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FULL PAPER

Mathematical Properties and Computations of Banahatti indices for a Nano-Structure "Toroidal Polyhex Network"

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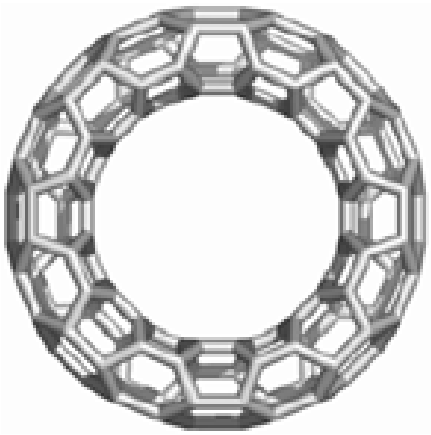
ABSTRACT: Let G be the connected graph with vertex set V(G) and edge set E(G).The first and second K Banhatti indices of G are defined as $B_1(G)=\sum_{ue}[d_G(u)+d_G(e)]$ and $B_2(G)=\sum_{ue}[d_G(u)d_G(e)]$ where ue means that the vertex u and edge e are incident in G.The first and second K hyper Banhatti indices of G are defined as $HB_1(G)=\sum_{ue}[d_G(u)+d_G(e)]^2$ and $HB_2(G)=\sum_{ue}[d_G(u)d_G(e)]^2$ respectively . In this paper, we compute the first and second K Banhatti indices of toroidal polyhex network. In addition, the first and second K hyper Banhatti indices of toroidal polyhex networks are determined.

KEYWORDS: carbon quantum dots, citrus lemon juice, fluorescent, hydrothermal method, cell imaging.

GRAPPHICAL ABSTACT:



1 - Introduction

Let G be a connected graph with vertex set V(G) and edge set E(G).The $d_G(v)$ of a vertex v is the number of edges 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 in G, which is defined by $d_G(e)=d_G(u)+d_G(v)-2$ with $e=uv$. For details about graph theory we refer [1]. Chemical reaction network theory is an area of applied mathematics that attempts to model the behaviour of real world chemical systems since its foundations in 1960s; it has

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attracted a growing research community, mainly due to its applications in biochemistry and theoratical chemistry. It has also attracted from pure mathematicians due to interesting problems that arise from the mathematical patterns in structure of materials.

Ceheminformatics is an emerging field in which quantitative structure-activity (QSAR) and sructure-property (QSPR) relationships predict the biological activities and properties of nanomaterial. In these studies, some physcio-chemical properties and topological indices are used to predict the bioactivity of chemical compounds [2,3]. The branch of chemistry which deals with the chemical structures with the help of mathematical tools is called mathematical chemistry. Chemical graph theory is the branch of mathematical chemistry that applies graph theory to the mathematical modeling of chemical phenomenan. In chemical graph theory, a molecular graph is asimple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges respectively. Topological index of a graph is a number that describe topology of understudy molecular structure [4,5].

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

$$B_1(G)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(e)\right],\ \text{and}\ B_2(G)=\sum_{uv\in E(G)}\left[d_G(u)\times d_G(e)\right].$$

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

$$HB_1(G)=\sum_{uv\in E(G)}\left[d_G(u)+d_G(e)\right]^2,\ \text{and}\ HB_2(G)=\sum_{uv\in E(G)}\left[d_G(u)\times d_G(e)\right]^2.$$

We refer [6] for details about these indices.In this article, we compute first and second K Banhatti index and first and second hyper K-Banhatti index of toroidal polyhex network.

2. Toroidal Polyhex Network

The discovery of the fullerene molecules has stimulated many interests in other possibilities for carbons. Many properties of fullerenes can be studied using mathematical tools such as graph theory. A fullerene can be represented by a trivalent graph on a closed surface with pentagonal and hexagonal faces, such that its vertices are carbon atoms of the molecule. Two vertices are adjacent if there is a bond between corresponding atoms. In [7], authors considered fullerene's extension to other closed surfaces and showed that only four surfaces, sphere, torus, Klein bottle and projective (elliptic) plane, are possible. The spherical and elliptic fullerenes have 12 and 6 pentagons respectively. There are no pentagons in the toroidal's and the Klein bottle's fullerenes [8].

A *toroidal fullerene* (toroidal polyhex), obtained from 3D Polyhex Torus Figure 1, is a cubic bipartite graph embedded on the torus such that each face is a hexagon. The torus is a closed surface that can carry the graphs of the toroidal polyhex in which all faces are hexagons and the degree of all vertices is 3. The optical and vibrational properties of toroidal carbon nanotubes can be found in [9]. There have appeared a few works in the enumeration of perfect matchings of toroidal polyhexes by applying various techniques, such as transfer-matrix and permanent of the adjacency matrix. Ye et al. [10] have studied a k-resonance of toroidal polyhexes. Classifications of all possible structures of fullerene Cayley graphs is given in [11] by Kang. The atom-bond connectivity index (ABC) and geometric–arithmetic index (GA) of the toroidal polyhex are computed in [12] by Baca et al. In [13-23], authors computed distance-based topological indices of eight infinite sequences of 3-generalized fullerenes. In [14], authors presented a new extension of the generalized topological indices (GTI) approach to represent topological indices in a unified way. Let L be a regular hexagonal lattice and $^{n}P_{m}$ be a $m\times n$ quadrilateral section (with m hexagons on the top and bottom sides and n hexagons on the lateral sides, n is even) cut from the regular hexagonal lattice L. First identify two

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lateral sides of ${}^{n}P_m$ to form a cylinder, and finally identify the top and bottom sides of ${}^{n}P_m$ at their corresponding points, see Figure 1. From this we get a toroidal polyhex $H_{\{m,n\}}$ with *mn* hexagons.

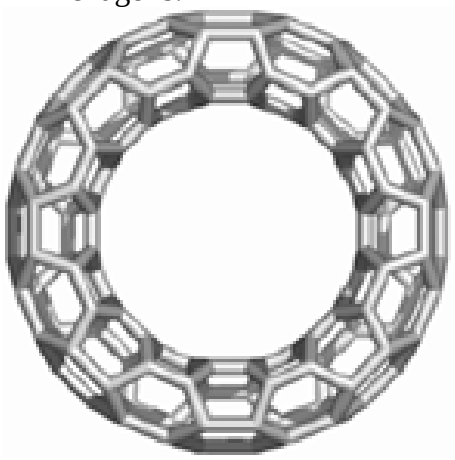

Fig 1. Polyhex Torus.

The set of vertices of the toroidal polyhex is: $V(H_{\{m,n\}}) = \{v_j^i, v_j^i : 0 \le i \le n-1, 0 \le j \le m-1\}$.

The set of edges of the toroidal polyhex is splitted into mutually disjoint subsets such that for even i such that $0 \le i \le n-2$, we have $A_i = \{u_j^i v_j^i : 0 \le j \le m-1\}$ and $A'_i = \{v_j^i u_{j+1}^i : 0 \le j \le m-1\}$. For i odd and $1 \le i \le n-1$, we have $B_i = \{v_j^i u_j^i : 0 \le j \le m-1\}$ and $B'_i = \{u_j^i v_{j+1}^i : 0 \le j \le m-1\}$. For $0 \le i \le n-1$ we have $C_i = \{v_j^i u_j^{i+1} : 0 \le j \le m-1\}$, where i is taken modulo n and j is taken modulo m. Hence

$$E(H_{\{m,n\}}) = \bigcup_{i=0}^{\frac{n}{2}-1} (A_{2i} \cup A'_{2i} \cup B_{2i+1} \cup B'_{2i+1}) \bigcup_{i=0}^{n-1} C_i.$$

We can easily observe from figure 2 that the number of vertices in $H_{\{m,n\}}$ are $2mn$ and the number of edges in $H_{\{m,n\}}$ are $3mn$.

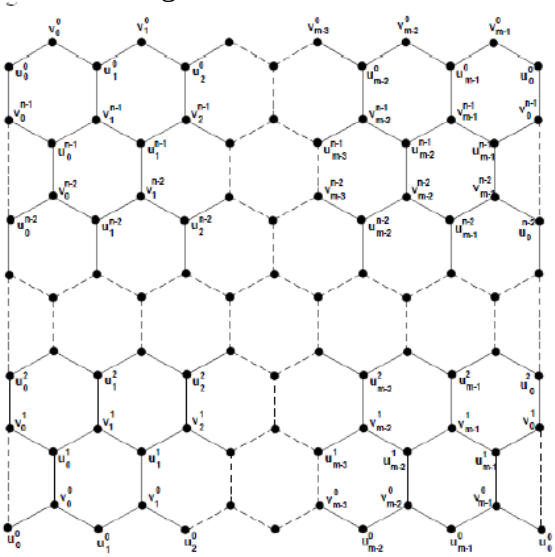

Fig 2. 2D-lattice graph of the toroidal polyhex.

1. Computational results

2. Theorem 1. Let $H_{\{m,n\}}$ be the toroidal polyhex network. Then its first and second K Banhatti indices are;

$B_1(H_{\{m,n\}}) = 42mn$ and $B_2(H_{\{m,n\}}) = 72mn$

Proof: Let $H_{\{m,n\}}$ be the toroidal polyhex network. There is only one type of edges in toroidal polyhex network based on degrees of end vertices of each edge. The edge partition $E_1(H_{\{m,n\}})$ contains $3mn$ edges uv, where $d_u = d_v = 3$.

So, by definition

$$\begin{aligned} B_1(H_{\{m,n\}}) &= \sum\nolimits_{ue} [d_G(u) + d_G(e)] \\ &= \sum\nolimits_{e=uv \in E(H_{\{m,n\}})} [(d_G(u) + d_G(e)) + (d_G(v) + d_G(e))] \\ &= 3mn[(3+4)+(3+4)] = 42mn. \end{aligned}$$

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$$B_2(H_{\{m,n\}}) = \sum_{ue}[d_G(u)d_G(e)]$$
$$= \sum_{e=uv\in E(H_{\{m,n\}})}[(d_G(u)d_G(e)) + (d_G(v)d_G(e))]$$
$$= 3mn[(3.4) + (3.4)] = 72mn.$$

Theorem 2. Let $H_{\{m,n\}}$ be the toroidal polyhex network. Then its K hyper Banhatti indices are; $HB_1(H_{\{m,n\}}) = 294mn$ and $HB_2(H_{\{m,n\}}) = 864mn$

Proof: By definition we have,

$$HB_1(H_{\{m,n\}}) = \sum_{ue}[d_G(u) + d_G(e)]^2$$
$$= \sum_{e=uv\in E(H_{\{m,n\}})}[(d_G(u) + d_G(e))^2 + (d_G(v) + d_G(e))^2]$$
$$= 3mn[(3+4)^2 + (3+4)^2] = 294mn.$$

Now,

$$HB_2(H_{\{m,n\}}) = [d_G(u)d_G(e)]^2$$
$$= \sum_{e=uv\in E(H_{\{m,n\}})}[(d_G(u)d_G(e))^2 + (d_G(v)d_G(e))^2]$$
$$= 3mn[(3.4)^2 + (3.4)^2] = 864mn.$$

■

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