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Forgotten topological on the First leap zagreb index of chemical structure in drugs

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Abstract. A massive of early drug tests implies that there exist strong inner relationships between the bio-medical and pharmacology characteristics of drugs and their molecular structures. The forgotten topological first leap index was defined to be used in the analysis of drug molecular structures, which is quite helpful for pharmaceutical and medical scientists to grasp the biological and chemical characteristics of new drugs. Such tricks are popularly employed in developing countries where enough money is lacked to afford the relevant chemical reagents and equipment. In our article, by means of drug molecular structure analysis and edge dividing technology, we present the forgotten topological index of several widely used chemical structures which often appear in drug molecular graphs.
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1. Introduction

In this paper, G is a simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The *order* $|V|$ of G is denoted by $n = n(G)$. For every vertex $v \in V$, the *open neighborhood* of v is the set $N(v) = \{u \in V(G) : uv \in E(G)\}$ and the *closed neighborhood* of v is the set $N[v] = N(v) \cup \{v\}$. The *degree* of a vertex $v \in V$ is $\deg_G(v) = |N(v)|$. C_n for the cycle of length n, and P_n for the path of order n. For details see [3].

Definition 1.1. [1] The first leap zagreb index $LM_1(G)$ is equal to the sum of squares of the second degrees of vertices($LM_1(G) = \sum_{v \in V} d_2^2(v)$)

2. Forgotten topological index of graphene G(m,n)

As a Kind of two-dimensional material, graphene is a planar sheet of carbon atoms that is densely packed in a honeycomb crystal lattice, and it is the main element of certain carbon allotropes including charcoal, fullerenes and graphite, see Fig 1.

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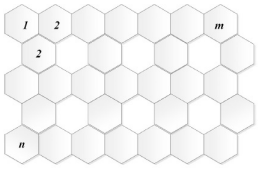

FIGURE 1. 2-Dimensional graph of graphene sheet

THEOREM 2.1. *Let $G(m,n)$ be a graphene sheet with n rows and m columns. We obtain*
$$LM_1(G(m,n)) = 72mn - 4(m+n+12).$$

PROOF. In terms of structure analysis, we get:

$$|V(G(m,n))| = \begin{cases} \lceil \frac{n}{2} \rceil (3m+1) + \lfloor \frac{n}{2} \rfloor (m+3) + m + 1 \text{ if } & \text{n} \equiv 1(mod\ 2) \\ \lceil \frac{n}{2} \rceil (3m+1) + \lfloor \frac{n}{2} \rfloor (m+3) + 2m \text{ if } & \text{n} \equiv 0(mod\ 2) \end{cases}$$

If $n \equiv 1(mod\ 2)$, then

$$\begin{aligned} |V(G(m,n))| &= \lceil \tfrac{n}{2} \rceil (3m+1) + \lfloor \tfrac{n}{2} \rfloor (m+3) + m + 1 \\ &= \tfrac{n+1}{2}(3m+1) + \tfrac{n-1}{2}(m+3) + m + 1 \\ &= 2mn + 2m + 2n. \end{aligned}$$

If $n \equiv 0(mod\ 2)$, then

$$\begin{aligned} |V(G(m,n))| &= \lceil \tfrac{n}{2} \rceil (3m+1) + \lfloor \tfrac{n}{2} \rfloor (m+3) + 2m \\ &= \tfrac{n}{2}(3m+1) + \tfrac{n}{2}(m+3) + 2m \\ &= 2mn + 2m + 2n. \end{aligned}$$

In view of further calculating, we have $n_2 = 2, n_3 = 2n+4, n_4 = 4(m-1), n_5 = 2n-4, n_6 = |V(G(m,n))| - 4n - 4m + 2 = 2mn - 2m - 2n + 2$ that $n_i = |d_2(v) = i|$. Therefore, using the definition of forgotten topological first leap index, we obtain

$$\begin{aligned} LM_1(G(m,n)) &= \textstyle\sum_{v \in V(G)} d_2^2(v) \\ &= 2(2)^2 + (2n+4)(3)^2 + (4m-4)(4)^2 + (2n-4)(5)^2 + (2mn-2m-2n+2)(6)^2 \\ &= 72mn - 8m - 4n - 48. \end{aligned}$$

Hence, we obtain the expected result. □

3. Forgotten topological index of polyomino chains of n-cycles and triangular benzenoid

From a mathematical point of view, polyomino system is a finite 2-connected plane graph in which each interior face is surrounded by a C_4. It is an edge-connected union of cells, and more details can be found in [2]. As an example, the polyomino chains of 8-cycles can be shown in Fig 2 .

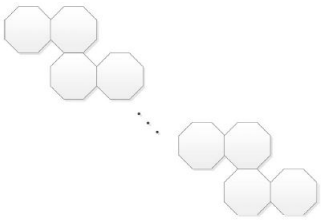

FIGURE 2. The zig-zag chain of 8-cycles.

THEOREM 3.1. *Let G be a polyomino chains of 8-cycles . We have $LM_1(G) = 304n - 52$.*

PROOF. By means of structure analysis, we infer $n_2 = 8n + 4, n_3 = 8n, n_4 = 2, n_5 = 8n - 4$. Therefore, using the definition of forgotten topological first leap index, we obtain

$$\begin{aligned} LM_1(G) &= \sum_{v \in V(G)} d_2^2(v) \\ &= (8n+4)(2)^2 + 8n(3)^2 + 2(4)^2 + (8n-4)(5)^2 \\ &= 304n - 52. \end{aligned}$$

Hence, we obtain the expected result. □

Next, we compute forgotten topological index of triangular benzenoid molecular graph $T(n)$. It,s structure can be referred to Fig 3 .

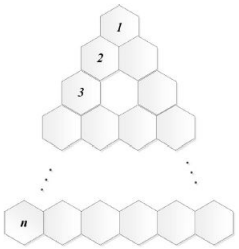

FIGURE 3. Molecular graph of triangular benzenoid.

THEOREM 3.2. *Let $T(n)$ be a triangular benzenoid. We deduce $LM_1(T_n) = 36n^2 + 24n - 42$.*

PROOF. By means of structure analysis, we infer $n_2 = 3, n_3 = 6, n_4 = 6n - 9, n_6 = (n-1)^2$. Therefore, using the definition of forgotten topological first leap index, we obtain

$$\begin{aligned} LM_1(T_n) &= \sum_{v \in V(G)} d_2^2(v) \\ &= 3(2)^2 + 6(3)^2 + (6n-9)(4)^2 + (n-1)^2(6)^2 \\ &= 36n^2 + 24n - 42. \end{aligned}$$

Hence, we obtain the expected result. □

4. Forgotten topological first leap index of two classes of benzenoid series

Finally, we aim to determine the forgotten topological first leap index of two classes of benzenoid series. First, we consider circumcoronene series of benzenoid H_k, when $k = 1, 2, 3$, the structures are preseted Fig 4.

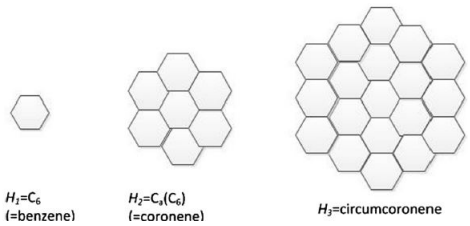

FIGURE 4. The first, second and third molecular graphs H_1, H_2 and H_3 from the circumcoronene series of benzenoid.

THEOREM 4.1. $LM_1(H_k) = 216k^2 - 240k + 36$.

PROOF. Consider circumcoronene series of benzenoid H_k for $k \geq 2$. It is not hard to check that $|V(H_k)| = 6k^2$ and $|E(H_k)| = 9k^2 - 3k$. Moreover, we deduce $n_3 = 12, n_4 = 6(2k-3), n_6 = 6(k-1)^2$. Thus, using the definition of forgotten topological first leap index, we obtain

$$\begin{aligned} LM_1(H_k) &= \sum_{v \in V(G)} d_2^2(v) \\ &= 12(3)^2 + 6(2k-3)(4)^2 + 6(k-1)(6)^2 \\ &= 216k^2 - 240k + 36. \end{aligned}$$

Hence, we obtain the expected result. □

Let P_n be the math n vertices. We have dn vertices and $dn-1$ edges for bridge molecular graph $G_d(P_n, v)$(see Fig 5).

FIGURE 5. The bridge molecular graph $G_d(P_n, v)$

THEOREM 4.2. $LM_1(G_d(P_n, v)) = 4nd + 20d - 60$

PROOF. Additionally, the edge set of bridge graph $G_d(P_n, v))$ can be divided in to four partitions: $n_1 = 2d, n_2 = (n-4)d+2, n_3 = d, n_4 = 2, n_5 = d-4$. Thus, using the definition of forgotten topological first leap index, we obtain

$$\begin{aligned} LM_1(G_d(P_n, v)) &= \sum_{v \in V(G)} d_2^2(v) \\ &= 2d(1)^2 + ((n-4)d+2)(2)^2 + d(3)^2 + 2(4)^2 + (d-4)(5)^2 \\ &= 20d + 4nd - 60. \end{aligned}$$

□

References

1. A.M. Naji ,N.D. Soner, *The First Leap Zagreb Index of Some Graph Operations*,International Journal of Applied Graph Theory,Vol.2, No.1 (2018), 07 - 18.
2. W. Gao, M.K.Siddiqui, M. Imran, M.K. Jamil, M.R. Farahani, *Forgotten topological index of chemical structure in drugs*,Saudi Pharmaceutical Journal (2016) 24, 258–264.
3. West, D.B, *Introduction to Graph Theory*, Prentice-Hall,2000.

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