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TOPOLOGICAL INVARIANTS OF MOLECULAR GRAPH OF GRAPHENE

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Abstract

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers and industrialists worldwide. The aim of this report is to compute the first and second *K* Banhatti indices of molecular graph of Graphene. We also compute the first and second *K*-hyper Banhatti indices of molecular graph of Graphene.

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 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 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 to 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 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, Randić introduced the Randić index [7].

Bollobás and Erdős [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

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

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

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

and

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

We refer [13] for details about these indices.

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industrialists worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors and biodevices. Also, it is the most effective material for electromagnetic interference (EMI) shielding. Now we focus on computation of topological indices of Graphene [14]. We refer [15-19] for details. In Figure 1, the molecular graph of Graphene is shown.

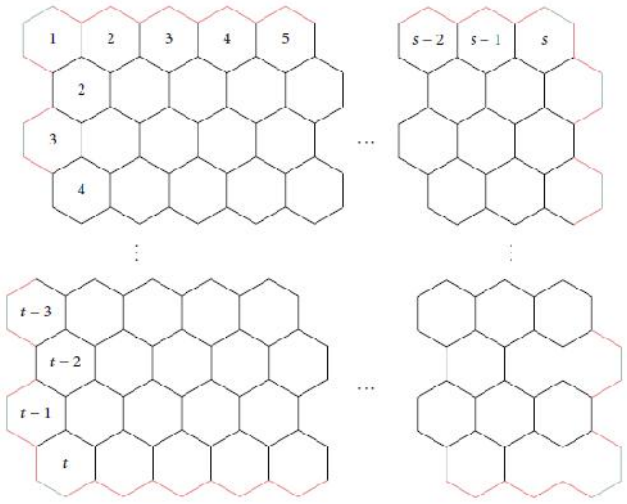

Figure 1. Molecular graph of Graphene.

In this report, we compute Banhatti indices of molecular graph of Graphene.

Throughout this report, G is a connected graph, $V(G)$ and $E(G)$ are the vertex set and the edge set, respectively, and d_v denotes the degree of a vertex v.

2. Computational Results

Theorem 1. *Let G be a molecular graph of Graphene having "t" rows of benzene rings with "s" benzene ring in each row. Then the first Banhatti index of G is* $B_1(G) = 42ts + 16s + 16t - 26$.

Proof. Let G be a molecular graph of Graphene (Figure 1). Then the edges of Graphene are divided into three types:

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

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

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

such that

$$|E_{\{2,2\}}| = t + 4,$$

$$|E_{\{2,3\}}| = 4s + 2t - 4,$$

$$|E_{\{3,3\}}| = 3ts - 2s - t - 1.$$

$d_{(G)}(u)$, $d_{(G)} = e \in E(G)$	$d_{(G)}(e)$	Numbers of edges
(2, 2)	2	$t + 4$
(2, 3)	3	$4s + 2t - 4$
(3, 3)	4	$3ts - 2s - t - 1$

Now by definition, we have

$$B_1(G) = \sum_{ue} [d_G(u) + d_G(e)]$$

$$= \sum_{ue \in |E_1|} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))]$$

$$+ \sum_{ue \in |E_2|} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))]$$

$$+ \sum_{ue \in |E_3|} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))]$$

$$= (t + 4)[(2 + 2) + (2 + 2)] + (4s + 2t - 4)[(2 + 3) + (3 + 3)]$$

$$+ (3ts - 2s - t - 1)[(3 + 4) + (3 + 4)]$$

$$= 42ts + 16s + 16t - 26.$$

Theorem 2. *Let G be a molecular graph of Graphene having "t" rows of benzene rings with "s" benzene ring in each row. Then the second K Banhatti index of G is* $B_2(G) = 96ts + 12s + 14t - 52$.

Proof. By the definition of the second *K* Banhatti index, we have

$$\begin{aligned}
B_2(G) &= \sum_{ue} d_G(u)d_G(e) \\
&= \sum_{ue\in|E_1|} [(d_G(u)d_G(e)) + (d_G(v)d_G(e))] \\
&\quad + \sum_{ue\in|E_2|} [(d_G(u)d_G(e)) + (d_G(v)d_G(e))] \\
&\quad + \sum_{ue\in|E_3|} [(d_G(u)d_G(e)) + (d_G(v)d_G(e))] \\
&= (t+4)[(2\times 2)+(2\times 2)] + (4s+2t-4)[(2\times 3)+(3\times 3)] \\
&\quad + (3ts-2s-t-1)[(3\times 4)+(3\times 4)] \\
&= 96ts + 12s + 14t - 52.
\end{aligned}$$

Theorem 3. *Let G be a molecular graph of Grapheme having "t" rows of benzene rings with "s" benzene ring in each row. Then the first K-hyper Banhatti index of G is* $HB_1(G) = 392ts + 48s + 56t - 214$.

Proof. By using the definition of first *K*-hyper Banhatti index, we have

$$\begin{aligned}
HB_1(G) &= \sum_{ue} [d_G(u) + d_G(e)]^2 \\
&= \sum_{ue\in|E_1|} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] \\
&\quad + \sum_{ue\in|E_2|} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] \\
&\quad + \sum_{ue\in|E_3|} [(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2] \\
&= (t+4)[(2+2)^2 + (2+2)^2] + (4s+2t-4)[(2+3)^2 + (3+3)^2] \\
&\quad + (3ts-2s-t-1)[(3+4)^2 + (3+4)^2] \\
&= 392ts + 48s + 56t - 214.
\end{aligned}$$

Theorem 4. *Let G be a molecular graph of Graphene having "t" rows of benzene rings with "s" benzene ring in each row. Then the second K-hyper Banhatti index of G is* $HB_2(G) = 864ts + 108s - 22t - 628$.

Proof. By using the definition of second *K*-hyper Banhatti index, we have

$$\begin{aligned} HB_2(G) &= \sum_{ue} (d_G(u)d_G(v))^2 \\ &= \sum_{ue\in|E_1|} [(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2] \\ &\quad + \sum_{ue\in|E_2|} [(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2] \\ &\quad + \sum_{ue\in|E_3|} [(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2] \\ &= (t+4)(16+16) + (4s+2t-4)(36+81) \\ &\quad + (3ts-2s-t-1)(144+144) \\ &= 864ts - 108s - 22t - 628. \end{aligned}$$

3. Conclusion

In this report, we computed *K* Banhatti and *K*-hyper Banhatti indices of molecular graph of Graphene. Our results may play a vital role in pharmacy.

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