Montes Taurus J. Pure Appl. Math. 2 (1), 81–86, 2020

Montes Taurus Journal of Pure and Applied Mathematics

https://www.mtjpamjournal.com

MTJPAM
ISSN: 2687-4814

Topological Indices of Collagen

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Abstract

Topological graph indices have been used in calculation of several chemical and physical properties of some molecular structures in QSAR and QSPR studies. The first example is the Wiener index which was used in determining the boiling points of the isomers of alkanes in 1947. Since then, a large number of topological graph indices are used to determine several properties of chemical molecules. In this paper, several topological graph indices are calculated for one of the important chemical substance class called collagen having extreme importance in the movement of body parts.

Keywords: Graph, collagen, Zagreb indices, topological indices

2010 MSC: 05C07, 05C30, 05C90, 94C15

1. Introduction

Collagen are class of macromolecules (a molecule formed by hundreds of atoms) which are a main compound of many tissues and bones in animals. Twenty-eight different types of collagen have been identified in vertebrates. Collagen types I to IV are the most frequent ones. The unique properties of each type are due to segments in the collagen molecules that disrupt the helical structure. These are caused by the amino acids in the X positions of the polypeptide sequence. Different tissues of the body may contain different amounts of each type of collagen. For example, cartilage contains a lot of type II, whereas type IV is mostly found in fundamental membranes. The most well-known and studied is the type II collagen. The type II collagen has the molecular formula $C_{65}H_{102}N_{18}O_{21}$, see Figure 1.

Collagen is mostly consumed in the cosmetic and pharmaceutical industries, where it is an important raw material in manufacturing cosmetic products or surgery equipments, and more importantly for implants. It is also consumed in food industry in producing gelatin and its derivatives.

Topological graph indices have been defined and had several usages in many areas to study some properties of different objects such as atoms and molecules. Several topological graph indices have been defined and studied by many mathematicians and chemists. This is because of the fact that most graphs are generated from molecules by replacing atoms and bonds between them with vertices and edges, respectively. They are defined as topological graph invariants measuring several chemical, physical, biological, pharmacological, pharmaceutical, etc. properties of graphs that are modelling real life examples. They can mainly be grouped into three classes according to the way they are defined:

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Received:15 December 2019, Accepted:26 March 2020
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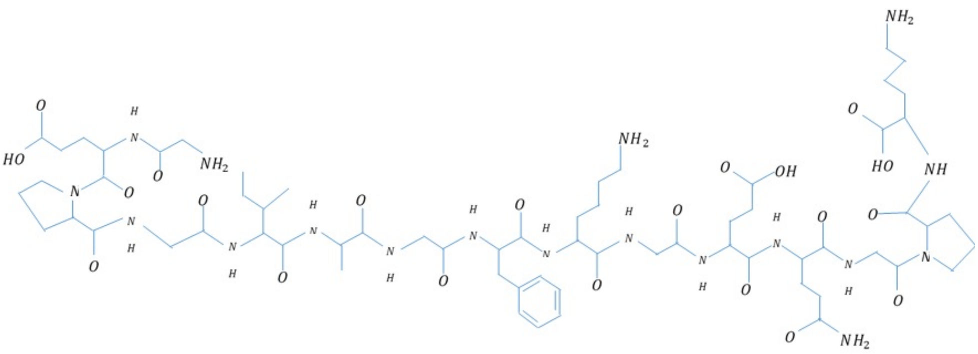

Figure 1. Collagen

by vertex degrees, by matrices or by distances.

Now let us recall some fundamental notions and results. Let $G = (V, E)$ be a simple graph with $| V(G) |= n$ vertices and $| E(G) |= m$ edges. n and m are respectively called as the order and size of the graph. Here, we do not allow neither loops nor multiple edges. For a vertex $v \in V(G)$, we denote the degree of v by $d_G(v)$ or d_v.

Two of the most important topological graph indices are called the first and second Zagreb indices denoted by $M_1(G)$ and $M_2(G)$, respectively:

$$M_1(G) = \sum_{u \in V(G)} d_G^2(u) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v). \tag{1.1}$$

These indices were defined in 1972 by Gutman and Trinajstic, [1], and are referred to due to their uses in chemistry with QSAR and QSPR studies. In [2], some results are given on the first and also some other Zagreb indices. These indices are calculated for some graph operations, in [3].

The F-index or with its better known name, the forgotten index of a graph G is denoted by $F(G)$ or $M_3(G)$ and defined as the sum of the cubes of the degrees of the vertices of the given graph. The chemical quantity called the total π-electron energy depends on the degree based sums $M_1(G)$ and $F(G) = \sum_{u \in V(G)} d_G^3(u)$. They first appeared in the study of structure-dependency of total π-electron energy in 1972, [1]. The first index was later named as the first Zagreb index and the second sum has never been further studied, [5], although it was shown to have an exceptional applicative potential.

The hyper-Zagreb index was defined as a new variety of the class of Zagreb indices by

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2,$$

see [5].

The study of the heat of formation for heptanes and octanes inspired Furtula et al. for defining a new index, called the augmented Zagreb index, resulting in better prediction power, [10]. It was defined by

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$

The harmonic index was introduced by Zhong, [6]. Zhong found that this index correlates well with Π-electron energy of benzenoid hydrocarbons and defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

Ranjini et al., [4], introduced the redefined Zagreb indices, i.e. the redefined first, second and third Zagreb indices for a graph G defined respectively by

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \cdot d_v},$$

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v},$$

and

$$ReZG_3(G) = \sum_{uv \in E(G)} (d_u \cdot d_v)(d_u + d_v).$$

Zagreb indices were reformulated in terms of the edge degrees instead of the vertex-degrees by Milicevic et. al., [7], as follows:

$$RM_1(G) = \sum_{uv \in E(G)} d(e)^2,$$

and

$$RM_2(G) = \sum_{e,e' \in E(G)} d(e)d(e')$$

where e, e' are pairs of incident edges of the graph G.

Aram and Dehgardi, [8], introduced the concept of reformulated F-index as

$$RF(G) = \sum_{uv \in E(G)} d(uv)^3.$$

Recently Kulli introduced the first and second K Banhatti indices to take into account the contributions of pairs of incident elements, [9]. They are defined as

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

and

$$B_2(G) = \sum_{u,e} d_G(u)d(e).$$

In this paper, we shall find some topological indices of type II collagen molecule which we denote by G^* throughout the paper.

2. Main Results

Now we will determine some well-known topological indices of G^*. First we have

Lemma 2.1. *The first and second Zagreb indices of G^* are $M_1(G^*) = 1166$ and $M_2(G^*) = 1510$.*

Proof. Let us partition the set of all edges of G^* into subsets $E_{(d_u,d_v)}$ where d_u and d_v denote the vertex degrees of the end vertices of an edge uv. In G^*, we get the partition of edges $E_{(1,2)}$, $E_{(1,3)}$, $E_{(1,4)}$, $E_{(2,3)}$, $E_{(3,3)}$, $E_{(3,4)}$ and $E_{(4,4)}$. The number of edges of these types for one unit are 3, 43, 74, 3, 21, 38 and 26, respectively.

Recall that $M_1(G) = \sum_{uv\in E(G)}(d_u + d_v)$. First, we will calculate $M_1(G)$ for one unit:

$$\begin{aligned} M_1(G^*) &= \mid E_{(1,2)} \mid (1+2)+ \mid E_{(1,3)} \mid (1+3)+ \mid E_{(1,4)} \mid (1+4) \\ &+ \mid E_{(2,3)} \mid (2+3)+ \mid E_{(3,3)} \mid (3+3) \\ &+ \mid E_{(3,4)} \mid (3+4)+ \mid E_{(4,4)} \mid (4+4) \\ &= 3\cdot(1+2) + 43\cdot(1+3) + 74\cdot(1+4) + 3\cdot(2+3) \\ &+ 21\cdot(3+3) + 38\cdot(3+4) + 26\cdot(4+4) \\ &= 1166. \end{aligned}$$

As $M_2(G) = \sum_{uv\in E(G)} d_u d_v$, we get the result by similar calculations:

$$\begin{aligned} M_2(G^*) &= \mid E_{(1,2)} \mid (1\cdot 2)+ \mid E_{(1,3)} \mid (1\cdot 3)+ \mid E_{(1,4)} \mid (1\cdot 4) \\ &+ \mid E_{(2,3)} \mid (2\cdot 3)+ \mid E_{(3,3)} \mid (3\cdot 3) \\ &+ \mid E_{(3,4)} \mid (3\cdot 4)+ \mid E_{(4,4)} \mid (4\cdot 4) \\ &= 3\cdot(1\cdot 2) + 43\cdot(1\cdot 3) + 74\cdot(1\cdot 4) + 3\cdot(2\cdot 3) \\ &+ 21\cdot(3\cdot 3) + 38\cdot(3\cdot 4) + 26\cdot(4\cdot 4) \\ &= 1510. \end{aligned}$$

□

Lemma 2.2. *The third Zagreb index (forgotten index) of G^* is $F(G^*) = 3902$.*

Proof. We know that $F(G) = \sum_{u\in V(G)} {d_u}^3$, i.e.,

$$F(G^*) = \sum_{u\in V} {d_u}^3 = 1^3\cdot 120 + 2^3\cdot 3 + 3^3\cdot 42 + 4^3\cdot 41 = 3902.$$

□

Lemma 2.3. *The hyper-Zagreb index of G^* is $HM(G^*) = 6922$.*

Proof. We know that $HM(G) = \sum_{uv\in E(G)}(d_u + d_v)^2$. Therefore

$$\begin{aligned} HM(G^*) &= \mid E_{(1,2)} \mid (1+2)^2+ \mid E_{(1,34)} \mid (1+3)^2 \\ &+ \mid E_{(1,4)} \mid (1+4)^2+ \mid E_{(2,3)} \mid (2+3)^2+ \mid E_{(3,3)} \mid (3+3)^2 \\ &+ \mid E_{(3,4)} \mid (3+4)^2+ \mid E_{(4,4)} \mid (4+4)^2 \\ &= 3(1+2)^2 + 43(1+3)^2 + 74(1+4)^2 \\ &+ 3(2+3)^2 + 21(3+3)^2 + 38(3+4)^2 + 26(4+4)^2 = 6922. \end{aligned}$$

□

Lemma 2.4. *The augmented Zagreb index of G^* is $AZI(G^*) =\approx 1626,087$.*

Proof. We recall that the augmented Zagreb index was defined by $AZI(G) = \sum_{uv\in E(G)}(\frac{d_u\cdot d_v}{d_u+d_v-2})^3$. Therefore we obtain

$$\begin{aligned} AZI(G^*) &= \mid E_{(1,2)} \mid (\frac{1\cdot 2}{1+2-2})^3+ \mid E_{(1,3)} \mid (\frac{1\cdot 3}{1+3-2})^3 \\ &+ \mid E_{(1,4)} \mid (\frac{1\cdot 4}{1+4-2})^3+ \mid E_{(2,3)} \mid (\frac{2\cdot 3}{2+3-2})^3 \\ &+ \mid E_{(3,3)} \mid (\frac{3\cdot 3}{3+3-2})^3+ \mid E_{(3,4)} \mid (\frac{3\cdot 4}{3+4-2})^3 \\ &+ \mid E_{(4,4)} \mid (\frac{4\cdot 4}{4+4-2})^3 \\ &= 3\cdot 2^3 + 43(\frac{3}{2})^3 + 74(\frac{4}{3})^3 + 3\cdot 2^3 + 21(\frac{9}{4})^3 + 38(\frac{12}{5})^3 + 26(\frac{8}{3})^3 \\ &= 1626,087\cdots. \end{aligned}$$

□

Lemma 2.5. *The harmonic index of G^* is $H(G^*) = 78,66$.*

Proof. Recall that $H(G) = \sum_{uv\in E(G)} \frac{2}{d_u+d_v}$. Hence

$$\begin{aligned} H(G^*) &= |E_{(1,2)}| \frac{2}{1+2} + |E_{(1,3)}| \frac{2}{1+3} + |E_{(1,4)}| \frac{2}{1+4} \\ &+ |E_{(2,3)}| \frac{2}{2+3} + |E_{(3,3)}| \frac{2}{3+3} + |E_{(3,4)}| \frac{2}{3+4} + |E_{(4,4)}| \frac{2}{4+4} \\ &= 2 + 43\cdot\frac{1}{2} + 74\cdot\frac{2}{5} + 3\cdot\frac{2}{5} + 21\cdot\frac{1}{3} + 38\cdot\frac{2}{7} + 26\cdot\frac{1}{4} \simeq 78,66. \end{aligned}$$

□

Lemma 2.6. *The redefined versions of Zagreb indices of G^* are $ReZG_1(G) \simeq 205,97$, $ReZG_2(G) \simeq 245,69$ and $ReZG_3(G) = 9758$.*

Proof. We recall that the first redefined Zagreb index was defined by $ReZG_1(G) = \sum_{uv\in E(G)} \frac{d_u+d_v}{d_u\cdot d_v}$. Hence we get

$$\begin{aligned} ReZG_1(G^*) &= |E_{(1,2)}| \frac{1+2}{1\cdot 2} + |E_{(1,3)}| \frac{1+3}{1\cdot 3} + |E_{(1,4)}| \frac{1+4}{1\cdot 4} \\ &+ |E_{(2,3)}| \frac{2+3}{2\cdot 3} + |E_{(3,3)}| \frac{3+3}{3\cdot 3} + + |E_{(3,4)}| \frac{3+4}{3\cdot 4} \\ &+ |E_{(4,4)}| \frac{4+4}{4\cdot 4} \\ &= 3\cdot\frac{3}{2} + 43\cdot\frac{4}{3} + 74\cdot\frac{5}{4} + 3\cdot\frac{5}{6} + 21\cdot\frac{2}{3} + 38\cdot\frac{7}{12} + 26\cdot\frac{1}{2} \\ &\simeq 205,97. \end{aligned}$$

Using similar methods, we get the other results for the second and third redefined Zagreb indices. □

Lemma 2.7. *The reformulated Zagreb indices of G^* are $RM_1(G^*) = 2951$ and $RM_2(G^*) = 3022$.*

Proof. In G^*, the degrees $d(uv)$ of the edges where uv is an edge are 1, 2, 3, 4, 5 and 6. The number of these edge degrees of G^* are $|d(uv) = 1| = 3, |d(uv) = 2| = 43, |d(uv) = 3| = 74, |d(uv) = 4| = 14, |d(uv) = 5| = 38$ and $|d(uv) = 6| = 26$.

Recall that $RM_1(G) = \sum_{uv\in E(G)} d(uv)^2$. Therefore, we find

$$RM_1(G^*) = 3\cdot 1^2 + 43\cdot 2^2 + 74\cdot 3^2 + 14\cdot 4^2 + 38\cdot 5^2 + 26\cdot 6^2 = 2951.$$

To calculate $RM_2(G^*)$, we partition the pairs of incident edges in G^* according to the product of their edge degrees $d(e)\cdot d(e')$ where $e, e' \in E$ and $e\ e'$. In G^*, we get $d(2)\cdot d(3), d(2)\cdot d(5), d(3)\cdot d(3), d(3)\cdot d(4), d(3)\cdot d(5), d(3)\cdot d(6), d(4)\cdot d(4), d(4)\cdot d(6), d(5)\cdot d(6)$ and $d(6)\cdot d(6)$. The number of these types of products are 6, 6, 54, 12, 18, 41, 7, 4, 6 and 25, respectively.

As $RM_2(G) = \sum_{e,e'\in E(G)} d(e)d(e')$, we find

$$\begin{aligned} RM_2(G^*) &= |d(2)\cdot d(3)|\cdot 2\cdot 3 + |d(2)\cdot d(5)|\cdot 2\cdot 5 \\ &+ |d(3)\cdot d(3)|\cdot 3\cdot 3 + |d(3)\cdot d(4)|\cdot 3\cdot 4 + |d(3)\cdot d(5)|\cdot 3\cdot 5 \\ &+ |d(3)\cdot d(6)|\cdot 3\cdot 6 + |d(4)\cdot d(4)|\cdot 4\cdot 4 + |d(4)\cdot d(6)|\cdot 4\cdot 6 \\ &+ |d(5)\cdot d(6)|\cdot 5\cdot 6 + |d(6)\cdot d(6)|\cdot 6\cdot 6 \\ &= 6\cdot 6 + 6\cdot 10 + 54\cdot 9 + 12\cdot 12 + 18\cdot 15 + 41\cdot 18 + 7\cdot 16 \\ &+ 4\cdot 24 + 6\cdot 30 + 25\cdot 36 \\ &= 3022. \end{aligned}$$

□

Lemma 2.8. *The reformulated F-index of G^* is $RF(G^*) = 13607$.*

Proof. Since $RF(G) = \sum_{uv\in E(G)} d(uv)^3$, the calculations are similar to $RM_1(G^*)$. □

Lemma 2.9. *The Banhatti indices of G^* are $B_1(G^*) = 2535$ and $B_2(G^*) = 4377$.*

Proof. We know that $B_1(G) = \sum_{u,e} d_G(u) + d(e)$. Therefore we find

$$\begin{aligned} B_1(G^*) &= 3[(1+1)+(1+2)] + 43[(2+1)+(2+3)] + 74[(3+1)+(3+4)] \\ &+ +14[(4+3)+(4+3)] + 38[(5+3)+(5+4)] + 26[(6+4)+(6+4)] \\ &= 2535 \end{aligned}$$

and

$$\begin{aligned} B_2(G^*) &= 3[(1\cdot 1)+(1\cdot 2)] + 43[(2\cdot 1)+(2\cdot 3)] + 74[(3\cdot 1)+(3\cdot 4)] \\ &+ 14[(4\cdot 3)+(4\cdot 3)] + 38[(5\cdot 3)+(5\cdot 4)] + 26[(6\cdot 4)+(6\cdot 4)] \\ &= 4377. \end{aligned}$$

□

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