LEAP ZAGREB INDICES OF VERAPAMIL

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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). Based on second distance degrees of the vertices, A.M. Naji et al. defined a topological index called Leap Zagreb indices of Graphs. In this article, we have computed first, second and third Leap Zagreb indices of Verapamil.

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I. INTRODUCTION

Qualitative predictions about reactivity of various compounds and the structure may obtained by chemists using simple rules provided by Graph theory. All the aspects of the application of graph theory to chemistry is concerned with chemical graph theory, which is a branch of mathematical chemistry. A molecular graph is a connected graph with atoms and chemical bonds as vertices and edges.

Verapamil is a medication that is used to control angina and treat excessive blood pressure (chest pain). The immediate-release tablets are also used to prevent and treat irregular heartbeats, either alone or in combination with other medications. Its molecular formula is $C_{27}H_{38}N_2O_4$.

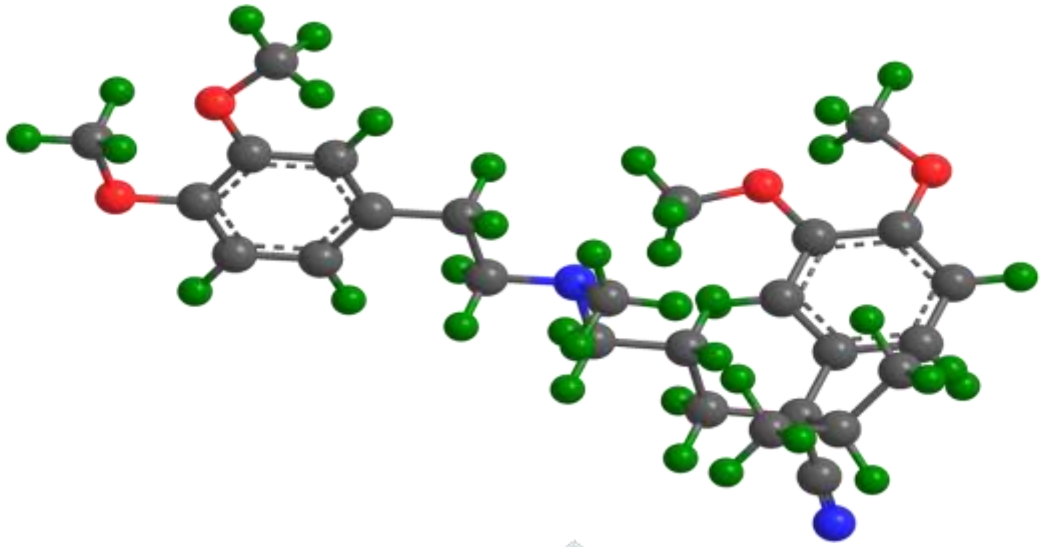

Figure 1 - Structural graph of Verapamil

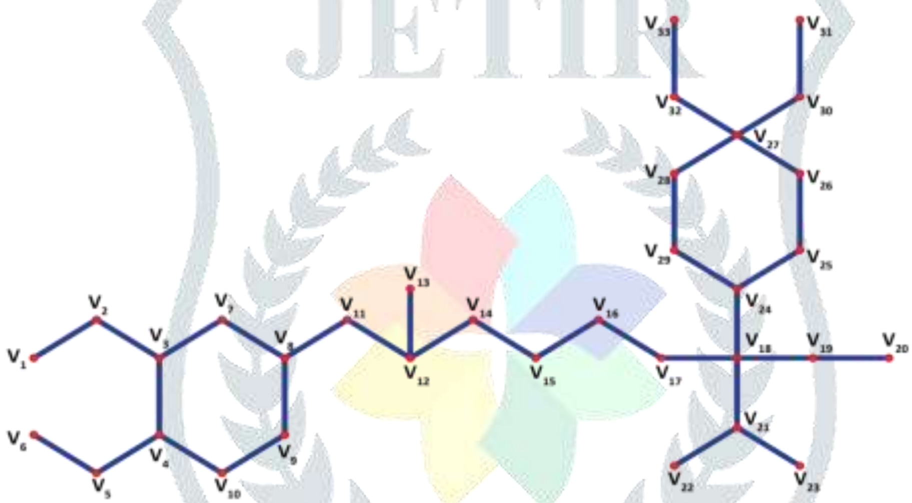

Figure 2 - Molecular graph of Verapamil

Topological indices are the molecular descriptors that describe the structures of chemical compounds and they help us to predict certain physic-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, loop less 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∈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.

The Zagreb indices were first introduced in [1] where the authors examined the dependence of total pi-electron energy of molecular structures. For a molecular graph, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined, respectively, as follows.

$$M_1(G) = \sum_{v \in V(G)} d^2(v)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Motivated by this, in 2017, Naji et al., [2] have introduced a new distance-degree-based topological indices conceived depending on the second degrees of vertices, and are so-called leap Zagreb indices of a graph G and are defined as:

$$LM_1(G) = \sum_{v \in V(G)} d_2^2(v/G)$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G)\, d_2(v/G)$$

$$LM_3(G) = \sum_{uv \in E(G)} (d_2(u/G) + d_2(v/G))$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compound, like boiling point, entropy, DHVAP, HVAP and eccentric factor .

II. Main Results and Discussion:

Theorem21: First Leap Zagreb index of Verapamil is 316.

Proof: Consider a molecular graph of Verapamil. It contains 33 vertices and 34 edges. Verapamil contains vertices of 2-degrees 1, 2, 3, 4, 5 and 6 only and we can partition the vertices of Verapamil into six sets, viz. V_1 , V_2 , V_3, V_4, V_5 and V_6, where each set V_i represents the collection of all vertices with 2-degree i. The number of vertices of 2-degree 1, 2, 3, 4, 5 and 6 are given in the following table -1.

Vertices of 2-degree i	$V_1(G)$	$V_2(G)$	$V_3(G)$	$V_4(G)$	$V_5(G)$	$V_6(G)$
Frequency	5	8	10	8	1	1

TABLE – 1

Consider,

$$LM_1(G) = \sum_{v\in V(G)} d_2^2(v/G)$$

$$= \sum_{v\in V_1(G)} d_2^2(v/G) + \sum_{v\in V_2(G)} d_2^2(v/G) + \sum_{v\in V_3(G)} d_2^2(v/G) + \sum_{v\in V_4(G)} d_2^2(v/G) + \sum_{v\in V_5(G)} d_2^2(v/G) + \sum_{v\in V_6(G)} d_2^2(v/G)$$

$$= 5(1)^2 + 8(2)^2 + 10(3)^2 + 8(4)^2 + 1(5)^2 + 1(6)^2$$

$$\therefore \quad LM_1(G) = 316$$

Theorem 2.2: Second Leap Zagreb index of Verapamil is 363.

Proof: Verapamil contains vertices of 2-degrees 1, 2, 3, 4, 5 and 6 and edges of the type $E_{1,2}$, $E_{1,3}$, $E_{2,2}$, $E_{2,3}$, $E_{2,4}$, $E_{3,3}$, $E_{3,4}$, $E_{3,5}$, $E_{3,6}$, $E_{4,4}$, $E_{4,6}$ and $E_{5,6}$ $respectively$. The frequency of such edges are shown in the following table-2, $where$ $E_{i,j}$ is the collection of all edges joining the vertices of 2-degrees i and j in G.

Edge type	$E_{1,2}$	$E_{1,3}$	$E_{2,2}$	$E_{2,3}$	$E_{2,4}$	$E_{3,3}$	$E_{3,4}$	$E_{3,5}$	$E_{3,6}$	$E_{4,4}$	$E_{4,6}$	$E_{5,6}$
Frequency	2	3	2	4	4	2	7	2	2	4	1	1

TABLE-2

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, d_2(v/G)$$

$$= \sum_{uv\in E_{1,2}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{1,3}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{2,2}(G)} d_2(u/G)\, d_2(v/G)$$

$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{2,4}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{3,3}(G)} d_2(u/G)\, d_2(G)$$

$$+ \sum_{uv\in E_{3,4}(G)} d_2(u/G)\, d_2(G) + \sum_{uv\in E_{3,5}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{3,6}(G)} d_2(u/G)\, d_2(v/G)$$

$$+ \sum_{uv\in E_{4,4}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{4,6}(G)} d_2(u/G)\, d_2(v/G) + \sum_{uv\in E_{5,6}(G)} d_2(u/G)\, d_2(v/G)$$

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

$$= 2\times 2 + 3\times 3 + 2\times 4 + 4\times 6 + 4\times 8 + 2\times 9 + 7\times 12 + 2\times 15 + 2\times 18 + 4\times 16 + 1\times 24 + 1\times 30$$

$$\therefore \quad LM_2(G) = 363.$$

Theorem 2.3: Third Leap Zagreb index of Verapamil is 218.

Proof: By definition of third Leap Zagreb index and by using table - 2 we have,

$$LM_3(G) = \sum_{uv\in E(G)} d_2(u/G) + d_2(v/G)$$

$$= \sum_{uv\in E_{1,2}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{1,3}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{2,2}(G)} d_2(u/G) + d_2(v/G)$$

$$+ \sum_{uv\in E_{2,3}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{2,4}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{3,3}(G)} d_2(u/G) + d_2(v/G)$$

$$+ \sum_{uv\in E_{3,4}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{3,5}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{3,6}(G)} d_2(u/G) + d_2(v/G)$$

$$+ \sum_{uv\in E_{4,4}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{4,6}(G)} d_2(u/G) + d_2(v/G) + \sum_{uv\in E_{5,6}(G)} d_2(u/G) + d_2(v/G)$$

$$= 2(1+2) + 3(1+3) + 2(2+2) + 4(2+3) + 4(2+4) + 2(3+3) + 7(3+4) + 2(3+5) + 2(3+6) + 4(4+4) + 1(4+6) + 1(5+6)$$

$$= 2\times 3 + 3\times 4 + 2\times 4 + 4\times 5 + 4\times 6 + 2\times 6 + 7\times 7 + 2\times 8 + 2\times 9 + 4\times 8 + 1\times 10 + 1\times 11$$

$\therefore\ LM_3(G) = 218.$

CONCLUSIONS:

The first, second and third Leap Zagreb indices of Verapamil are calculated without using computer.

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