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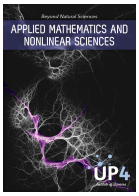

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Redefined Zagreb indices of Some Nano Structures

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Abstract

In theoretical chemistry, the researchers use graph models to express the structure of molecular, and the Zagreb indices and redefined Zagreb indices defined on molecular graph G are applied to measure the chemical characteristics of compounds and drugs. In this paper, we present the exact expressions of redefined Zagreb indices for certain important chemical structures like nanotube and nanostar. As supplement, the redefined Zagreb indices of polyomino chain and benzenoid series are manifested.

Keywords: molecular graph, redefined Zagreb index, nanotube, nanostar, polyomino chain, benzenoid series.
AMS 2010 codes: 05C70.

1 Introduction and Motivations

For the past 40 years, chemical graph theory, as an important branch of both computational chemistry and graph theory, has attracted much attention and the results obtained in this field have been applied in many chemical and pharmaceutical engineering applications. In these frameworks, the molecular is represented as a graph in which each atom is expressed as a vertex and covalent bounds between atoms are represented as edges between vertices. Topological indices were introduced to determine the chemical and pharmaceutical properties. Such indices can be regarded as score functions which map each molecular graph to a non-negative real number. There were many famous degree-based or distance-based indices such as Wiener index, PI index, Zagreb index, atom-bond connectivity index, Szeged index and eccentric connectivity index et al. Because of its

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wide engineering applications, many works contributed to determining the indices of special molecular graphs (See Yan et al., [24], Gao and Shi [7], Gao and Wang [8], [9] and [10] and Jamil et al. [13] for more details).

In our article, we only consider simple (molecular) graphs which are finite, loopless, and without multiple edges. Let $G = (V(G), E(G))$ be a graph in which the vertex set and edge set are expressed as $V(G)$ and $E(G)$, respectively. Readers can refer Bondy and Mutry [3] for any notations and terminologies used but not clearly explained in our paper.

The first Zagreb index can be regarded as one of the oldest graph invariants which was defined in 1972 by Gutman and Trinajsti [11] as

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

where $d(v)$ is the degree vertex v in G. Another alternative formulation for $M_1(G)$ is denoted as $\sum_{e=uv \in E(G)}(d(u)+d(v))$. And, the second Zagreb index was later introduced as

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

In 2005, Li and Zheng [14] introduced the first general Zagreb index as

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

where $\alpha \in R$. Obviously, $M_1^0(G) = |V(G)|$, $M_1^1(G) = 2|E(G)|$ and $M_1^2 \equiv M_1(G)$. Furthermore, we have

$$M_1^{\alpha+1}(G) = \sum_{v \in V(G)} d^{\alpha+1}(v) = \sum_{uv \in E(G)} (d^{\alpha}(u) + d^{\alpha}(v)). \tag{1}$$

Note that, when $\alpha = -1$ in (1) it is simply

$$M_1^0(G) = \sum_{v \in V(G)} d^0(v) = \sum_{uv \in E(G)} (d^{-1}(u) + d^{-1}(v)) = \sum_{uv \in E(G)} \frac{d(u)+d(v)}{d(u)d(v)} = n.$$

So the output of $ReZG_1(G)$ is always n, simply the vertices in the graph G. Note that their identities for $ReZG_1(G)$ in our paper is calculated in terms of the other graph parameters like p, q.

As degree-based topological indices, the redefined version of Zagreb indices of a graph G introduced by Ranjini et al., [19], and Usha et al., [20].

The Redefined first Zagreb index of a molecular graph G is defined by

$$ReZG_1(G) = \sum_{e=uv \in E(G)} \frac{d(u)+d(v)}{d(u)d(v)},$$

The Redefined second Zagreb index of a molecular graph G is defined by

$$ReZG_2(G) = \sum_{e=uv \in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}.$$

The Redefined third Zagreb index of a molecular graph G is defined by

$$ReZG_3(G) = \sum_{e=uv \in E(G)} (d(u)d(v))(d(u)+d(v)).$$

The Redefined third Zagreb index was also independently defined by Mansour and Song [15]. Moreover, the generalized version was presented in [23].

There have been many advances in Wiener index, Szeged index, PI index, and other degree-based or distance-based indices of molecular graphs, while the study of the redefined Zagreb indices of nano structures has been largely limited. Furthermore, nanotube, nanostar, polyomino chain and benzenoid series are critical and widespread molecular structures which have been widely applied in medical science, chemical engineering and pharmaceutical fields (see Mirzargar [18], Ashrafi and Karbasioun [1], Manuel et al., [16], Baca et al., [4], DeBorde et al., [5], Matsuno et al., [17], Vilela et al., [22], Velichko, Nosich [21], Haslam and Raeymaekers [12], Ashrafi and Karbasioun [2]). Also, these structures are the basic and primal structures of other more complicated chemical molecular structures and nano materials. Based on these grounds, we have attracted tremendous academic and industrial interests in determining the redefined Zagreb indices of special family of nanotube and nanostar from a computation point of view. In addition, the redefined Zagreb indices of polyomino chain and benzenoid series are considered.

The main contribution of our paper is two-folded. First, we focus on four classes of nanotubes: $VC_5C_7[p,q]$, $HC_5C_7[p,q]$, polyhex zigzag $TUZC_6$ and polyhex armchair $TUAC_6$, and theredefined Zagreb indices of these four classes of nanotubes are determined. Second, we compute the redefined Zagreb indices of dendrimer nanostar $D_3[n]$. As supplement, we calculate the redefined Zagreb indices of some special families of polyomino chains and benzenoid series.

2 Main Results and Proofs

2.1 redefined Zagreb indices of nanotubes

The purpose of this part is to yield the redefined Zagreb indices of certain special classes nanotubes. Our work in this part can be divided into two parts: (1) $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes; (2) zigzag $TUZC_6$ and armchair $TUAC_6$.

2.1.1 Nanotubes Covered by C_5 and C_7

In this subsection, we discuss $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes which consisting of cycles C_5 and C_7 (or it is a trivalent decoration constructed by C_5 and C_7 in turn, and thus called C_5C_7-net). It can cover either a cylinder or a torus.

The parameter p is denoted as the number of pentagons in the 1-st row of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$. The vertices and edges in first four rows are repeated alternatively. In these nanotubes, and we set q as the number of such repetitions. For arbitrary $p,q \in \mathbb{N}$, there exist $16p$ edges and $6p$ vertices in each period of $VC_5C_7[p,q]$ which are adjacent at the end of the molecular structure. By simple computation, we check that $|V(VC_5C_7[p,q])| = 16pq+6p$ and $|E(VC_5C_7[p,q])| = 24pq+6p$ since there are $6p$ vertices with $d(v) = 2$ and other $16pq$ vertices with $d(v) = 3$.

Furthermore, there are $8p$ vertices and $12p$ edges in any periods of $HC_5C_7[p,q]$. We get $|V(HC_5C_7[p,q])| = 8pq+5p$ and $|E(HC_5C_7[p,q])| = 12pq+5p$ since there are $5p$ vertices adjacent at the end of structure, and exists q repetition and $5p$ addition edges.

Let δ and Δ be the minimum and maximum degree of graph G, respectively. In the whole following context, for any graph G, its vertex set $V(G)$ and edge set $E(G)$ are divided into several partitions:

- for any i, $2\delta(G) \le i \le 2\Delta(G)$, let $E_i = \{e = uv \in E(G) | d(u)+d(v) = i\}$;
- for any j, $(\delta)^2 \le j \le (\Delta)^2$, let $E_j^* = \{e = uv \in E(G) | d(u)d(v) = j\}$;
- for any k, $\delta \le k \le \Delta$, let $V_k = \{v \in V(G) | d(v) = k\}$.

Therefore, by omitting the single carbon atoms and the hydrogen, we infer two partitions $V_2 = \{v \in V(G) | d(v) = 2\}$ and $V_3 = \{v \in V(G) | d(v) = 3\}$ for $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$. Moreover, the edge set of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ can be divided into the following three edge sets.

- E_4 (or E_4^*): $d(u) = d(v) = 2$;
- E_6 (or E_9^*): $d(u) = d(v) = 3$;

- E_5 (or E_6^*), $d(u)=2$ and $d(v)=3$.

Now, we state the main results in this subsection.

Theorem 1.

$$\begin{aligned}
ReZG_1(VC_5C_7[p,q]) &= 16pq+6p,\\
ReZG_2(VC_5C_7[p,q]) &= 36pq-\frac{27}{5}p,\\
ReZG_3(VC_5C_7[p,q]) &= 1296pq+36p,\\
ReZG_1(HC_5C_7[p,q]) &= 8pq+5p,\\
ReZG_2(HC_5C_7[p,q]) &= 18pq+\frac{23}{5}p,\\
ReZG_3(HC_5C_7[p,q]) &= 648pq+40p.
\end{aligned}$$

Proof. First, considering nanotubes $VC_5C_7[p,q]$ for arbitrary $p,q\in\mathbb{N}$. By analyzing its structure, we have $|V_2|=6p$, $|V_3|=16pq$, $|E_5|=|E_6^*|=12p$ and $|E_6|=|E_9^*|=24pq-6p$. In terms of the definitions of redefined Zagreb indices, we infer

$$\begin{aligned}
ReZG_1(VC_5C_7[p,q]) &= \sum_{e=uv\in E_6}\frac{d(u)+d(v)}{d(u)d(v)}+\sum_{e=uv\in E_5}\frac{d(u)+d(v)}{d(u)d(v)}\\
&= \frac{2}{3}|E_6|+\frac{5}{6}|E_5|.
\end{aligned}$$

$$\begin{aligned}
ReZG_2(VC_5C_7[p,q]) &= \sum_{e=uv\in E_6}\frac{d(u)d(v)}{d(u)+d(v)}+\sum_{e=uv\in E_5}\frac{d(u)d(v)}{d(u)+d(v)}\\
&= \frac{3}{2}|E_6|+\frac{6}{5}|E_5|.
\end{aligned}$$

$$\begin{aligned}
ReZG_3(VC_5C_7[p,q]) &= \sum_{e=uv\in E_6}(d(u)d(v))(d(u)+d(v))+\sum_{e=uv\in E_5}\frac{d(u)+d(v)}{d(u)d(v)}\\
&= 54|E_6|+30|E_5|.
\end{aligned}$$

Second, we consider nanotube $HC_5C_7[p,q]$ for arbitrary $p,q\in\mathbb{N}$. According to its chemical structure, we verify $|V_2|=5p$, $|V_3|=8pq$, $|E_4|=|E_4^*|=p$, $|E_5|=|E_6^*|=8p$, and $|E_6|=|E_9^*|=12pq-4p$. Therefore, by means of the definitions of redefined Zagreb indices, we infer

$$\begin{aligned}
&ReZG_1(HC_5C_7[p,q])\\
&= \sum_{e=uv\in E_6}(d(u)+d(v))+\sum_{e=uv\in E_5}(d(u)+d(v))+\sum_{e=uv\in E_4}(d(u)+d(v))\\
&= \frac{2}{3}|E_6|+\frac{6}{5}|E_5|+|E_4|.
\end{aligned}$$

$$\begin{aligned}
&ReZG_2(HC_5C_7[p,q])\\
&= \sum_{e=uv\in E_6}(d(u)d(v))+\sum_{e=uv\in E_5}(d(u)+d(v))+\sum_{e=uv\in E_4}(d(u)d(v))\\
&= \frac{3}{2}|E_6|+\frac{6}{5}|E_5|+|E_4|.
\end{aligned}$$

$$\begin{aligned}
&ReZG_3(HC_5C_7[p,q])\\
&= \sum_{e=uv\in E_6}(d(u)d(v))+\sum_{e=uv\in E_5}(d(u)+d(v))+\sum_{e=uv\in E_4}(d(u)d(v))\\
&= 54|E_6|+30|E_5|+16|E_4|.
\end{aligned}$$

2.1.2 Two Classes of Polyhex Nanotubes

We study the redefined Zagreb indices of polyhex nanotubes: zigzag $TUZC_6$ and armchair $TUAC_6$ in this subsection. We use parameter $m \in \mathbb{N}$ to denote the number of hexagons in the 1-st row of the $TUZC_6$ and $TUAC_6$. Analogously, the positive integer n is used to express the number of hexagons in the 1-st column of the 2D-lattice of $TUZC_6$ and $TUAC_6$. In view of structure analysis, we conclude $|V(TUZC_6)| = |V(TUAC_6)| = 2m(n+1)$ and $|E(TUZC_6)| = |E(TUAC_6)| = 3mn+2m$.

Clearly, the degree of vertex in polyhex nanotubes can't exceed three. For nanotubes $TUZC_6[m,n]$ with any $m,n \in \mathbb{N}$, we infer $|V_2| = 2m$, $|V_3| = 2mn$, $|E_5| = |E_6^*| = 4m$ and $|E_6| = |E_9^*| = 3mn-2m$. Moreover, for nanotube $TUAC_6[m,n]$ with any $m,n \in \mathbb{N}$, we get $|V_2| = 2m$, $|V_3| = 2mn$, $|E_4| = |E_4^*| = m$, $|E_5| = |E_6^*| = 2m$ and $|E_6| = |E_9^*| = 3mn-m$. Therefore, the results stated as follows are obtained by means of above discussions and the definitions of redefined Zagreb indices.

Theorem 2.

$$ReZG_1(TUZC_6[m,n]) = 2mn+2m,$$
$$ReZG_2(TUZC_6[m,n]) = \frac{9}{2}mn-\frac{9}{5}m,$$
$$ReZG_3(TUZC_6[m,n]) = 162mn+12m,$$
$$ReZG_1(TUAC_6[m,n]) = 2mn+2m,$$
$$ReZG_2(TUAC_6[m,n]) = \frac{9}{2}mn\frac{19}{10}m,$$
$$ReZG_3(TUAC_6[m,n]) = 162mn+22m.$$

2.2 Redefined Zagreb indices of dendrimer nanostars

Dendrimer is a basic structure in nanomaterials. In this section, for any $n \in \mathbb{N}$, $D_3[n]$ is denoted as the n-th growth of dendrimer nanostar. We aim to determine the redefined Zagreb indices of dendrimer nanostar $D_3[n]$ (its structure can be referred to Figure 1 for more details).

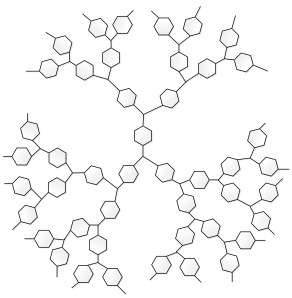

Fig. 1 The structure of 2-dimensional of dendrimer nanostar $D_3[n]$.

This class of dendrimer nanostar has a core presented in Figure 1 and we call an element as a leaf. It is not difficult to check that a leaf is actually consisted of C_6 or chemically benzene, and $D_3[n]$ is constituted by adding $3\cdot 2^n$ leafs in the n-th growth of $D_3[n-1]$. Therefore, there are in all $3\cdot 2^{n+1}-3$ leafs (C_6) in the dendrimer $D_3[n]$. The main contribution in this section can be stated as follows.

Theorem 3.

$$ReZG_1(D_3[n]) = 42\cdot 2^n - 20,$$
$$ReZG_2(D_3[n]) = \frac{1131}{20}\cdot 2^n - \frac{147}{5},$$
$$ReZG_2(D_3[n]) = 1410\cdot 2^n - 768.$$

Proof. Let $V_i[n]$ be the number of vertices with degree i ($i \in \{1,2,3,4\}$) in $D_3[n]$. In terms of hierarchy structural of $D_3[n]$, we deduce $V_1[n+1] = 2V_1[n] = 3\cdot 2^{n+1}$, $V_2[n+1] = V_2[n] + 12\cdot 2^{n+1}$ and $V_3[n+1] = V_3[n] + 6\cdot 2^{n+1} + V_1[n]$. Hence, by means of the induction on n with $V_1[0] = 3$, $V_2[0] = 12$ and $V_3[0] = 7$, we get $V_2[n+1] = 12(2^{n+2}-1)$ and $V_3[n+1] = 15\cdot 2^{n+1} - 8$.

Set $E_3^* = \{e = uv \in E(D_3[n]) | d(u) = 3, d(v) = 1\}$. We infer

$$|E_3^*| = 3\cdot 2^n,$$

$$|E_4^*| = |E_4| = 6(2^{n+1}-1),$$
$$|E_6^*| = |E_5| = 12(2^{n+1}-1),$$
$$|E_9^*| = |E_6| = 9\cdot 2^n - 6,$$
$$|E_4| = |E_3^*| + |E_4^*| = 15\cdot 2^n - 6.$$

Therefore, the expected results are obtained by the definition of the first, the second and the third redefined Zagreb indices. □

3 More Findings

3.1 Redefined Zagreb indices of polymino chains

From the perspective of mathematical, a polyomino system can be considered as a finite 2-connected plane graph in which each interior cell is surrounded by a C_4. In other words, it can be regarded as an edge-connected union of cells in the planar square lattice. For instance, polyomino chain is a special polyomino system in which the joining of the centers (denoted c_i as the center of the i-th square) of its adjacent regular forms a path $c_1c_2\cdots c_n$. Let $\mathscr{P}_n$ be the set of polyomino chains with n squares. We have $|E(PC_n)| = 3n+1$ for each $PC_n \in \mathscr{P}_n$. PC_n is called a linear chain expressed as LC_n if the subgraph of PC_n induced by V_3 has exactly $n-2$ squares. Moreover, PC_n is called a zig-zag chain denoted as ZC_n if the subgraph of PC_n induced by $V_{>2}$ (all the vertices with degree larger than two) is a path has exactly $n-1$ edges.

The branched or angularly connected squares in a polyomino chain are called a kink, and a maximal linear chain in a polyomino chain including the kinks and terminal squares at its end is called a segment represented by S. We use $l(S)$ to denote the length of S which is determined by the number of squares in S. Assume a polyomino chain consists of a sequence of segments $S_1, S_2, \cdots, S_m$ with $m \geq 1$, and we denote $l(S_i) = l_i$ for $i \in \{1,2,\cdots,m\}$ with property that $\sum_{i=1}^{m} l_i = n+m-1$. For arbitrary segment S in a polyomino chain, we have $2 \leq l(S) \leq n$. Specially, we get $m = 1$ and $l_1 = n$ for a linear chain LC_n, and $m = n-1$ and $l_i = 2$ for a zig-zag chain ZC_n.

The theorems presented in the below reveal clearly how the redefined Zagreb indices of certain families of polyomino chain are expressed.

Theorem 4. *Let LC_n, ZC_n be the polyomino chains presented above. Then, we get*

$$ReZG_1(LC_n) = \begin{cases} 4, & n = 1 \\ 2n+2, & n \geq 2. \end{cases}$$

$$ReZG_2(LC_n) = \begin{cases} 4, & n = 1 \\ \frac{9n}{2} - \frac{7}{10}, & n \geq 2. \end{cases}$$

$$ReZG_3(LC_n) = \begin{cases} 64, & n = 1 \\ 162n - 118, & n \geq 2. \end{cases}$$

$$ReZG_1(ZC_n) = \begin{cases} 4, & n = 1 \\ \frac{11}{6}n + \frac{7}{3}, & n \geq 2. \end{cases}$$

$$ReZG_2(ZC_n) = \begin{cases} 4, & n = 1 \\ 5n + \frac{58}{21}, & n \geq 2. \end{cases}$$

$$ReZG_3(ZC_n) = \begin{cases} 64, & n = 1 \\ 236n - 280, & n \geq 2. \end{cases}$$

Proof. The results are obvious for $n = 1$, and we only focus on $n \geq 2$ in the following discussion. It is not hard to check that $|E(LC_n)| = |E(ZC_n)| = 3n + 1$.

For the polyomino chain LC_n, we obtain $|E_4| = |E_4^*| = 2$, $|E_5| = |E_6^*| = 4$ and $|E_6| = |E_9^*| = 3n - 5$. By the definitions of redefined Zagreb indices, we have

$$ReZG_1(LC_n) = 2 + 4 \cdot \frac{5}{6} + (3n-5)\frac{2}{3},$$

$$ReZG_2(LC_n) = 2 + 4 \cdot \frac{6}{5} + (3n-5)\frac{3}{2},$$

$$ReZG_3(LC_n) = 2 \cdot 16 + 4 \cdot 30 + (3n-5)54.$$

By the same fashion, we yield

$$ReZG_1(ZC_n) = 2 + 4 \cdot \frac{5}{6} + 2(m-1)\frac{2}{3} + 2 \cdot \frac{7}{12} + (3n-2m-5)\frac{1}{2},$$

$$ReZG_2(ZC_n) = 2 + 4 \cdot \frac{6}{5} + 2(m-1)\frac{3}{2} + 2 \cdot \frac{12}{7} + (3n-2m-5) \cdot 2,$$

$$ReZG_3(ZC_n) = 2 \cdot 16 + 4 \cdot 30 + 2(m-1) \cdot 54 + 2 \cdot 84 + (3n-2m-5) \cdot 128.$$

The expected results are got from the fact $m = n - 1$ for ZC_n. □

Theorem 5. *Let PC_n^1 ($n \geq 3$) be a polyomino chain with n squares and two segments which $l_1 = 2$ and $l_2 = n - 1$. Then, we have*

$$ReZG_1(PC_n^1) = \begin{cases} 8, & n = 3 \\ 2n + 2, & n \geq 4. \end{cases}$$

$$ReZG_2(PC_n^1) = \begin{cases} \frac{1354}{105}, & n = 3 \\ \frac{9}{2}n - \frac{11}{21}, & n \geq 4. \end{cases}$$

$$ReZG_3(PC_n^1) = \begin{cases} 416, & n = 3 \\ 162n - 28, & n \geq 4. \end{cases}$$

Proof. For $n = 3$, it is trivial. For $n \geq 4$, we obtain $|E_4| = |E_4^*| = 2$, $|E_5| = |E_6^*| = 5$, $|E_8^*| = 1$, $|E_7| = |E_{12}^*| = 3$, $|E_9^*| = 3n - 10$ and $|E_6| = |E_9^*| + |E_8^*| = 3n - 9$. Therefore, by means of simply calculation, we obtain the desired results. □

Theorem 6. *Let PC_n^2 be a polyomino chain with n squares and m segments $S_1, S_2, \cdots, S_m$ ($m \geq 3$) such that $l_1 = l_m = 2$ and $l_2, \cdots, l_{m-1} \geq 3$. Then*

$$ReZG_1(PC_n^2) = \frac{3}{2}n + m + \frac{3}{2},$$

$$ReZG_2(PC_n^2) = 6n - \frac{96}{35}m + \frac{8}{21},$$

$$ReZG_3(PC_n^2) = 384n - 372m + 8.$$

Proof. For this chemical structure, we get $|E_4| = |E_4^*| = 2$, $|E_5| = |E_6^*| = 2m$, $|E_8^*| = 2$, $|E_7| = |E_{12}^*| = 4m-6$, $|E_9^*| = 3n-6m+3$ and $|E_6| = |E_9^*| + |E_8^*| = 3n-6m+5$. Therefore, in view of the definitions of redefined Zagreb indices, we obtain the desired results. □

The last two results obtained using similarly tricks.

Theorem 7. *Let PC_n^3 ($n \geq 4$) be a polyomino chain with n squares and m segments $S_1, S_2, \cdots, S_m$ ($m \geq 3$) such that $l_1 = 2$, $l_2, \cdots, l_m \geq 3$ or $l_m = 2$, $l_1, l_2 \cdots, l_{m-1} \geq 3$. Then*

$$ReZG_1(PC_n^3) = 2n + \frac{31}{12},$$

$$ReZG_2(PC_n^3) = \frac{9}{2}n + \frac{9}{35}m + \frac{22}{35},$$

$$ReZG_2(PC_n^3) = 162n + 72m - 142.$$

Theorem 8. *Let PC_n^4 be a polyomino chain with n squares and m segments $S_1, S_2, \cdots, S_m$ ($m \geq 3$) such that $l_i \geq 3$ ($i = \{1, \cdots, m\}$). Then*

$$ReZG_1(PC_n^4) = 2n + 2,$$

$$ReZG_2(PC_n^4) = \frac{9}{2}n + \frac{9}{35}m - \frac{67}{70},$$

$$ReZG_3(PC_n^4) = 162n + 72m - 190.$$

3.2 Redefined Zagreb indices of two classes of benzenoid series

The last part of our paper is to determine the redefined Zagreb indices of two classes of benzenoid series.

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

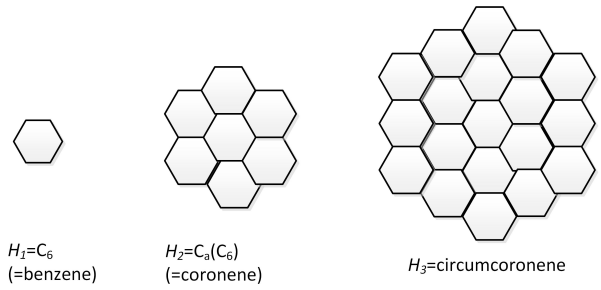

Fig. 2 The structure of H_k when $k = 1, 2, 3$.

Thus, this family of circumcoronene homologous series of benzenoid is consisted several copy of benzene C_6 on circumference, the more details for this structure can refer to Figure 3.

Clearly, its vertex set can be divided into two part: V_2 and V_3 such that $|V_2| = 6k$ and $|V_3| = 6k(k-1)$. Moreover, by simply calculation, we have $|E_4| = |E_4^*| = 6$, $|E_6| = |E_9^*| = 9k^2 - 15k + 6$ and $|E_5| = |E_6^*| = 12(k-1)$. Hence, we immediately deduce the following conclusion.

Theorem 9.

$$ReZG_1(H_k) = 6k^2,$$

$$ReZG_2(H_k) = \frac{27}{2}k^2 - \frac{81}{10}k + \frac{3}{5},$$

$$ReZG_3(H_k) = 486k^2 - 450k + 60.$$

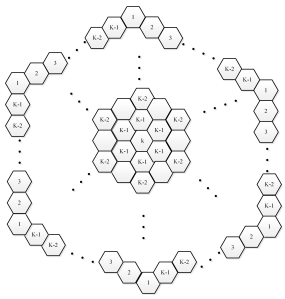

Fig. 3 The circumcoronene series of benzenoid H_k.

Next, we consider capra-designed planar benzenoid series $Ca_k(C_6)$ (the structure can refer to Farahani and Vlad [6] for more details). By means of intermediate results presented in Farahani and Vlad [6], we present the redefined Zagreb indices of $Ca_k(C_6)$ which are stated as follows.

Theorem 10.

$$ReZG_1(Ca_k(C_6)) = 2 \cdot 7^k + 3^{k+1} + 1,$$

$$ReZG_2(Ca_k(C_6)) = \frac{9}{2}7^k + \frac{14}{5}3^k - \frac{3}{2},$$

$$ReZG_3(Ca_k(C_6)) = 162 \cdot 7^k + 28 \cdot 3^k - 114.$$

4 Conclusion

The purpose of this paper is to discuss the redefined Zagreb indices of several nano structures, and these molecular graphs we considered here are fundamentally and commonly used in chemical and nano engineering. Specifically, the main contributions in this report can be concluded into two aspects: first, we compute the redefined Zagreb indices of four classes of nanotubes; then, the redefined Zagreb indices of dendrimer nanostars $D_3[n]$ are calculated. As supplement, we also discuss some families of polyomino chains and benzenoid series. As redefined Zagreb indices can been used in QSPR/QSAR study and play a crucial role in analyzing both the boiling point and melting point for medicinal drugs and chemical compounds, the results obtained in our paper illustrate the promising prospects of application for medical, pharmacal, biological, chemical and nanosciences.

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