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SOME TOPOLOGICAL INDICES OF CHOLESTEROL

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Abstract: In this paper we compute the First Zagreb index, Second Zagreb index, First multiple Zagreb index, Second multiple Zagreb index, Augmented Zagreb index, Harmonic index and Hyper Zagreb index of Cholesterol. These are some topological indices based on degrees.

AMS Subject Classification: 05C12, 05C90

Key Words: Zagreb indices, multiple Zagreb indices, augmented Zagreb index, harmonic index, hyper Zagreb index, cholesterol

1. Introduction

The cholesterol is made in the body by the liver, but it is also formed in some foods. This substance is expected to be essentially free sterol isomers as it is

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of natural origin. Hydrogen bonds are formed by the hydroxyl group using the carbonyl oxygen of phospholipid and sphingolipid head groups available in its vicinity. The cholesterol is very much essential for the normal levels for the body's normal functioning. The abnormal levels are quite dangerous and lead to heart attacks. The thermodynamic properties of this material are, therefore, important in the study of the biochemical processes in which it is involved.

The topological indices are the molecular descriptors that describes the structures of chemical compounds and it help us to predict certain physico-chemical properties like boiling point, enthalpy of vaporization, stability etc. In this paper, we determine the topological indices like Atom-bond connectivity index, Fourth Atom-bond connectivity index, Sum connectivity index, Randic connectivity index, Geometric-arithmetic connectivity index and Fifth Geometric-arithmetic connectivity index of Cholesterol.

All molecular graphs considered in this paper are finite, connected, loop less and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ 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. Using these terminologies, certain topological indices are defined in the following manner.

A graph invariant is any function on a graph that does not depend on a labeling of its vertices. A topological index is a graph invariant applicable in chemistry. By IUPAC terminology, a topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. In an exact phrase, if Graph denotes the class of all finite graphs then a topological index is a function Top from Graph into real numbers with this property that $\mathrm{Top}(G) = \mathrm{Top}(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological indices.

The 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. Recently Rajesh Kanna and his students [11] determined ABC index, ABC_4 index, Randic connectivity index, Sum connectivity index, GA index and GA_5 index of Cholesterol. In this paper, we determine the topological indices like Zagreb indices, Multiple Zagreb indices, Augmented Zagreb index, Harmonic index and Hyper Zagreb index of Cholesterol.

1.1. Zagreb Indices

Much studied and in chemistry much applied graph invariants are the pair of molecular descriptors (or topological index), known as the First Zagreb index $M_1(G)$ and Second Zagreb index $M_2(G)$. They first appeared in the topological formula for total φ-energy of conjugated molecules that has been derived in 1972 by I. Gutman and N. Trinajstić [5]. 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, such as POLLY, OASIS, DRAGON, CERIUS, TAM, DISSIM etc. $M_1(G)$ and $M_2(G)$ are, in fact, measures of branching of the molecular carbonatom skeleton [8] and can thus be viewed as molecular structure descriptors. The Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism and heterosystems, etc. Overall, Zagreb indices exhibited a potential applicability for deriving multi-linear regression models. Details on the chemical applications of the two Zagreb indices can be found in the books [12, 13]. Further studies on Zagreb indices can be found in [1, 6, 16, 17, 18].

Definition 1. For a simple connected graph G, the first and second Zagreb indices were defined as follows

$$M_1(G) = \sum_{e=uv\in E(G)} (d_u + d_v), \quad M_2(G) = \sum_{e=uv\in E(G)} d_u d_v,$$

where d_v denotes the degree(number of first neighbors) of vertex v in G.

1.2. Multiple Zagreb Indices

In 2012, M. Ghorbani and N. Azimi [4] defined the Multiple Zagreb topological indices of a graph G, based on degree of vertices of G.

Definition 2. For a simple connected graph G, the first and second multiple Zagreb indices were defined as follows:

$$PM_1(G) = \prod_{e=uv\in E(G)} (d_u + d_v), \quad PM_2(G) = \prod_{e=uv\in E(G)} d_u d_v.$$

The properties of the first and second Multiple Zagreb indices may be found in [2, 7] .

1.3. Augmented Zagreb Index

The Augmented Zagreb index was introduced by Furtula et al. [3]. 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.

Definition 3. 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

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

Further studies can be found in [9] and the references cited there in.

1.4. Harmonic Index

The Harmonic index was introduced by Zhong [15]. It has been found that the harmonic index correlates well with the Randic index and with the π-electron energy of benzenoid hydrocarbons.

Definition 4. 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 [14, 17].

1.5. Hyper Zagreb Index

G. H. Shirdel et al. [10] introduced a new distance-based of Zagreb indices of a graph G named Hyper-Zagreb index.

Definition 5. The hyper Zagreb index is defined as

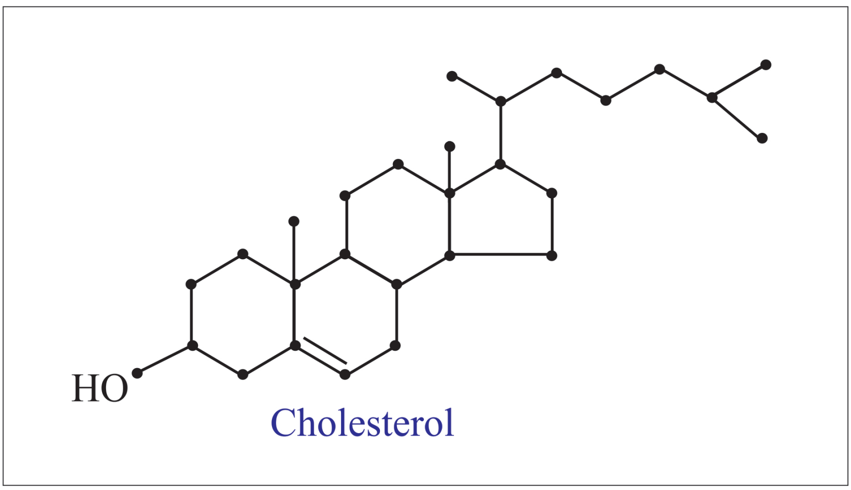
$$HM(G) = \sum_{e=uv \in E(G)} (d_u + d_v)^2.$$

2. Main Results

Theorem 6. *The First Zagreb index of Cholesterol is*

$$M_1(C_{27}H_{46}O) = 158.$$

Proof. Consider a cholesterol $C_{27}H_{46}O$. We partition the edges of $C_{27}H_{46}O$ into edges of the type $E_{(d_u,d_v)}$ where uv is an edge. In $C_{27}H_{46}O$ we get edges of the type $E_{(1,3)}$, $E_{(1,4)}$, $E_{(2,2)}$, $E_{(2,3)}$, $E_{(2,4)}$, $E_{(3,3)}$ and $E_{(3,4)}$. The number of edges of these types are 4, 2, 6, 10, 2, 3 and 4 respectively.



We know that $M_1(G) = \sum_{e=uv\in E(G)} (d_u + d_v)$, i.e.,

$$\begin{aligned} M_1(C_{27}H_{46}O) =& |E_{(1,3)}| \sum_{uv\in E_{(1,3)}(G)} (d_u + d_v) + |E_{(1,4)}| \sum_{uv\in E_{(1,4)}(G)} (d_u + d_v) \\ &+ |E_{(2,2)}| \sum_{uv\in E_{(2,2)}(G)} (d_u + d_v) + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}(G)} (d_u + d_v) \\ &+ |E_{(2,4)}| \sum_{uv\in E_{(2,4)}(G)} (d_u + d_v) \\ &+ |E_{(3,3)}| \sum_{uv\in E_{(3,3)}(G)} (d_u + d_v) + |E_{(3,4)}| \sum_{uv\in E_{(3,4)}(G)} (d_u + d_v) \\ &= 4(1+3) + 2(1+4) + 6(2+2) + 10(2+3) + 2(2+4) \\ &+ 3(3+3) + 4(3+4) = 158. \end{aligned}$$

□

Theorem 7. *The Second Zagreb index of Cholesterol is*

$$M_2(C_{27}H_{46}O) = 195.$$

Proof. We know that $M_2(G) = \sum_{e=uv\in E(G)} d_u d_v$, i.e.,

$$\begin{aligned} M_2(C_{27}H_{46}O) =& |E_{(1,3)}| \sum_{uv\in E_{(1,3)}(G)} d_u d_v + |E_{(1,4)}| \sum_{uv\in E_{(1,4)}(G)} d_u d_v \\ &+ |E_{(2,2)}| \sum_{uv\in E_{(2,2)}(G)} d_u d_v + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}(G)} d_u d_v \\ &+ |E_{(2,4)}| \sum_{uv\in E_{(2,4)}(G)} d_u d_v \\ &+ |E_{(3,3)}| \sum_{uv\in E_{(3,3)}(G)} d_u d_v + |E_{(3,4)}| \sum_{uv\in E_{(3,4)}(G)} d_u d_v \\ =& 4(1\cdot 3) + 2(1\cdot 4) + 6(2\cdot 2) + 10(2\cdot 3) \\ &+ 2(2\cdot 4) + 3(3\cdot 3) + 4(3\cdot 4) \\ =& 195. \end{aligned}$$

□

Theorem 8. *The First multiple Zagreb index of Cholesterol is*

$$PM_1(C_{27}H_{46}O) = 2322432000.$$

Proof. We know that $PM_1(G) = \prod_{e=uv\in E(G)} (d_u + d_v)$, i.e.,

$$\begin{aligned}
PM_1(C_{27}H_{46}O) =& |E_{(1,3)}| \prod_{uv\in E_{(1,3)}(G)} (d_u + d_v) \times |E_{(1,4)}| \prod_{uv\in E_{(1,4)}(G)} (d_u + d_v) \\
& \times |E_{(2,2)}| \prod_{uv\in E_{(2,2)}(G)} (d_u + d_v) \\
& \times |E_{(2,3)}| \prod_{uv\in E_{(2,3)}(G)} (d_u + d_v) \times |E_{(2,4)}| \prod_{uv\in E_{(2,4)}(G)} (d_u + d_v) \\
& \times |E_{(3,3)}| \prod_{uv\in E_{(3,3)}(G)} (d_u + d_v) \times |E_{(3,4)}| \prod_{uv\in E_{(3,4)}(G)} (d_u + d_v) \\
=& 4(1+3) \times 2(1+4) \times 6(2+2) \times 10(2+3) \times 2(2+4) \times \\
& 3(3+3) \times 4(3+4) \\
=& 2322432000.
\end{aligned}$$

□

Theorem 9. *The Second multiple Zagreb index of Cholesterol is*

$$PM_2(C_{27}H_{46}O) = 2866544640.$$

Proof. We know that $PM_2(G) = \prod_{e=uv\in E(G)} d_u d_v$, i.e.,

$$\begin{aligned}
PM_2(C_{27}H_{46}O) =& |E_{(1,3)}| \prod_{uv\in E_{(1,3)}(G)} d_u d_v \times |E_{(1,4)}| \prod_{uv\in E_{(1,4)}(G)} d_u d_v \\
& + |E_{(2,2)}| \prod_{uv\in E_{(2,2)}(G)} d_u d_v \times |E_{(2,3)}| \prod_{uv\in E_{(2,3)}(G)} d_u d_v \\
& \times |E_{(2,4)}| \prod_{uv\in E_{(2,4)}(G)} d_u d_v \\
& \times |E_{(3,3)}| \prod_{uv\in E_{(3,3)}(G)} d_u d_v \times |E_{(3,4)}| \prod_{uv\in E_{(3,4)}(G)} d_u d_v \\
=& 4(1\cdot 3) \times 2(1\cdot 4) \times 6(2\cdot 2) \times 10 \\
& (2\cdot 3) \times 2(2\cdot 4) \times 3(3\cdot 3) \times 4(3\cdot 4) \\
=& 2866544640.
\end{aligned}$$

□

Theorem 10. *The Augmented Zagreb index of Cholesterol is*

$$AZI_4(C_{27}H_{46}O) = 251.7086157.$$

Proof. We know that $AZI(G) = \sum_{e=uv\in E(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$, i.e.,

$$\begin{aligned}
M_2(C_{27}H_{46}O) =& |E_{(1,3)}| \sum_{uv\in E_{(1,3)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
&+ |E_{(1,4)}| \sum_{uv\in E_{(1,4)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
&+ |E_{(2,2)}| \sum_{uv\in E_{(2,2)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
&+ |E_{(2,3)}| \sum_{uv\in E_{(2,3)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
&+ |E_{(2,4)}| \sum_{uv\in E_{(2,4)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
&+ |E_{(3,3)}| \sum_{uv\in E_{(3,3)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
&+ |E_{(3,4)}| \sum_{uv\in E_{(3,4)}(G)} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3 \\
=& 4\left[\frac{1\times 3}{1+3-2}\right]^3 + 2\left[\frac{1\times 4}{1+4-2}\right]^3 + 6\left[\frac{2\times 2}{2+2-2}\right]^3 \\
&+ 10\left[\frac{2\times 3}{2+3-2}\right]^3 + 2\left[\frac{2\times 4}{2+4-2}\right]^3 + 3\left[\frac{3\times 3}{3+3-2}\right]^3 \\
&+ 4\left[\frac{3\times 4}{3+4-2}\right]^3 \\
=& 251.7086157.
\end{aligned}$$

□

Theorem 11. *The harmonic index of Cholesterol is* $H(C_{27}H_{46}O) =$ *12.13333.*

Proof. We know that $H(G) = \sum_{e=uv\in E(G)} \frac{2}{d_u+d_v}$, i.e.,

$$\begin{aligned}
H(C_{27}H_{46}O) =&|E_{(1,3)}| \sum_{uv\in E_{(1,3)}(G)} \frac{2}{d_u+d_v} + |E_{(1,4)}| \sum_{uv\in E_{(1,4)}(G)} \frac{2}{d_u+d_v} \\
&+ |E_{(2,2)} \sum_{uv\in E_{(2,2)}(G)} \frac{2}{d_u+d_v} + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}(G)} \frac{2}{d_u+d_v} \\
&+ |E_{(2,4)}| \sum_{uv\in E_{(2,4)}(G)} \frac{2}{d_u+d_v} \\
&+ |E_{(3,3)}| \sum_{uv\in E_{(3,3)}(G)} \frac{2}{d_u+d_v} + |E_{(3,4)}| \sum_{uv\in E_{(3,4)}(G)} \frac{2}{d_u+d_v} \\
=&4\times\frac{2}{1+3} + 2\times\frac{2}{1+4} + 6\times\frac{2}{2+2} + 10\times\frac{2}{2+3} \\
&+ 2\times\frac{2}{2+4} + 3\times\frac{2}{3+3} + 4\times\frac{2}{3+4} = 12.13333. \qquad \square
\end{aligned}$$

Theorem 12. *The hyper Zagreb index of Cholesterol is* $HM(C_{27}H_{46}O) = 836$.

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

$$\begin{aligned}
HM(C_{27}H_{46}O) =&|E_{(1,3)}| \sum_{uv\in E_{(1,3)}(G)} (d_u+d_v)^2 + |E_{(1,4)}| \sum_{uv\in E_{(1,4)}(G)} (d_u+d_v)^2 \\
&+|E_{(2,2)}| \sum_{uv\in E_{(2,2)}(G)} (d_u+d_v)^2 + |E_{(2,3)}| \sum_{uv\in E_{(2,3)}(G)} (d_u+d_v)^2 \\
&+|E_{(2,4)}| \sum_{uv\in E_{(2,4)}(G)} (d_u+d_v)^2 \\
&+|E_{(3,3)}| \sum_{uv\in E_{(3,3)}(G)} (d_u+d_v)^2 + |E_{(3,4)}| \sum_{uv\in E_{(3,4)}(G)} (d_u+d_v)^2 \\
=&4(1+3)^2 + 2(1+4)^2 + 6(2+2)^2 + 10(2+3)^2 + 2(2+4)^2 \\
&+ 3(3+3)^2 + 4(3+4)^2 = 836. \qquad \square
\end{aligned}$$

References

[1] J. Braun, A. Kerber, M. Meringer and C. Rücker, Similarity of molecular descriptors: The equivalence of Zagreb indices and walk counts, *MATCH Commun. Math. Comput. Chem.*, **54** (2005), 163-176.

[2] M. Eliasi, A. Iranmanesh and I. Gutman, Multiplicative versions of first Zagreb index, *MATCH Commun. Math. Comput. Chem.*, **68** (2012), 217-230.

[3] B. Furtula, A. Graovac and D. Vukičević, Augmented Zagreb index, *J. of Mathematical Chemistry*, **48** (2010), 370-380.

[4] M. Ghorbani and N. Azimi, Note on multiple Zagreb indices, *Iranian J. of Mathematical Chemistry*, **3**, No 2 (2012), 137-143.

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

[6] I. Gutman and K.C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.*, **50** (2004), 83-92.

[7] I. Gutman, Multiplicative Zagreb indices of trees, *Bulletin of Soc. of Mathematicians Banja Luka*, **18** (2011), 17-23.

[8] I. Gutman, B. Ruščić, N. Trinajstić and C.F. Wilcox, Graph theory and molecular orbitals, XII. Acyclic polyenes, *J. Chem. Phys.*, **62** (1975), 3399-3405.

[9] Y. Huang, B. Liu† and Lu Gan, Augumented Zagreb Index of connected graphs, *MATCH Commun. Math. Comput. Chem.*, **67** (2012), 483-494.

[10] G.H. Shirdel, H. Rezapour and A.M. Sayadi, The Hyper-Zagreb Index of Graph Operations, *Iranian J. of Mathematical Chemistry*, **4**, No 2 (2013), 213-220.

[11] G. Sridhara, M.R. Rajesh Kanna and R.S. Indumathi, Computation of topological indices of graphene, *Journal of Nanomaterial*, **2015** (2015), Article ID 969348, 8 pages.

[12] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim (2000).

[13] R. Todeschini and V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, Vols. I and II (2009).

[14] R. Wu, Z. Tang and H. Deng, A lower bound for the harmonic index of a graph with minimum degree at least two, *Faculty of Sciences and Mathematics, University of Nis (Serbia)*, **27** (2013), 51-55.

[15] L. Zhong, The harmonic index on graphs, *Applied Mathematics Letters*, **25** (2012), 561-566.

[16] B. Zhou and I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, *Chemical Physics Letters*, **394** (2004), 93-95.

[17] B. Zhou and N. Trinajstić, On a novel connectivity index, *J. of Mathematical Chemistry*, **46** (2009) 1252-1270.

[18] B. Zhou and N. Trinajstić, On general sum-connectivity index, *Journal of Mathematical Chemistry*, **47** (2010), 210-218.