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Research paper

Topological Indices of Vitamin D_3

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Abstract

Graph theory has provided chemists with a variety of useful tools, such as topological indices. A topological index $Top(G)$ of a graph G is a number with the property that for every graph H isomorphic to G, $Top(H) = Top(G)$. In this paper, we compute ABC index, ABC_4 index, Randić connectivity index, Sum connectivity index, GA index , GA_5 index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index and Hyper Zagreb index, First Zagreb polynomial, Second Zagreb polynomial, Third Zagreb polynomial, Forgotten polynomials, Forgotten topological index and Symmetric division index of vitamin D_3.

Keywords: *ABC index, ABC_4 index, Randić connectivity index, Sum connectivity index, GA index , GA_5 index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index, Hyper Zagreb index, First Zagreb polynomial, Second Zagreb polynomial, Third Zagreb polynomial, Forgotten polynomial, Forgotten topological index, Symmetric division index and vitamin D_3.*

1. Introduction

Vitamin D_3 is the common name for cholecalciferol. It's molecular formula is $C_{27}H_{44}O$. Its structure is shown in the following figure. Vitamin D_3 is made by the body naturally when skin is exposed to the sun. It is more natural and easier for the body to absorb. Vitamin D_3 can be taken as a supplement to improve overall health.Vitamin D3 also encourages the kidneys to recycle phosphate back into the blood, which helps the blood stay at the right ph. Historically, vitamin D_3 loss has been associated with rickets, a disease caused by low levels of vitamin D_3 that commonly affects children. Oily fish like salmon, codfish, mackerel, and blue fish are great natural sources of vitamin D_3.

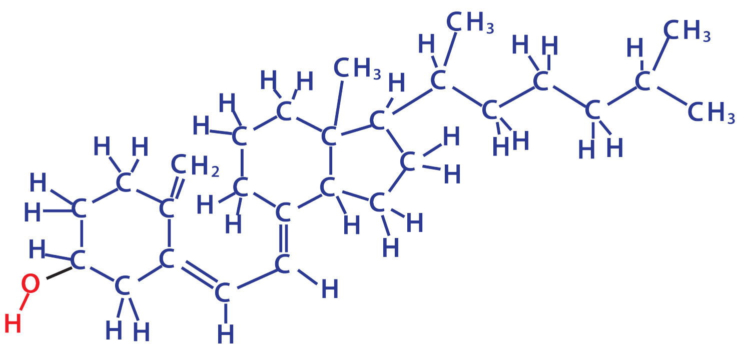

Figure-1

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physico-chemical properties like boiling point, enthalpy of vaporization, stability, etc. Molecules and molecular compounds are often modeled by molecular graph. 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 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.

In this paper, we determine the topological indices like atom-bond connectivity index, Fourth atom-bond connectivity index, Sum connectivity index, Randić connectivity index, Geometric- arithmetic connectivity index and Fifth geometric- arithmetic connectivity index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index and Hyper Zagreb index of Caffeine. Also we determine certain polynomials.

The Atom-bond connectivity index, ABC index is one of the degree based molecular descripter, which was introduced by Estrada et al. [8] in late $1990's$ and it can be used for modelling thermodynamic properties of organic chemical compounds, it is also used as a tool for explaining the stability of branched alkanes [9].

Some upper bounds for the atom-bond connectivity index of graphs can be found in [4], The atom-bond connectivity index of chemical bicyclic graphs, connected graphs can be seen in [5, 31]. For further results on ABC index of trees see the papers [12, 22, 30, 32] and the references cited there in.

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, $ABC(G)=\sum_{uv\in E}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$
The fourth atom bond connectivity index, $ABC_4(G)$ index was introduced by M. Ghorbani et al. [16] in 2010. Further studies on $ABC_4(G)$ index can be found in [10, 11].

Let G be a graph, then its fourth ABC index is defined as , $ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$, 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 first and oldest degree based topological index is Randić index [24] denoted by $\chi(G)$ and was introduced by Milan Randić in 1975. It provides a quantitative assessment of branching of molecules. For the graph G Randić index is defined as, $\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_ud_v}}$ Sum connectivity index belongs to a family of Randić like indices and it was introduced by Zhou and N. Trinajstić [34]. Further studies on Sum connectivity index can be found in [35, 36]. For a simple connected graph G, its sum connectivity index $S(G)$ is defined as, $S(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_u+d_v}}$
The Geometric-arithmetic index, $GA(G)$ index of a graph G was introduced by D. Vukičević et.al[28]. Further studies on GA index can be found in [3, 6, 33]
Let G be a graph and $e=uv$ be an edge of G then,
$$GA(G)=\sum_{e=uv\in E(G)}\frac{2\sqrt{d_ud_v}}{d_u+d_v}.$$
The fifth geometric-arithmetic index, $GA_5(G)$ was introduced by A.Graovac et al [17] in 2011. For a Graph G, the fifth geometric-arithmetic index is defined as $GA_5(G)=\sum_{uv\in E(G)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}$, where S_u is the sum of the degrees of all neighbors of the vertex u in G, similarly S_v.

A pair of molecular descriptors (or topological index), known as the first Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$, first appeared in the topological formula for the total π-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N.Trinajstic[18]. Soon after these indices have been used as branching indices. Later the Zagreb indices found applications in QSPR and QSAR studies. Zagreb indices are included in a number of programs used for the routine computation of topological indices POLLY, DRAGON, CERIUS, TAM, DISSI. $M_1(G)$ and $M_2(G)$ were recognize as measures of the branching of the carbon atom molecular skeleton [21], and since then these are frequently used for structure property modeling. Details on the chemical applications of the two Zagreb indices can be found in the books [26, 27]. Further studies on Zagreb indices can be found in [2, 19, 34, 35, 36].
For a simple connected graph G, the first and second Zagreb indices were defined as follows
$$M_1(G)=\sum_{e=uv\in E(G)}(d_u+d_v), \qquad M_2(G)=\sum_{e=uv\in E(G)}d_ud_v.$$
where d_v denotes the degree(number of first neighbors) of vertex v in G.
In 2012, M. Ghorbani and N. Azimi [15] 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
$$PM_1(G)=\prod_{e=uv\in E(G)}(d_u+d_v), \qquad PM_2(G)=\prod_{e=uv\in E(G)}d_ud_v.$$
Properties of the first and second multiple Zagreb indices may be found in [7, 20]

The augmented Zagreb index was introduced by Furtula et al [13]. This graph invariant has proven to be a valuable predictive index in the study of the heat of formation in octanes and heptanes, is a novel topological index in chemical graph theory, whose prediction power is better than atom-bond connectivity index. Some basic investigation implied that AZI index has better correlation properties and structural sensitivity among the very well established degree based topological indices.
Let $G=(V,E)$ be a graph and d_u be the degree of a vertex u, then augmented Zagreb index is denoted by $AZI(G)$ and is defined as $AZI(G)=\sum_{uv\in E}\left[\frac{d_ud_v}{d_u+d_v-2}\right]^3$. Further studies can be found in [23] and the references cited there in.
The Harmonic index was introduced by Zhong [37]. It has been found that the harmonic index correlates well with the Randić index and with the π-electron energy of benzenoid hydrocarbons.
Let $G=(V,E)$ be a graph and d_u be the degree of a vertex u then Harmonic index is defined as $H(G)=\sum_{e=uv\in E(G)}\frac{2}{d_u+d_v}$. Further studies on $H(G)$ can be found in [29, 35].

G.H. Shirdel et.al[25] introduced a new distance-based of Zagreb indices of a graph G named Hyper-Zagreb Index The hyper Zagreb index is defined as, $HM(G)=\sum_{e=uv\in E(G)}(d_u+d_v)^2$.
Fath-Tabar [1] introduced the third Zagreb indix in 2011. which is defined by, For a simple connected graph G, the third Zagreb index is defined as

$$ZG_3(G)=\sum_{e=uv\in E(G)}|d_u-d_v|.$$

Again in 2011Fath-Tabar [1] introduced the first, second and third Zagreb polynomials which are defined as follows. The first, second and third Zagreb polynomials for a simple connected graph G is defined as

$$ZG_1(G,x)=\sum_{e=uv\in E(G)}x^{d_u+d_v}.$$
$$ZG_2(G,x)=\sum_{e=uv\in E(G)}x^{d_ud_v}.$$
$$ZG_3(G,x)=\sum_{e=uv\in E(G)}x^{|d_u-d_v|}.$$

The forgotten topological index is also a degree based topological index, denoted by $F(G)$ for simple graph G. It was encountered in [14], defined as

$$F(G)=\sum_{e=uv\in E(G)}[(d_u)^2+(d_v)^2].$$

The forgotten polynomial for a graph G is defined as

$$F(G,x)=\sum_{e=uv\in E(G)}x^{[(d_u)^2+(d_v)^2]}.$$

Symmetric division index is defined by

$SDD(G)=\sum_{e=uv\in E(G)}\left\{\frac{min(d_u,d_v)}{max(d_u,d_v)}+\frac{max(d_u,d_v)}{min(d_u,d_v)}\right\}$. This topological index is useful for determining total surface area and heat formation of some chemical compounds.

2. Main results

Theorem 2.1. *Atom bond connectivity index of vitamin D_3 is* 21.674532.

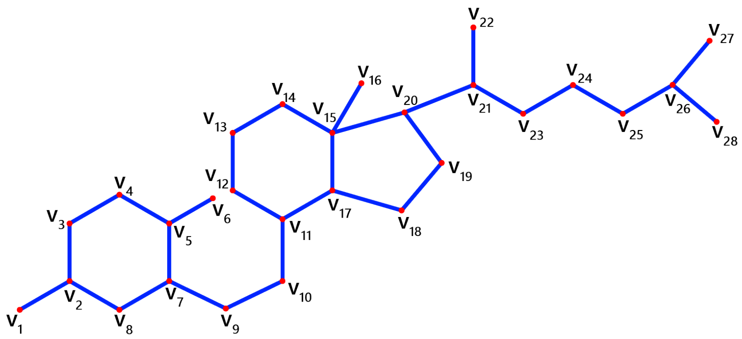

Figure-2

Proof. Consider a molecular graph of vitamin D_3 as shown in figure−2. Let $E_{i,j}$ denotes edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of vitamin D_3 (as shown in the Figure−1) contains edges of the type $E_{1,3}$, $E_{1,4}$, $E_{2,2}$, $E_{2,3}$, $E_{2,4}$, $E_{3,3}$ and $E_{3,4}$. From the figure, the number edges of these types are as follows.
$|E_{1,3}|$=5, $|E_{1,4}|$=1, $|E_{2,2}|$=7, $|E_{2,3}|$=11, $|E_{2,4}|$=1, $|E_{3,3}|$=3 and $|E_{3,4}|$=2.
∴ The atom-bond connectivity index of vitamin D_3

$$=ABC(C_{27}H_{44}O)$$

$$=\sum_{uv\in E}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}.$$

$$=|E_{1,3}|\sqrt{\frac{1+3-2}{1.3}}+|E_{1,4}|\sqrt{\frac{1+4-2}{1.4}}+|E_{2,2}|\sqrt{\frac{2+2-2}{2.2}}+|E_{2,3}|\sqrt{\frac{2+3-2}{2.3}}+$$
$$|E_{2,4}|\sqrt{\frac{2+4-2}{2.4}}+|E_{3,3}|\sqrt{\frac{3+3-2}{3.3}}+|E_{3,4}|\sqrt{\frac{3+4-2}{3.4}}.$$

$$=5\times(\sqrt{\frac{2}{3}})+1\times(\sqrt{\frac{3}{4}})+7\times(\sqrt{\frac{1}{2}})+11\times(\sqrt{\frac{1}{2}})+1\times(\sqrt{\frac{1}{2}})+3\times(\sqrt{\frac{4}{9}})+2\times(\sqrt{\frac{5}{12}}).$$

$ABC(C_{27}H_{44}O) = 21.674532.$ □

Theorem 2.2. *Fourth atom bond connectivity index of vitamin D_3 is* 16.574627.

Proof. Let $e_{i,j}$ denotes the edges of vitamin D_3 with $i = S_u$ and $j = S_v$. It is easy to see that the summation of degrees of edge endpoints of vitamin D_3 have 14 edge types $e_{3,4}$, $e_{3,5}$, $e_{3,6}$, $e_{4,5}$, $e_{4,6}$, $e_{4,9}$, $e_{5,5}$, $e_{5,6}$, $e_{5,7}$, $e_{5,9}$, $e_{6,7}$, $e_{6,9}$, $e_{7,9}$ and $e_{9,9}$ as shown in the figure−2.
clearly from the figure −2, $|e_{3,4}| = 2$, $|e_{3,5}| = 1$, $|e_{3,6}| = 2$, $|e_{4,5}| = 4$, $|e_{4,6}| = 1$, $|e_{4,9}| = 1$, $|e_{5,5}| = 4$, $|e_{5,6}| = 3$, $|e_{5,7}| = 3$, $|e_{5,9}| = 2$, $|e_{6,7}| = 2$, $|e_{6,9}| = 2$, $|e_{7,9}| = 1$ and $|e_{9,9}| = 2$.
The fourth atom-bond connectivity index of vitamin D_3

$$= ABC_4(C_{27}H_{44}O)$$

$$= \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

$$=|e_{3,4}|\Big(\sqrt{\frac{3+4-2}{3\cdot 4}}\Big)+|e_{3,5}|\Big(\sqrt{\frac{3+5-2}{3\cdot 5}}\Big)+|e_{3,6}|\Big(\sqrt{\frac{3+6-2}{3\cdot 6}}\Big)+|e_{4,5}|\Big(\sqrt{\frac{4+5-2}{4\cdot 5}}\Big)+$$
$$|e_{4,6}|\Big(\sqrt{\frac{4+6-2}{4\cdot 6}}\Big)+|e_{4,9}|\Big(\sqrt{\frac{4+9-2}{4\cdot 9}}\Big)+|e_{5,5}|\Big(\sqrt{\frac{5+5-2}{5\cdot 5}}\Big)+|e_{5,6}|\Big(\sqrt{\frac{5+6-2}{5\cdot 6}}\Big)+$$
$$|e_{5,7}|\Big(\sqrt{\frac{5+7-2}{5\cdot 7}}\Big)+|e_{5,9}|\Big(\sqrt{\frac{5+9-2}{5\cdot 9}}\Big)+|e_{6,7}|\Big(\sqrt{\frac{6+7-2}{6\cdot 7}}\Big)+|e_{6,9}|\Big(\sqrt{\frac{6+9-2}{6\cdot 9}}\Big)+$$
$$|e_{7,9}|\Big(\sqrt{\frac{7+9-2}{7\cdot 9}}\Big)+|e_{9,9}|\Big(\sqrt{\frac{9+9-2}{9\cdot 9}}\Big)$$

.

$$=2\times\sqrt{\frac{5}{12}}+1\times\sqrt{\frac{6}{15}}+2\times\sqrt{\frac{7}{18}}+4\times\sqrt{\frac{7}{20}}+1\times\sqrt{\frac{8}{24}}+1\times\sqrt{\frac{11}{36}}+4\times\sqrt{\frac{8}{25}}$$
$$+3\times\sqrt{\frac{9}{30}}+3\times\sqrt{\frac{10}{35}}+2\times\sqrt{\frac{12}{45}}+2\times\sqrt{\frac{11}{42}}+2\times\sqrt{\frac{13}{54}}+1\times\sqrt{\frac{14}{63}}+2\times\sqrt{\frac{16}{81}}$$

.

$ABC_4(C_{27}H_{44}O) = 16.574627.$ □

Theorem 2.3. *Randić connectivity index of vitamin D_3 is* 13.308386.

Proof. Randić connectivity index of vitamin D_3

$$= \chi(C_{27}H_{44}O)$$

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

$$=|E_{1,3}|\Big(\frac{1}{\sqrt{1\cdot 3}}\Big)+|E_{1,4}|\Big(\frac{1}{\sqrt{1\cdot 4}}\Big)+|E_{2,2}|\Big(\frac{1}{\sqrt{2\cdot 2}}\Big)+|E_{2,3}|\Big(\frac{1}{\sqrt{2\cdot 3}}\Big)+|E_{2,4}|\Big(\frac{1}{\sqrt{2\cdot 4}}\Big)+$$
$$|E_{3,3}|\Big(\tfrac{1}{\sqrt{3\cdot 3}}\Big)+|E_{3,4}|\Big(\tfrac{1}{\sqrt{3\cdot 4}}\Big)$$

$$=5\times\Big(\frac{1}{\sqrt{3}}\Big)+1\times\Big(\frac{1}{2}\Big)+7\times\Big(\frac{1}{2}\Big)+11\times\Big(\frac{1}{\sqrt{6}}\Big)+1\times\Big(\frac{1}{\sqrt{8}}\Big)+3\times\Big(\frac{1}{\sqrt{9}}\Big)+2\times\Big(\frac{1}{\sqrt{12}}\Big)$$

$\therefore \chi(C_{27}H_{44}O)$= 13.308386. □

Theorem 2.4. *Sum connectivity index of vitamin D_3 is* 13.755485.

Proof. Sum connectivity index of vitamin D_3

$$= S(C_{27}H_{44}O)$$

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

$$=|E_{1,3}|\Big(\frac{1}{\sqrt{1+3}}\Big)+|E_{1,4}|\Big(\frac{1}{\sqrt{1+4}}\Big)+|E_{2,2}|\Big(\frac{1}{\sqrt{2+2}}\Big)+|E_{2,3}|\Big(\frac{1}{\sqrt{2+3}}\Big)+|E_{2,4}|\Big(\frac{1}{\sqrt{2+4}}\Big)+$$
$$|E_{3,3}|\Big(\tfrac{1}{\sqrt{3+3}}\Big)+|E_{3,4}|\Big(\tfrac{1}{\sqrt{3+4}}\Big).$$

$$=5\times\Big(\frac{1}{2}\Big)+1\times\Big(\frac{1}{\sqrt{5}}\Big)+7\times\Big(\frac{1}{2}\Big)+11\times\Big(\frac{1}{\sqrt{5}}\Big)+1\times\Big(\frac{1}{\sqrt{6}}\Big)+3\times\Big(\frac{1}{\sqrt{6}}\Big)+2\times\Big(\frac{1}{\sqrt{7}}\Big)$$

$\therefore S(C_{27}H_{44}O)$=13.755485. □

Theorem 2.5. *Geometric-Arithmetic index of vitamin D_3 is* 28.830178.

Proof. Geometric-Arithmetic index of vitamin D_3

$= GA(C_{27}H_{44}O)$

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

$= |E_{1,3}|\left(\frac{2\sqrt{1\cdot 3}}{1+3}\right)+|E_{1,4}|\left(\frac{2\sqrt{1\cdot 4}}{1+4}\right)+|E_{2,2}|\left(\frac{2\sqrt{2\cdot 2}}{2+2}\right)+|E_{2,3}|\left(\frac{2\sqrt{2\cdot 3}}{2+3}\right)+|E_{2,4}|\left(\frac{2\sqrt{2\cdot 4}}{2+4}\right)+$
$|E_{3,3}|\left(\frac{2\sqrt{3\cdot 3}}{3+3}\right)+|E_{3,4}|\left(\frac{2\sqrt{3\cdot 4}}{3+4}\right).$

$5\times\frac{\sqrt{3}}{2}+1\times\frac{4}{5}+7+11\times 2\times\frac{\sqrt{6}}{5}+1\times\frac{4\sqrt{2}}{6}+3\times\frac{6}{6}+2\times\frac{2\sqrt{12}}{7}$

$GA(C_{27}H_{44}O)$ =28.830178 □

Theorem 2.6. *Fifth geometric-arithmetic index of vitamin D_3 is* 29.519525.

Proof. Fifth geometric-arithmetic index of vitamin D_3

$= GA_5(C_{27}H_{44}O)$

$= \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u+S_v}$

$=|e_{3,4}|\left(\frac{2\sqrt{3\cdot 4}}{3+4}\right)+|e_{3,5}|\left(\frac{2\sqrt{3\cdot 5}}{3+5}\right)+|e_{3,6}|\left(\frac{2\sqrt{3\cdot 6}}{3+6}\right)+|e_{4,5}|\left(\frac{2\sqrt{4\cdot 5}}{4+5}\right)+|e_{4,6}|\left(\frac{2\sqrt{4\cdot 6}}{4+6}\right)+$
$|e_{4,9}|\left(\frac{2\sqrt{4\cdot 9}}{4+9}\right)+|e_{5,5}|\left(\frac{2\sqrt{5\cdot 5}}{5+5}\right)+|e_{5,6}|\left(\frac{2\sqrt{5\cdot 6}}{5+6}\right)+|e_{5,7}|\left(\frac{2\sqrt{5\cdot 7}}{5+7}\right)+|e_{5,9}|\left(\frac{2\sqrt{5\cdot 9}}{5+9}\right)+$
$|e_{6,7}|\left(\frac{2\sqrt{6\cdot 7}}{6+7}\right)+|e_{6,9}|\left(\frac{2\sqrt{6\cdot 9}}{6+9}\right)+|e_{7,9}|\left(\frac{2\sqrt{7\cdot 9}}{7+9}\right)+|e_{9,9}|\left(\frac{2\sqrt{9\cdot 9}}{9+9}\right)$

$=2\times\left(\frac{2\sqrt{12}}{7}\right)+1\times\left(\frac{2\sqrt{15}}{8}\right)+2\times\left(\frac{2\sqrt{18}}{9}\right)+4\times\left(\frac{2\sqrt{20}}{9}\right)+1\times\left(\frac{2\sqrt{24}}{10}\right)+$
$1\times\left(\frac{2\sqrt{36}}{13}\right)+4\times\left(\frac{2\sqrt{25}}{10}\right)+3\times\left(\frac{2\sqrt{30}}{11}\right)+3\times\left(\frac{2\sqrt{35}}{12}\right)+2\times\left(\frac{2\sqrt{45}}{14}\right)+$
$2\times\left(\frac{2\sqrt{42}}{13}\right)+2\times\left(\frac{2\sqrt{54}}{15}\right)+1\times\left(\frac{2\sqrt{63}}{16}\right)+2\times\left(\frac{2\sqrt{81}}{18}\right)$

$\therefore GA_5(C_{27}H_{44}O)$ =29.519525. □

Theorem 2.7. *First Zagreb index of vitamin D_3 is* 146.

Proof. First Zagreb index of vitamin D_3

$= M_1(C_{27}H_{44}O)$

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

$=| E_{1,3} | (1+3)+ | E_{1,4} | (1+4)+ | E_{2,2} | (2+2)+ | E_{2,3} | (2+3)+ | E_{2,4} | (2+4)+$

$| E_{3,3} | (3+3)+ | E_{3,4} | (3+4)$

$=5\times 4+1\times 5+7\times 4+11\times 5+1\times 6+3\times 6+2\times 7$

$\therefore M_1(C_{27}H_{44}O)$=146. □

Theorem 2.8. *Second Zagreb index of vitamin D_3 is* 172.

Proof. Second Zagreb index of vitamin D_3

$= M_2(C_{27}H_{44}O)$

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

$=| E_{1,3} | (1\cdot 3)+ | E_{1,4} | (1\cdot 4)+ | E_{2,2} | (2\cdot 2)+ | E_{2,3} | (2\cdot 3)+ | E_{2,4} | (2\cdot 4)+$

$| E_{3,3} | (3\cdot 3) + | E_{3,4} | (3\cdot 4)$

$=5\times 3+1\times 4+7\times 4+11\times 6+1\times 8+3\times 9+2\times 12$

$\therefore M_2(C_{27}H_{44}O) = 172.$ □

Theorem 2.9. *First multiple Zagreb index of vitamin* D_3 *is* 2.601×10^{20}.

Proof. First multiple Zagreb index of vitamin D_3

$= PM_1(C_{27}H_{44}O)$

$$= \prod_{e=uv\in E(G)} (d_u+d_v)$$
$$= \prod_{e=uv\in E_{1,3}} (d_u+d_v) \prod_{e=uv\in E_{1,4}} (d_u+d_v) \prod_{e=uv\in E_{2,2}} (d_u+d_v) \prod_{e=uv\in E_{2,3}} (d_u+d_v)$$
$$\prod_{e=uv\in E_{2,4}} (d_u+d_v) \prod_{e=uv\in E_{3,3}} (d_u+d_v) \prod_{e=uv\in E_{3,4}} (d_u+d_v) \prod$$
$$=4^5\times 5^1\times 4^7\times 5^{11}\times 6^1\times 6^3\times 7^2$$

$PM_1(C_{27}H_{44}O)=2\cdot 601\times 10^{20}.$ □

Theorem 2.10. *Second multiple Zagreb index of vitamin* D_3 *is* 4.852×10^{21}.

Proof. Second multiple Zagreb index of vitamin D_3

$= PM_2(C_{27}H_{44}O)$

$$= \prod_{e=uv\in E(G)} d_u d_v$$
$$= \prod_{e=uv\in E_{1,3}} (d_u d_v) \prod_{e=uv\in E_{1,4}} (d_u d_v) \prod_{e=uv\in E_{2,2}} (d_u d_v) \prod_{e=uv\in E_{2,3}} (d_u d_v)$$
$$\prod_{e=uv\in E_{2,4}} (d_u d_v) \prod_{e=uv\in E_{3,3}} (d_u d_v) \prod_{e=uv\in E_{3,4}} (d_u d_v)$$
$$=3^5\times 4^1\times 4^7\times 6^{11}\times 8^1\times 9^3\times 12^2$$

$PM_2(C_{27}H_{44}O) = 4\cdot 852\times 10^{21}.$ □

Theorem 2.11. *Augmented Zagreb index of vitamin* D_3 *is* 233.06525.

Proof. Augmented Zagreb index of vitamin D_3

$= AZI(G)$

$$= \sum_{e=uv\in E(G)} \left[\frac{d_u d_v}{d_u+d_v-2}\right]^3$$
$$=| E_{1,3} | \left(\frac{1\cdot 3}{1+3-2}\right)^3 + | E_{1,4} | \left(\frac{1\cdot 4}{1+4-2}\right)^3 + | E_{2,2} | \left(\frac{2\cdot 2}{2+2-2}\right)^3 + | E_{2,3} | \left(\frac{2\cdot 3}{2+3-2}\right)^3 +$$
$$| E_{2,4} | \left(\frac{2\cdot 4}{2+4-2}\right)^3 + | E_{3,3} | \left(\frac{3\cdot 3}{3+3-2}\right)^3 + | E_{3,4} | \left(\frac{3\cdot 4}{3+4-2}\right)^3$$
$$=5\times\left(\frac{3}{2}\right)^3 + 1\times\left(\frac{4}{3}\right)^3 + 7\times\left(\frac{4}{2}\right)^3 + 11\times\left(\frac{6}{3}\right)^3 + 1\times\left(\frac{8}{4}\right)^3 + 3\times\left(\frac{9}{4}\right)^3 + 2\times\left(\frac{12}{5}\right)^3$$

$\therefore AZI(C_{27}H_{44}O) = 233.06525.$ □

Theorem 2.12. *Harmonic index of vitamin* D_3 *is* 12.704762.

Proof. Harmonic index of vitamin D_3

$= H(C_{27}H_{44}O)$

$$= \sum_{e=uv\in E(G)} \frac{2}{d_u+d_v}$$
$$=| E_{1,3} | \left(\frac{2}{1+3}\right) + | E_{1,4} | \left(\frac{2}{1+4}\right) + | E_{2,2} | \left(\frac{2}{2+2}\right) + | E_{2,3} | \left(\frac{2}{2+3}\right) +$$
$$| E_{2,4} | \left(\frac{2}{2+4}\right) + | E_{3,3} | \left(\frac{2}{3+3}\right) + | E_{3,4} | \left(\frac{2}{3+4}\right)$$

$$=5\times\left(\frac{2}{4}\right)+1\left(\frac{2}{5}\right)+7\times\left(\frac{2}{4}\right)+11\times\left(\frac{2}{5}\right)+1\times\left(\frac{2}{6}\right)+3\times\left(\frac{2}{6}\right)+2\times\left(\frac{2}{7}\right)$$

$\therefore H(C_{27}H_{44}O) = 12.704762.$ □

Theorem 2.13. *Hyper Zagreb index of vitamin D_3 is* 734.

Proof. The hyper Zagreb index of vitamin D_3

$$= HM(C_{27}H_{44}O)$$

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

$$=\mid E_{1,3}\mid(1+3)^2+\mid E_{1,4}\mid(1+4)^2+\mid E_{2,2}\mid(2+2)^2+\mid E_{2,3}\mid(2+3)^2+\mid E_{2,4}\mid(2+4)^2+$$

$$\mid E_{3,3}\mid(3+3)^2+\mid E_{3,4}\mid(3+4)^2$$

$$=5\times4^2+1\times5^2+7\times4^2+11\times5^2+1\times6^2+3\times6^2+2\times7^2$$

$\therefore H(C_{27}H_{44}O) = 734.$ □

Theorem 2.14. *First Zagreb polynomials of vitamin D_3 is* $2x^7+4x^6+12x^5+12x^4$.

Proof. First Zagreb polynomials of vitamin D_3

$$= ZG_1(C_{27}H_{44}O,x)$$

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

$$=\mid E_{1,3}\mid x^{(1+3)}+\mid E_{1,4}\mid x^{(1+4)}+\mid E_{2,2}\mid x^{(2+2)}+\mid E_{2,3}\mid x^{(2+3)}+$$

$$\mid E_{2,4}\mid x^{(2+4)}+\mid E_{3,3}\mid x^{(3+3)}+\mid E_{3,4}\mid x^{(3+4)}$$

$$=5\times x^4+1\times x^5+7\times x^4+11\times x^5+1\times x^6+3\times x^6+2\times x^7$$

$\therefore ZG_1(C_{27}H_{44}O,x)=2x^7+4x^6+12x^5+12x^4.$ □

Theorem 2.15. *Second Zagreb polynomials of vitamin D_3 is* $2x^{12}+3x^9+x^8+11x^6+8x^4+5x^3$.

Proof. Second Zagreb polynomials of vitamin D_3

$$= ZG_2(C_{27}H_{44}O,x)$$

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

$$=\mid E_{1,3}\mid x^{(1\times3)}+\mid E_{1,4}\mid x^{(1\times4)}+\mid E_{2,2}\mid x^{(2\times2)}+\mid E_{2,3}\mid x^{(2\times3)}+$$

$$\mid E_{2,4}\mid x^{(2\times4)}+\mid E_{3,3}\mid x^{(3\times3)}+\mid E_{3,4}\mid x^{(3\times4)}$$

$$=5\times x^3+1\times x^4+7\times x^4+11\times x^6+1\times x^8+3\times x^9+2\times x^{12}$$

$\therefore ZG_1(C_{27}H_{44}O,x)=2x^{12}+3x^9+x^8+11x^6+8x^4+5x^3.$ □

Theorem 2.16. *Third Zagreb polynomials of vitamin D_3 is* $x^3+6x^2+13x+10$.

Proof. Third Zagreb polynomials of vitamin D_3

$$= ZG_3(C_{27}H_{44}O,x)$$

$$=\sum_{e=uv\in E(G)}x^{|d_u-d_v|}$$

$$=\mid E_{1,3}\mid x^{|1-3|}+\mid E_{1,4}\mid x^{|1-4|}+\mid E_{2,2}\mid x^{|2-2|}+\mid E_{2,3}\mid x^{|2-3|}+$$

$$\mid E_{2,4}\mid x^{|2-4|}+\mid E_{3,3}\mid x^{|3-3|}+\mid E_{3,4}\mid x^{|3-4|}$$

$=5\times x^2+1\times x^3+7\times x^0+11\times x^1+1\times x^2+3\times x^0+2\times x^1$

$\therefore ZG_1(C_{27}H_{44}O,x)=x^3+6x^2+13x+10.$ □

Theorem 2.17. *Forgotten topological index of vitamin D_3 is* 390.

Proof. Forgotten topological index of vitamin D_3

$=F(C_{27}H_{44}O)$

$$=\sum_{e=uv\in E(G)}[(d_u)^2+(d_v)^2]$$

$=|E_{1,3}|(1^2+3^2)+|E_{1,4}|(1^2+4^2)+|E_{2,2}|(2^2+2^2)+|E_{2,3}|(2^2+3^2)+$

$|E_{2,4}|(2^2+4^2)+|E_{3,3}|(3^2+3^2)+|E_{3,4}|(3^2+4^2)$

$=5\times 10+1\times 17+7\times 8+11\times 13+1\times 20+3\times 18+2\times 25$

$\therefore F(C_{27}H_{44}O)=390.$ □

Theorem 2.18. *Forgotten polynomial of vitamin D_3 is*
$2x^{25}+x^{20}+3x^{18}+x^{17}+11x^{13}+5x^{10}+7x^8$.

Proof. Forgotten polynomial of vitamin D_3

$=F(C_{27}H_{44}O,x)$

$$=\sum_{e=uv\in E(G)}x^{[(d_u)^2+(d_v)^2]}$$

$=|E_{1,3}|x^{(1^2+3^2)}+|E_{1,4}|x^{(1^2+4^2)}+|E_{2,2}|x^{(2^2+2^2)}+|E_{2,3}|x^{(2^2+3^2)}+$

$|E_{2,4}|x^{(2^2+4^2)}+|E_{3,3}|x^{(3^2+3^2)}+|E_{3,4}|x^{(3^2+4^2)}$

$=5\times x^{10}+1\times x^{17}+7\times x^8+11\times x^{13}+1\times x^{20}+3\times x^{18}+2\times x^{25}$

$\therefore F(C_{27}H_{44}O,x)=2x^{25}+x^{20}+3x^{18}+x^{17}+11x^{13}+5x^{10}+7x^8.$ □

Theorem 2.19. *Symmetric division index of vitamin D_3 is* 71.416667.

Proof. Symmetric division index of vitamin D_3

$=SDD(C_{27}H_{44}O)$

$$=\sum_{e=uv\in E(G)}\left\{\frac{min(d_u,d_v)}{max(d_u,d_v)}+\frac{max(d_u,d_v)}{min(d_u,d_v)}\right\}$$

$$=|E_{1,3}|\left\{\frac{min(1,3)}{max(1,3)}+\frac{max(1,3)}{min(1,3)}\right\}+|E_{1,4}|\left\{\frac{min(1,4)}{max(1,4)}+\frac{max(1,4)}{min(1,4)}\right\}$$
$$+|E_{2,2}|\left\{\frac{min(2,2)}{max(2,2)}+\frac{max(2,2)}{min(2,2)}\right\}+|E_{2,3}|\left\{\frac{min(2,3)}{max(2,3)}+\frac{max(2,3)}{min(2,3)}\right\}$$
$$+|E_{2,4}|\left\{\frac{min(2,4)}{max(2,4)}+\frac{max(2,4)}{min(2,4)}\right\}+|E_{3,3}|\left\{\frac{min(3,3)}{max(3,3)}+\frac{max(3,3)}{min(3,3)}\right\}$$
$$+|E_{3,4}|\left\{\frac{min(3,4)}{max(3,4)}+\frac{max(3,4)}{min(3,4)}\right\}$$
$$=5\times\frac{10}{3}+1\times\frac{17}{4}+7\times 2+11\times\frac{13}{6}+1\times\frac{20}{8}+3\times 2+2\times\frac{25}{12}$$

$\therefore F(C_{27}H_{44}O)=71.416667.$ □

3. Conclusion:

ABC index, ABC_4 index, Randić connectivity index, Sum connectivity index, *GA* index , GA_5 index, First Zagreb index, Second Zagreb index, First Multiple Zagreb index, Second Multiple Zagreb index, Augmented Zagreb index, Harmonic index and Hyper Zagreb index, First Zagreb polynomial, Second Zagreb polynomial, Third Zagreb polynomial, Forgotten polynomial, Forgotten topological index and Symmetric division index of vitamin D_3 was computed.

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