Generalized Zagreb index of polyomino chains and nanotubes

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The Zagreb index is a distance-based topological index which reflects certain structural features of organic molecules. In this article, in terms of molecular structural analysis, we report the generalized Zagreb index of polyomino chains and two kinds of nanotubes. Moreover, the Randic related indices of polyomino chains are also discussed.

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1. Introduction

Investigations of degree or distance based topological indices have been conducted over 35 years. Topological indices are numerical parameters of molecular graph, and play significant roles in physics, chemistry and pharmacology science.

Specifically, let G be a molecular graph, then a topological index can be regarded as a score function f: $G \rightarrow R^{+}$, with this property that $f(G_1) = f(G_2)$ if G_1 and G_2 are isomorphic. As numerical descriptors of the molecular structure obtained from the corresponding molecular graph, topological indices are widely used in theoretical chemistry, especially in QSPR/QSAR study. For instance, Wiener index, Zagreb index, harmonic index and sum connectivity index are introduced to reflect certain structural features of organic molecules. There are several papers contributing to determine these distance-based indices of special molecular graph (See Hosamani [1], Yan et al. [2], Jamil et al. [3], and Gao et al., [4-10] for more detail). The notation and terminology used but undefined in this paper can be found in [11].

The first and second Zagreb indices was introduced by Gutman and Trinajstic [12] which denoted by

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

and

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

respectively. Here $d(v)$ denotes the degree of vertex v in molecular graph G.

The modified second Zagreb index for molecular graph G is defined by

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

Azari and Iranmanesh [13] introduced generalized Zagreb index of molecular graph G which is stated as:

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

where t_1 and t_2 are arbitrary non-negative integers.

Bollobas and Erdos [14] introduced the general Randic index $R_k(G)$ for a molecular graph G, i.e.,

$$R_k(G) = \sum_{uv \in E(G)} (d(u)d(v))^k,$$

where $k \neq 0$ is a real number .

Li and Liu [15] determined the first three minimum general Randic indices among trees, and the corresponding extremal trees are characterized. Liu and Gutman [16] reported several novel estimates of the general Randic index and of its special cases – the ordinary and modified Zagreb indices.

If $k=-\frac{1}{2}$, then the general Randic index is just the Randic index which is introduced by Randic [17] in 1975:

$$R(G)=\sum_{uv\in E(G)}(d(u)d(v))^{-\frac{1}{2}}.$$

Although there have been several advances in Wiener index, Zagreb index, PI index, harmonic index and sum connectivity index of molecular graphs, the study of generalized Zagreb index and Randic related indices for special chemical structures has been largely limited. In addition, as widespread and critical chemical structures, polyomino system and nanotubes are widely used in medical science and pharmaceutical field. As an example, polyomino chain is one of the basic chemical structures and exists widely in benzene and alkali molecular structures. For these reasons, it has attracted tremendous academic and industrial interests to research the generalized Zagreb index of these molecular structures from a mathematical point of view. As supplement, we derive the Randic related indices of polyomino chains.

In this paper, we first present the generalized Zagreb index and Randic related indices of several polyomino chains. Then, the expressions of $M_{\{t_1,t_2\}}(VC_5C_7[p,q])$ and $M_{\{t_1,t_2\}}(HC_5C_7[p,q])$ are manifested.

2. Indices of polyomino chains

From the view of graph theory, a polyomino system is a finite 2-connected plane graph, and each interior cell is encircled by a regular square with length 1. That is to say, it is an edge-connected union of cells in the planar square lattice. One special polyomino system is polyomino chain, in which the joining of the centers (let c_i be the center of the i-th square) of its adjacent regular composes a path $c_1c_2\cdots c_n$. Let $\boldsymbol{B}_n$ be the set of polyomino chains with n squares. The number of edges in each $B_n\in\boldsymbol{B}_n$ is $3n$+1. B_n is called a linear chain and denoted by L_n if the subgraph of B_n induced by the vertices with degree 3 is a molecular graph with exactly n−2 squares. B_n is called a zig-zag chain and denoted by Z_n if the subgraph of B_n induced by the vertices with degree >2 is a path with n−1 edges.

A kind of a polyomino chain is the branched or angularly connected squares. A segment of a polyomino chain is a maximal linear chain in the polyomino chains, including the kinks and terminal squares at its end. Let $l(S)$ be the length of S and computed by the number of squares in S. We infer $2\le l(S)\le n$ for any segment S of a polyomino chain. In particular, we deduce m=1 and $l_1=n$ for a linear chain L_n with n squares. And, $m=n-1$ and $l_i=2$ for a zig-zag chain Z_n with n squares.

We always suppose that a polyomino chain consists of a sequence of segments $S_1,S_2,\cdots S_m$, $m\ge 1$ and $l(S_i)=l_i$, $i\in\{1,2,\cdots,m\}$. By the fact that two neighboring segments have one square in common, we obtain $\sum_{i=1}^{m}l_i=n+m-1$.

The theorems stated in the follows give the expression of generalized Zagreb index of polyomino chains.

Theorem 1. Let L_n, Z_n be the polyomino chains described above. Then, we yield

$$M_{\{t_1,t_2\}}(L_n)=\begin{cases}8\cdot 2^{t_1+t_2}, & n=1\\ 4\cdot 2^{t_1+t_2}+4\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1}), & \\ +2(3n-5)\cdot 3^{t_1+t_2}, & n\ge 2\end{cases}$$

$$M_{\{t_1,t_2\}}(Z_n)=\begin{cases}8\cdot 2^{t_1+t_2}, & n=1\\ 4\cdot 2^{t_1+t_2}+4\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1}) & \\ +2\cdot 3^{t_1+t_2}, & n=2\\ 4\cdot 2^{t_1+t_2}+4\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1}) & \\ +2(n-2)\cdot(2^{t_1}4^{t_2}+2^{t_2}4^{t_1}) & \\ +2\cdot(3^{t_1}4^{t_2}+3^{t_2}4^{t_1})+ & \\ 2(n-3)\cdot 4^{t_1+t_2}, & n\ge 3\end{cases}.$$

Proof. For n=1, 2, it is easy to check the results. In the following discussion, we assume that $n\ge 3$.

We verify that $|E(L_n)|=|E(Z_n)|=3n+1$. Let n_{ij} be the number of edges with degree i, j. Hence

(i) For the polyomino chain L_n, we get $n_{22}=2$, $n_{23}=4$ and $n_{33}=3n-5$. By the definition of generalized Zagreb index, we have

$$M_{\{t_1,t_2\}}(L_n)=4\cdot 2^{t_1+t_2}+4\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})$$
$$+2(3n-5)\cdot 3^{t_1+t_2}.$$

(ii) Using the same fashion, we infer

$$M_{\{t_1,t_2\}}(Z_n) = 4\cdot 2^{t_1+t_2} + 4\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1})$$
$$+2(m-1)\cdot(2^{t_1}4^{t_2} + 2^{t_2}4^{t_1}) + 2\cdot(3^{t_1}4^{t_2} + 3^{t_2}4^{t_1})$$
$$+2(3n-2m-5)\cdot 4^{t_1+t_2}.$$

Note that m=n−1 for Z_n. We get the desired results.

Remark 1. By the discussion in the proof of Theorem 1, we obtain the computational formulas of general Randic index as follows:

$$R_k(L_n) = \begin{cases} 4^{k+1}, & n=1 \\ 2\cdot 4^k + 4\cdot 6^k + (3n-5)\cdot 9^k, & n\ge 2 \end{cases},$$

$$R_k(Z_n) = \begin{cases} 4^{k+1}, & n=1 \\ 2\cdot 4^k + 4\cdot 6^k + 9^k, & n=2 \\ 2\cdot 4^k + 4\cdot 6^k + 2(n-2)\cdot 8^k & \\ +2\cdot 12^k + (n-3)\cdot 16^k, & n\ge 3 \end{cases}.$$

Take k=1, -1 and $-\frac{1}{2}$ in the above formulas, we get

$$M_2(L_n) = \begin{cases} 16, & n=1 \\ 27n-13, & n\ge 2 \end{cases},$$

$$M_2(Z_n) = \begin{cases} 16, & n=1 \\ 41, & n=2 \\ 32n-24, & n\ge 3 \end{cases},$$

$$M_2^*(L_n) = \begin{cases} 1, & n=1 \\ \frac{n}{3}+\frac{11}{18}, & n\ge 2 \end{cases},$$

$$M_2^*(Z_n) = \begin{cases} 1, & n=1 \\ \frac{23}{18}, & n=2 \\ \frac{5n}{16}+\frac{31}{48}, & n\ge 3 \end{cases},$$

$$R(L_n) = \begin{cases} 2, & n=1 \\ n+\frac{4}{\sqrt{6}}-\frac{2}{3}, & n\ge 2 \end{cases},$$

$$R(Z_n) = \begin{cases} 2, & n=1 \\ \frac{4}{\sqrt{6}}+\frac{4}{3}, & n=2 \\ \frac{n+1}{4}+\frac{4}{\sqrt{6}}+\frac{1}{\sqrt{3}}+\frac{n-2}{\sqrt{2}}, & n\ge 3 \end{cases}.$$

Theorem 2. Let B_n^1 ($n\ge 3$) be a polyomino chain with n squares and consisting of m segments S_1, S_2 with lengths l_1=2, l_2 = n− 1. Then

$$M_{\{t_1,t_2\}}(B_n^1) = \begin{cases} 4\cdot 2^{t_1+t_2} + 4\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + 4\cdot 3^{t_1+t_2} & \\ +2\cdot(3^{t_1}4^{t_2} + 3^{t_2}4^{t_1}), & n=3 \\ 4\cdot 2^{t_1+t_2} + 5\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + & \\ 3\cdot(3^{t_1}4^{t_2} + 3^{t_2}4^{t_1}) + 2(3n-10)\cdot 3^{t_1+t_2} & \\ +(2^{t_1}4^{t_2} + 2^{t_2}4^{t_1}), & n\ge 4 \end{cases}.$$

Proof. It is trivial for n=3, we skip it here. For $n\ge 4$, we have n_{22} = 2, n_{23} = 5, n_{24} = 1, n_{34} = 3, n_{33} = 3n−10. Thus, by virtue of the definitions, we obtain the desired results.

Remark 2. By the discussion in the proof of Theorem 2, the computational formula of general Randic index is inferred as follows:

$$R_k(B_n^1) = \begin{cases} 2\cdot 4^k + 4\cdot 6^k + 2\cdot 9^k & \\ +2\cdot 12^k, & n=3 \\ 2\cdot 4^k + 5\cdot 6^k + 3\cdot 12^k & \\ +(3n-10)\cdot 9^k + 8^k, & n\ge 4 \end{cases}.$$

By taking k=1, -1 and $-\frac{1}{2}$ in the above formula, we deduce the expression of second Zagreb index, modified second Zagreb index and Randic index

$$M_2(B_n^1) = \begin{cases} 74, & n=3 \\ 27n-8, & n\ge 4 \end{cases},$$

$$M_2^*(B_n^1) = \begin{cases} \frac{14}{9}, & n=3 \\ \frac{n}{3}+\frac{43}{72}, & n\ge 4 \end{cases},$$

$$R(B_n^1)=\begin{cases}\frac{4}{\sqrt{6}}+\frac{5}{3}+\frac{1}{\sqrt{3}}, & n=3\\ n+\frac{5}{\sqrt{6}}+\frac{3}{2\sqrt{3}}-\frac{7}{3}+\frac{1}{2\sqrt{2}}, & n\geq 4\end{cases}.$$

In the following consideration of this section, we assume that $2\leq l(i)\leq n-1$ with $1\leq i\leq m$.

Theorem 3. Let B_n^2 $(n\geq 4)$ be a polyomino chain with n squares consisting of m segments S_1, $S_2,\cdots,S_m$ $(m\geq 3)$ with lengths $l_1=l_m=2$, $l_2,\cdots$, $l_{m-1}\geq 3$. Then

$$M_{\{t_1,t_2\}}(B_n^2)=4\cdot 2^{t_1+t_2}+2m\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})$$

$$+2\cdot(2^{t_1}4^{t_2}+2^{t_2}4^{t_1})+(4m-6)\cdot(3^{t_1}4^{t_2}+3^{t_2}4^{t_1})$$

$$+2(3n-6m+3)\cdot 4^{t_1+t_2}.$$

Proof. In B_n^2, we get $n_{22}=2$, $n_{23}=2m$, $n_{24}=2$, $n_{34}=4m-6$, $n_{33}=3n-6m+3$. Thus, by virtue of the definition, we get the desired results.

Remark 3. By the discussion in the proof of Theorem 3, we obtain the computational formula of general Randic index below:

$$R_k(B_n^2)=2\cdot 4^k+2m\cdot 6^k+2\cdot 8^k$$

$$+(4m-6)\cdot 12^k+(3n-6m+3)\cdot 16^k.$$

The following formulas are yielded by taking k=1, -1 and $-\frac{1}{2}$ respectively in the above formula:

$$M_2(B_n^2)=48n-36m,$$

$$M_2^*(B_n^2)=\frac{7}{16}+\frac{3n}{16}+\frac{7m}{24},$$

$$R(B_n^2)=\frac{2m}{\sqrt{6}}+\frac{1}{\sqrt{2}}+\frac{2m-3}{\sqrt{3}}+\frac{3n-6m+7}{4}.$$

In similar ways, we have

Theorem 4. Let B_n^3 be a polyomino chain with n squares consisting of m segments S_1, $S_2,\cdots,S_m$ $(m\geq 3)$ with lengths $l_1=2$, $l_2,\cdots$, l_{m-1}, $l_m\geq 3$ or $l_m=2$, l_1, $l_2,\cdots$, $l_{m-1}\geq 3$. Then

$$M_{\{t_1,t_2\}}(B_n^3)=4\cdot 2^{t_1+t_2}+(2m+1)\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})$$

$$+2(3n-6m+4)\cdot 3^{t_1+t_2}+(4m-5)\cdot(3^{t_1}4^{t_2}+3^{t_2}4^{t_1}).$$

Theorem 5. Let B_n^4 be a polyomino chain with n squares consisting of m segments S_1, $S_2,\cdots,S_m$ $(m\geq 3)$ with lengths $l_i\geq 3$(i=1, 2, $\cdots$,m). Then

$$M_{\{t_1,t_2\}}(B_n^4)=4\cdot 2^{t_1+t_2}+(2m+2)\cdot(2^{t_1}3^{t_2}+2^{t_2}3^{t_1})$$

$$+2(3n-6m+1)\cdot 3^{t_1+t_2}+(4m-4)\cdot(3^{t_1}4^{t_2}+3^{t_2}4^{t_1}).$$

Remark 4. By the discussions in the proofs of Theorem 4 and Theorem 5, we verify the computational formulas of general Randic index in the following:

$$R_k(B_n^3)=2\cdot 4^k+(2m+1)\cdot 6^k$$

$$+(3n-6m+4)\cdot 9^k+(4m-5)\cdot 12^k,$$

$$R_k(B_n^4)=2\cdot 4^k+(2m+2)\cdot 6^k$$

$$+(3n-6m+1)\cdot 9^k+(4m-4)\cdot 12^k.$$

Again, the formulas stated as follows are obtained by taking k=1, -1 and $-\frac{1}{2}$ in the above formulas:

$$M_2(B_n^3)=27n+6m-10,$$

$$M_2^*(B_n^3)=\frac{n}{3}+\frac{25}{36},$$

$$R(B_n^3)=\frac{2m+1}{\sqrt{6}}+\frac{3n-6m+7}{3}+\frac{4m-5}{2\sqrt{3}}.$$

$$M_2(B_n^4) = 27n + 6m - 19,$$

$$M_2^*(B_n^4) = \frac{n}{3} + \frac{11}{18},$$

$$R(B_n^4) = \frac{2m+2}{\sqrt{6}} + \frac{3n-6m+4}{3} + \frac{2m-2}{\sqrt{3}}.$$

3. Indices of nanotubes

The purpose of this section is to calculate the generalized Zagreb index of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes. The structures of these nanotubes consist of cycles with length 5 and 7 (or C_5C_7 net, which is a trivalent decoration made by alternating C_5 and C_7) by different compound. It can cover either a torus or a cylinder.

Let *p* be the number of pentagons in the first row of the 2D-lattice of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$. In these nanotubes, the first four rows of vertices and edges are repeated alternatively, and let *q* be the number of this repetition. For any *p*, $q \in □$, in each period of $VC_5C_7[p,q]$, there are 16*p* vertices and 6*p* vertices which are taken to the end of the molecular structure. Hence, we have $|V(VC_5C_7[p,q])|$ =16*pq*+6*p*. In view of 3*p*+3*p* vertices have degree two and other 16*pq* vertices have degree three, we get $|E(VC_5C_7[p,q])|$ = 24*pq* + 6*p*.

Moreover, there are 8*p* vertices in each period of $HC_5C_7[p,q]$. We obtain $|V(HC_5C_7[p,q])|$ = 8*pq* + 5*p*, where 5*p* vertices which are taken to the end of structure. Furthermore, there are 12*p* edges in each period, and *q* repetition and 5*p* addition edges. We conclude that $|E(HC_5C_7[p,q])|$ =12*pq*+5*p*.

Let $\delta(G)$ and $\Delta(G)$ be the minimum and maximum degree of *G*. We divide edge set *E*(*G*) and vertex set *V* (*G*) into several partitions: for any *i*, $2\delta(G) \le i \le 2\Delta(G)$, let E_i = {e=*uv* ∈ *E*(*G*)| $d(v) + d(u) = i$}; for any *j*, $(\delta(G))^2 \le j \le (\Delta(G))^2$, let E_j^* ={*e*=*uv* ∈ *E*(*G*)| $d(v)d(u) = j$} and for any *k*, $\delta(G) \le k \le \Delta(G)$, let $V_k = \{ v \in V(G) \mid d(v) = k\}$.

Obviously, the degree of vertex in nanotubes is belonging to {1, 2, 3, 4}. Thus, we infer two partitions V_3 = {$v \in V(G)$| $d(v)$ = 3} and V_2 = {$v \in V(G)$| $d(v)$ = 2}.

Since the hydrogen and single carbon atoms can be omitted. We yield three partitions of edge set: E_4, $d(u) = d(v) = 2$; E_6, $d(u) = d(v) = 3$; E_5, $d(u) = 2$ and $d(v) = 3$.

Now, we present the main results in this section.

Theorem 6. $M_{\{t_1,t_2\}}(VC_5C_7[p,q]) =$

$$2(24pq-6p)\cdot 3^{t_1+t_2} + 12p\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}).$$

Proof. Consider nanotubes $VC_5C_7[p,q]$ for any *p*, $q \in □$, we deduce $|V_2|$ =6*p*, $|V_3|$ =16*pq*, $|E_5| = |E_6^*|$ = 6*p* + 6*p*, and $|E_6| = |E_9^*|$ =24*pq*-6*p*.

According to definitions of generalized Zagreb index, we have

$$M_{\{t_1,t_2\}}(VC_5C_7[p,q])$$

$$= \sum_{e=uv\in E_6} (d(u)^{t_1} d(v)^{t_2} + d(u)^{t_2} d(v)^{t_1})$$

$$+ \sum_{e=uv\in E_5} (d(u)^{t_1} d(v)^{t_2} + d(u)^{t_2} d(v)^{t_1})$$

$$= 2|E_6|\cdot 3^{t_1+t_2} + |E_5|\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}).$$

Theorem 7.

$$M_{\{t_1,t_2\}}(HC_5C_7[p,q]) = 2(12pq-4p)\cdot 3^{t_1+t_2} + 8p\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + 2p\cdot 2^{t_1+t_2}.$$

Proof. Consider nanotube $HC_5C_7[p,q]$ for any *p*, $q \in □$. We obtain $|V_2|$ =5*p*, $|V_3|$ = 8*pq*, $|E_4| = |E_4^*|$ = *p*, $|E_5| = |E_6^*|$ = 8*p*, and $|E_6| = |E_9^*|$ = 12*pq*−4*p*.

Therefore, in terms of definitions of generalized Zagreb index, we get

$$M_{\{t_1,t_2\}}(HC_5C_7[p,q])$$

$$= \sum_{e=uv\in E_6} (d(u)^{t_1} d(v)^{t_2} + d(u)^{t_2} d(v)^{t_1})$$

$$+ \sum_{e=uv\in E_5} (d(u)^{t_1} d(v)^{t_2} + d(u)^{t_2} d(v)^{t_1})$$

$$+ \sum_{e=uv\in E_4} (d(u)^{t_1} d(v)^{t_2} + d(u)^{t_2} d(v)^{t_1})$$

$$= 2|E_6|\cdot 3^{t_1+t_2} + |E_5|\cdot(2^{t_1}3^{t_2} + 2^{t_2}3^{t_1}) + 2|E_4|\cdot 2^{t_1+t_2}.$$

4. Conclusion

In this paper, in view of mathematical derivation and molecular graph structural analysis, we obtain the generalized Zagreb index of polyomino chains and two classes of nanotubes. Furthermore, the general Randic indices of polyomino chains are presented. The results achieved in our paper illustrate the promising application prospects for chemical engineering.

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