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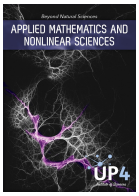

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# Note on forgotten topological index of chemical structure in drugs

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## Abstract

The forgotten topological index of a graph $G$ is defined as the sum of the cube of the degrees of its vertices. In the recent paper [6], [W. Gao et al. (2016), *Forgotten topological index of chemical structure in drugs*, Saudi Pharmaceutical Journal, 24, 258-264], the forgotten topological index of some chemical structures has been obtained. In this note, we correct their result regarding triangular benzenoid. Also, we have given the expression for the forgotten topological index of graphene structure which is more compact than the one was obtained in the paper above.

**Keywords:** Forgotten topological index; degree of a vertex; computational medical; chemical structure
**AMS 2010 codes:** 05C07, 92E10

## 1 Introduction

Development of drugs in medicine industry has more demand to determine the pharmacological, chemical and biological characteristics of the drugs. Many previous studies have pointed out that chemical and pharmacodynamics characteristics of drugs and their molecular structures are closely correlated [2, 4, 5, 9, 13].

In mathematical medicine, structure of the drug is represented as an undirected graph, where each vertex indicates an atom and each edge represents a chemical bond between the atoms.

Let $G$ be a simple graph corresponding to a drug structure with vertex (atom) set $V(G)$ and edge (bond) set $E(G)$. The edge joining the vertices $u$ and $v$ is denoted by $uv$. Thus, if $uv \in E(G)$ then $u$ and $v$ are adjacent in $G$. The degree of a vertex $u$, denoted by $d(u)$, is the number of edges incident to $u$. Several topological indices such as Estrada index [1], Zagreb index [8], PI index [10], eccentric index [11], and Wiener index [12] have been introduced in the literature to study the chemical and pharmacological properties of molecules.

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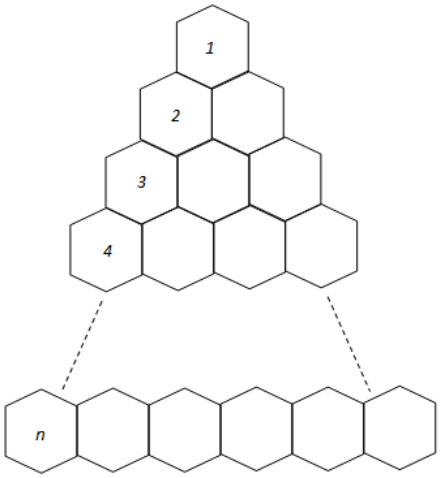


**Fig. 1** Molecular graph of triangular benzenoid $T(n)$.

Furtula and Gutman [3] introduced the forgotten topological index of a graph $G$, also called as $F-$index, which is defined as

$$F(G) = \sum_{u \in V(G)} (d(u))^3 = \sum_{uv \in E(G)} \left[ (d(u))^2 + (d(v))^2 \right].$$

The study of forgotten topological index of the chemical structure in drugs is carried out in [6, 7]. Recently, Gao et al. [6] have obtained the forgotten topological index of some drug structures. The expression for the forgotten topological index of triangular benzenoid in their paper is erroneous. In this note we correct it. Also, we give the expression for forgotten topological index of graphene sheet which is more compact than the one obtained by Gao et al. [6].

## 2 Forgotten index of triangular benzenoid

The structure of the triangular benzenoid molecular graph $T(n)$ is shown in Fig. 1. It has $n(n+1)/2$ hexagons.

In Gao et al. [6], the following result was obtained.

**Theorem 1.** *Let $T(n)$ be a triangular benzenoid. Then*

$$F(T(n)) = \frac{39}{2}n^2 + \frac{177}{2}n - 60.$$

Expression in Theorem 1 is not correct. In the following theorem, we give the correct expression for $F(T(n))$.

**Theorem 2.** *Let $T(n)$ be a triangular benzenoid. Then the forgotten index of $T(n)$ is*

$$F(T(n)) = 27n^2 + 51n - 30.$$

*Proof.* Partition the vertex set $V(T(n))$ into two subsets $V_1$ and $V_2$ such that $V_1 = \{u \mid d(u) = 2\}$ and $V_2 = \{u \mid d(u) = 3\}$.

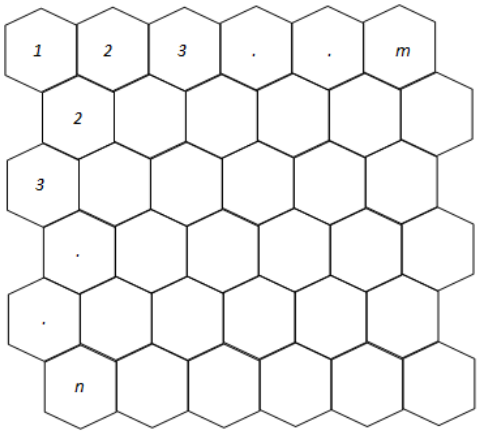


**Fig. 2** 2−Dimensional graph of graphene sheet $G(m,n)$.

By means of structure analysis of $T(n)$, we have $|V_1| = 3n+3$ and $|V_2| = n(n+1)-2$. Therefore, by the definition of forgotten topological index, we get

$$\begin{aligned} F(T(n)) &= \sum_{u\in V(T(n))} (d(u))^3 \\ &= \sum_{u\in V_1} (d(u))^3 + \sum_{u\in V_2} (d(u))^3 \\ &= (3n+3)(8) + (n(n+1)-2)(27) \\ &= 27n^2 + 51n - 30. \end{aligned}$$

## 3 Forgotten index of graphene

Graphene is a planar sheet of carbon atoms that is densely placed in a honeycomb crystal lattice. It is the main element of certain carbon allotropes. The structure of graphene $G(m,n)$ with $n$ rows and $m$ columns is shown in Fig. 2. It has $mn$ hexagons.

In Gao et al. [6], the following result was obtained.

**Theorem 3.** *Let $G(m,n)$ be a graphene sheet with n rows and m columns. Then*

$$F(G(m,n)) = \begin{cases} 18\left(\left\lceil \frac{n}{2}\right\rceil (5m+1) + \left\lfloor \frac{n}{2}\right\rfloor (m+3)\right) - 20m - 20n - 20 & \text{if } n \equiv 1 (mod\ 2) \\ 18\left(\left\lceil \frac{n}{2}\right\rceil (5m+1) + \left\lfloor \frac{n}{2}\right\rfloor (m+3)\right) + 16m - 20n - 38 & \text{if } n \equiv 0 (mod\ 2). \end{cases}$$

In the following theorem, we give a simple expression for the forgotten index of graphene $G(m,n)$.

**Theorem 4.** *Let $G(m,n)$ be a graphene sheet with n rows and m columns. Then*

$$F(G(m,n)) = 54mn + 16m + 16n - 38.$$

*Proof.* If $n = 1$ and $m \geq 1$, then we get the result by direct observation.

Now for $n \geq 2$ and $m \geq 1$, by analysis of structure of graphene sheet $G(m,n)$, we partition the edge set of the graph $G(m,n)$ into the following three subsets: $E_1 = \{uv \mid d(u) = d(v) = 2\}$, $E_2 = \{uv \mid d(u) = 2 \text{ and } d(v) = 3\}$ and $E_3 = \{uv \mid d(u) = d(v) = 3\}$. Let $e_{ij}$ denote the number of edges whose one end vertex has degree $i$ and other end vertex has degree $j$. The number of edges in each row of graphene sheet $G(m,n)$ is given in Table1.

**Table 1** Number of edges in each row of $G(m,n)$.

| Row | $e_{22}$ | $e_{23}$ | $e_{33}$ |
|---|---|---|---|
| 1 | 3 | $2m$ | $3m-2$ |
| 2 | 1 | 2 | $3m-1$ |
| 3 | 1 | 2 | $3m-1$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $n-1$ | 1 | 2 | $3m-1$ |
| $n$ | 3 | $2m$ | $m-1$ |

Using the data of Table 1, we can easily write $|E_1| = n+4$, $|E_2| = 4m+2n-4$ and $|E_3| = 3mn-2m-n-1$. Therefore, by the definition of forgotten topological index, we obtain

$$\begin{aligned} F(G(m,n)) &= \sum_{uv\in E(G(m,n))} \left[(d(u))^2+(d(v))^2\right] \\ &= \sum_{uv\in E_1} \left[(d(u))^2+(d(v))^2\right] + \sum_{uv\in E_2} \left[(d(u))^2+(d(v))^2\right] + \sum_{uv\in E_3} \left[(d(u))^2+(d(v))^2\right] \\ &= (n+4)(8)+(4m+2n-4)(13)+(3mn-2m-n-1)(18) \\ &= 54mn+16m+16n-38. \end{aligned}$$

## 4 Conclusions

In this note, we have given the correct expression for the forgotten topological index of triangular benzenoid. Also, a simple expression for the forgotten topological index of graphene sheet is derived.

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