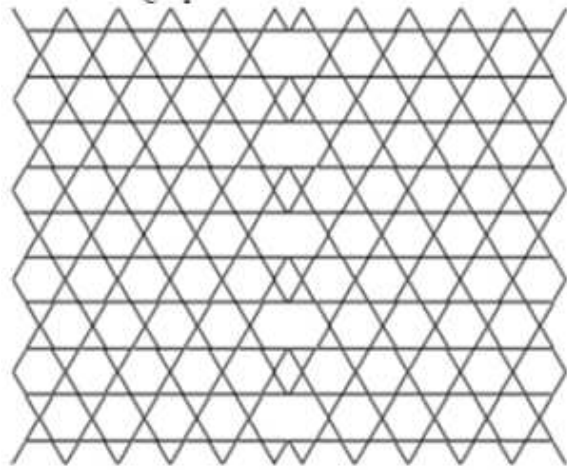


Figure 2. The line graph of H-Pantacenic nanotube  $K[p, q]$ .

## 2. COMPUTATIONAL RESULTS

In this section we will give our main results.

**2.1. Banhatti Indices.** In this section, we compute first and second K Banhatti indices and K hyper Banhatti indices of the line graph of H-Pantacenic nanotube.

**Theorem 2.** *Let  $G = L(K[p, q])$  be a line graph of H-Pantacenic nanotube. Then*

- (1)  $B_1(G) = 1320pq - 20q,$
- (2)  $B_2(G) = 1500q + 3168pq.$

*Proof.* The line graph of H-Pantacenic Nanotubes is shown in figure 2. It can be observed from the Figure 2 and Lemma 1 that

$$V(G) = 33pq - 2q,$$

$$E(G) = 66pq - 8q.$$

We can divide the edge set of the line graph of H-Pantacenic Nanotube into following three classes depending on the degree of end vertices of each edge:

$$E_{\{2,3\}}(G) = \{e = uv \in E(G) : d_u = 2, d_v = 3\},$$

$$E_{\{3,4\}}(G) = \{e = uv \in E(G) : d_u = 3, d_v = 4\},$$

and

$$E_{\{4,4\}}(G) = \{e = uv \in E(G) : d_u = 4, d_v = 4\}.$$

Now

$$|E_{\{2,3\}}| = 4q,$$

$$|E_{\{3,4\}}| = 8q,$$

$$|E_{\{4,4\}}| = 66pq - 20q.$$

<b>Table 1:</b>		
$(d_G(u), d_G(v)) = e \in E(G)$	$d_G(e)$	Number of edges
(2,3)	3	$4q$
(3,4)	5	$8q$
(4,4)	6	$66pq - 20q$

(1) 1. From the definition of first K Banhatti index, we have

$$\begin{aligned}
B_1(G) &= \sum_{uv \in E(G)} [d_G(u) + d_G(e)] \\
&= \sum_{uv \in E_{\{2,3\}}(G)} [d_G(u) + d_G(e)] + \sum_{uv \in E_{\{3,4\}}(G)} [d_G(u) + d_G(e)] \\
&\quad + \sum_{uv \in E_{\{4,4\}}(G)} [d_G(u) + d_G(e)] \\
&= \sum_{uv \in E_{\{2,3\}}(G)} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] \\
&\quad + \sum_{uv \in E_{\{3,4\}}(G)} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] \\
&\quad + \sum_{uv \in E_{\{4,4\}}(G)} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] \\
&= 4q[(2 + 3) + (3 + 3)] + 8q[(3 + 5) + (4 + 5)] \\
&\quad + (66pq - 20q)[(4 + 6) + (4 + 6)] \\
&= 1320pq - 20q.
\end{aligned}$$

(2) From the definition of second K Banhatti index, we have

$$\begin{aligned}
 B_2(G) &= \sum_{uv \in E(G)} [d_G(u) \cdot d_G(e)] \\
 &= \sum_{uv \in E_{\{2,3\}}(G)} [d_G(u) \cdot d_G(e)] + \sum_{uv \in E_{\{3,4\}}(G)} [d_G(u) \cdot d_G(e)] \\
 &\quad + \sum_{uv \in E_{\{4,4\}}(G)} [d_G(u) \cdot d_G(e)] \\
 &= \sum_{uv \in E_{\{2,3\}}(G)} [(d_G(u) \cdot d_G(e)) + (d_G(v) \cdot d_G(e))] \\
 &\quad + \sum_{uv \in E_{\{3,4\}}(G)} [(d_G(u) \cdot d_G(e)) + (d_G(v) \cdot d_G(e))] \\
 &\quad + \sum_{uv \in E_{\{4,4\}}(G)} [(d_G(u) \cdot d_G(e)) + (d_G(v) \cdot d_G(e))] \\
 &= 4q[(2 \cdot 3) + (3 \cdot 3)] + 8q[(3 \cdot 5) + (4 \cdot 5)] \\
 &\quad + (66pq - 20q)[(4 \cdot 6) + (4 \cdot 6)] \\
 &= 1500q + 3168pq.
 \end{aligned}$$

□

**Theorem 3.** Let  $G = L(K[p, q])$  be a line graph of H-Pantacenic nanotube. Then

- (1)  $HB_1(G) = 13200pq - 2596q,$
- (2)  $HB_2(G) = 76032pq - 21939q.$

*Proof.* Using the Table 1 given in theorem 2, we have

(1) 1. From the definition of first K hyper Bhanhatti index, we have

$$\begin{aligned}
HB_1(G) &= \sum_{uv \in E(G)} [d_G(u) + d_G(e)]^2 \\
&= \sum_{uv \in E_{\{2,3\}}(G)} [d_G(u) + d_G(e)]^2 + \sum_{uv \in E_{\{3,4\}}(G)} [d_G(u) + d_G(e)]^2 \\
&\quad + \sum_{uv \in E_{\{4,4\}}(G)} [d_G(u) + d_G(e)]^2 \\
&= \sum_{uv \in E_{\{2,3\}}(G)} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] \\
&\quad + \sum_{uv \in E_{\{3,4\}}(G)} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] \\
&\quad + \sum_{uv \in E_{\{4,4\}}(G)} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] \\
&= 4q[(2 + 3)^2 + (3 + 3)^2] + 8q[(3 + 5)^2 + (4 + 5)^2] \\
&\quad + (66pq - 20q)[(4 + 6)^2 + (4 + 6)^2] \\
&= 13200pq - 2596q.
\end{aligned}$$

(2) From the definition of second K hyper Bhanhatti index, we have

$$\begin{aligned}
HB_2(G) &= \sum_{uv \in E(G)} [d_G(u) \cdot d_G(e)]^2 \\
&= \sum_{uv \in E_{\{2,3\}}(G)} [d_G(u) \cdot d_G(e)]^2 + \sum_{uv \in E_{\{3,4\}}(G)} [d_G(u) \cdot d_G(e)]^2 \\
&\quad + \sum_{uv \in E_{\{4,4\}}(G)} [d_G(u) \cdot d_G(e)]^2 \\
&= \sum_{uv \in E_{\{2,3\}}(G)} [(d_G(u) \cdot d_G(e))^2 + (d_G(v) \cdot d_G(e))^2] \\
&\quad + \sum_{uv \in E_{\{3,4\}}(G)} [(d_G(u) \cdot d_G(e))^2 + (d_G(v) \cdot d_G(e))^2] \\
&\quad + \sum_{uv \in E_{\{4,4\}}(G)} [(d_G(u) \cdot d_G(e))^2 + (d_G(v) \cdot d_G(e))^2] \\
&= 4q[(2 \cdot 3)^2 + (3 \cdot 3)^2] + 8q[(3 \cdot 5)^2 + (4 \cdot 5)^2] \\
&\quad + (66pq - 20q)[(4 \cdot 6)^2 + (4 \cdot 6)^2] \\
&= 76032pq - 21939q.
\end{aligned}$$

□

**2.2. Multiplicative Banahatti Indices.** In this section, we compute multiplicative versions of first and second K Banahatti indices and K hyper Banahatti indices of the line graph of H-Pantacenic nanotube.

**Theorem 4.** *Let  $G = L(K[p, q])$  be a line graph of H-Pantacenic nanotube. Then*

$$(1) \ BII_1(G) = 5^{4q} \cdot 6^{4q} \cdot 8^{8q} \cdot 9^{8q} \cdot 10^{2q(66p-20)},$$

$$(2) \ BII_2(G) = 6^{4q} \cdot 9^{4q} \cdot 15^{8q} \cdot 20^{8q} \cdot 24^{2q(66p-20)}.$$

*Proof.* Using the Table 1 given in theorem 2, we have

(1) From the definition of first multiplicative K Banahatti index

$$\begin{aligned} BII_1(G) &= \prod_{uv \in E(G)} [d_G(u) + d_G(e)] \\ &= \prod_{uv \in E_{\{2,3\}}(G)} [d_G(u) + d_G(e)] \cdot \prod_{uv \in E_{\{3,4\}}(G)} [d_G(u) + d_G(e)] \\ &\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [d_G(u) + d_G(e)] \\ &= \prod_{uv \in E_{\{2,3\}}(G)} [(d_G(u) + d_G(e)) \cdot (d_G(v) + d_G(e))] \\ &\quad \cdot \prod_{uv \in E_{\{3,4\}}(G)} [(d_G(u) + d_G(e)) \cdot (d_G(v) + d_G(e))] \\ &\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [(d_G(u) + d_G(e)) \cdot (d_G(v) + d_G(e))] \\ &= [(2 + 3) \cdot (3 + 3)]^{4q} \cdot [(3 + 5) \cdot (4 + 5)]^{8q} \\ &\quad \cdot [(4 + 6) \cdot (4 + 6)]^{(66pq-20q)} \\ &= 5^{4q} \cdot 6^{4q} \cdot 8^{8q} \cdot 9^{8q} \cdot 10^{2q(66p-20)}. \end{aligned}$$



(2) From the definition of second multiplicative K Banahatti index

$$\begin{aligned}
BII_2(G) &= \prod_{uv \in E(G)} [d_G(u) \cdot d_G(e)] \\
&= \prod_{uv \in E_{\{2,3\}}(G)} [d_G(u) \cdot d_G(e)] \cdot \prod_{uv \in E_{\{3,4\}}(G)} [d_G(u) \cdot d_G(e)] \\
&\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [d_G(u) \cdot d_G(e)] \\
&= \prod_{uv \in E_{\{2,3\}}(G)} [(d_G(u) \cdot d_G(e)) \cdot (d_G(v) \cdot d_G(e))] \\
&\quad \cdot \prod_{uv \in E_{\{3,4\}}(G)} [(d_G(u) \cdot d_G(e)) \cdot (d_G(v) \cdot d_G(e))] \\
&\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [(d_G(u) \cdot d_G(e)) \cdot (d_G(v) \cdot d_G(e))] \\
&= [(2 \cdot 3) \cdot (3 \cdot 3)]^{4q} \cdot [(3 \cdot 5) \cdot (4 \cdot 5)]^{8q} \\
&\quad \cdot [(4 \cdot 6) \cdot (4 \cdot 6)]^{(66pq-20q)} \\
&= 6^{4q} \cdot 9^{4q} \cdot 15^{8q} \cdot 20^{8q} \cdot 24^{2q(66p-20)}.
\end{aligned}$$

□

**Theorem 5.** Let  $G = L(K[p, q])$  be a line graph of  $H$ -Pantacenic nanotube. Then

$$\begin{aligned}
(1) \quad HBII_1(G) &= 5^{8q} \cdot 6^{8q} \cdot 8^{16q} \cdot 9^{16q} \cdot 10^{4q(66p-20)}, \\
(2) \quad HBII_2(G) &= 6^{8q} \cdot 9^{8q} \cdot 15^{16q} \cdot 20^{16q} \cdot 24^{4q(66p-20)}.
\end{aligned}$$

*Proof.* Using the Table 1 given in theorem 2, we have

(1)

$$\begin{aligned}
HBII_1(G) &= \prod_{uv \in E(G)} [d_G(u) + d_G(e)]^2 \\
&= \prod_{uv \in E_{\{2,3\}}(G)} [d_G(u) + d_G(e)]^2 \cdot \prod_{uv \in E_{\{3,4\}}(G)} [d_G(u) + d_G(e)]^2 \\
&\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [d_G(u) + d_G(e)]^2 \\
&= \prod_{uv \in E_{\{2,3\}}(G)} [(d_G(u) + d_G(e))^2 \cdot (d_G(v) + d_G(e))^2] \\
&\quad \cdot \prod_{uv \in E_{\{3,4\}}(G)} [(d_G(u) + d_G(e))^2 \cdot (d_G(v) + d_G(e))^2] \\
&\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [(d_G(u) + d_G(e))^2 \cdot (d_G(v) + d_G(e))^2] \\
&= [(2+3)^2 \cdot (3+3)^2]^{4q} \cdot [(3+5)^2 \cdot (4+5)^2]^{8q} \\
&\quad \cdot [(4+6)^2 \cdot (4+6)^2]^{(66pq-20q)} \\
&= 5^{8q} \cdot 6^{8q} \cdot 8^{16q} \cdot 9^{16q} \cdot 10^{4q(66p-20)}.
\end{aligned}$$

(2)

$$\begin{aligned}
HBII_2(G) &= \prod_{uv \in E(G)} [d_G(u) \cdot d_G(e)]^2 \\
&= \prod_{uv \in E_{\{2,3\}}(G)} [d_G(u) \cdot d_G(e)]^2 \cdot \prod_{uv \in E_{\{3,4\}}(G)} [d_G(u) \cdot d_G(e)]^2 \\
&\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [d_G(u) \cdot d_G(e)]^2 \\
&= \prod_{uv \in E_{\{2,3\}}(G)} [(d_G(u) \cdot d_G(e))^2 \cdot (d_G(v) \cdot d_G(e))^2] \\
&\quad \cdot \prod_{uv \in E_{\{3,4\}}(G)} [(d_G(u) \cdot d_G(e))^2 \cdot (d_G(v) \cdot d_G(e))^2] \\
&\quad \cdot \prod_{uv \in E_{\{4,4\}}(G)} [(d_G(u) \cdot d_G(e))^2 \cdot (d_G(v) \cdot d_G(e))^2] \\
&= [(2 \cdot 3)^2 \cdot (3 \cdot 3)^2]^{4q} \cdot [(3 \cdot 5)^2 \cdot (4 \cdot 5)^2]^{8q} \\
&\quad \cdot [(4 \cdot 6)^2 \cdot (4 \cdot 6)^2]^{(66pq-20q)} \\
&= 6^{8q} \cdot 9^{8q} \cdot 15^{16q} \cdot 20^{16q} \cdot 24^{4q(66p-20)}.
\end{aligned}$$

□

### 3. CONCLUSIONS

Topological indices are numerical parameter that help to predict properties of molecular compounds. In the present report, we computed K Banahatti indices and K hyper Banahatti indices of line graph of H-Pantacenic nanotube.

### COMPETING INTERESTS

The authors declare that they have no competing interests.

### AUTHOR'S CONTRIBUTIONS

All authors contributed equally to the writing of this paper. All authors read and approved the final manuscript.

### REFERENCES

- [1] West, D. B. Introduction to graph theory (Vol. 2). Upper Saddle River: Prentice hall. (2001).
- [2] Rücker, G., & Rücker, C. On topological indices, boiling points, and cycloalkanes. *Journal of chemical information and computer sciences*, 39(5), 788-802. (1999).
- [3] Klavzar, S., & Gutman, I. A comparison of the Schultz molecular topological index with the Wiener index. *Journal of chemical information and computer sciences*, 36(5), 1001-1003. (1996).
- [4] Wiener, H. Structural determination of paraffin boiling points. *Journal of the American Chemical Society*, 69(1), 17-20. (1947).
- [5] Dobrynin, A. A., Entringer, R., & Gutman, I. Wiener index of trees: theory and applications. *Acta Applicandae Mathematica*, 66(3), 211-249. (2001).
- [6] Gutman, I., & Polansky, O. E. *Mathematical concepts in organic chemistry*. Springer Science & Business Media. (2012).
- [7] Randić, M. Characterization of molecular branching. *Journal of the American Chemical Society*, 97(23), 6609-6615. (1975).
- [8] Bollobás, B., & Erdős, P. Graphs of extremal weights. *Ars Combinatoria*, 50, 225-233. (1998).
- [9] Amic, D., Bešlo, D., Lucic, B., Nikolić, S., & Trinajstić, N. The vertex-connectivity index revisited. *Journal of chemical information and computer sciences*, 38(5), 819-822. (1998).
- [10] Hu, Y., Li, X., Shi, Y., Xu, T., & Gutman, I. On molecular graphs with smallest and greatest zeroth-order general Randić index. *MATCH Commun. Math. Comput. Chem*, 54(2), 425-434. (2005).
- [11] Sardar, M. S., Zafar, S., & Farahani, M. R. (2017). The Generalized Zagreb Index of Capra-Designed Planar Benzenoid Series  $Ca_k(C_6)$ , *Open J. Math. Sci.*, Vol. 1(2017), No. 1, pp. 44 - 51
- [12] Mutee ur Rehman, H., Sardar, R., & Raza, A. (2017). Computing Topological Indices of Hex Board and its Line Graph, *Open J. Math. Sci.*, Vol. 1(2017), No. 1, pp. 62 - 71.

- [13] Kulli, V. R., Chaluvvaraju, B., & Boregowda, H. S. (2017). Connectivity Banhatti indices for certain families of benzenoid systems. *Journal of Ultra Chemistry*, 13(4), 81-87.
- [14] Kulli, V. R. (2016). Multiplicative K Hyper-Banhatti Indices And Coindices Of Graphs. *International Journal of Mathematical Archive ISSN 2229-5046 [A UGC Approved Journal]*, 7(6).