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V 型潘式纳米管线图的特定 Banhatti 指数

瓦格斯·纳泽尔
（拉合尔教育大学 科学与技术部，拉合尔 54000）

摘要：拓扑指数是与图表关联的数字量，其表征图的拓扑在图自同构下是不变的. 拓扑指数被用作结构－活性定量关系（QSAR）的例子，其中分子的生物活性或其他性质与其化学结构相关. 因此，计算了 V 型潘氏纳米管线图的第 1 和第 2 的 K Banhatti 指数，以及 V 型潘氏纳米管线图的第 1 和第 2 的 K 超 Banhatti 指数.
关键词：K Banhatti 指数；K 超 Banhatti 指数；线图；亚苯基；V 型潘式纳米管
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The Certain Banhatti Indices of the Line Graph of V-pantacenic Nanotube

WAQAS Nazeer
（Division of Science and Technology，University of Education Lahore，Lahore，Pakistan　54000）

Abstract：A topological index is a numeric quantity associated with a graph which characterizes the topology of the graph and is invariant under graph automorphism. Topological indices are used as an 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 V-Pantacenic Nanotubes. We also compute the first and second K hyper Banhatti indices of the Line Graphs of V-Pantacenic Nanotubes.
Key words：K Banhatti index；K-hyper Banhatti index；line graph；phenylenes；V-Pantacenic

0　Introduction

Chemical graph theory is a branch of graph theory in which a chemical compound is represented by a 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 at least 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 $d(u,v)=d_G(u,v)$ in graph G. For a vertex v of G the "degree" d_v is the number of vertices attached to 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 to each other. We refer to 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].

The number that describes the topology of a graph is called topological index. In 1947, the first and most studied topological index was introduced by Weiner[4]. More details about this index can be found in[5-6]. In 1975, Milan Randic introduced the Randic index[7].

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作者简介：瓦格斯·纳泽尔，男，巴基斯坦人，副教授，博士，主要从事图论和理论化学研究.

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 to[11-15]. The first and second K-Banhatti indices of G are defined as

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

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

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

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

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

We refer to[16-17] for details about these indices.

The first and second multiplicative K Banhatti indices are defined as[18]

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

$$BII_2(G)=\prod_{ue}[d_G(u)d_G(e)].$$

The first and second multiplicative K hyper Banhatti indices are defined as[18]

$$HBII_1(G)=\prod_{ue}(d_G(u)+d_G(e))^2,$$

$$HBII_2(G)=\prod_{ue}(d_G(u)d_G(e))^2.$$

The line graph $L(G)$ of a graph G is the graph each of whose vertices, representing 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 V-Pantacenic nanotube[19]. The graph of V-Pantacenic nanotube is given in figure 1 and the line graph of V-Pantacenic nanotube is given in figure 2.

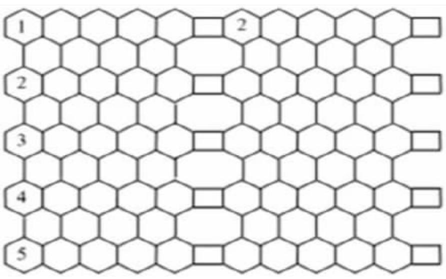

Figure 1 The V-Pantacenic nanotube $F[2,5]$

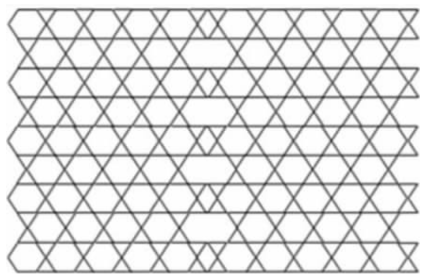

Figure 2 The line graph of V-Pantacenic nanotube $F[2,5]$

1 Computational Results

In this section we will give our main results.

Theorem 1 Let $G=L(F[p,q])$ be a line graph of V-Pantacenic nanotube. Then

$$B_1(G)=1\ 320pq-568p,$$

$$B_2(G)=3\ 168pq-1\ 652p,$$

$$HB_1(G)=13\ 200pq-6\ 936p,$$

$$HB_2(G)=76\ 032pq-49\ 132p.$$

Proof The line graph of V-Pantancenic Nanotubes is shown in figure 2. It can be observed from the figure 2 and lemma 1 that

$$|V(G)| = 33pq - 5p,$$

There are two types of vertices based on the degree, i. e

$$V_1(G) = \{v \in V(G) : d_v = 3\},$$
$$V_2(G) = \{v \in V(G) : d_v = 4\},$$

Such that

$$|V_1(G)| = 20p,$$
$$|V_2(G)| = 33pq - 25p.$$

Also

$$|E(G)| = 66pq - 20p.$$

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

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

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

Now

$$|E_{\{3,3\}}(G)| = 18p,$$
$$|E_{\{3,4\}}(G)| = 20p,$$
$$|E_{\{4,4\}}(G)| = 66pq - 58p.$$

The detailed edge set dividing can refer to Table 1.

Tab. 1 The edge set dividing of $L(F[p, q])$

$d_{(G)}(u), d_{(G)} = e \in E(G)$	$d_{(G)}(e)$	Numbers of edges
(3, 3)	4	$18p$
(3, 4)	5	$20p$
(4, 4)	6	$66pq - 58p$

1) From the definition of first K Banhatti index

$B_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(e)] = \sum_{ue \in E_{\{3,3\}}} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] + \sum_{ue \in E_{\{3,4\}}} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] + \sum_{ue \in E_{\{4,4\}}} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] = 18p[(3+4) + (3+4)] + 20[(3+5) + (4+5)] + (66pq - 58p)[(4+6) + (4+6)] = 1\,320pq - 568p.$

2) From the definition of second K Banhatti index

$B_2(G) = \sum_{uv \in E(G)} [d_G(u) \times d_G(e)] = \sum_{ue \in E_{\{3,3\}}} [(d_G(u)d_G(e)) + (d_G(v)d_G(e))] + \sum_{ue \in E_{\{3,4\}}} [(d_G(u)d_G(e)) + (d_G(v)d_G(e))] + \sum_{ue \in E_{\{4,4\}}} [(d_G(u)d_G(e)) + (d_G(v)d_G(e))] = 12[(3 \times 4) + (3 \times 4)] + 20p[(3 \times 5) + (4 \times 5)] + (66pq - 58p)[(4 \times 6) + (4 \times 6)] = 3\,168pq - 1\,652p.$

3) From the definition of first K hyper Banhatti index

$HB_1(G) \sum_{uv \in E(G)} [d_G(u) + d_G(e)]^2 = \sum_{ue \in E_{\{2,3\}}} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] + \sum_{ue \in E_{\{3,4\}}} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] + \sum_{ue \in E_{\{4,4\}}} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] = 12p[(3+4)^2 + (3+4)^2] + 20p[(3+5)^2 + (4+5)^2] + (66pq - 58p)[(4+6)^2 + (4+6)^2] = 13\,200pq - 6\,936p.$

4) From the definition of second K hyper Banhatti index

$HB_2(G) = \sum_{ue} [d_G(u)d_G(e)]^2 = \sum_{ue \in E_{\{2,3\}}} [(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2] + \sum_{ue \in E_{\{3,4\}}} [(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2] + \sum_{ue \in E_{\{4,4\}}} [(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2] = 12p[(3 \times 4)^2 + (3 \times 4)^2] + 20p[(3 \times 5)^2 +$

$(4\times5)^2]+(66pq-58p)[(4\times6)^2+(4\times6)^2]=76\,032pq-49\,132p$.

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

$$BII_1(G)=7^{24p}\times8^{20p}\times9^{20p}\times10^{2(66pq-58p)},$$

$$BII_2(G)=12^{24p}\times(15)^{20p}\times(20)^{20p}\times(24)^{2(66pq-58p)},$$

$$HBII_1(G)=7^{48p}\times8^{40p}\times9^{40p}\times10^{4(66pq-58p)},$$

$$HBII_2(G)=12^{48p}\times15^{40p}\times20^{40p}\times24^{4(66pq-58p)}.$$

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

$BII_1(G)=\prod_{ue}[d_G(u)+d_G(e)]=\prod_{e=uv\in E_{\{2,3\}}}[d_G(u)+d_G(e)][d_G(v)+d_G(e)]\times\prod_{e=uv\in E_{\{3,4\}}}[d_G(u)+d_G(e)][d_G(v)+d_G(e)]\times\prod_{e=uv\in E_{\{4,4\}}}[d_G(u)+d_G(e)][d_G(v)+d_G(e)]=(3+4)^{12p}\times(3+4)^{12p}\times(3+5)^{20p}\times(4+5)^{20p}\times(4+6)^{(66pq-58p)}\times(4+6)^{(66pq-58p)}=7^{24p}\times8^{20p}\times9^{20p}\times10^{2(66pq-58p)}$.

2) From the definition of second multiplicative K Banahatti index

$BII_2(G)=\prod_{ue}d_G(u)d_G(e)=\prod_{e=uv\in E_{\{3,3\}}}[(d_G(u)d_G(e))\times(d_G(v)d_G(e))]\times\prod_{e=uv\in E_{\{3,4\}}}[(d_G(u)d_G(e))\times(d_G(v)d_G(e))]\times\prod_{e=uv\in E_{\{4,4\}}}[(d_G(u)d_G(e))\times(d_G(v)d_G(e))]=(3\times4)^{12p}\times(3\times4)^{12p}\times(3\times5)^{20p}\times(4\times5)^{20p}\times(4\times6)^{(66pq-58p)}\times(4\times6)^{(66pq-58p)}=12^{24p}\times(15)^{20p}\times(20)^{20p}\times(24)^{2(66pq-58p)}$.

3) From the definition of first multiplicative K hyper Banahatti index

$HBII_1(G)=\prod_{ue}[d_G(u)+d_G(e)]^2=\prod_{e=uv\in E_{\{3,3\}}}[d_G(u)+d_G(e)]^2[d_G(v)+d_G(e)]^2\times\prod_{e=uv\in E_{\{3,4\}}}[d_G(u)+d_G(e)]^2[d_G(v)+d_G(e)]^2\times\prod_{e=uv\in E_{\{4,4\}}}[d_G(u)+d_G(e)]^2[d_G(v)+d_G(e)]^2=[(3+4)^2]^{12p}\times[(3+4)^2]^{12p}\times[(3+5)^2]^{20p}\times[(4+5)^2]^{20p}\times[(4+6)^2]^{(66pq-58p)}\times[(4+6)^2]^{(66pq-58p)}=7^{48p}\times8^{40p}\times9^{40p}\times10^{4(66pq-58p)}$.

4) From the definition of second multiplicative K hyper Banahatti index

$HBII_2(G)=\prod_{ue}(d_G(u)d_G(e))^2=\prod_{e=uv\in E_{\{3,3\}}}[(d_G(u)d_G(e))^2\times(d_G(v)d_G(e))^2]\times\prod_{e=uv\in E_{\{3,4\}}}[(d_G(u)d_G(e))^2\times(d_G(v)d_G(e))^2]\times\prod_{e=uv\in E_{\{4,4\}}}[(d_G(u)d_G(e))^2\times(d_G(v)d_G(e))^2]=[(3\times4)^2]^{12p}\times[(3\times4)^2]^{12p}\times[(3\times5)^2]^{20p}\times[(4\times5)^2]^{20p}\times[(4\times6)^2]^{(66pq-58p)}\times[(4\times6)^2]^{(66pq-58p)}=12^{48p}\times15^{40p}\times20^{40p}\times24^{4(66pq-58p)}$.

2 Conclusion

In this report we computed first K Banahatti index, second K Banahatti index, first K hyper Banahatti index, second K hyper Banahatti index, first multiplicative K Banahatti index, second multiplicative K Banahatti index, first multiplicative K hyper Banahatti index and second multiplicative K hyper Banahatti index of the line graph of V-Pantacenic nanotube. The following figure 3 and figure 4 show the dependence of first K Banahatti index and second K Banahatti index on the involved structural parameters p and q.

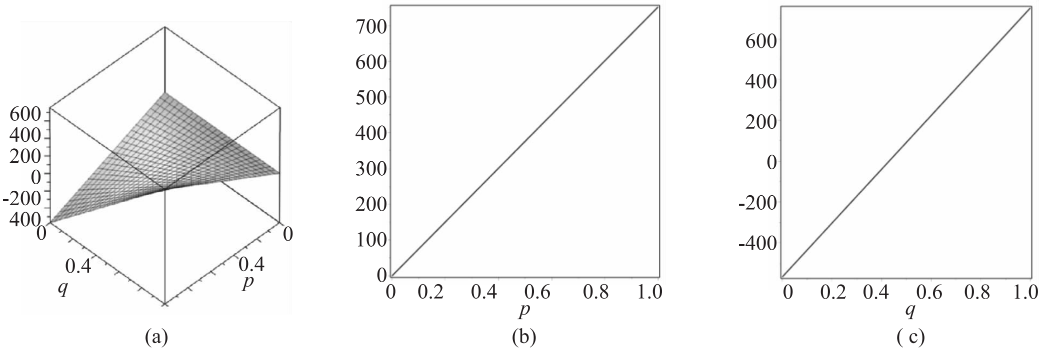

Figure 3 Plot of first K Banahatti index 3D(left), for p=1 (middle) and for q=1 (right)

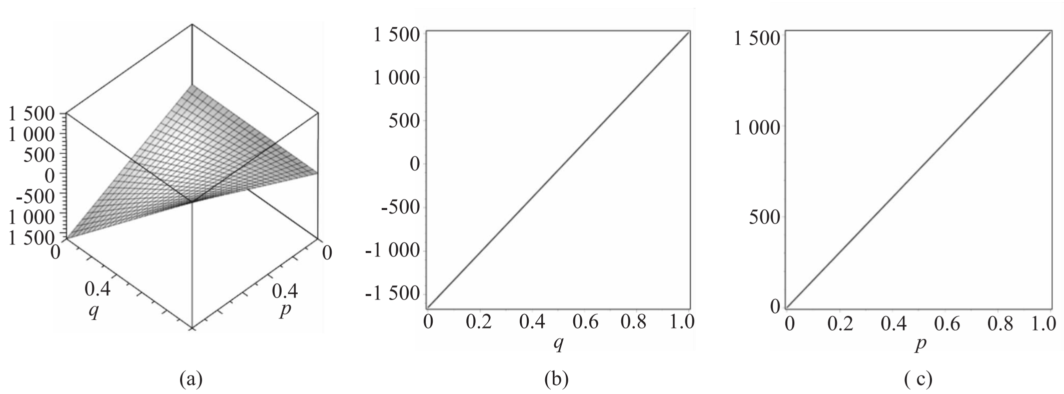

Figure 4 Plot of second K Banahatti index 3D(left), for p=1 (middle) and for q=1 (right)

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