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Computing Degree-Based Topological Indices for Molecular Graphs

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Abstract: In our paper, by means of drug's molecular structure analysis and edge dividing technology, we investigate the degree-based topological indices of several widely-used chemical structures which often appear in drug molecular graphs.

Keywords: Distance, degree, Topological index, Dendrimers.

1 Introduction

The branch of mathematical chemistry which applies graph theory to model the chemical structures is known as chemical graph theory [1]. This theory has a remarkable role in the development of chemical sciences. In chemistry, biochemistry and nanotechnology different topological indices are found to be useful in isomer discrimination, structure-property relationship, structure-activity relationship and pharmaceutical drug design. Developing structure-activity relationships for drug compounds using computational or theoretical methods relies on appropriate representations of molecular structure. This review focuses on the role of Topological Indices (TIs) from a drug design and discovery perspective. When a single number represents a graph invariant, it is known as topological index or topological descriptor.

Topological indices are mathematical tools that correlate the chemical structure with various physical properties, chemical reactivity or biological activity numerically. A topological index is a function having a set of molecular graphs as its domain and a set of real numbers as its range. In QSAR/QSPR study, a prediction about the bioactivity of chemical compounds is made on the basis of physico-chemical properties and topological indices such as Zagreb and multiple Zagreb indices. The reduced forgotten topological index is used in the analysis of drug designing for pharmaceutical and medical scientists to grasp the biological and chemical characteristics of new drugs. The topological and graph invariants based on distances between vertices of a graph are widely used for characterizing molecular graphs, establishing relationships between structures and properties of molecules, predicting biological activities of chemical compounds and making their chemical applications. Topological indices have some major classes but among these classes degree-based topological indices have a prominent role in chemical graph theory.

Let G be a molecular graph [2,3] with vertex set $V(G)$ and edge set $E(G)$.If u and v are two adjacent vertices of G, then the edge connecting them will be denoted by uv. By $deg(v)$ we denote the degree (number of first neighbors) of the vertex v of the graph G .

There are two Zagreb indices [4,5] the first M_1 and the second M_2, defined as $M_1 = M_1(G) = \sum_{v \in V(G)} deg(v)^2$ and $M_2 = M_2(G) = \sum_{uv \in E(G)} deg(u)deg(v)$ respectively.

The first Zagreb index can be rewritten also as [6]
$M_1 = M_1(G) = \sum_{uv \in E(G)} [deg(u) + deg(v)]$.

With the notation, the forgotten topological index is defined as [7]
$F = F(G) = \sum_{v \in V(G)} deg(v)^3 = \sum_{uv \in E(G)} [deg(u)^2 + deg(v)^2]$.

After appearing in the work , the quantity F was never again considered in the chemical and/or mathematical literature.

The forgotten topological index involves the number of vertices, edges, and maximum and minimum vertex degree. They showed that the predictive ability of this index is almost similar to that of first Zagreb index and

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for the entropy and acentric factor, both of them yield correlation coefficients greater than 0.95.They named this index as "forgotten topological index" or "F-index." Topological indices are abundantly used in the QSPR and QSAR researches. So far, many various types of topological indices have been described. Topological indices are defined and used in many areas to study several properties of different objects such as atoms and molecules. Several topological indices have been defined and studied by mathematicians and chemists .

The reduced second Zagreb index is defined as [8]
$RM_2 = RM_2(G) = \sum_{ij\in E(G)} (d_i - 1)(d_j - 1)$.

Because of the identity
$RM_2(G) = M_2(G) - M_1(G) + m$.

This graph invariant is necessarily encountered within studies of the difference between the two Zagreb indices. In addition, if the graph G is a tree, then $RM_2(G)$ is equal to the number of pairs of vertices at distance 3, which, in mathematical chemistry, is often referred to as the "wiener polarity index".

In [9] A. Subhashini and J. Baskar Babujee introduced reduced forgotten topological index stated as
$RF = RF(G) = \sum_{uv\in E(G)} [(d_u - 1)^2 + (d_v - 1)^2]$

Bollobas and Erdos [10] introduced general randic index stated as
$R_k(G) = \sum_{uv\in E(G)} (d_u d_v)^k$. Where k is a real number.

General sum connectivity index [11] is stated as
$\psi_k(G) = \sum_{uv\in E(G)} (d_u + d_v)^k$.

Shirdel et al [12] introduced a new version of Zagreb index named Hyper Zagreb index stated as,
$HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2$.

Hyper Zagreb index is a special case of general Sum connectivity index when $k = 2$. L. Yan, W. Gao, and J.S. Li [13] introduced Harmonic index and it is stated as,
$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}$.

In this paper, We would like to study the "Degree-Based Topological Indices", and establish some of its basic properties in graphs. In addition, we would like to study the physico-chemical properties of some chemical structures.

2 Chemical Structures taken for study

2.1 Regular hexagonal lattice

There are various types of lattices which are under study, some topological indices are obtained for hexagonal lattices.

If L is a regular hexagonal lattice, let P_m^n be $m \times n$ quadrilateral section cut from L where $m,n \geq 2$. Here m represents the number of hexagons on the top and bottom sides and n is the number of hexagons on the lateral sides. see Fig. 1 illustrates detailed chemical structure [14].

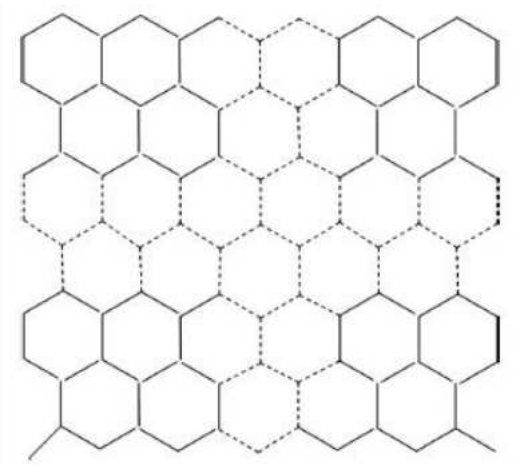

Fig. 1: Quadrilateral section P_m^n cuts from the regular hexagonal lattice

The tube NA_m^n with $2m(n+1)$ vertices and $(3n+2)m$ edges is obtained by identifying two lateral sides of P_m^n via identifying the vertices u_0^j and u_m^j $(j = 0,1,\ldots,n)$[15].

Let $n \in N$ be even so that $n,m \geq 2$. The tube NC_m^n of order $n(2m+1)$ with size $n(3m+1/2)$ can be yielded by identifying the top and bottom sides of the quadrilateral section P_m^n in a similar way in which the vertices u_i^n for $i = 0,1,\ldots,m$ vertic v_i^0 and v_i^n for $i = 0,1,\ldots,m$ are identified [16].

2.2 Dendrimer stars $D_3[n]$

We discuss an important chemical structure $D_3[n]$ which denotes the n-th growth of star dendrimer $\forall\ n \in N \cup \{0\}$. See Figure 2 for more details on the structure of this chemical molecular graph which widely appears in drug structures.

According to the analysis in [17,18,19] we know that $E(D_3[n])$ can be divided into four parts:. $n_{13} = 3.2^n$, $n_{22} = 6(2^{n+1} - 1)$, $n_{23} = 12(2^{n+1} - 1)$, and $n_{33} = 9.2^n - 6$. Hence, we directly get the following conclusion for these molecular structures.

2.3 Two classes of benzenoid series

We aim to determine the reduced forgotten topological index of two classes of benzenoid series [15].

First, we consider circumcoronene series of benzenoid H_k, when $k = 1,2,3$ the structures are presented in Figure 3.

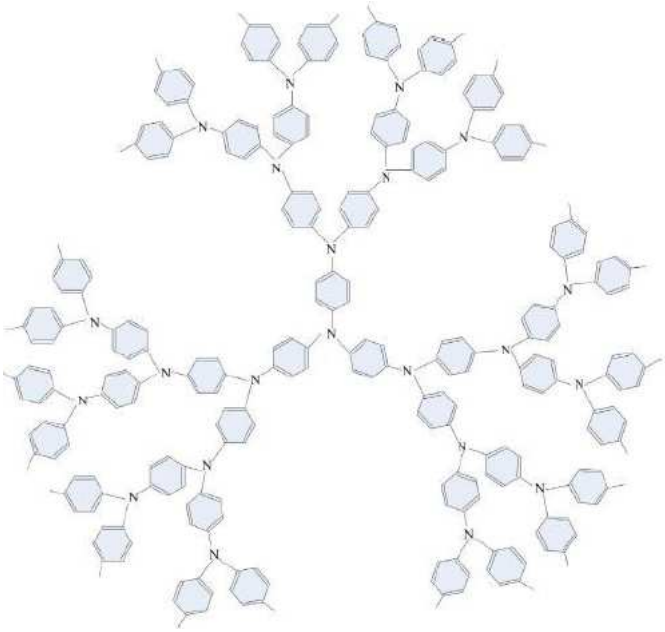

Fig. 2: The 2D of the n^{th} growth of star dendrimer $D_3[n]$

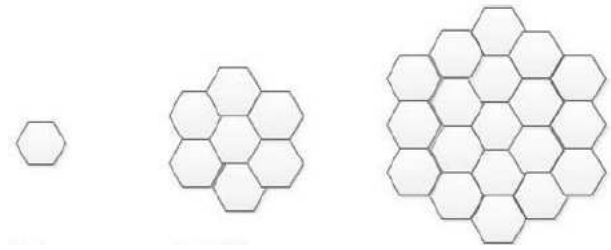

Fig. 3: The first, second and third molecular graphs $H_1 = C_6$ (= benzene), $H_2 = C_2(C_6)$ (= coronene) and H_3 (= circumcoronene) from the circumcoronene series of benzenoid

Thus, this family of circumcoronene homologous series of benzenoid consists of several copies of benzene C_6 on circumference, and the more details for this structure [16,20] can be referred to in Figure 4.

3 Degree-based topological index

Theorem 1.
$RF(NA_m^n) = 24mn + 4m.$
$RF(NC_m^n) = 24mn - 8n.$

*Proof.*For the tube NA_m^n, we derive $n_{23} = 4m$, and $n_{33} = m(3n-2)$. Hence, by means of the definition of reduced forgotten topological index, we get

$$\begin{aligned} RF(NA_m^n) &= \sum_{uv\in E_{23}} [(d_u-1)^2 + (d_v-1)]^2 \\ &= \sum_{uv\in E_{23}} [(2-1)^2 + (3-1)^2] \\ &\quad + \sum_{uv\in E_{33}} [(3-1)^2 + (3-1)^2]. \\ &= 5.4m + 8m(3n-2) \\ &= 20m + 24mn - 16m \\ &= 24mn + 4m \end{aligned}$$

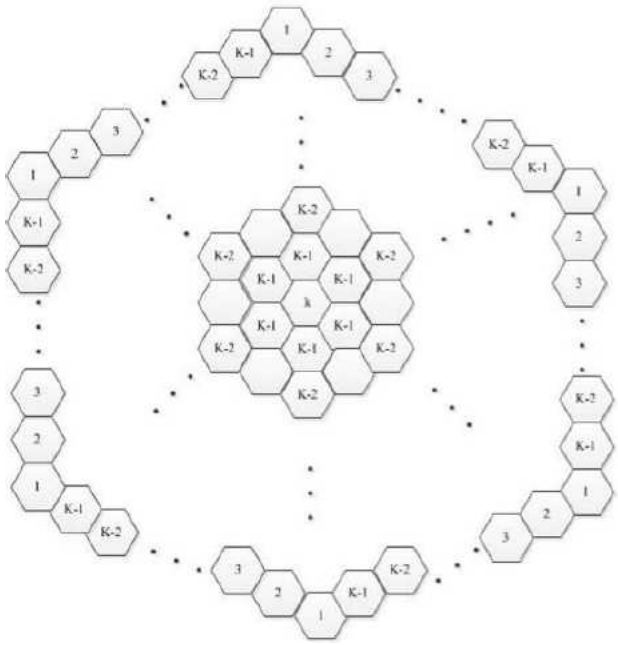

Fig. 4: The circumcoronene series of benzenoid H_k for $k \geq 1$

For the tube NC_m^n, we derive $n_{22} = n$, $n_{23} = 2n$ and $n_{33} = n\left(3m - \frac{5}{2}\right)$. Hence, by means of the definition of reduced forgotten topological index, we get

$$\begin{aligned} RF(NC_m^n) &= \sum_{uv\in E(NC_m^n)} [(d_u-1)^2 + (d_v-1)]^2. \\ &= \sum_{uv\in E_{22}} [(2-1)^2 + (2-1)^2] \\ &\quad + \sum_{uv\in E_{23}} [(2-1)^2 + (3-1)^2] \\ &\quad + \sum_{uv\in E_{33}} [(3-1)^2 + (3-1)^2]. \\ &= 2n + 5\times 2n + 8n\left(3m - \frac{5}{2}\right). \\ &= 2n + 10n + 24mn - \frac{40n}{2}. \end{aligned}$$

$$= 12n + 24mn - \frac{40n}{2}.$$
$$= 24mn - \frac{40n+24n}{2}.$$
$$= 24mn - \frac{16n}{2}.$$
$$= 24mn - 8n.$$

Theorem 2.
$RF(H_k) = 72k^2 - 60k.$

*Proof.*Consider circumcoronene series of benzenoid H_k for $k \geq 1$.

$$|V(H_k)| = 6k^2 \text{ and } |E(H_k)| = 9k^2 - 3k$$

Moreover, we deduce $n_{33} = 9k^2 - 15k + 6$, $n_{23} = 12(k-1)$ and $n_{22} = 6$.
Thus, by using the definition of Reduced forgotten topological index we get,

$$\begin{aligned} RF(H_k) &= \sum_{uv \in E(H_k)} [(d_u - 1)^2 + (d_v - 1)]^2. \\ &= \sum_{uv \in E_{22}} [(2-1)^2 + (2-1)^2] \\ &\quad + \sum_{uv \in E_{23}} [(2-1)^2 + (3-1)^2] \\ &\quad + \sum_{uv \in E_{33}} [(3-1)^2 + (3-1)^2]. \\ &= 2 \times 6 + 5 \times 12(k-1) + 8(9k^2 - 15k + 6). \\ &= 12 + 5 \times (12k - 12) + 72k^2 - 120k + 48. \\ &= 72k^2 + 60k - 60 - 120k + 60. \\ &= 72k^2 - 60k. \end{aligned}$$

Theorem 3.
$RF(Ca_k(C_6)) = 24.7^k + 6.3^k - 18.$

*Proof.*By analyzing the molecular structure of $Ca_k(C_6)$, The edge set of $Ca_k(C_6)$ can be divided into three partitions:

$$n_{22} = 3^k + 3, n_{23} = 4.3^k \text{ and } n_{33} = 3.7^k - 2.3^k - 3.$$

Thus, by using the definition of Reduced Forgotten topological index, we get,

$$\begin{aligned} RF(Ca_k(C_6)) &= \sum_{uv \in E(Ca_k(C_6))} [(d_u - 1)^2 + (d_v - 1)]^2. \\ &= \sum_{uv \in E_{22}} [(2-1)^2 + (2-1)^2] \\ &\quad + \sum_{uv \in E_{23}} [(2-1)^2 + (3-1)^2] \\ &\quad + \sum_{uv \in E_{33}} [(3-1)^2 + (3-1)^2]. \\ &= 2(3^k + 3) + 20.3^k + 8(3.7^k - 2.3^k - 3). \\ &= 24.7^k + 6.3^k - 18. \end{aligned}$$

Theorem 4.
$R_k(NA_m^n) = 4m.6^k + m(3n-2).9^k$
$R_k(NC_m^n) = n.4^k + 2n.6^k + n\left(3m - \frac{5}{2}\right).9^k$

*Proof.*For the tube NA_m^n, we derive $n_{23} = 4m$, and $n_{33} = m(3n-2)$.
Hence, by means of the definition of general randic index, we get

$$\begin{aligned} R_k(NA_m^n) &= \sum_{uv \in E(NA_m^n)} [(d_u.d_v)]^k. \\ &= \sum_{uv \in E_{23}} (2.3)^k + \sum_{uv \in E_{33}} (3.3)^k. \\ &= 4m.6^k + m(3n-2).9^k \end{aligned}$$

For the tube NC_m^n, We derive $n_{22} = n$, $n_{23} = 2n$ and $n_{33} = n\left(3m - \frac{5}{2}\right)$.

$$\begin{aligned} R_k(NC_m^n) &= \sum_{uv \in E(NC_m^n)} [(d_u.d_v)]^k. \\ &= \sum_{uv \in E_{22}} (2.2)^k + \sum_{uv \in E_{23}} (2.3)^k + \sum_{uv \in E_{33}} (3.3)^k. \\ &= n.4^k + 2n.6^k + n.\left(3m - \frac{5}{2}\right).9^k. \end{aligned}$$

Theorem 5.
$\psi_k(NA_m^n) = 4m.5^k + m(3n-2).6^k.$
$\psi_k(NC_m^n) = n.4^k + 2n.5^k + n\left(3m - \frac{5}{2}\right).6^k$

*Proof.*For the tube NA_m^n, we derive $n_{23} = 4m$ and $n_{33} = m(3n-2)$.
Hence, by means of the definition of general sum connectivity index, we get

$$\begin{aligned} \psi_k(NA_m^n) &= \sum_{uv \in E(NA_m^n)} [(d_u + d_v)]^k. \\ &= \sum_{uv \in E_{23}} (2+3)^k + \sum_{uv \in E_{33}} (3+3)^k. \\ &= 4m.5^k + m(3n-2).6^k \end{aligned}$$

For the tube NC_m^n, We derive $n_{22} = n$, $n_{23} = 2n$ and $n_{33} = n\left(3m - \frac{5}{2}\right)$.

$$\begin{aligned} \psi_k(NC_m^n) &= \sum_{uv \in E(NC_m^n)} (d_u + d_v)^k. \\ &= \sum_{uv \in E_{22}} (2+2)^k + \sum_{uv \in E_{23}} (2+3)^k + \sum_{uv \in E_{33}} (3+3)^k. \\ &= n.4^k + 2n.5^k + n.\left(3m - \frac{5}{2}\right).6^k. \end{aligned}$$

Theorem 6.
$HM(NA_m^n) = 4m.5^2 + m(3n-2).6^2$
$HM(NC_m^n) = n.4^2 + 2n.5^2 + n.\left(3m - \frac{5}{2}\right).6^2.$

*Proof.*For the tube NA_m^n, we derive $n_{23} = 4m$ and $n_{33} = m(3n-2)$.

Hence, by means of the definition of Hyper Zagreb index, We get

$$\begin{aligned} HM(NA_m^n) &= \sum_{uv\in E(NA_m^n)} [(d_u+d_v)]^2. \\ &= \sum_{uv\in E_{23}} (2+3)^2 + \sum_{uv\in E_{33}} (3+3)^2. \\ &= 4m.5^2 + m(3n-2).6^2. \end{aligned}$$

For the tube NC_m^n, We derive $n_{22} = n$, $n_{23} = 2n$ and $n_{33} = n\left(3m-\frac{5}{2}\right)$.

$$\begin{aligned} HM(NC_m^n) &= \sum_{uv\in E(NC_m^n)} (d_u+d_v)^2. \\ &= \sum_{uv\in E_{22}} (2+2)^2 + \sum_{uv\in E_{23}} (2+3)^2 \\ &\quad + \sum_{uv\in E_{33}} (3+3)^2. \\ &= n.4^2 + 2n.5^2 + n.\left(3m-\frac{5}{2}\right).6^2. \end{aligned}$$

Theorem 7.
$H(NA_m^n) = 4m.\frac{2}{5} + m(3n-2).\frac{2}{6}$.
$H(NC_m^n) = \frac{n}{2} + \frac{4n}{5} + \frac{2n}{6}\left(3m-\frac{5}{2}\right)$.

*Proof.*For the tube NA_m^n, we derive $n_{23} = 4m$ and $n_{33} = m(3n-2)$.
Hence, by means of the definition of Harmonic index, We get

$$\begin{aligned} H(NA_m^n) &= \sum_{uv\in E(NA_m^n)} \left(\frac{2}{d_u+d_v}\right) \\ &= \sum_{uv\in E_{23}} \frac{2}{5} + \sum_{uv\in E_{33}} \frac{2}{6}. \\ &= 4m.\frac{2}{5} + m(3n-2).\frac{2}{6} \end{aligned}$$

For the tube NC_m^n, We derive $n_{22} = n$, $n_{23} = 2n$ and $n_{33} = n\left(3m-\frac{5}{2}\right)$.

$$\begin{aligned} H(NC_m^n) &= \sum_{uv\in E(NC_m^n)} \left(\frac{2}{d_u+d_v}\right) \\ &= \sum_{uv\in E_{22}} \frac{2}{4} + \sum_{uv\in E_{23}} \frac{2}{5} + \sum_{uv\in E_{33}} \frac{2}{6}. \\ &= n.\frac{1}{2} + 2n.\frac{2}{5} + n.\left(3m-\frac{5}{2}\right).\frac{1}{3} \end{aligned}$$

Theorem 8.
$\psi_k(H_k) = 6.4^k + 12(k-1).5^k + (9k^2-15k+6).6^k$

*Proof.*Consider circumcoronene series of benzenoid H_k for $k \geq 1$.

$$|V(H_k)| = 6k^2 \text{ and } |E(H_k)| = 9k^2 - 3k$$

Moreover, we deduce $n_{33} = 9k^2-15k+6$, $n_{23} = 12(k-1)$ and $n_{22} = 6$. Thus, by using the definition of general sum connectivity index, we get,

$$\begin{aligned} \psi_k(H_k) &= \sum_{uv\in E(H_k)} [(d_u+d_v)]^k. \\ &= \sum_{uv\in E_{22}} (2+2)^k + \sum_{uv\in E_{23}} (2+3)^k + \sum_{uv\in E_{33}} (3+3)^k. \\ &= 6.4^k + 12(k-1).5^k + (9k^2-15k+6).6^k. \end{aligned}$$

Theorem 9.
$R_k(H_k) = 6.4^k + 12(k-1).6^k + (9k^2-15k+6).9^k$

*Proof.*Consider circumcoronene series of benzenoid H_k for $k \geq 1$.

$$|V(H_k)| = 6k^2 \text{ and } |E(H_k)| = 9k^2 - 3k$$

Moreover, we deduce $n_{33} = 9k^2-15k+6$, $n_{23} = 12(k-1)$ and $n_{22} = 6$.
Thus, by using the definition of general randic index, we get,

$$\begin{aligned} R_k(H_k) &= \sum_{uv\in E(H_k)} [(d_u.d_v)]^k. \\ &= \sum_{uv\in E_{22}} (2.2)^k + \sum_{uv\in E_{23}} (2.3)^k + \sum_{uv\in E_{33}} (3.3)^k. \\ &= 6.4^k + 12(k-1).6^k + (9k^2-15k+6).9^k. \end{aligned}$$

Theorem 10.
$HM(H_k) = 6.4^2 + 12(k-1).5^2 + (9k^2-15k+6).6^2$

*Proof.*Consider circumcoronene series of benzenoid H_k for $k \geq 1$.

$$|V(H_k)| = 6k^2 \text{ and } |E(H_k)| = 9k^2 - 3k$$

Moreover, we deduce $n_{33} = 9k^2-15k+6$, $n_{23} = 12(k-1)$ and $n_{22} = 6$.
Thus, by using the definition of Hyper Zagreb index, we get,

$$\begin{aligned} HM(H_k) &= \sum_{uv\in E(H_k)} ((d_u+d_v))^2. \\ &= \sum_{uv\in E_{22}} (2+2)^2 + \sum_{uv\in E_{23}} (2+3)^2 + \sum_{uv\in E_{33}} (3+3)^2. \\ &= 6.4^2 + 12(k-1).5^2 + (9k^2-15k+6).6^2. \end{aligned}$$

Theorem 11.
$H(H_k) = 6.\frac{2}{4} + 12(k-1).\frac{2}{5} + (9k^2-15k+6).\frac{2}{6}$.

*Proof.*Consider circumcoronene series of benzenoid H_k for $k \geq 1$.

$$|V(H_k)| = 6k^2 \text{ and } |E(H_k)| = 9k^2 - 3k$$

Moreover, we deduce $n_{33} = 9k^2 - 15k + 6, n_{23} = 12(k-1)$ and $n_{22} = 6$.
Thus, by using the definition of harmonic index, we get,

$$\begin{aligned} H(H_k) &= \sum_{uv \in E_{22}} \left(\frac{2}{2+2}\right) + \sum_{uv \in E_{23}} \left(\frac{2}{2+3}\right) \\ &\quad + \sum_{uv \in E_{33}} \left(\frac{2}{3+3}\right). \\ &= 6.\frac{2}{4} + 12(k-1).\frac{2}{5} + (9k^2 - 15k + 6).\frac{2}{6}. \end{aligned}$$

Theorem 12.

$$\begin{aligned} R_k(Ca_k(C_6)) &= (3^k+3).4^k + (4.3^k).6^k \\ &\quad + (3.7^k - 2.3^k - 3).9^k. \end{aligned}$$

*Proof.*By analyzing the molecular structure of $Ca_k(C_6)$, The edge set of $Ca_k(C_6)$ can be divided into three partitions: $n_{22} = 3^k + 3$, $n_{23} = 4.3^k$ and $n_{33} = 3.7^k - 2.3^k - 3$.
Thus, by using the definition of general randic index, we get,

$$\begin{aligned} R_k(Ca_k(C_6)) &= \sum_{uv \in E(Ca_k(C_6))} (d_u.d_v)^k. \\ &= \sum_{uv \in E_{22}} (2.2)^k + \sum_{uv \in E_{23}} (2.3)^k + \sum_{uv \in E_{33}} (3.3)^k. \\ &= (3^k+3).4^k + (4.3^k).6^k \\ &\quad + (3.7^k - 2.3^k - 3).9^k. \end{aligned}$$

Theorem 13.

$$\begin{aligned} \psi_k(Ca_k(C_6)) &= (3^k+3).4^k + (4.3^k).5^k \\ &\quad + (3.7^k - 2.3^k - 3).6^k. \end{aligned}$$

*Proof.*By analyzing the molecular structure of $Ca_k(C_6)$, The edge set of $Ca_k(C_6)$ can be divided into three partitions: $n_{22} = 3^k + 3$, $n_{23} = 4.3^k$ and $n_{33} = 3.7^k - 2.3^k - 3$.
Thus, by using the definition of General Sum Connectivity index, we get,

$$\begin{aligned} \psi_k(Ca_k(C_6)) &= \sum_{uv \in E(Ca_k(C_6))} (d_u + d_v)^k. \\ &= \sum_{uv \in E_{22}} (2+2)^k + \sum_{uv \in E_{23}} (2+3)^k \\ &\quad + \sum_{uv \in E_{33}} (3+3)^k. \\ &= (3^k+3).4^k + (4.3^k).5^k \\ &\quad + (3.7^k - 2.3^k - 3).6^k. \end{aligned}$$

Theorem 14.

$$\begin{aligned} HM(Ca_k(C_6)) &= (3^k+3).4^2 + (4.3^k).5^2 \\ &\quad + (3.7^k - 2.3^k - 3).6^2. \end{aligned}$$

*Proof.*By analyzing the molecular structure of $Ca_k(C_6)$, The edge set of $Ca_k(C_6)$ can be divided into three partitions: $n_{22} = 3^k + 3$, $n_{23} = 4.3^k$ and $n_{33} = 3.7^k - 2.3^k - 3$.
Thus, by using the definition of Hyper Zagreb index, we get,

$$\begin{aligned} HM(Ca_k(C_6)) &= \sum_{uv \in E(Ca_k(C_6))} (d_u + d_v)^2. \\ &= \sum_{uv \in E_{22}} (2+2)^2 + \sum_{uv \in E_{23}} (2+3)^2 \\ &\quad + \sum_{uv \in E_{33}} (3+3)^2. \\ &= (3^k+3).4^2 + (4.3^k).5^2 \\ &\quad + (3.7^k - 2.3^k - 3).6^2. \end{aligned}$$

Theorem 15.

$$\begin{aligned} H(Ca_k(C_6)) &= (3^k+3).\frac{1}{2} + (4.3^k).\frac{2}{5} \\ &\quad + (3.7^k - 2.3^k - 3).\frac{1}{3}. \end{aligned}$$

*Proof.*By analyzing the molecular structure of $Ca_k(C_6)$, The edge set of $Ca_k(C_6)$ can be divided into three partitions: $n_{22} = 3^k + 3$, $n_{23} = 4.3^k$ and $n_{33} = 3.7^k - 2.3^k - 3$.
Thus, by using the definition of harmonic index, we get,

$$\begin{aligned} H(Ca_k(C_6)) &= \sum_{uv \in E(Ca_k(C_6)} \left(\frac{2}{d_u + d_v}\right). \\ &= \sum_{uv \in E_{22}} \left(\frac{2}{4}\right) + \sum_{uv \in E_{23}} \left(\frac{2}{5}\right) \\ &\quad + \sum_{uv \in E_{33}} \left(\frac{2}{6}\right). \\ &= (3^k+3).\left(\frac{1}{2}\right) + (4.3^k).\left(\frac{2}{5}\right) \\ &\quad + (3.7^k - 2.3k - 3).\left(\frac{1}{3}\right). \end{aligned}$$

4 Conclusion

Degree-based topological indices are introduced to measure the medicinal properties of new drugs which is largely popular in developing areas. In our paper, in terms of drug structure analysis and edge dividing trick, we determine the degree-based topological indices of certain molecular graphs which widely appear in drug structures.

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