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Degree-based indices computation for special chemical molecular structures using edge dividing method

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Abstract

In computational chemistry, the molecular structures are modelled as graphs which are called the molecular graphs. In these graphs, each vertex represents an atom and each edge denotes covalent bound between atoms. It is shown that the topological indices defined on the molecular graphs can reflect the chemical characteristics of chemical compounds and drugs. In this paper, we report several degree based indices of some widely used chemical molecular structures by means of edge dividing technology.

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1 Introduction

Topological indices, as numerical parameters of molecular structures, play a vital role in chemistry, and medicine science. It has been proved that topological indices reflect biochemical properties (such as the melting point, boiling point, toxicity and QSPR/QSAR study) of their corresponding compounds and drugs(see Wiener [1] and Katritzky et al., [2] for more details). Several articles contributed to determining the topological indices of special molecular graphs (See Yan et al. [3] and [4], Gao and Shi [5] and [6], Gao and Wang [7], [8] and [9], Xi and Gao [10], Gao et al. [11], Gao et al., [12] and [13], Gao and Farahani [14], Farahani and Gao [15],

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and Farahani [16], [17], [18], [19], [20], [21], [22], [23], [24] and [25] for more details). The notations and terminologies that were used but were undefined in this paper can be found in [26].

All the molecular graphs considered in our paper are simple graphs. Let G be a (molecular) graph with vertex and edge sets being denoted by $V(G)$ and $E(G)$, respectively. Bollobas and Erdos [27] defined the general Randic index which was stated as

$$R_k(G) = \sum_{e=uv} (d(u)d(v))^k, \tag{1}$$

where k is a real number and $d(u)$ denotes the degree of vertex u in G. Li and Liu [28] proposed the first three minimum general Randic indices of tree structure, and they also determined the corresponding extremal trees. Liu and Gutman [29] characterized several estimating on general Randic index. Throughout our paper, we always assume that k is a real number.

By setting $k = 1$ and $k = -1$ respectively in formula (1), then it becomes the second Zagreb index ($M_2(G)$) and the modified second Zagreb index ($M_2^*(G)$):

$$M_2(G) = \sum_{e=uv} d(u)d(v),$$

$$M_2^*(G) = \sum_{e=uv} \frac{1}{d(u)d(v)}.$$

The sum connectivity index ($\chi(G)$) of molecular graph G can be formulated as:

$$\chi(G) = \sum_{e=uv} (d(u)+d(v))^{-\frac{1}{2}}.$$

Zhou and Trinajstic [30] introduced the general sum connectivity index as

$$\chi_k(G) = \sum_{e=uv} (d(u)+d(v))^k.$$

Note that a new version of Zagreb indices named Hyper-Zagreb index was introduced by Shirdel et al. [31] as

$$HM(G) = \sum_{e=uv} (d(u)+d(v))^2.$$

However, Hyper-Zagreb index is only a special case of general sum connectivity when $k = 2$.

As a famous degree-based index, the harmonic index of molecular graph is denoted as:

$$H(G) = \sum_{e=uv} \frac{2}{d(u)+d(v)}.$$

Favaron et al. [32] manifested the relation between the eigenvalues and harmonic index of molecular graphs. Zhong [33] reported the minimum and maximum values of the harmonic index for connected molecular graphs and trees, and the corresponding extremal molecular graphs are also described. Wu et al. [34] derived the minimum value of the harmonic index with the minimum degree at least two. Liu [35] yielded the relationship between the diameter and the harmonic index of molecular graphs.

Very recently, Yan et al. [4] introduced the general harmonic index for extending harmonic index in more chemical engineering applications which can be stated as

$$H_k(G) = \sum_{e=uv} (\frac{2}{d(u)+d(v)})^k.$$

Vukicevic and Furtula [36] raised the Geometric-arithmetic index (in short, GA index) denoted by

$$GA(G)=\sum_{e=uv}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}.$$

Furthermore, Eliasi and Iranmanesh [42] defined its general version which was stated as follows:

$$OGA_k(G)=\sum_{e=uv}(\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)})^k.$$

The atom-bond connectivity index (in short, ABC index) was introduced by by Estrada et al. [37] as

$$ABC(G)=\sum_{e=uv}\sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.$$

Das et al. [38] identified the extremal molecular graph with regard to this index. Furtula et al. [39] studied the chemical trees with extremal ABC index. Vassilev and Huntington [40] obtained the chemical trees with extremal ABC index in view of considering how the removal of a certain edge takes place. Chen et al. [41] characterized the atom-bond connectivity index of the zig-zag chain polyomino molecular structures. Additional, they obtained the tight upper bound on the atom-bond connectivity index of catacon densed polyomino molecular graphs.

Azari and Iranmanesh [43] proposed the generalized Zagreb index of molecular graph G which can be formulated by

$$M_{t_1,t_2}(G)=\sum_{e=uv}(d(u)^{t_1}d(v)^{t_2}+d(u)^{t_2}d(v)^{t_1}),$$

where t_1 and t_2 are arbitrary non-negative integers.

Several polynomials related to degree based indices are also introduced. For instance, the first and the second Zagreb polynomials are expressed by

$$M_1(G,x)=\sum_{e=uv}x^{d(u)+d(v)}$$

and

$$M_2(G,x)=\sum_{e=uv}x^{d(u)d(v)},$$

respectively.

Moreover, the third Zagreb index and third Zagreb polynomial are defined as

$$M_3(G)=\sum_{e=uv}|d(u)-d(v)|,$$

and

$$M_3(G,x)=\sum_{e=uv}x^{|d(u)-d(v)|}.$$

The multiplicative version of first and second Zagreb indices were introduced by Gutman [44], and Ghorbani and Azimi [45] as:

$$PM_1(G)=\prod_{e=uv\in E(G)}(d(u)+d(v)),$$

$$PM_2(G)=\prod_{e=uv\in E(G)}(d(u)d(v)).$$

Several conclusions on $PM_1(G)$ and $PM_2(G)$ can be refered to Eliasi et al., [46], Xu et al., [47], and Farahani [48].

Furthermore, Ranjini et al., [49] re-defined the Zagreb indices, i.e., the redefined first, second and third Zagreb indices of a graph G were manifested as

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

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

and

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

respectively.

Although several advances have been made in distance-based indices (such as Wiener index, PI index and degree distance) of molecular graph, the study of degree-based indices for special chemical structures has been largely limited. Because of these, tremendous academic and industrial interest has been attracted to research the vertex-weighted Wiener number of this molecular structure from a mathematical point of view.

The purpose of this paper is to study the degree-based indices (including general Randic index, Zagreb indices, sum connectivity index, harmonic indices, GA related indices, ABC index, some polynomials, multiplicative Zagreb indices and redefined Zagreb indices) of some wildly used chemical structures. The technology used to get these conclusions is followed by edge dividing trick.

2 A Small Example

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

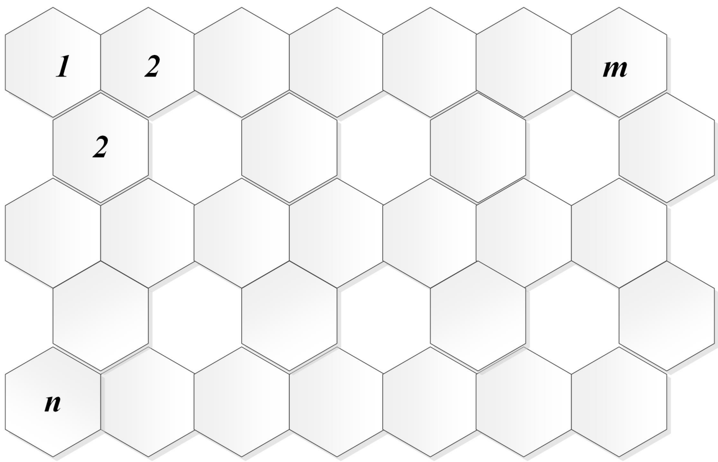

Fig. 1 2-Dimensional graph of graphene sheet

In the following example, we determine several topological indices for some graphene sheets which will be used to serve as basic building blocks in the graphene graphs. Let $G(m,n)$ be a graphene sheet with n rows and m columns.

Let δ and Δ be the minimum and maximum degree of (molecular) graph G, respectively. In the whole following context, for any (molecular) 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 $V_k = \{v \in V(G)|d(v) = k\}$.

It is easy to see that

$$|E(G(m,n))| = \begin{cases} \lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3), & n \equiv 1(\text{mod}2) \\ \lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) + 2m - 1, & n \equiv 0(\text{mod}2). \end{cases}$$

Furthermore, we have

$$|E_4| = |E_4^*| = n+4,$$

$$|E_5| = |E_6^*| = 4m+2n-4,$$

and

$$|E_6| = |E_9^*| = |E(G(m,n))| - 4m - 3n.$$

Therefore, according to the definition of degree-based indices, we deduce

$$R_k(G(m,n)) = \begin{cases} (n+4)4^k + (4m+2n-4)6^k + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 4m - 3n)9^k, & n \equiv 1(\text{mod}2) \\ (n+4)4^k + (4m+2n-4)6^k + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 2m - 3n - 1)9^k, & n \equiv 0(\text{mod}2). \end{cases}$$

$$M_2(G(m,n)) = \begin{cases} 9(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)) - 12m - 11n - 8, & n \equiv 1(\text{mod}2) \\ 6m - 11n - 17 + 9(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)), & n \equiv 0(\text{mod}2). \end{cases}$$

$$M_2^*(G(m,n)) = \begin{cases} \frac{n}{4} + \frac{1}{3} + \frac{2m}{9} + \frac{1}{9}(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)), & n \equiv 1(\text{mod}2) \\ \frac{n}{4} + \frac{2}{9} + \frac{4m}{9} + \frac{1}{9}(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)), & n \equiv 0(\text{mod}2). \end{cases}$$

$$\chi(G(m,n)) = \begin{cases} \frac{n+4}{2} + \frac{4m+2n-4}{\sqrt{5}} + \frac{\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 4m - 3n}{\sqrt{6}}, & n \equiv 1(\text{mod}2) \\ \frac{n+4}{2} + \frac{4m+2n-4}{\sqrt{5}} + \frac{\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 2m - 3n - 1}{\sqrt{6}}, & n \equiv 0(\text{mod}2). \end{cases}$$

$$\chi_k(G(m,n)) = \begin{cases} (n+4)4^k + (4m+2n-4)5^k + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 4m - 3n)6^k, & n \equiv 1(\text{mod}2) \\ (n+4)4^k + (4m+2n-4)5^k + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 2m - 3n - 1)6^k, & n \equiv 0(\text{mod}2). \end{cases}$$

$$HM(G(m,n)) = \begin{cases} 36(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)) - 42n - 44m - 36, & n \equiv 1(\text{mod}2) \\ 36(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)) - 42n + 28m - 72, & n \equiv 0(\text{mod}2). \end{cases}$$

$$H(G(m,n)) = \begin{cases} \frac{8m+9n+12}{30} + \frac{1}{3}(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)), & n \equiv 1(\text{mod}2) \\ \frac{38m-9n+2}{30} + \frac{1}{3}(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3)), & n \equiv 0(\text{mod}2). \end{cases}$$

$$H_k(G(m,n)) = \begin{cases} \frac{1}{2^k}(n+4) + (\frac{2}{5})^k (4m+2n-4) + \frac{1}{3^k}(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 4m - 3n), & n \equiv 1(\text{mod}2) \\ \frac{1}{2^k}(n+4) + (\frac{2}{5})^k (4m+2n-4) + \frac{1}{3^k}(\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 2m - 3n - 1), & n \equiv 0(\text{mod}2). \end{cases}$$

$$GA(G(m,n)) = \begin{cases} (4m+2n-4)\frac{2\sqrt{6}}{5} + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 4m - 2n + 4), & n \equiv 1(\text{mod}2) \\ (4m+2n-4)\frac{2\sqrt{6}}{5} + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 2m - 2n + 3), & n \equiv 0(\text{mod}2). \end{cases}$$

$$GA_k(G(m,n)) = \begin{cases} (4m+2n-4)(\frac{2\sqrt{6}}{5})^k + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 4m - 2n + 4), & n \equiv 1(\text{mod}2) \\ (4m+2n-4)(\frac{2\sqrt{6}}{5})^k + (\lceil \frac{n}{2} \rceil (5m+1) + \lfloor \frac{n}{2} \rfloor (m+3) - 2m - 2n + 3), & n \equiv 0(\text{mod}2). \end{cases}$$

$$M_1(G(m,n),x)=\begin{cases}(n+4)x^4+(4m+2n-4)x^5+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-4m-3n)x^6, & n\equiv 1(\text{mod}2)\\(n+4)x^4+(4m+2n-4)x^5+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-2m-3n-1)x^6, & n\equiv 0(\text{mod}2).\end{cases}$$

$$M_2(G(m,n),x)=\begin{cases}(n+4)x^4+(4m+2n-4)x^6+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-4m-3n)x^9, & n\equiv 1(\text{mod}2)\\(n+4)x^4+(4m+2n-4)x^6+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-2m-3n-1)x^9, & n\equiv 0(\text{mod}2).\end{cases}$$

$$M_3(G(m,n))=4m+2n-4.$$

$$M_3(G(m,n),x)=\begin{cases}(4m+2n-4)x+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-4m-2n+4), & n\equiv 1(\text{mod}2)\\(4m+2n-4)x+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-2m-2n+3), & n\equiv 0(\text{mod}2).\end{cases}$$

$$M_{t_1,t_2}(G(m,n))=\begin{cases}(n+4)2^{t_1+t_2+1}+(4m+2n-4)(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})\\+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-4m-3n)3^{t_1+t_2+1}, & n\equiv 1(\text{mod}2)\\(n+4)2^{t_1+t_2+1}+(4m+2n-4)(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})\\+(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-2m-3n-1)3^{t_1+t_2+1}, & n\equiv 0(\text{mod}2).\end{cases}$$

$$PM_1(G(m,n))=\begin{cases}4^{n+4}5^{4m+2n-4}6^{\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-4m-3n}, & n\equiv 1(\text{mod}2)\\4^{n+4}5^{4m+2n-4}6^{\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-2m-3n-1}, & n\equiv 0(\text{mod}2).\end{cases}$$

$$PM_2(G(m,n))=\begin{cases}4^{n+4}6^{4m+2n-4}9^{\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-4m-3n}, & n\equiv 1(\text{mod}2)\\4^{n+4}6^{4m+2n-4}9^{\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)-2m-3n-1}, & n\equiv 0(\text{mod}2).\end{cases}$$

$$ReZG_1(G(m,n))=\begin{cases}\frac{2}{3}(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)+m+n+1), & n\equiv 1(\text{mod}2)\\n\frac{5}{3}+2m+\frac{2}{3}(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)), & n\equiv 0(\text{mod}2).\end{cases}$$

$$ReZG_2(G(m,n))=\begin{cases}\frac{3}{2}(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3))-\frac{6m}{5}-\frac{11n}{10}-\frac{4}{5}, & n\equiv 1(\text{mod}2)\\m\frac{9}{5}-\frac{11}{10}n-\frac{23}{10}+\frac{3}{2}(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)), & n\equiv 0(\text{mod}2).\end{cases}$$

$$ReZG_3(G(m,n))=\begin{cases}-86n-96m-56+54(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)), & n\equiv 1(\text{mod}2)\\12m-86m-110+54(\lceil\frac{n}{2}\rceil(5m+1)+\lfloor\frac{n}{2}\rfloor(m+3)), & n\equiv 0(\text{mod}2).\end{cases}$$

3 Degree Based Indices of Three Families of Dendrimer Nanostars

We now discuss three famous infinite classes $NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ of dendrimer nanostars. The aim of this section is to compute the degree-based indices of these dendrimer nanostars.

Consider the molecular graph of $NS_1[n]$, where n is the number of steps of growth in this type of dendrimer nanostars. By computation, we get $|E_6^*|=18\cdot 2^n-12$, $|E_4|=|E_4^*|=9\cdot 2^n+3$, $|\{(u,v)|d(u)=3,d(v)=1\}|=1$ and $|E_7|=|E_{12}^*|=3$. Hence, by the definition of degree based indices, we infer

$$R_k(NS_1[n])=3^k+3\cdot 12^k+(18\cdot 2^n-12)6^k+(9\cdot 2^n+3)4^k,$$

$$M_2(NS_1[n])=144\cdot 2^n-21.$$

$$M_2^*(NS_1[n])=\frac{21}{4}\cdot 2^n-\frac{2}{3},$$

$$\chi(NS_1[n])=2+\frac{3}{\sqrt{7}}+\frac{18\cdot 2^n-12}{\sqrt{5}}+\frac{9}{2}\cdot 2^n,$$

$$\chi_k(NS_1[n]) = 3\cdot 7^k + (18\cdot 2^n - 12)5^k + (9\cdot 2^n + 4)4^k,$$

$$HM(NS_1[n]) = 594\cdot 2^n - 89,$$

$$H(NS_1[n]) = \frac{117}{10}\cdot 2^n - \frac{68}{35},$$

$$H_k(NS_1[n]) = 3\cdot(\frac{2}{7})^k + (18\cdot 2^n - 12)(\frac{2}{5})^k + (9\cdot 2^n + 4)(\frac{1}{2})^k,$$

$$GA(NS_1[n]) = \frac{31\sqrt{3}}{14} + (18\cdot 2^n - 12)\frac{2\sqrt{6}}{5} + (9\cdot 2^n + 3),$$

$$GA_k(NS_1[n]) = (\frac{\sqrt{3}}{2})^k + 3(\frac{4\sqrt{3}}{7})^k + (18\cdot 2^n - 12)(\frac{2\sqrt{6}}{5})^k + (9\cdot 2^n + 3),$$

$$M_1(NS_1[n],x) = 3x^7 + (18\cdot 2^n - 12)x^5 + (9\cdot 2^n + 4)x^4,$$

$$M_2(NS_1[n],x) = x^3 + 3x^{12} + (18\cdot 2^n - 12)x^6 + (9\cdot 2^n + 3)x^4,$$

$$M_3(NS_1[n]) = 18\cdot 2^n - 7,$$

$$M_3(NS_1[n],x) = x^2 + (18\cdot 2^n - 9)x + (9\cdot 2^n + 3),$$

$$M_{t_1,t_2}(NS_1[n]) = (3^{t_1} + 3^{t_2}) + 3(3^{t_1}4^{t_2} + 3^{t_2}4^{t_1}) + (18\cdot 2^n - 12)(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + (9\cdot 2^n + 3)2^{t_1+t_2+1},$$

$$PM_1(NS_1[n]) = 7^3\cdot 5^{18\cdot 2^n - 12}\cdot 4^{9\cdot 2^n + 4},$$

$$PM_2(NS_1[n]) = 3\cdot 12^3\cdot 6^{18\cdot 2^n - 12}\cdot 4^{9\cdot 2^n + 3},$$

$$ReZG_1(NS_1[n]) = 24\cdot 2^n - \frac{47}{12},$$

$$ReZG_2(NS_1[n]) = \frac{153}{5}\cdot 2^n - \frac{771}{140},$$

$$ReZG_3(NS_1[n]) = 684\cdot 2^n - 48.$$

We now consider the second class $NS_2[n]$, where n is the number of steps of growth in this type of dendrimer nanostar. In view of structure analysis and computation, we get $|E_5| = |E_6^*| = 24\cdot 2^n - 8$, $|E_4| = |E_4^*| = 12\cdot 2^n + 2$ and $|E_6| = |E_9^*| = 1$. Hence, by the definition of degree based indices, we infer

$$R_k(NS_2[n]) = 9^k + (24\cdot 2^n - 8)6^k + (12\cdot 2^n + 2)4^k,$$

$$M_2(NS_2[n]) = 192\cdot 2^n - 31.$$

$$M_2^*(NS_2[n]) = 5\cdot 2^n - \frac{13}{18},$$

$$\chi(NS_2[n]) = 168\cdot 2^n - 26,$$

$$\chi_k(NS_2[n]) = 6^k + (24\cdot 2^n - 8)5^k + (12\cdot 2^n + 2)4^k,$$

$$HM(NS_2[n]) = 792\cdot 2^n - 132,$$

$$H(NS_2[n]) = \frac{78}{5}\cdot 2^n - \frac{28}{15},$$

$$H_k(NS_2[n]) = (\frac{1}{3})^k + (24\cdot 2^n - 8)(\frac{2}{5})^k + (12\cdot 2^n + 2)(\frac{1}{2})^k,$$

$$GA(NS_2[n]) = (24\cdot 2^n - 8)\frac{2\sqrt{6}}{5} + (12\cdot 2^n + 3),$$

$$GA_k(NS_2[n]) = (24\cdot 2^n - 8)(\frac{2\sqrt{6}}{5})^k + (12\cdot 2^n + 3),$$
$$M_1(NS_2[n],x) = x^6 + (24\cdot 2^n - 8)x^5 + (12\cdot 2^n + 2)x^4,$$
$$M_2(NS_2[n],x) = x^9 + (24\cdot 2^n - 8)x^6 + (12\cdot 2^n + 2)x^4,$$
$$M_3(NS_2[n]) = 24\cdot 2^n - 8,$$
$$M_3(NS_2[n],x) = (24\cdot 2^n - 8)x + (12\cdot 2^n + 3),$$
$$M_{t_1,t_2}(NS_2[n]) = 3^{t_1+t_2+1} + (24\cdot 2^n - 8)(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + (12\cdot 2^n + 2)2^{t_1+t_2+1},$$
$$PM_1(NS_2[n]) = 6\cdot 5^{24\cdot 2^n-8}\cdot 4^{12\cdot 2^n+2},$$
$$PM_2(NS_2[n]) = 9\cdot 6^{24\cdot 2^n-8}\cdot 4^{12\cdot 2^n+2},$$
$$ReZG_1(NS_2[n]) = 32\cdot 2^n - 4,$$
$$ReZG_2(NS_2[n]) = \frac{204}{5}\cdot 2^n - \frac{61}{10},$$
$$ReZG_3(NS_2[n]) = 912\cdot 2^n - 154.$$

Next, we consider the second class $NS_3[n]$, where n is the number of steps of growth in this type of dendrimer nanostar. By means of similar way, we get $|E_5| = |E_6^*| = 28\cdot 2^n - 6$, $|E_6| = |E_9^*| = 6\cdot 2^n$, $|E_4^*| = 22\cdot 2^n - 7$ and $|\{(u,v)|d(u) = 3, d(v) = 1\}| = 2^{n+1}$. Hence, by the definition of degree based indices, we infer

$$R_k(NS_3[n]) = 9^k(6\cdot 2^n) + 3^k(2^{n+1}) + (28\cdot 2^n - 6)6^k + (22\cdot 2^n - 7)4^k,$$
$$M_2(NS_3[n]) = 316\cdot 2^n - 64.$$
$$M_2^*(NS_3[n]) = \frac{23}{2}\cdot 2^n - \frac{11}{4},$$
$$\chi(NS_3[n]) = 272\cdot 2^n - 58,$$
$$\chi_k(NS_3[n]) = 6^k(6\cdot 2^n) + (28\cdot 2^n - 6)5^k + (24\cdot 2^n - 7)4^k,$$
$$HM(NS_3[n]) = 1300\cdot 2^n - 262,$$
$$H(NS_3[n]) = \frac{126}{5}\cdot 2^n - \frac{59}{10},$$
$$H_k(NS_3[n]) = (\frac{1}{3})^k(6\cdot 2^n) + (28\cdot 2^n - 6)(\frac{2}{5})^k + (24\cdot 2^n - 7)(\frac{1}{2})^k,$$
$$GA(NS_3[n]) = \sqrt{3}\cdot 2^n + (28\cdot 2^n - 6)\frac{2\sqrt{6}}{5} + (28\cdot 2^n - 7),$$
$$GA_k(NS_3[n]) = (\frac{\sqrt{3}}{2})^k(2^{n+1}) + (28\cdot 2^n - 6)(\frac{2\sqrt{6}}{5})^k + (28\cdot 2^n - 7),$$
$$M_1(NS_3[n],x) = x^6(6\cdot 2^n) + (28\cdot 2^n - 6)x^5 + (24\cdot 2^n - 7)x^4,$$
$$M_2(NS_3[n],x) = x^9(6\cdot 2^n) + x^3(2^{n+1}) + (28\cdot 2^n - 6)x^6 + (22\cdot 2^n - 7)x^4,$$
$$M_3(NS_3[n]) = 32\cdot 2^n - 6,$$
$$M_3(NS_3[n],x) = 2^{n+1}\cdot x^2 + (28\cdot 2^n - 6)x + (28\cdot 2^n - 7),$$
$$M_{t_1,t_3}(NS_2[n]) = 3^{t_1+t_2+1}(6\cdot 2^n) + (3^{t_1} + 3^{t_2})(2^{n+1}) + (28\cdot 2^n - 6)(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + (22\cdot 2^n - 7)2^{t_1+t_2+1},$$
$$PM_1(NS_3[n]) = 6^{6\cdot 2^n}\cdot 5^{28\cdot 2^n-6}\cdot 4^{24\cdot 2^n-7},$$
$$PM_2(NS_3[n]) = 9^{6\cdot 2^n}\cdot 3^{2^{n+1}}\cdot 6^{28\cdot 2^n-6}\cdot 4^{22\cdot 2^n-7},$$
$$ReZG_1(NS_3[n]) = 52\cdot 2^n - 12,$$
$$ReZG_2(NS_3[n]) = \frac{661}{2}\cdot 2^n - \frac{71}{5},$$
$$ReZG_3(NS_3[n]) = 1540\cdot 2^n) - 292.$$

4 Degree Based Indices of Polyomino Chains of k-Cycles and Triangular Benzenoid

From a mathematical point of view, k-polyomino system is a finite 2-connected plane graph in which each interior face (i.e. cell) is surrounded by a C_4. That is to say, it is an edge-connected union of cells, see Klarner [50] and Ghorbani and Ghazi [51]. As an instance, the polyomino chains of 8-cycles can be seen in Figure 2.

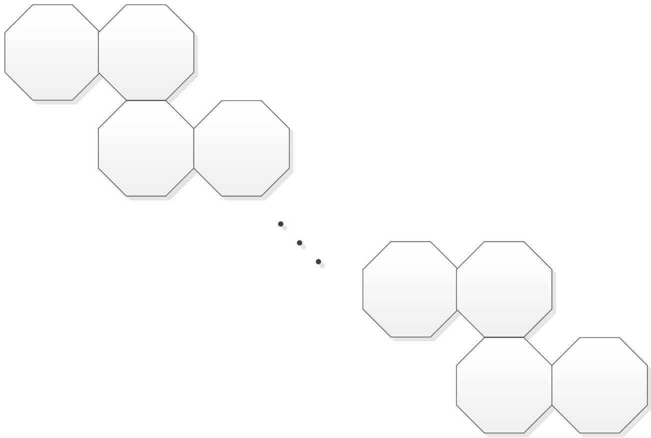

Fig. 2 The zig-zag chain of 8-cycles

This graph has n^2+4n+1 vertices and $\frac{3(n^2+3n)}{2}$ edges. Furthermore, we obtain $|E_4| = |E_4^*| = 12n+4$, $|E_6| = |E_9^*| = 8n-3$, and $|E_5| = |E_6^*| = 8n$. Hence, in view of definition of degree based indices, we have

$$R_k(G) = 9^k(8n-3) + 8n\cdot 6^k + (12n+4)4^k,$$

$$M_2^*(G) = \frac{47}{9}n + \frac{2}{3},$$

$$\chi(G) = 136n-2,$$

$$\chi_k(G) = 6^k(8n-3) + 8n\cdot 5^k + (12n+4)4^k,$$

$$HM(G) = 680n-44,$$

$$H(G) = \frac{178}{15}n+1,$$

$$H_k(G) = (\frac{1}{3})^k(8n-3) + 8n\cdot(\frac{2}{5})^k + (12n+4)(\frac{1}{2})^k,$$

$$GA_k(G) = (20n+1) + 8n(\frac{2\sqrt{6}}{5})^k,$$

$$M_1(G,x) = (8n-3)x^6 + 8nx^5 + (12n+4)x^4,$$

$$M_2(G,x) = (8n-3)x^9 + 8nx^6 + (12n+4)x^4,$$

$$M_3(G) = (20n+1) + 8nx,$$

$$M_3(G,x) = 8n,$$

$$M_{t_1,t_3}(G) = 3^{t_1+t_2+1}(8n-3) + 8n(2^{t_1}3^{t_2} + 3^{t_1}2^{t_2}) + (12n+4)2^{t_1+t_2+1},$$

$$PM_1(G) = 6^{8n-3}\cdot 5^{8n}\cdot 4^{12n+4},$$

$$PM_2(G) = 9^{8n-3}\cdot 6^{8n}\cdot 4^{12n+4},$$

$$ReZG_1(G) = 24n + 2,$$

$$ReZG_2(G) = \frac{168}{5}n - \frac{1}{2},$$

$$ReZG_3(G) = 864n - 98.$$

Next, we compute four topological indices of triangular benzenoid graph $T(n)$ with $n^2 + 4^n + 1$ vertices and $\frac{3(n^2+3n)}{2}$ edges which is depicted in Figure 3.

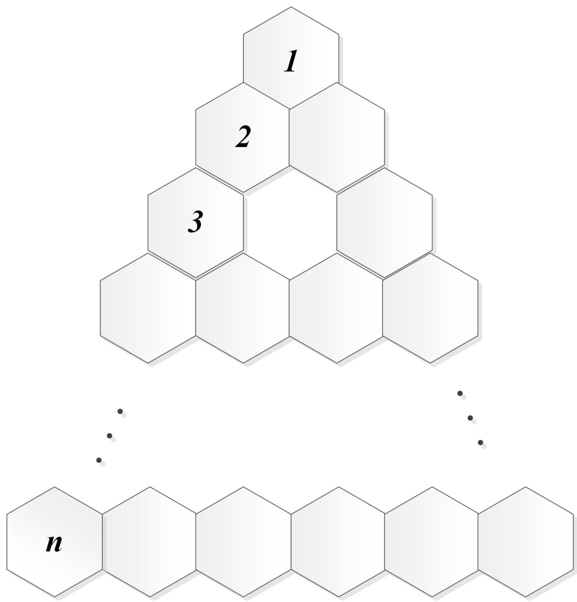

Fig. 3 Graph of triangular benzenoid $T(n)$

For triangular benzenoid $T(n)$, we deduce $|E_4| = |E_4^*| = 6$, $|E_6| = |E_9^*| = 6(n-1)$, and $|E_5| = |E_6^*| = \frac{3n(n-1)}{2}$. Hence, in view of definition of degree based indices, we derive

$$R_k(T(n)) = 9^k(6n-1) + \frac{3n(n-1)}{2} \cdot 6^k + 6 \cdot 4^k,$$

$$M_2^*(T(n)) = \frac{1}{4}n^2 + \frac{5}{12}n + \frac{25}{18},$$

$$\chi(T(n)) = \frac{15}{2}n^2 - \frac{57}{2}n + 18,$$

$$\chi_k(T(n)) = 6^k(6n-1) + \frac{3n(n-1)}{2} \cdot 5^k + 6 \cdot 4^k,$$

$$HM(T(n)) = \frac{75}{2}n^2 - \frac{357}{2}n + 60,$$

$$H(T(n)) = \frac{3}{5}n^2 - \frac{7}{5}n + \frac{8}{3},$$

$$H_k(T(n)) = (\frac{1}{3})^k(6n-1) + \frac{3n(n-1)}{2} \cdot (\frac{2}{5})^k + 6 \cdot (\frac{1}{2})^k,$$

$$GA_k(T(n)) = \frac{3n^2 - 3n + 12}{2} + 6(n-1)(\frac{2\sqrt{6}}{5})^k,$$

$$M_1(T(n),x) = (6n-1)x^6 + \frac{3n(n-1)}{2}x^5 + 6x^4,$$

$$M_2(T(n),x) = (6n-1)x^9 + \frac{3n(n-1)}{2}x^6 + 6x^4,$$

$$M_3(T(n)) = (6n+5) + \frac{3n(n-1)}{2}x,$$

$$M_3(T(n),x) = \frac{3n(n-1)}{2},$$

$$M_{t_1,t_3}(T(n)) = 3^{t_1+t_2+1}(6n-1) + \frac{3n(n-1)}{2}\cdot(2^{t_1}3^{t_2}+3^{t_1}2^{t_2}) + 6\cdot 2^{t_1+t_2+1},$$

$$PM_1(T(n)) = 6^{6n-1}\cdot 5^{\frac{3n(n-1)}{2}}\cdot 4^6,$$

$$PM_2(T(n)) = 9^{6n-1}\cdot 6^{\frac{3n(n-1)}{2}}\cdot 4^6,$$

$$ReZG_1(T(n)) = \frac{5}{4}n^2 - \frac{11}{4}n + \frac{16}{3},$$

$$ReZG_2(T(n)) = \frac{9}{5}n^2 - \frac{36}{5}n + \frac{9}{2},$$

$$ReZG_3(T(n)) = 45n^2 + 279n + 42.$$

5 Degree Based Indices of Bridge Graph

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The bridge (molecular) graph $B(G_1,G_2,\cdots,G_d) = B(G_1,G_2,\cdots,G_d;v_1,v_2,\cdots,v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is yielded from the graphs $G_1,G_2,\cdots,G_d$ in which the vertices v_i and v_{i+1} are connected by an edge for $i=1,2,\cdot,d-1$. The main result of this section is determining the formulas of some degree based indices for the infinite family of nano structures of bridge graph with $G_1,G_2,\cdots,G_d$(see Figure 4). We set $G_d(H,v) = B(H,H,\cdots,H;v,v,\cdots,v)$ for special situations of bridge graphs.

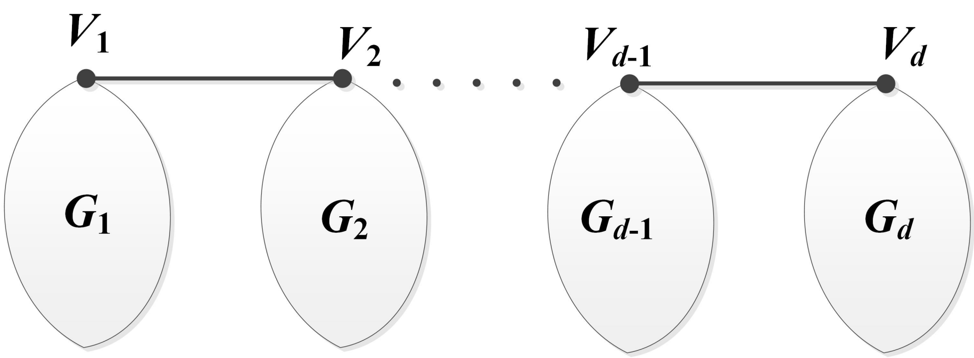

Fig. 4 The bridge graph $T(n)$

In the following context of this section, we discuss the bridge graphs in which the main parts of graphs are path, cycle and complete graph, respectively.

Case 1. Let P_n be the path with n vertices. We have dn vertices and $dn-1$ edges for bridge graph $G_d(P_n,v)$ (see Figure 5 for more details). Additionally, the edge set of bridge graph $G_d(P_n,v)$ can be divided into four

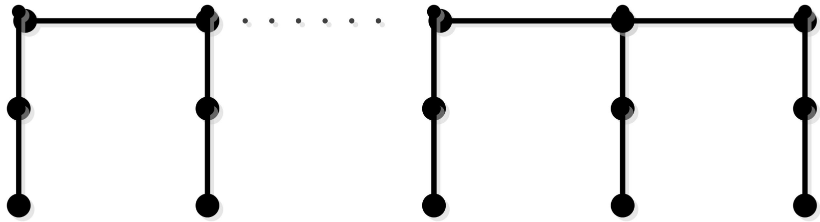

Fig. 5 The nano structures bridge graph $G_d(P_n, v_1)$

partitions. By computation, we get $|E_5| = |E_6^*| = d$, $|E_6| = |E_9^*| = d-3$, $|E_4| = |E_4^*| = d(n-3)+2$, $|E_3| = |E_2^*| = d$.

Hence, in view of definition of degree-based indices, we deduce

$$R_k(G_d(P_n,v)) = d\cdot 6^k + (d-3)9^k + (d(n-3)+2)4^k + d\cdot 2^k,$$

$$M_2^*(G_d(P_n,v)) = \frac{dn}{4} + \frac{d}{36} + \frac{1}{6},$$

$$\chi(G_d(P_n,v)) = 4dn + 2d - 10,$$

$$\chi_k(G_d(P_n,v)) = d\cdot 5^k + (d-3)6^k + (d(n-3)+2)4^k + d\cdot 3^k,$$

$$HM(G_d(P_n,v)) = 16dn + 22d - 76,$$

$$H(G_d(P_n,v)) = \frac{dn}{2} - \frac{d}{10},$$

$$H_k(G_d(P_n,v)) = d(\frac{2}{5})^k + (d-3)(\frac{1}{3})^k + (d(n-3)+2)(\frac{1}{2})^k + d(\frac{2}{3})^k,$$

$$GA_k(G_d(P_n,v)) = d(\frac{2\sqrt{6}}{5})^k + dn - 2d - 1 + d(\frac{2\sqrt{2}}{3})^k,$$

$$M_1(G_d(P_n,v),x) = dx^5 + (d-3)x^6 + (d(n-3)+2)x^4 + dx^3,$$

$$M_2(G_d(P_n,v),x) = dx^6 + (d-3)x^9 + (d(n-3)+2)x^4 + dx^2,$$

$$M_3(G_d(P_n,v)) = 2d,$$

$$M_3(G_d(P_n,v),x) = 2dx + dn - 2d - 1,$$

$$M_{t_1,t_2}(G_d(P_n,v)) = d(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + (d-3)3^{t_1+t_2+1} + (d(n-3)+2)2^{t_1+t_2+1} + d(2^{t_1} + 2^{t_2}),$$

$$PM_1(G_d(P_n,v)) = 5^d 6^{d-3} 4^{d(n-3)+2} 3^d,$$

$$PM_2(G_d(P_n,v)) = 6^d 9^{d-3} 4^{d(n-3)+2} 2^d,$$

$$ReZG_1(G_d(P_n,v)) = dn,$$

$$ReZG_2(G_d(P_n,v)) = dn + \frac{11}{30}d - \frac{5}{2},$$

$$ReZG_3(G_d(P_n,v)) = 42d - 130 + 16dn.$$

Case 2. Let C_n be the cycle with n vertices. There are dn vertices and $dn+d-1$ edges for bridge graph $G_d(C_n,v)$ (see Figure 6 for its structure). Moreover, the edge set of bridge graph $G_d(C_n,v)$ can be divided into five partitions which are stated as follows: $|E_5| = |E_6^*| = 4$, $|E_6| = |E_8^*| = 2d-4$, $|E_4| = |E_4^*| = d(n-2)$, $|E_8| = |E_{16}^*| = d-3$ and $|E_7| = |E_{12}^*| = 2$.

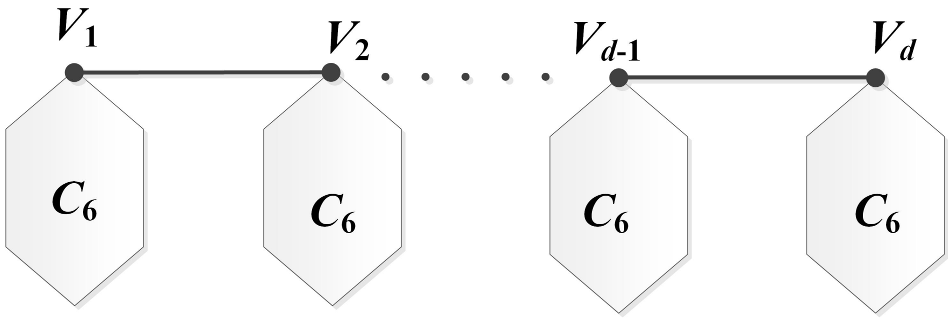

Fig. 6 The nano structures bridge graph $G_d(C_6,v)$

Thus, by means of definition of degree-based indices, we get

$$R_k(G_d(C_n,v)) = 4\cdot 6^k + (2d-4)8^k + (d(n-2))4^k + (d-3)16^k + 2\cdot 12^k,$$

$$M_2^*(G_d(C_n,v)) = \frac{dn}{4} - \frac{3}{16}d + \frac{7}{48},$$

$$\chi(G_d(C_n,v)) = 4dn + 12d - 14,$$

$$\chi_k(G_d(C_n,v)) = 4\cdot 5^k + (2d-4)6^k + (d(n-2))4^k + (d-3)8^k + 2\cdot 7^k,$$

$$HM(G_d(G_d(C_n,v)) = 16dn + 104d - 138,$$

$$H(G_d(G_d(C_n,v)) = \frac{dn}{2} - \frac{d}{12} + \frac{37}{420},$$

$$H_k(G_d(C_n,v)) = 4(\frac{2}{5})^k + (2d-4)(\frac{1}{3})^k + (d(n-2))(\frac{1}{2})^k + (d-3)(\frac{1}{4})^k + 2(\frac{2}{7})^k,$$

$$GA_k(G_d(C_n,v)) = 4(\frac{2\sqrt{6}}{5})^k + (2d-4)(\frac{2\sqrt{2}}{3})^k + (dn-d-3) + 2(\frac{4\sqrt{3}}{7})^k,$$

$$M_1(G_d(C_n,v),x) = 4x^5 + (2d-4)x^6 + (d(n-2))x^4 + (d-3)x^8 + 2x^7,$$

$$M_2(G_d(C_n,v),x) = 4x^6 + (2d-4)x^8 + (d(n-2))x^4 + (d-3)x^{16} + 2x^{12},$$

$$M_3(G_d(C_n,v)) = 4d-2,$$

$$M_3(G_d(C_n,v),x) = 6x + (2d-4)x^2 + (dn-d-3),$$

$$M_{t_1,t_2}(G_d(C_n,v)) = 4(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + (2d-4)(2^{t_1}4^{t_2} + 2^{t_2}4^{t_1}) + (d(n-2))2^{t_1+t_2+1} + (d-3)4^{t_1+t_2+1} + 2(3^{t_1}4^{t_2} + 3^{t_2}4^{t_1}),$$

$$PM_1(G_d(G_d(C_n,v)) = 30625\cdot 6^{2d-4}4^{d(n-2)}8^{d-3},$$

$$PM_2(G_d(G_d(C_n,v)) = 186624\cdot 9^{2d-4}4^{d(n-2)}16^{d-3},$$

$$ReZG_1(G_d(G_d(C_n,v)) = dn,$$

$$ReZG_2(G_d(G_d(C_n,v)) = dn + \frac{8d}{3} - \frac{326}{105},$$

$$ReZG_3(G_d(G_d(C_n,v)) = 16dn + 282d - 292.$$

Case 3. Let K_n be the compete graph with n vertices. Hence, there are dn vertices and $\frac{dn(n-1)}{2} + d - 1$ edges for bridge graph $G_d(K_n,v)$ (see Figure 7 for its structure) and its edge set of graph can be divided into five partitions: $|E_{10}| = |E_{25}^*| = d-2$, $|E_9| = |E_{20}^*| = 2$, $|E_{n+3}| = |E_{4(n-1)}^*| = 2$, $|E_{n+4}| = |E_{5(n-1)}^*| = d-2$ and $|E_{2n-2}| = |E_{(n-1)^2}^*| = \frac{d(n-1)(n-2)}{3}$.

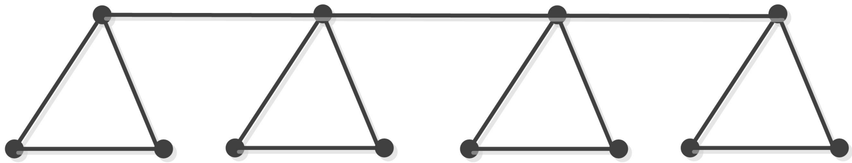

Fig. 7 The nano structures bridge graph $G_d(K_3,v)$

Hence, in view of definition of degree based indices, we get

$$R_k(G_d(K_n,v)) = (d-2)25^k + 2\cdot 20^k + 2(4(n-1))^k + (d-2)(5(n-1))^k + \frac{d(n-1)(n-2)}{3}(n-1)^{2k},$$

$$M_2^*(G_d(K_n,v)) = \frac{d-2}{25} + \frac{1}{10} + \frac{1}{2(n-1)} + \frac{d-2}{5(n-1)} + \frac{d(n-2)}{3(n-1)},$$

$$\chi(G_d(K_n,v)) = dn + 14d - 4 + \frac{2d(n-1)^2(n-2)}{3},$$

$$\chi_k(G_d(K_n,v)) = (d-2)10^k + 2\cdot 9^k + 2(n+3)^k + (d-2)(n+4)^k + \frac{d(n-1)(n-2)}{3}(2n-2)^k,$$

$$HM(G_d(G_d(K_n,v)) = 100d - 38 + 2(n+3)^2 + (d-2)(n+4)^2 + \frac{4d(n-1)^3(n-2)}{3},$$

$$H(G_d(G_d(K_n,v)) = \frac{dn}{3} - \frac{7d}{15} + \frac{2}{45} + \frac{4}{n+3} + \frac{2(d-2)}{n+4},$$

$$H_k(G_d(K_n,v)) = (d-2)(\frac{1}{5})^k + 2(\frac{2}{9})^k + 2(\frac{2}{n+3})^k + (d-2)(\frac{2}{n+4})^k + \frac{d(n-1)(n-2)}{3}(\frac{1}{n-1})^k,$$

$$GA_k(G_d(K_n,v)) = 2(\frac{4\sqrt{5}}{9})^k + 2(\frac{4\sqrt{n-1}}{n+3})^k + (d-2)(\frac{2\sqrt{5(n-1)}}{n+4})^k + \frac{d(n-1)(n-2)}{3} + d - 2,$$

$$M_1(G_d(K_n,v),x) = (d-2)x^{10} + 2x^9 + 2x^{n+3} + (d-2)x^{n+4} + \frac{d(n-1)(n-2)}{3}x^{2(n-1)},$$

$$M_2(G_d(K_n,v),x) = (d-2)x^{25} + 2x^{20} + 2x^{4(n-1)} + (d-2)x^{5(n-1)} + \frac{d(n-1)(n-2)}{3}x^{(n-1)^2},$$

$$M_3(G_d(K_n,v)) = \frac{d(n-1)(n-2)}{3} + d - 2,$$

$$M_3(G_d(K_n,v),x) = 2x + 2x^{n-5} + (d-2)x^{n-6} + \frac{d(n-1)(n-2)}{3} + d - 2,$$

$$\begin{aligned} M_{t_1,t_2}(G_d(K_n,v)) &= (d-2)5^{t_1+t_2+1} + 2(4^{t_1}5^{t_2} + 4^{t_2}5^{t_1}) + 2(4^{t_1}(n-1)^{t_2} + 4^{t_2}(n-1)^{t_1}) \\ &+ (d-2)(5^{t_1}(n-1)^{t_2} + 5^{t_2}(n-1)^{t_1}) + \frac{d(n-1)(n-2)}{3}(n-1)^{t_1+t_2+1}, \end{aligned}$$

$$PM_1(G_d(G_d(K_n,v)) = 81\cdot 10^{d-2}(n+3)^2(n+4)^{d-2}(2n-2)^{\frac{d(n-1)(n-2)}{3}},$$

$$PM_2(G_d(G_d(K_n,v)) = 400\cdot 25^{d-2}(4(n-1))^2(5(n-1))^{d-2}(n-1)^{\frac{2d(n-1)(n-2)}{3}},$$

$$ReZG_1(G_d(G_d(K_n,v)) = (d-2)\frac{2}{5} + \frac{9}{10} + 2\frac{n+3}{4(n-1)} + (d-2)\frac{n+4}{5(n-1)} + \frac{d(n-1)(n-2)}{3}\frac{2}{n-1},$$

$$ReZG_2(G_d(G_d(K_n,v)) = (d-2)\frac{5}{2} + \frac{40}{9} + 2\frac{4(n-1)}{n+3} + (d-2)\frac{5(n-1)}{n+4} + \frac{d(n-1)(n-2)}{3}\frac{n-1}{2},$$

$$ReZG_3(G_d(G_d(K_n,v)) = 250(d-2) + 360 + 8(n-1)(n+3) + 5(n-1)(d-2)(n+4) + \frac{2d(n-1)^4(n-2)}{3}.$$

6 Degree Based Indices of Carbon Nanotube Network

In this section, we focus on the $m \times n$ quadrilateral section P_m^n with $m \geq 2$ hexagons on the top and bottom sides and $n \geq 2$ hexagons on the lateral sides cut from the regular hexagonal lattice L, see Figure 8 for its detailed chemical structure.

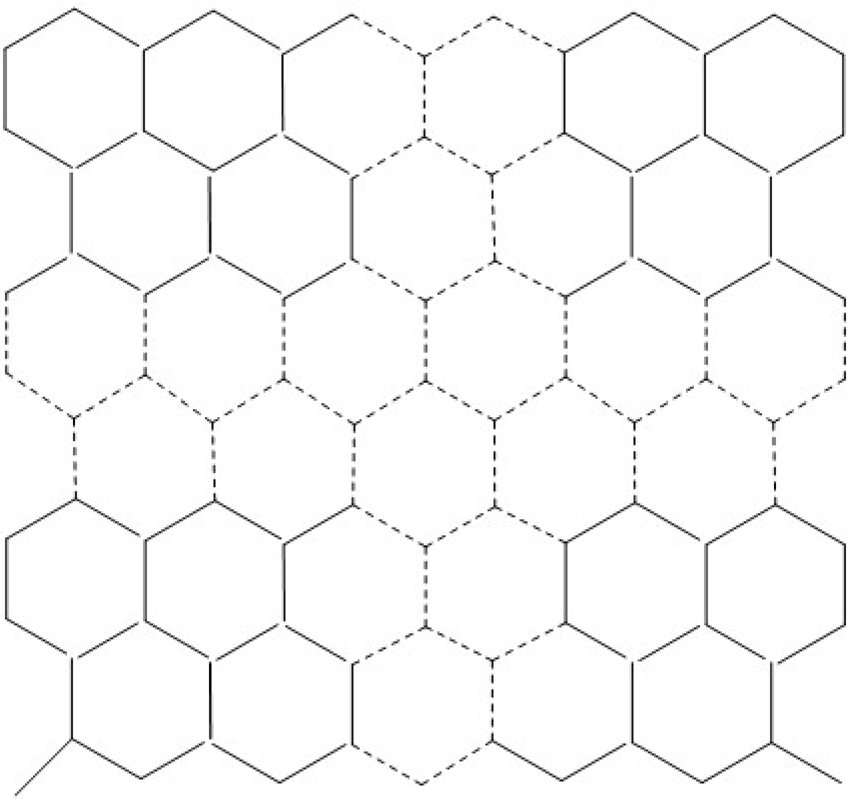

Fig. 8 Quadrilateral section P_m^n cuts from the regular hexagonal lattice

The nanotube 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 $(j = 0,1,2,\cdots,n)$.

Let $n \in \mathbb{N}$ be even so that $n,m \geq 2$. The nanotube NC_m^n of order $n(2m+1)$ with size $n(3m+\frac{1}{2})$ can be yielded by identifying the top and bottom sides of the quadrilateral section P_m^n in a similarly way in which the vertices u_i^0 and u_i^n for $i = 0,1,2,\cdots,m$ and vertices v_i^0 and v_i^n for $i = 0,1,2,\cdots,m$ are identified. See Baca et al., [52] for more details.

By analysis, the edge set of NA_m^n can be divided into two parts: $E_6 = E_9^*$ and $E_5 = E_6^*$ with $m(3n-2)$ and $4m$ edges respectively. Therefore, by the definition of degree-based indices, we get

$$\chi(NA_m^n) = 18mn + 8m,$$

$$\chi_k(NA_m^n) = m(3n-2)\cdot 6^k + 4m\cdot 5^k,$$

$$HM(NA_m^n) = 108mn + 28m,$$

$$H(NA_m^n) = nm - \frac{14}{15}m,$$

$$H_k(NA_m^n) = m(3n-2)(\frac{1}{3})^k + 4m(\frac{2}{5})^k,$$

$$GA_k(NA_m^n) = m(3n-2) + 4m(\frac{2\sqrt{6}}{5})^k,$$
$$M_1(NA_m^n, x) = m(3n-2)x^6 + 4mx^5,$$
$$M_2(NA_m^n, x) = m(3n-2)x^9 + 4mx^6,$$
$$M_3(NA_m^n) = 4m,$$
$$M_3(NA_m^n, x) = m(3n-2) + 4mx,$$
$$M_{t_1,t_3}(NA_m^n) = m(3n-2)3^{t_1+t_2+1} + 4m(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}),$$
$$PM_1(NA_m^n) = 6^{m(3n-2)}5^{4m},$$
$$PM_2(NA_m^n) = 9^{m(3n-2)}6^{4m},$$
$$ReZG_1(NA_m^n) = 2mn + 2m,$$
$$ReZG_2(NA_m^n) = \frac{9mn}{2} + \frac{9m}{5},$$
$$ReZG_3(NA_m^n) = 162mn + 12m.$$

For NC_m^n, its edge set can be divided into three parts: $|E_4| = |E_4^*| = n$, $|E_5| = |E_6^*| = 2n$ and $|E_6| = |E_9^*| = n(3m - \frac{5}{2})$. Hence, according to the definition of degree based indices, we infer

$$\chi(NC_m^n) = 18mn - n,$$
$$\chi_k(NC_m^n) = n(3m - \frac{5}{2})6^k + 2n \cdot 5^k + n \cdot 4^k,$$
$$HM(NC_m^n) = 108mn - 24n,$$
$$H(NC_m^n) = nm - \frac{7}{15}m,$$
$$H_k(NC_m^n) = n(3m - \frac{5}{2})(\frac{1}{3})^k + 2n(\frac{2}{5})^k + n(\frac{1}{2})^k,$$
$$GA_k(NC_m^n) = n(3m - \frac{3}{2}) + 2n(\frac{2\sqrt{6}}{5})^k,$$
$$M_1(NC_m^n, x) = n(3m - \frac{5}{2})x^6 + 2nx^5 + nx^4,$$
$$M_2(NC_m^n, x) = n(3m - \frac{5}{2})x^9 + 2nx^6 + nx^4,$$
$$M_3(NC_m^n) = 2n,$$
$$M_3(NC_m^n, x) = n(3m - \frac{3}{2}) + 2nx,$$
$$M_{t_1,t_3}(NC_m^n) = n(3m - \frac{5}{2})3^{t_1+t_2+1} + 2n(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + n \cdot 2^{t_1+t_2+1},$$
$$PM_1(NC_m^n) = 6^{n(3m-\frac{5}{2})}5^{2n}4^n,$$
$$PM_2(NC_m^n) = 9^{n(3m-\frac{5}{2})}6^{2n}4^n,$$
$$ReZG_1(NC_m^n) = 2mn + \frac{13}{3}n,$$
$$ReZG_2(NC_m^n) = \frac{9}{2}mn - \frac{7}{20}n,$$
$$ReZG_3(NC_m^n) = 162mn - 59n.$$

7 Degree Based Indices of Dendrimer Nanostars $D_3[n]$

In this section, we discuss an important chemical structure $D_3[n]$ which denotes the n-th growth of nanostar dendrimer for $\forall n \in \mathbb{N} \cup \{0\}$. See Figure 9 for more details on the structure of this chemical graph.

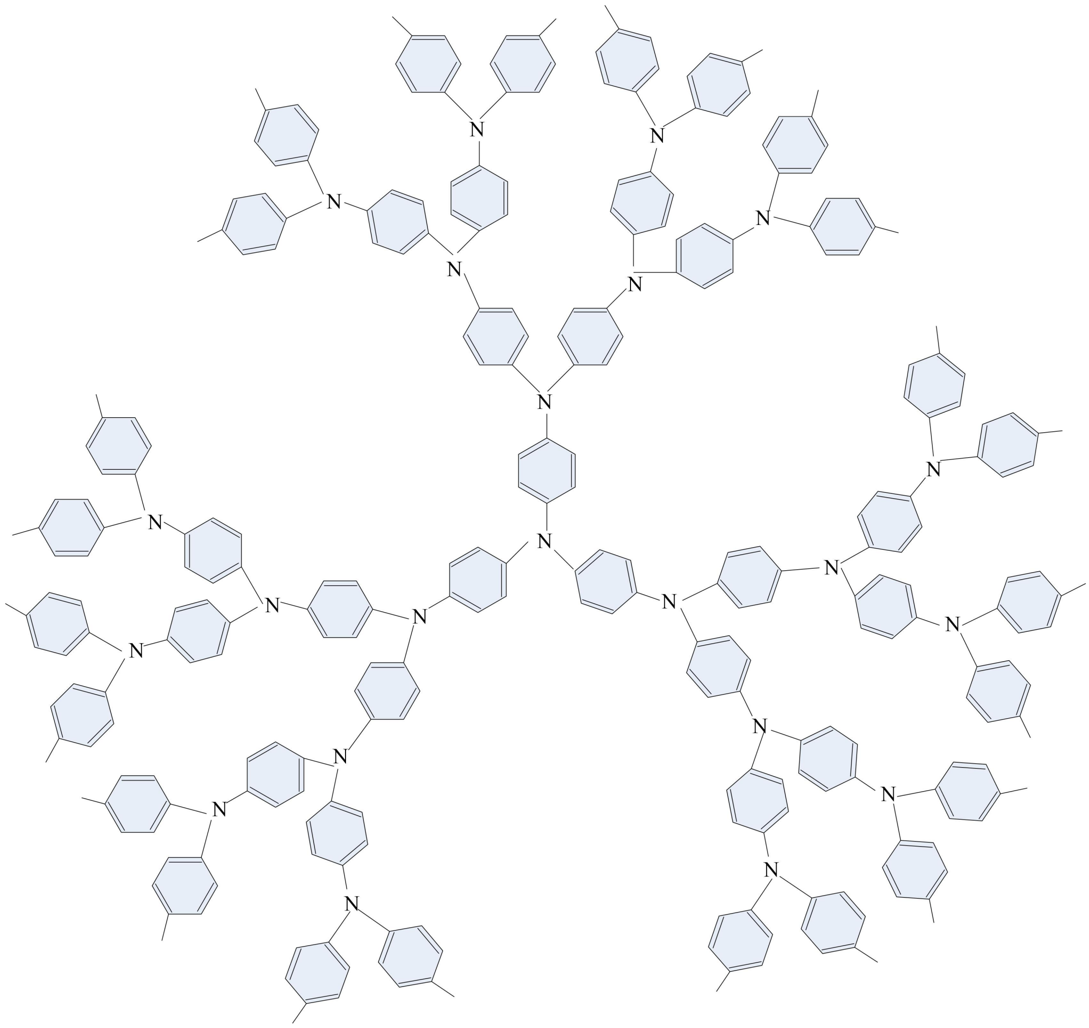

Fig. 9 The 2-Dimensional of the n-th growth of nanostar dendrimer $D_3[n]$.

Farahani [23] determined multiple Zagreb indices of $D_3[n]$. However, there are typos on the computation formulates. In this section, we calculate the degree based indices of dendrimer nanostars $D_3[n]$. Also, the typos in expression of multiple Zagreb indices of $D_3[n]$ in Farahani [23] are corrected. According to the analysis in Farahani [23], we know that $|V(D_3[n])| = 4(3 \cdot 2^{n+1} - 5)$, $|E(D_3[n])| = 24(2^{n+1} - 1)$ and $E(D_3[n])$ can be divided into four parts. Specifically, we have $|E_3^*| = 3 \cdot 2^n$, $|E_4^*| = 6(2^{n+1} - 1)$, $|E_4| = |E_3^*| + |E_4^*| = 15 \cdot 2^n - 6$, $|E_5| = |E_6^*| = 12(2^{n+1} - 1)$ and $|E_6| = |E_9^*| = 9 \cdot 2^n - 6$. Hence, by the definition of degree based indices, we infer

$$R_k(D_3[n]) = 9^k(9 \cdot 2^n - 6) + 3^k(3 \cdot 2^n) + (12(2^{n+1} - 1))6^k + (6(2^{n+1} - 1))4^k,$$

$$M_2^*(D_3[n]) = 9 \cdot 2^n - \frac{25}{6},$$

$$\chi_k(D_3[n]) = 6^k(9 \cdot 2^n - 6) + (12(2^{n+1} - 1))5^k + (15 \cdot 2^n - 6)4^k,$$

$$HM(D_3[n]) = 964 \cdot 2^n - 612,$$

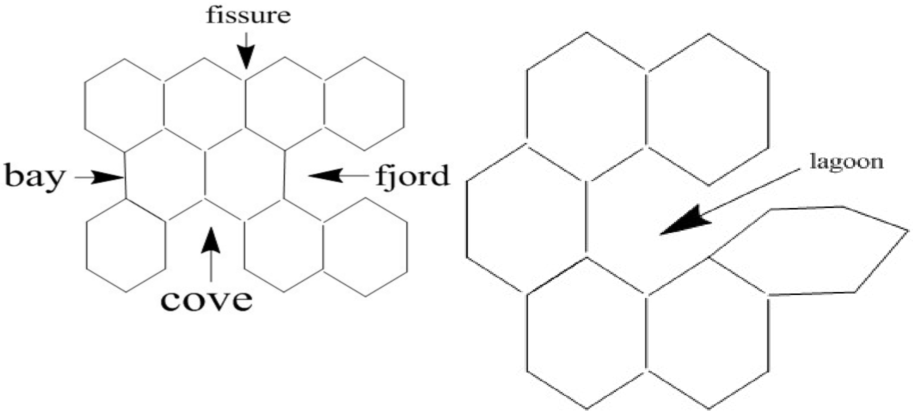

Fig. 10 Classes of inlets occurring on the perimeter of a benzenoid system.

$$H(D_3[n]) = \frac{201}{10}\cdot 2^n - \frac{49}{5},$$

$$H_k(D_3[n]) = (\frac{1}{3})^k(9\cdot 2^n - 6) + (12(2^{n+1}-1))(\frac{2}{5})^k + (15\cdot 2^n - 6)(\frac{1}{2})^k,$$

$$GA(D_3[n]) = (21\cdot 2^n - 12) + \frac{2\sqrt{2}}{3}(3\cdot 2^n) + (12(2^{n+1}-1))\frac{2\sqrt{6}}{5},$$

$$GA_k(D_3[n]) = (21\cdot 2^n - 12) + (\frac{2\sqrt{2}}{3})^k(3\cdot 2^n) + (12(2^{n+1}-1))(\frac{2\sqrt{6}}{5})^k,$$

$$ABC(D_3[n]) = (6\cdot 2^n - 4) + \sqrt{\frac{1}{2}}(39\cdot 2^n - 18),$$

$$M_3(D_3[n]) = 21\cdot 2^n - 12,$$

$$M_3(D_3[n],x) = (3\cdot 2^n)x^2 + (12(2^{n+1}-1))x + (21\cdot 2^n - 12),$$

$$M_{t_1,t_3}(D_3[n]) = 3^{t_1+t_2+1}(9\cdot 2^n - 6) + (3^{t_1}+3^{t_2})(3\cdot 2^n) + (12(2^{n+1}-1))(2^{t_1}3^{t_2}+2^{t_2}3^{t_1}) + (6(2^{n+1}-1))2^{t_1+t_2+1},$$

$$PM_1(D_3[n]) = 6^{9\cdot 2^n-6}\cdot 5^{12(2^{n+1}-1)}\cdot 4^{15\cdot 2^n-6},$$

$$PM_2(D_3[n]) = 9^{9\cdot 2^n-6}\cdot 3^{3\cdot 2^n}\cdot 6^{12(2^{n+1}-1)}\cdot 4^{6(2^{n+1}-1)},$$

$$ReZG_1(D_3[n]) = 42\cdot 2^n - 20,$$

$$ReZG_2(D_3[n]) = \frac{1131}{20}2^n - \frac{147}{5},$$

$$ReZG_3(D_3[n]) = 1434\cdot 2^n - 780.$$

8 Degree Based Indices of Benzenoid Systems and Phenylenes

In this section, we consider the degree based indices of benzenoid systems and phenylenes (the structure can refer to Rada et al., [53], Cyvin and Brunvoll [54], Pavlovic and Gutman [55], Yousefi-Azari et al., [56], and Xiao et al., [57]). Note that coves, fjords, fissures, bays and lagoons are basic structural characteristics of the perimeter of the benzenoid systems which can refer to Figure 10.

For the rest context of this section, we set S as a benzenoid system with n vertices, h hexagons and r inlets. By calculating, we verify that $|E_4| = |E_4^*| + |E_4^*| = n - 2h - r + 2$, $|E_5| = |E_6^*| = 2r$ and $|E_6| = |E_9^*| = 3h - r - 3$. Thus, following the definition of degree-based indices, we infer

$$R_k(NS_3[n]) = 9^k(3h - r - 3) + (2r)6^k + (n - 2h - r + 2)4^k,$$

$$M_2(NS_3[n]) = 4n + 19h - r - 19.$$

$$M_2^*(NS_3[n]) = \frac{n}{4} - \frac{h}{6} - \frac{r}{36} + \frac{1}{6},$$

$$\chi(NS_3[n]) = 4n + 10h - 10,$$

$$\chi_k(NS_3[n]) = 6^k(3h - r - 3) + (2r)5^k + (n - 2h - r + 2)4^k,$$

$$HM(NS_3[n]) = 16n - 2r + 76h - 76,$$

$$H(NS_3[n]) = \frac{n}{2} - \frac{r}{30},$$

$$H_k(NS_3[n]) = (\frac{1}{3})^k(3h - r - 3) + (2r)(\frac{2}{5})^k + (n - 2h - r + 2)(\frac{1}{2})^k,$$

$$ABC(NS_3[n]) = \sqrt{\frac{1}{2}}(n + h - 1),$$

$$GA_k(NS_3[n]) = (\frac{\sqrt{3}}{2})^k(2^{n+1}) + (28 \cdot 2^n - 6)(\frac{2\sqrt{6}}{5})^k + (28 \cdot 2^n - 7),$$

$$M_1(NS_3[n], x) = (3h - r - 3)x^6 + (2r)x^5 + (n - 2h - r + 2)x^4,$$

$$M_2(NS_3[n], x) = (3h - r - 3)x^9 + (2r)x^6 + (n - 2h - r + 2)x^4,$$

$$M_3(NS_3[n]) = 2r,$$

$$M_3(NS_3[n], x) = (n + h - 2r - 1) + (2r)x,$$

$$M_{t_1,t_3}(NS_2[n]) = 3^{t_1+t_2+1}(3h - r - 3) + (2r)(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + (n - 2h - r + 2)2^{t_1+t_2+1},$$

$$PM_1(NS_3[n]) = 6^{3h-r-3}5^{2r}4^{n-2h-r+2},$$

$$PM_2(NS_3[n]) = 9^{3h-r-3}6^{2r}4^{n-2h-r+2},$$

$$ReZG_1(NS_3[n]) = n,$$

$$ReZG_2(NS_3[n]) = n + \frac{5h}{2} - \frac{5}{2} - \frac{r}{10},$$

$$ReZG_3(NS_3[n]) = 16n - 30r + 130h + 32.$$

For phenylene chemical structure, we set PH as a phenylene with h hexagons and r inlets. The detailed structure can refer to Figure 11.

By structure analysis and computation, we obtain $|E_4| = |E_4^*| + |E_4^*| = 2h - r + 4$, $|E_5| = |E_6^*| = 2r$ and $|E_6| = |E_9^*| = 6h - r - 6$. Again, using the definition of degree based indices, we yield

$$R_k(NS_3[n]) = 9^k(6h - r - 6) + (2r)6^k + (2h - r + 4)4^k,$$

$$M_2(NS_3[n]) = 62h - r - 38,$$

$$M_2^*(NS_3[n]) = \frac{7h}{6} - \frac{r}{36} + \frac{1}{3},$$

$$\chi(NS_3[n]) = 44h + 20,$$

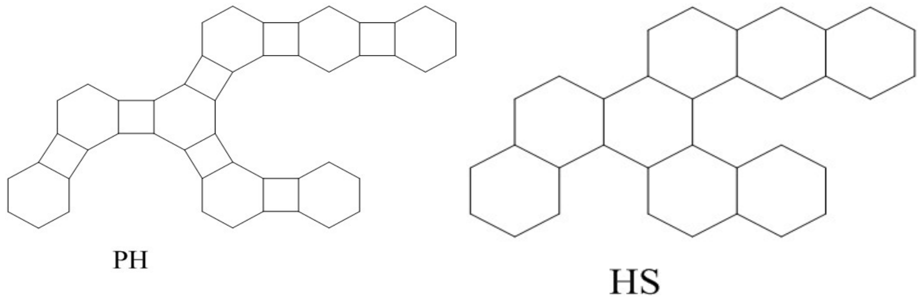

Fig. 11 A phenylene (PH) and its hexagonal squeeze (HS).

$$\chi_k(NS_3[n]) = 6^k(6h-r-6)+(2r)5^k+(2h-r+4)4^k,$$
$$HM(NS_3[n]) = 248h-2r-152,$$
$$H(NS_3[n]) = 3h-\frac{r}{30},$$
$$H_k(NS_3[n]) = (\frac{1}{3})^k(6h-r-6)+(2r)(\frac{2}{5})^k+(2h-r+4)(\frac{1}{2})^k,$$
$$ABC(NS_3[n]) = 4h-\frac{2}{3}r-4+\sqrt{\frac{1}{2}}(2h+r+4),$$
$$GA_k(NS_3[n]) = (8h-2r-2)+(2r)(\frac{2\sqrt{6}}{5})^k,$$
$$M_1(NS_3[n],x) = (6h-r-6)x^6+(2r)x^5+(2h-r+4)x^4,$$
$$M_2(NS_3[n],x) = (6h-r-6)x^9+(2r)x^6+(2h-r+4)x^4,$$
$$M_3(NS_3[n]) = 2r,$$
$$M_3(NS_3[n],x) = (8h-2r-2)+2rx,$$
$$M_{t_1,t_3}(NS_2[n]) = 3^{t_1+t_2+1}(6h-r-6)+(2r)(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})+(2h-r+4)2^{t_1+t_2+1},$$
$$PM_1(NS_3[n]) = 6^{6h-r-6}5^{2r}4^{2h-r+4},$$
$$PM_2(NS_3[n]) = 9^{6h-r-6}6^{2r}4^{2h-r+4},$$
$$ReZG_1(NS_3[n]) = 6h,$$
$$ReZG_2(NS_3[n]) = 11n-\frac{r}{25}-5,$$
$$ReZG_3(NS_3[n]) = 356h-10r-260.$$

9 Degree Based Indices of Polycyclic Aromatic Hydrocarbons PAH_n

Polycyclic aromatic hydrocarbons PAH_s is a family of hydrocarbon molecules which is consisted of cycles with length six (Benzene) and can be considered as small pieces of graphene sheets with the free valences of the dangling bonds saturated by H. Vice versa, a graphene sheet can be interpreted as an infinite PAH molecule. In this section, the first members of this hydrocarbon family are stated as follows which are shown in Figure 12: let PAH_1 be the Benzene with six carbon (C) and six hydrogen (H) atoms, PAH_2 be the Coronene with 24 carbon and twelve hydrogen atoms and PAH_3 be the Circumcoronene with 54 carbon and eighteen hydrogen atoms.

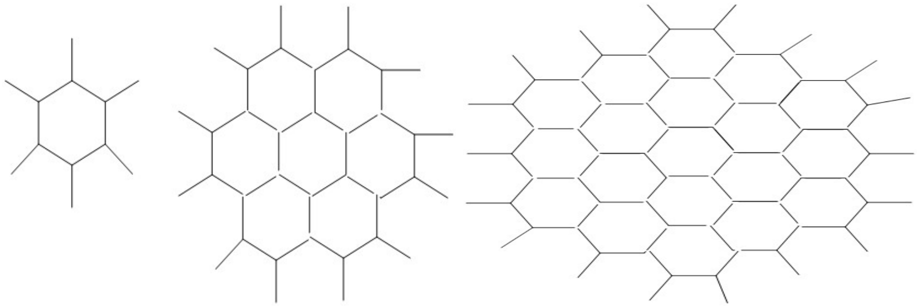

Fig. 12 A phenylene (PH) and its hexagonal squeeze (HS).

It is not hard to check that the general representation of polycyclic aromatic hydrocarbon PAH_n has $6n^2$ carbon (C) atoms and $6n$ hydrogen (H) atoms. By the analysis given by Farahani [58], we know that $|V(PAH_n)| = 6n^2+6n$, $|E(PAH_n)| = 9n^2+3n$, and the edge set of PAH_n can be divided into two parts: $E_4 = E_3^*$ and $E_6 = E_9^*$ such that $|E_4| = |E_3^*| = 6n$ and $|E_6| = |E_9^*| = 9n^2-3n$. Therefore, by the definition of degree-based indices, we infer

$$R_k(NS_3[n]) = 9^k(9n^2-3n)+(6n)3^k,$$

$$M_2^*(NS_3[n]) = n^2+\frac{5n}{3},$$

$$\chi_k(NS_3[n]) = 6^k(9n^2-3n)+(6n)4^k,$$

$$HM(NS_3[n]) = 228n^2-108n,$$

$$H(NS_3[n]) = 3n^2+2n,$$

$$H_k(NS_3[n]) = (\frac{1}{3})^k(9n^2-3n)+(6n)(\frac{1}{2})^k,$$

$$ABC(NS_3[n]) = 6n^2-1n+(6n)\sqrt{\frac{1}{2}},$$

$$GA(NS_3[n]) = (9n^2-3n)+3n\sqrt{3},$$

$$GA_k(NS_3[n]) = (9n^2-3n)+(6n)(\frac{\sqrt{3}}{2})^k,$$

$$M_3(NS_3[n]) = 12n,$$

$$M_3(NS_3[n],x) = (9n^2-3n)+(6n)x^2,$$

$$M_{t_1,t_3}(NS_2[n]) = 3^{t_1+t_2+1}(9n^2-3n)+(6n)(3^{t_1}+3^{t_2}),$$

$$PM_1(NS_3[n]) = 6^{9n^2-3n}4^{6n},$$

$$PM_2(NS_3[n]) = 9^{9n^2-3n}\cdot 3^{6n},$$

$$ReZG_1(NS_3[n]) = 6n^2+6n,$$

$$ReZG_2(NS_3[n]) = \frac{27}{2}n^2,$$

$$ReZG_3(NS_3[n]) = 486n^2-90n.$$

10 Conclusion

In our article, we mainly report the degree-based indices of some widely used chemical structures with the help of molecular graph structure analysis, edge dividing technology and mathematical derivation. These molecular structures are widely used in the analysis of both the melting point, boiling point, QSPR/QSAR study and other chemical proptoses for chemical compounds and drugs. Thus, the promising prospects of the application for the chemical and pharmacy engineering will be illustrated in the theoretical conclusion that is obtained in this article.

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