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SOME TOPOLOGICAL INDICES OF VITAMIN K

[1]Dr. M. GAYATHRI
Associate Professor
[1]Department of Mathematics, Government First Grade College, Varthur, Bangalore-87

Abstract: In this paper, I computed topological indices of Vitamin K such as ABC index, Fourth atom bond connectivity index, Randic connectivity index, Sum connectivity index,Geometric arithmetic index, Fifth Geometric arithmetic index, First Zagreb index, Second Zagreb index, First multiple Zagreb index, Second multiple Zagreb index,Augmented Zagreb index, Harmonic index, Hyper-Zagreb index, First modified Zagreb index,Second modofied Zagreb index,Symmetric division deg index, Redefined First, Second, Third Zagreb index, Arithmetic-Geometric index.

Index Terms: ABC index, Fourth atom bond connectivity index, Randic connectivity index, Sum connectivity index,Geometric arithmetic index, Fifth Geometric arithmetic index, First Zagreb index, Second Zagreb index, First multiple Zagreb index, Second multiple Zagreb index,Augmented Zagreb index, Harmonic index, Hyper-Zagreb index, First modified Zagreb index,Second modofied Zagreb index,Symmetric division deg index, Redefined First, Second, Third Zagreb index, Arithmetic-Geometric index and Vitamin K.

1. Introduction:

Vitamin K plays a key role in helping the blood clot, preventing excessive bleeding. Unlike many other vitamins, vitamin K is not typically used as a dietary supplement.

Vitamin K is actually a group of compounds. The most important of these compounds appears to be Vitamin K1 and Vitamin K2. Vitamin K1 is obtained from leafy greens and some other vegetables. Vitamin K2 is a group of compounds largely obtained from meats, cheeses, and eggs, and synthesized by bacteria.

Vitamin K is found throughout the body including the liver, brain, heart, pancreas, and bone. It is broken down very quickly and excreted in urine or stool. Because of this, it rarely reaches toxic levels in the body even with high intakes, as may sometimes occur with other fat-soluble vitamins.

Vitamin K deficiency in adults is rare, but may occur in people taking medications that block vitamin K metabolism such as antibiotics, or in those with conditions that cause malabsorption of food and nutrients. A deficiency is also possible in new born infants because vitamin K does not cross the placenta, and breast milk contains a low amount. The limited amount of blood clotting proteins at birth increases the risk of bleeding in infants if they are not given vitamin K supplements. The following are the most common signs of a deficiency.

A topological graph index, also called a molecular descriptor, is a mathematical formula that can be applied to any graph which models some molecular structure. From this index, it is possible to analyse mathematical values and further investigate some physicochemical properties of a molecule like boiling point, enthalpy of vaporization, stability etc.,. Therefore, it is an efficient method in avoiding expensive and time-consuming laboratory experiments.

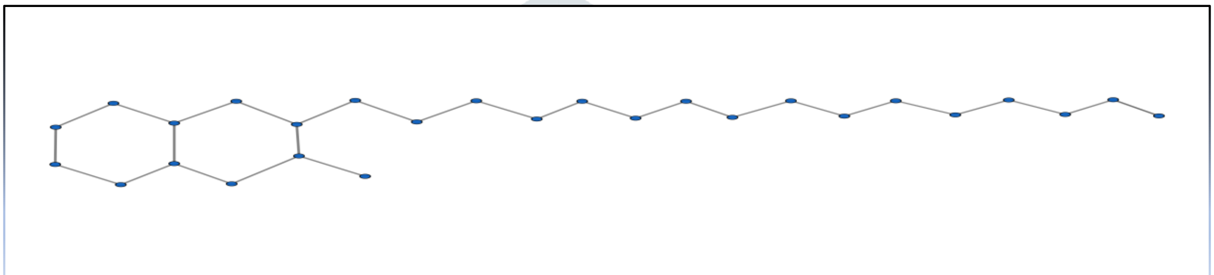
A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Note that hydrogen atoms are often omitted. All molecular graphs considered in this paper are finite, connected, loopless and without multiple edges. Let $G=(V,E)$ be a graph with vertex set V and an edge set E. The degree of a vertex

$u \in E(G)$ is denoted by d_u and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv.

Nowadays, there are numerous topological indices, some applied in chemistry. They can be classified by the structural properties of the graphs used for their calculation. Since then, over 3000 topological graph indices are registered in Chemical Data Bases. This research area is studied by mathematicians and chemists. There is a rapidly increasing interest in this topic, therefore topological graph indices are researched worldwide.

In this paper, we determine the topological indices[1] like ABC index[2], Fourth atom bond connectivity index[3], Randic connectivity index[4], Sum connectivity index[5],Geometric arithmetic index[6], Fifth Geometric arithmetic index, First Zagreb index[5], Second Zagreb index[5], First multiple Zagreb index[5], Second multiple Zagreb index[5],Augmented Zagreb index[5], Harmonic index[8], Hyper-Zagreb index[7], First modified Zagreb index[7],Second modified Zagreb index[7],Symmetric division deg index, Redefined First, Second, Third Zagreb index, Arithmetic-Geometric index[9] and Vitamin K.

Structure of Vitamin K:



Vitamin K Structure

2.1 Definition:

Let $G=(V,E)$ be a molecular graph and d_u is the degree of the vertex u, then ABC index of G is defined as, $ABC(G)=\sum_{uv\in E}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$. In 2009, Furtula et al. introduced Atom Bond Connectivity (ABC) index, which it has been applied up until now to study the stability of alkanes and strain energy of cyclo alkanes. The ABC index has proven to be a valuable predictive index in the study of the heat of formation in alkanes.

2.2 Definition :

Let G be a graph, then its fourth ABC index is defined as, $ABC_4(G)=\sum_{uv\in E}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$, Where S_u is sum of the degrees of all neighbours of vertex u in G. In other words $S_u=\sum_{uv\in E(G)} d_v$, Similarly for S_v. The fourth atom bond connectivity index $ABC_4(G)$ was introduced by M. Ghorbani et al. in 2010.

2.3 Definition :

The Randic connectivity index $\chi(G)$ is one of the classical graph based molecular structure descriptors that found countless applications in chemistry and pharmacology. In particular for designing quantitative structure property and structure activity relations. The randic connectivity index is also known as product connectivity index. It was invented in 1976 by Milan Randic and is defined as

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}$$

2.4 Definition:

The sum connectivity index was proposed by Zhou and Trinajstic in 2009, which is defined as the sum over all the edges of the graph of the terms $\left(d_G(a_1)+d_G(a_2)\right)^{-\frac{1}{2}}$. This concept was extended to the general sum connectivity index in 2010 which is defined as follows

$$\chi_\alpha(G)=\sum_{a_1a_2\in E(G)}\left(d_G(a_1)+d_G(a_2)\right)^\alpha$$

Where α is a real number. Then $\chi_{-\frac{1}{2}}(G)$ is the classical sum connectivity index.

2.5 Definition:

In 2009, Vukičević and Furtula introduced the geometric-arithmetic index. Geometric-arithmetic index is one of the most studied graph invariant to characterize the topological aspects of underlying interconnection networks or graphs.

Let G be a graph and $e=uv$ be an edge of G then $GA(G)=\sum_{e=uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}$

2.6 Definition:

The fifth geometric-arithmetic index is used to test the chemical properties of chemical compounds, nanomaterials and drugs. The Fifth geometric-arithmetic topological indices was introduced by A. Graovac et al. For a graph G, the fifth Geometric arithmetic index is defined as $GA(G)=\sum_{e=uv\in E(G)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}$

Where S_u is sum of the degrees of all neighbours of vertex u in G. In other words $S_u=\sum_{uv\in E(G)}d_v$, Similarly for S_v.

2.7 Definition :

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestic. The Zagreb indices are the oldest graph invarients used in mathematical chemistry to predict the chemical phenomena. For a simple connected graph G, the first Zagreb index is equal to the sum of squares of the degrees of vertices and the second Zagreb index is equal to the sum of the products of the degrees of pairs of adjacent vertices.

$$M_1(G)=\sum_{e=uv\in E(G)}(d_u+d_v)$$

$$M_2(G)=\sum_{e=uv\in E(G)}(d_ud_v)$$

Where d_v denotes the degree of vertex *v* in G.

2.8 Definition:

In 2012, M. Ghorbani and N. Azimi defined the Multiple Zagreb topological indices of a graph G, based on degree of vertices of G. For a simple connected graph G, the first and second multiple Zagreb indices were defined as follows

$$PM_1(G)=\prod_{e=uv\in E(G)}(d_u+d_v)$$

$$PM_2(G)=\prod_{e=uv\in E(G)}(d_ud_v)$$

2.9 Definition:

The Augmented Zagreb index (AZI) possess the best correlating ability among several topological indices. Boris Furtula proposed a topological index called Augmented Zagreb index, defined as

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

Boris Furtula et al. proved that AZI is a valuable predictive index in the study of the heat of formation in heptanes and octanes. Boris Furtula et al have studied extremal properties of AZI index of trees and chemical trees, they proved that among all trees the star has the minimum AZI value.

2.10 Definition:

Favaron et al. considered the relationship between the harmonic index and the eigen values of graphs. Zhong determined the minimum and maximum values of harmonic index on simple connected graphs,trees, unicyclic graphs and bicyclic graphs respectively, and characterized the corresponding extremal graphs. Some upper and lower bounds on the harmonic index of a graph were obtained by Ilic. Xu and Deng et al. established some relationship between the harmonic index of a graph and its topological indices, such as Randic index, atom bond connectivity index, chromatic number and radius respectively. Wu et al. determined the graph with minimum harmonic index among all the graphs with minimum degree at least two.

Let $G = (V, E)$ be a graph and d_u be the degree of a vertex u then Harmonic index is defined as $H(G) = \sum_{e=uv \in E(G)} \frac{2}{d_u + d_v}$

2.11 Definition:

G.H. Shirdel et.al introduced a new distance based of Zagreb indices of a graph G named Hyper- Zagreb index.

The Hyper Zagreb index is defined as, $HM(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^2$

2.12 Definition:

The first Zagreb and the second Zagreb index give greater weights to the inner vertices and edges, and smaller weights to outer vertices and edges which opposes intuitive reasoning. Hence, they were amended as, for a simple connected graph G, let ${}^{m}M_1(G) = \sum_{v \in v(G)} \frac{1}{[d(v)]^2}$ which was called the first modified Zagreb index, ${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$ which was called the second modified Zagreb index.

2.13 Definition:

The symmetric division deg index(or simply sdd-index) was proposed byVukicevic et.al. as a remarkable predictor of total surface area of polychlorobiphenyls. It is one of discrete Adriatic indices that showed good predictive properties on the testing sets provided by international Academy of Mathematical Chemistry.

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right) = \sum_{uv \in E(G)} \left(\frac{d_r^2 + d_s^2}{d_u d_v} \right)$$

2.14 Definition :

Ranjini et al redefined the Zagreb indice, i.e., the redefined first, second and third Zagreb indices for a graph G and these are defined as

$$\operatorname{Re} ZG_1(G) = \sum_{uv\in E(G)} \frac{d(u)+d(v)}{d(u)d(v)}$$

$$\operatorname{Re} ZG_2(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$$

$$\operatorname{Re} ZG_3(G) = \sum_{uv\in E(G)} d(u)d(v)\left(d(u)+d(v)\right)$$

2.15 Definition:

The arithmetic-geometric index AG(G) was recently introduced as a modification of the well known geometric arithmetic index. The arithmetic-geometricindex is defined as

$$AG(G) = \sum_{uv\in E(G)} \frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}}$$

3. Main Results:

3.1 Theorem: The Atom bond connectivity index of Vitamin K is given by $ABC(C_{31}H_{46}O_2) = 23.2028$

Proof: Consider a vitamin K $C_{31}H_{46}O_2$. Let $m_{i,j}$ denotes edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of Vitamin K(as shown in the Figure-1) contains edges of the type $m_{2,2}$, $m_{2,3}$, $m_{3,3}$, $m_{3,1}$. From the figure, the number edges of these types are as follows. $|m_{2,2}| = 10$, $|m_{2,3}| = 14$, $|m_{3,3}| = 2$, $|m_{3,1}| = 6$. Therefore the atom-bond connectivity index of Vitamin K is

$$ABC(C_{31}H_{46}O_2) = \sum_{uv\in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$ABC(C_{31}H_{46}O_2) = |m_{2,2}| \sqrt{\frac{2+2-2}{2.2}} + |m_{2,3}| \sqrt{\frac{2+3-2}{2.3}} + |m_{3,3}| \sqrt{\frac{3+3-2}{3.3}} + |m_{3,1}| \sqrt{\frac{3+1-2}{3.1}}$$

$$= 10(0.7071) + 14(0.7071) + 2(0.6667) + 6(0.8165) = 23.2028$$

3.2 Theorem: The fourth atom bond connectivity index of Vitamin K is $ABC_4(C_{31}H_{46}O_2) = 18.3477$

Proof: Let $e_{i,j}$ denotes the edges of Vitamin K with $i = S_u$ and $j = S_v$. It is easy to see that the summation of degrees of edge endpoints of Vitamin K have twelve edge types $e_{3,4}$, $e_{3,5}$, $e_{3,6}$, $e_{4,4}$, $e_{4,5}$, $e_{5,5}$, $e_{5,7}$, $e_{5,8}$, $e_{6,6}$, $e_{6,7}$, $e_{6,8}$, $e_{7,7}$ as shown in the following Figure 1. Clearly from the figure 1, $|e_{3,4}| = 2$, $|e_{3,5}| = 3$, $|e_{3,6}| = 1$, $|e_{4,4}| = 1$, $|e_{4,5}| = 9$, $|e_{5,5}| = 7$, $|e_{5,7}| = 2$, $|e_{5,8}| = 1$, $|e_{6,6}| = 1$, $|e_{6,7}| = 2$, $|e_{6,8}| = 2$, $|e_{7,7}| = 1$. The fourth atom-bond connectivity index of vitamin K.

$$ABC_4(C_{31}H_{46}O_2) = |e_{3,4}|\sqrt{\frac{3+4-2}{3.4}} + |e_{3,5}|\sqrt{\frac{3+5-2}{3.5}} + |e_{3,6}|\sqrt{\frac{3+6-2}{3.6}} + |e_{4,4}|\sqrt{\frac{4+4-2}{4.4}}$$

$$+ |e_{4,5}|\sqrt{\frac{4+5-2}{4.5}} + |e_{5,5}|\sqrt{\frac{5+5-2}{5.5}} + |e_{5,7}|\sqrt{\frac{5+7-2}{5.7}} + |e_{5,8}|\sqrt{\frac{5+8-2}{5.8}}$$

$$+ |e_{6,6}|\sqrt{\frac{6+6-2}{6.6}} + |e_{6,7}|\sqrt{\frac{6+7-2}{6.7}} + |e_{6,8}|\sqrt{\frac{6+8-2}{6.8}} + |e_{7,7}|\sqrt{\frac{7+7-2}{7.7}}$$

$$ABC_4(C_{31}H_{46}O_2) = 2(0.6455)+3(0.3625)+1(0.6236)+1(0.6124)+9(0.5916)$$
$$+7(0.5657)+2(0.5345)+1(0.5244)+1(0.5270)+2(0.5118)$$
$$+2(0.5)+1(0.4949)$$

$$ABC_4(C_{31}H_{46}O_2) = 18.3477$$

3.3Theorem: The Randic connectivity index of Vitamin K is $\chi\left(C_{31}H_{46}O_2\right)=14.8458$

Proof: Consider Randic connectivity index of Vitamin K

$$\chi\left(C_{31}H_{46}O_2\right)=\left|m_{2,2}\right|\sqrt{\frac{1}{2.2}}+\left|m_{2,3}\right|\sqrt{\frac{1}{2.3}}+\left|m_{3,3}\right|\sqrt{\frac{1}{3.3}}+\left|m_{3,1}\right|\sqrt{\frac{1}{3.1}}$$
$$=10(0.5)+14(0.4082)+2(0.3333)+6(0.5774)$$
$$=14.8458$$

3.4 Theorem: The sum connectivity index of Vitamin K is $\chi_\alpha\left(C_{31}H_{46}O_2\right)=15.0772$

Proof: Consider the sum connectivity index of vitamin K,

$$\chi_\alpha\left(C_{31}H_{46}O_2\right)=\sum_{e=uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}$$
$$=\left|m_{2,2}\right|\sqrt{\frac{1}{2+2}}+\left|m_{2,3}\right|\sqrt{\frac{1}{2+3}}+\left|m_{3,3}\right|\sqrt{\frac{1}{3+3}}+\left|m_{3,1}\right|\sqrt{\frac{1}{3+1}}$$
$$=10(0.5)+14(0.4472)+2(0.4082)+6(0.5)$$
$$=15.0772$$

3.5 Theorem: The Geometric-arithmetic index of Vitamin K is $GA(C_{31}H_{46}O_2)=30.9132$

Proof: Consider the Geometric-arithmetic index of Vitamin K

$$GA(C_{31}H_{46}O_2)=\sum_{e=uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$$
$$=\left|m_{2,2}\right|\frac{2\sqrt{2.2}}{2+2}+\left|m_{2,3}\right|\frac{2\sqrt{2.3}}{2+3}+\left|m_{3,3}\right|\frac{2\sqrt{3.3}}{3+3}+\left|m_{3,1}\right|\frac{2\sqrt{3.1}}{3+1}$$
$$=10(1)+14(0.9798)+2(1)+6(0.8660)$$
$$=30.9132$$

3.6 Theorem: The Fifth Geometric-arithmetic index of Vitamin K is $GA_5(C_{31}H_{46}O_2)=31.6894$

Proof: Consider the Fifth Geometric-arithmetic index of Vitamin K

$$GA_5(C_{31}H_{46}O_2)=\left|e_{3,4}\right|\sqrt{\frac{3+4-2}{3.4}}+\left|e_{3,5}\right|\sqrt{\frac{3+5-2}{3.5}}+\left|e_{3,6}\right|\sqrt{\frac{3+6-2}{3.6}}+\left|e_{4,4}\right|\sqrt{\frac{4+4-2}{4.4}}$$
$$+\left|e_{4,5}\right|\sqrt{\frac{4+5-2}{4.5}}+\left|e_{5,5}\right|\sqrt{\frac{5+5-2}{5.5}}+\left|e_{5,7}\right|\sqrt{\frac{5+7-2}{5.7}}+\left|e_{5,8}\right|\sqrt{\frac{5+8-2}{5.8}}$$

$$+\left|e_{6,6}\right|\sqrt{\frac{6+6-2}{6.6}}+\left|e_{6,7}\right|\sqrt{\frac{6+7-2}{6.7}}+\left|e_{6,8}\right|\sqrt{\frac{6+8-2}{6.8}}+\left|e_{7,7}\right|\sqrt{\frac{7+7-2}{7.7}}$$

$$GA_5(C_{31}H_{46}O_2)=2(0.6455)+3(0.3625)+1(0.6236)+1(0.6124)+9(0.5916)$$

$$+7(0.5657)+2(0.5345)+1(0.5244)+1(0.5270)+2(0.5118)$$

$$+2(0.5)+1(0.4949)$$

$$GA_5(C_{31}H_{46}O_2)=18.3477$$

3.7 Theorem: The First Zagreb index of Vitamin K is $M_1(C_{31}H_{46}O_2)=146$

Proof: First Zagreb index = $\sum_{e=uv\in E(G)}(d_u+d_v)$

$$=\left|m_{2,2}\right|(2+2)+\left|m_{2,3}\right|(2+3)+\left|m_{3,3}\right|(3+3)+\left|m_{3,1}\right|(3+1)$$

$$=\left|m_{2,2}\right|(4)+\left|m_{2,3}\right|(5)+\left|m_{3,3}\right|(6)+\left|m_{3,1}\right|(4)$$

$$=10(4)+14(5)+2(6)+6(4)$$

$$=40+70+12+24=146$$

3.8 Theorem: The Second Zagreb index of Vitamin K is $M_1(C_{31}H_{46}O_2)=140$

Proof: Second Zagreb index = $\sum_{e=uv\in E(G)}(d_u.d_v)$

$$=\left|m_{2,2}\right|(2.2)+\left|m_{2,3}\right|(2.3)+\left|m_{3,3}\right|(3.3)+\left|m_{3,1}\right|(3.1)$$

$$=\left|m_{2,2}\right|(4)+\left|m_{2,3}\right|(6)+\left|m_{3,3}\right|(9)+\left|m_{3,1}\right|(3)$$

$$=10(4)+14(6)+2(9)+6(3)$$

$$=40+64+18+18=140$$

3.9 Theorem: The First Multiple Zagreb index of Vitamin K is $PM_1(C_{31}H_{46}O_2)=9.437184\times10^{20}$

Proof: The First Multiple Zagreb index of vitamin K is

$$PM_1(C_{31}H_{46}O_2)=\prod_{e=uv\in E(G)}(d_u+d_v)$$

$$=\prod_{e=uv\in m_{2,2}}(d_u+d_v)+\prod_{e=uv\in m_{2,3}}(d_u+d_v)+\prod_{e=uv\in m_{3,3}}(d_u+d_v)+\prod_{e=uv\in m_{3,1}}(d_u+d_v)$$

$$=4^{10}\times5^{14}\times6^2\times4^6$$

$$=9.437184\times10^{20}$$

3.10 Theorem: The Second Multiple Zagreb index of Vitamin K is $PM_2(C_{31}H_{46}O_2) = 4.8521 \times 10^{21}$

Proof: The Second Multiple Zagreb index of vitamin K is

$$PM_2(C_{31}H_{46}O_2) = \prod_{e=uv\in E(G)} (d_u \times d_v)$$

$$= \prod_{e=uv\in m_{2,2}} (d_u \times d_v) + \prod_{e=uv\in m_{2,3}} (d_u \times d_v) + \prod_{e=uv\in m_{3,3}} (d_u \times d_v) + \prod_{e=uv\in m_{3,1}} (d_u \times d_v)$$

$$= 4^{10} \times 6^{14} \times 9^2 \times 3^6 = 4.8521 \times 10^{21}$$

3.11 Theorem: The Augmented Zagreb index of Vitamin K is $AZI(C_{31}H_{46}O_2) = 235.0312$

Proof: Augmented Zagreb index $AZI(G) = \sum_{uv\in E} \left[\frac{d_u d_v}{d_u + d_v - 2} \right]^3$

$$= |m_{2,2}| \left[\frac{2.2}{2+2-2} \right]^3 + |m_{2,3}| \left[\frac{2.3}{2+3-2} \right]^3 + |m_{3,3}| \left[\frac{3.3}{3+3-2} \right]^3 + |m_{3,1}| \left[\frac{3.1}{3+1-2} \right]^3$$

$$= 10(8) + 14(8) + 2\left(\frac{729}{64} \right) + 6\left(\frac{27}{8} \right)$$

$$= 235.0312$$

3.12 Theorem: The Harmonic index of Vitamin K is $H(C_{31}H_{46}O_2) = 14.2667$

Proof: The Harmonic index $H(G) = \sum_{e=uv\in E(G)} \frac{2}{d_u + d_v}$

$$= |m_{2,2}| \left[\frac{2}{2+2} \right] + |m_{2,3}| \left[\frac{2}{2+3} \right] + |m_{3,3}| \left[\frac{2}{3+3} \right] + |m_{3,1}| \left[\frac{2}{3+1} \right]$$

$$= 10\left(\frac{1}{2} \right) + 14\left(\frac{2}{5} \right) + 2\left(\frac{2}{6} \right) + 6\left(\frac{1}{2} \right)$$

$$= \frac{214}{15} = 14.2667$$

3.13 Theorem: The Hyper Zagreb index of Vitamin K is $HM(C_{31}H_{46}O_2) = 832$

Proof: Hyper Zagreb index = $\sum_{e=uv\in E(G)} (d_u + d_v)^2$

$$= |m_{2,2}| [2+2]^2 + |m_{2,3}| [2+3]^2 + |m_{3,3}| [3+3]^2 + |m_{3,1}| [3+1]^2$$

$$= 10(16) + 14(36) + 2(36) + 6(16) = 832$$

3.14 Theorem: The First Modified Zagreb index of Vitamin K is ${}^{m}M_1(C_{31}H_{46}O_2)=11.1389$

Proof: First Modified Zagreb index ${}^{m}M_1(G)=\sum_{v\in v(G)}\frac{1}{[d(v)]^2}$

$$=\frac{1}{2^2}(17)+\frac{1}{3^2}(8)+\frac{1}{1^2}(6)=11.1389$$

3.15 Theorem: The Second Modified Zagreb index of Vitamin K is ${}^{m}M_2(C_{31}H_{46}O_2)=7.0556$

Proof: Second Modified Zagreb index ${}^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d(u)d(v)}$

$$=|m_{2,2}|\frac{1}{2.2}+|m_{2,3}|\frac{1}{2.3}+|m_{3,3}|\frac{1}{3.3}+|m_{3,1}|\frac{1}{3.1}$$

$$=\frac{10}{4}+\frac{14}{6}+\frac{2}{9}+\frac{6}{3}=\frac{127}{18}=7.0556$$

3.16 Theorem: The symmetric division deg index of Vitamin K is $SDD(C_{31}H_{46}O_2)=74.3333$

Proof: The symmetric division deg index $SDD(G)=\sum_{uv\in E(G)}\left(\frac{d_r^2+d_s^2}{d_u d_v}\right)$

$$=|m_{2,2}|\left(\frac{4+4}{2.2}\right)+|m_{2,3}|\left(\frac{4+9}{2.3}\right)+|m_{3,3}|\left(\frac{9+9}{3.3}\right)+|m_{3,1}|\left(\frac{9+1}{3.1}\right)$$

$$=10\left(\frac{8}{4}\right)+14\left(\frac{13}{6}\right)+2\left(\frac{18}{9}\right)+6\left(\frac{10}{3}\right)=74.3333$$

3.17 Theorem: The redefined first Zagreb index Vitamin K is $\operatorname{Re}ZG_1(C_{31}H_{46}O_2)=31$

Proof: The redefined first Zagreb index $\operatorname{Re}ZG_1(G)=\sum_{uv\in E(G)}\frac{d(u)+d(v)}{d(u)d(v)}$

$$=|m_{2,2}|\left(\frac{2+2}{2.2}\right)+|m_{2,3}|\left(\frac{2+3}{2.3}\right)+|m_{3,3}|\left(\frac{3+3}{3.3}\right)+|m_{3,1}|\left(\frac{3+1}{3.1}\right)$$

$$=10\left(\frac{4}{4}\right)+14\left(\frac{5}{6}\right)+2\left(\frac{6}{9}\right)+6\left(\frac{4}{3}\right)=31$$

3.18 Theorem: The redefined second Zagreb index Vitamin K is $\operatorname{Re}ZG_2(C_{31}H_{46}O_2)=34.3$

Proof: The redefined second Zagreb index $\operatorname{Re}ZG_2(G)=\sum_{uv\in E(G)}\frac{d(u).d(v)}{d(u)+d(v)}$

$$=|m_{2,2}|\left(\frac{2.2}{2+2}\right)+|m_{2,3}|\left(\frac{2.3}{2+3}\right)+|m_{3,3}|\left(\frac{3.3}{3+3}\right)+|m_{3,1}|\left(\frac{3.1}{3+1}\right)$$

$$=10\left(\frac{4}{4}\right)+14\left(\frac{6}{5}\right)+2\left(\frac{9}{6}\right)+6\left(\frac{3}{4}\right)=34.3$$

3.19 Theorem: The redefined third Zagreb inedx Vitamin K is $\operatorname{Re} ZG_3(C_{31}H_{46}O_2)=760$

Proof: The redefined second Zagreb index

$$\operatorname{Re} ZG_3(G)=\sum_{uv\in E(G)} d(u)d(v)(d(u)+d(v))$$

$$=|m_{2,2}|(2.2)(2+2)+|m_{2,3}|(2.3)(2+3)+|m_{3,3}|(3.3)(3+3)+|m_{3,1}|(3.1)(3+1)$$

$$=10(4)(4)+14(6)(5)+2(9)(6)+6(3)(4)=760$$

3.20 Theorem: The arithmetic geometric index Vitamin K is $AG(C_{31}H_{46}O_2)=33.2169$

Proof: The arithmetic geometric index $AG(G)=\sum_{uv\in E(G)}\frac{d(u)+d(v)}{2\sqrt{d(u)d(v)}}$

$$=10\frac{(2+2)}{2\sqrt{2.2}}+14\frac{(2+3)}{2\sqrt{2.3}}+2\frac{(3+3)}{2\sqrt{3.3}}+6\frac{(3+1)}{2\sqrt{3.1}}$$

$$=10+\frac{35}{\sqrt{6}}+\frac{6}{\sqrt{9}}+\frac{12}{\sqrt{3}}=33.2169$$

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