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MORE TOPOLOGICAL INDICES OF TOROIDAL POLYHEX NETWORK

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Abstract

A topological index of graph G is a numerical parameter related to G which characterizes its topology and is preserved under isomorphism of graphs. Properties of the chemical compounds and topological

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indices are correlated. In this work, we compute newly defined topological indices, namely, arithmetic-geometric index (AG_1 index), SK index, SK_1 index and SK_2 index of toroidal polyhex network. We also compute sum connectivity index and modified Randić index of underlying graph.

1. Introduction

Cheminformatics is an emerging field in which quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) predict the biological activities and properties of nanomaterial, see [1-4]. In these studies, some physico-chemical properties and topological indices are used to predict bioactivity of the chemical compounds, see [5-7].

The branch of chemistry which deals with the chemical structures with the help of mathematical tools is called *mathematical chemistry*. Chemical graph theory is that branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges, respectively. A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a connection between any pair of vertices in G. The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4. The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex, and will be denoted by d_v. The concept of degree in graph theory is closely related (but not identical) to the concept of valence in chemistry. For details on basics of graph theory, any standard text such as [3] can be of great help.

The first Zagreb index and the second Zagreb index introduced by Gutman and Trinajstic [8] are defined as:

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 \text{ and } M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

Sum connectivity index is defined as:

$$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

and modified Randić index is defined as:

$$mR(G) = \sum_{uv \in E(G)} \frac{1}{\max\{d_u, d_v\}}.$$

Shigehalli and Kanabur [9] introduced the following new degree-based topological indices:

$$AG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}, \quad SK(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{2},$$

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{2}, \quad SK_2(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2.$$

In this paper, we compute some degree-based topological indices of toroidal polyhex network. Moreover, we plot our results to see the dependences of these topological indices on the parameters involved.

2. Computational Results

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 [10], the 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 toroidal and Klein bottle's fullerenes [11].

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 graph of toroidal polyhex in which all faces are hexagons and the degree of all vertices is 3. We refer [12, 13] for further studies about toroidal polyhexes, and for further studies about degree-based topological indices, we refer [14, 15] and the references therein. 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. [16] have studied a k-resonance of toroidal polyhexes. Classification of all possible structures of fullerene Cayley graphs is given in [17] by Kang. The atom-bond connectivity index (ABC) and geometric-arithmetic index (GA) of toroidal polyhex are computed in [18] by Baca et al. In [19], the authors computed distance-based topological indices of eight infinite sequences of 3-generalized fullerenes. In [20], the authors presented a new extension of the generalized topological indices (GTI) approach representing topological indices in a unified way.

Figure 1. Polyhex torus.

Let L be a regular hexagonal lattice and ${}^{n}P_{m}$ be an $m \times n$ 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 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. From this, we get a toroidal polyhex $H_{\{m,n\}}$ with mn hexagons.

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 split 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 $A_i' = \{v_j^i u_{j+1}^i : 0 \le j \le m-1\}$ and 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 $B_i' = \{u_j^i v_{j+1}^i : 0 \le j \le m-1\}$ and 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 $H_{\{m,n\}}$ is $2mn$ and the number of edges in $H_{\{m,n\}}$ is $3mn$. Note that there is only one type of edges in toroidal polyhex based on degrees of end vertices of each edge. The edge partition $E_1(H_{\{m,n\}})$ contains $3mn$ edges uv, where $d_u = d_v = 3$.

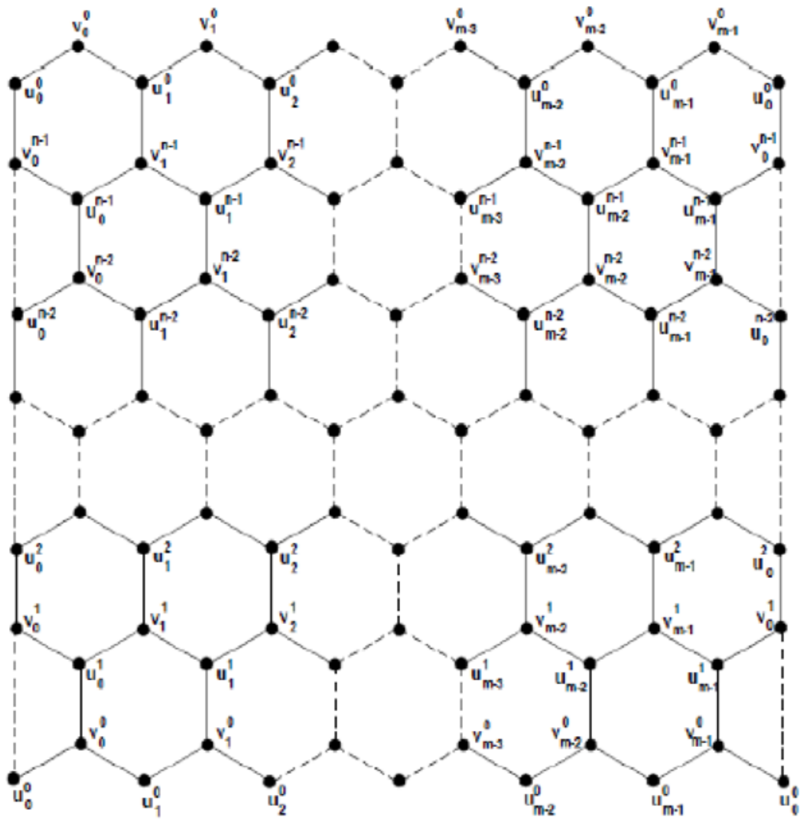

Figure 2. 2D lattice graph of toroidal polyhex.

Theorem 1. *Let* $H_{\{m,n\}}$ *be the toroidal polyhex. Then*

$$SC(H_{\{m,n\}}) = \frac{2mn}{\sqrt{6}},$$

$$mR(H_{\{m,n\}}) = \frac{2nm}{3}.$$

Proof. Let $H_{\{m,n\}}$ be toroidal polyhex with defining parameters m and n. Then

$$SC(H_{\{m,n\}}) = \sum_{uv \in E(H_{\{m,n\}})} \frac{1}{\sqrt{d_u + d_v}}$$

$$= \sum_{uv \in E_1(H_{\{m,n\}})} \frac{1}{\sqrt{d_u + d_v}}$$

$$= |E(H_{\{m,n\}})| \frac{1}{\sqrt{3+3}}$$

$$= \frac{2mn}{\sqrt{6}},$$

$$mR(H_{\{m,n\}}) = \sum_{uv \in E(H_{\{m,n\}})} \frac{1}{\max\{d_u, d_v\}}$$

$$= \sum_{uv \in E_1(H_{\{m,n\}})} \frac{1}{\max\{d_u, d_v\}}$$

$$= \frac{2nm}{3}.$$

Theorem 2. *Let* $H_{\{m,n\}}$ *be the toroidal polyhex. Then*

$$AG_1(H_{\{m,n\}}) = 2mn,$$

$$SK(H_{\{m,n\}}) = 6mn,$$

$$SK_1(H_{\{m,n\}}) = 9mn,$$

$$SK_2(H_{\{m,n\}}) = 18mn.$$

Proof. Let $H_{\{m,n\}}$ be toroidal polyhex with defining parameters m and n. Then

$$AG_1(H_{\{m,n\}}) = \sum_{uv \in E(H_{\{m,n\}})} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}}$$

$$= \sum_{uv \in E_1(H_{\{m,n\}})} \frac{d_u + d_v}{2\sqrt{d_u \cdot d_v}}$$

$$= |E(H_{\{m,n\}})| \frac{3+3}{2\sqrt{9}}$$

$$= 2mn,$$

$$SK(H_{\{m,n\}}) = \sum_{uv \in E(H_{\{m,n\}})} \frac{d_u + d_v}{2}$$

$$= \sum_{uv \in E_1(H_{\{m,n\}})} \frac{d_u + d_v}{2}$$

$$= |E(H_{\{m,n\}})| \frac{3+3}{2}$$

$$= 6mn,$$

$$SK_1(H_{\{m,n\}}) = \sum_{uv \in E(H_{\{m,n\}})} \frac{d_u \cdot d_v}{2}$$

$$= \sum_{uv \in E_1(H_{\{m,n\}})} \frac{d_u \cdot d_v}{2}$$

$$= |E(H_{\{m,n\}})| \frac{9}{2}$$

$$= 9mn,$$

$$SK_2(H_{\{m,n\}}) = \sum_{uv \in E(H_{\{m,n\}})} \left(\frac{d_u + d_v}{2}\right)^2$$

$$= \sum_{uv \in E_1(H_{\{m,n\}})} \left(\frac{d_u + d_v}{2}\right)^2$$

$$= |E(H_{\{m,n\}})| \left(\frac{3+3}{2}\right)^2$$

$$= 18mn.$$

3. Conclusions and Discussion

In this article, we computed arithmetic-geometric index (AG_1 index), SK index, SK_1 index and SK_2 index, sum connectivity index and modified Randić index of toroidal polyhex. These results can play a vital role in determining properties of this network and its uses in industry, electronics, and pharmacy.

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References

[1] D. Stover and D. Normile, Buckytubes, Popular Science 240(4) (1992), 31.

[2] The many faces of nanotech, Nature Nanotechnology 2(10) (2007), p. 585. doi:10.1038/nnano.2007.308

[3] D. B. West, An Introduction to Graph Theory, Prentice-Hall, 1996.

[4] E. Deutsch and S. Klavzar, *M*-polynomial and degree-based topological indices, Iranian Journal of Mathematical Chemistry 6(2) (2015), 93-102.

[5] I. Gutman, Molecular graphs with minimal and maximal Randić indices, Croat. Chem. Acta 75 (2002), 357-369.

[6] I. Gutman, Degree-based topological indices, Croat. Chem. Acta 86 (2013), 351-361.

[7] D. Vukičević, On the edge degrees of trees, Glas. Mat. Ser. III 44(64) (2009), 259-266.

[8] I. Gutman and N. Trinajstic, Graph theory and molecular orbitals total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 (1972), 535-538.

[9] V. S. Shigehalli and R. Kanabur, Computation of new degree-based topological indices of graphene, J. Math. 2016 (2016), Article ID 4341919, 6 pages.

[10] M. Deza, P. W. Fowler, A. Rassat and K. M. Rogers, Fullerenes as tilings of surfaces, J. Chem. Inf. Comput. Sci. 40 (2000), 550-558.

[11] E. C. Kirby and P. Pollak, How to enumerate the connectional isomers of a toroidal polyhex fullerene, J. Chem. Inf. Comput. Sci. 38(6) (1998), 1256. doi: 10.1021/ci980486r.

[12] D. J. Klein, Elemental benzenoids, J. Chem. Inf. Comput. Sci. 34(2) (1994), 453-459. DOI: 10.1021/ci00018a037.

[13] F. Beuerle, C. Herrmann, A. C. Whalley, C. Valente, A. Gamburd, M. A. Ratner and J. F. Stoddart, Optical and vibrational properties of toroidal carbon nanotubes, Chem. Eur. J. 17 (2011), 3868-3875.

[14] Muhammad S. Sardar, Sohail Zafar and Mohammad R. Farahani, The generalized Zagreb index of Capra-designed planar benzenoid series $Ca_k(C_6)$, Open J. Math. Sci. 1(1) (2017), 44-51.

[15] Hafiz Mutee ur Rehman, Riffat Sardar and Ali Raza, Computing topological indices of hex board and its line graph, Open J. Math. Sci. 1(1) (2017), 62-71.

[16] D. Ye, Z. Qi and H. Zhang, On *k*-resonant fullerene graphs, SIAM J. Discrete Math. 23(2) (2009), 1023-1044.

[17] M. H. Kang, Toroidal fullerenes with the Cayley graph structures, Discrete Math. 311 (2011), 2384-2395.

[18] M. Baca, J. Horvathova, M. Mokrisova and A. Suhanyiova, On topological indices of fullerenes, Appl. Math. Comput. 251 (2015), 154-161.

[19] Z. Mehranian and A. R. Ashrafi, Topological Indices of 3-generalized Fullerenes, Distance, Symmetry, and Topology in Carbon Nanomaterials, Springer International Publishing, 2016, pp. 281-301.

[20] E. Ernesto and A. R. Matamala, GTI-space: the space of generalized topological indices, Journal of Mathematical Chemistry 43(2) (2008), 508-517.