Biological Characteristics Analyzing of Molecular Structures via Topological Index Computation

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Abstract: It's revealed from the earlier studies that lots of biological characteristics of compound are closely related to the molecular structure of compound. For example, the structure-dependency of total π-electron energy E_π heavily depends on the sum of squares of the vertex degrees of the molecular graph. It provided us the trick to analyze the biological properties of compounds and materials by means of topological index calculating. In this paper, we study the biological characteristics of some important molecular structures from mathematical perspective. First, Nordhaus-Gaddum-type inequalities for some distance-based indices are presented; then, the reverse eccentric connectivity index of haphthylenic lattice is determined.

Keywords: Theoretical biology, biological characteristic, molecular graph, topological index, haphthylenic lattice

1. Introduction

In the past 40 years, a large number of biological experiments found that there is a closed connection between biological properties of compound and its molecular structure. As an instance, it's found that the sum of squares of the vertex degrees of the molecular graph reflects the structure-dependency of total π-electron energy E_π and measures the physical-biological properties of molecular structures (see Gutman et al. [1-5], Angelina et al. [6], Jones et al. [7], Peric et al. [8], Morales [9] and Markovic [10]).

In theoretical biology, each vertex expresses an atom and each edge represents a chemical bond between two atoms, thus the molecular structure can be modeled as a graph G with atom set $V(G)$ (i.e., vertex set) and chemical bound set $E(G)$ (i.e., edge set). A topological index defined on the molecular graph is regarded as a real-valued function f: $G \rightarrow R^+$ which maps each molecular structure to a positive real score. There are more than one thousand indices introduced in past 40 years, such as Wiener index, PI index, eccentric related index, harmonic index, Zagreb index, and sum connectivity index (Several results on these indices can refer to Gao et al. [11-19], and Hosamani [20] for more details). The terminologies and notations used but not clearly defined in this paper can be found in Bondy and Mutry [21].

As the extension of the Wiener index, the modified Wiener index was introduced as

$$W_\lambda(G)=\sum_{\{u,v\}\subseteq V(G)} d^\lambda(u,v).$$

The hyper-Wiener index and λ-modified hyper-Wiener index are defined as

$$WW(G)=\frac{1}{2}(\sum_{\{u,v\}\subseteq V(G)} d^2(u,v)+\sum_{\{u,v\}\subseteq V(G)} d(u,v))$$

and

$$WW_\lambda(G)=\frac{1}{2}(\sum_{\{u,v\}\subseteq V(G)} d^{2\lambda}(u,v)+\sum_{\{u,v\}\subseteq V(G)} d^\lambda(u,v)),$$

respectively.

The multiplicative Wiener index is stated as

$$\pi(G)=\prod_{\{u,v\}\subseteq V(G)} d(u,v).$$

Correspondingly, the logarithm of multiplicative Wiener index is expressed as

$$\Pi(G)=\ln(\sqrt{2\prod_{\{u,v\}\subseteq V(G)} d(u,v)})\cdot$$

The Harary index is denoted as

$$H(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d(u,v)},$$

The second and third Harary indices are defined as

$$H_1(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d(u,v)+1},$$

$$H_2(G)=\sum_{\{u,v\}\subseteq V(G)}\frac{1}{d(u,v)+2}.$$

More generally, generalized Harary index is denoted by

$$H_t(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)+t}$$

where t is any non-negative real number. The contributions on Wiener related indices and Harary related indices can refer to Knor et al. [22], Mujahed and Nagy [23], Quadras et al. [24], Ghorbani and Klavzar [25], Sedlar [26], Pattabiraman and Paulraja [27], Fazlollahi and Shabani [28], Ilic et al. [29], Heydari [30], Eliasi [31] and Lucic et al. [32].

For a fixed vertex $u \in V(G)$, the eccentricity $ec(u)$ of vertex u is defined as the largest distance between u and any other vertex v in G. Ediz [33] introduced a new distance-based topological index called reverse eccentric connectivity index which is stated as

$$^{RE}\xi^c(G) = \sum_{v \in V(G)} \frac{ec(v)}{S(v)},$$

where $S(v) = \sum_{u \in N_G(v)} d(u)$. Nejati and Mehdi [34] obtained the reverse eccentric connectivity index of tetragonal carbon nanocones. More results on eccentricity related indices can refer to Abraham and Weismann [35], McCrary et al. [36], Farooq et al. [37], Putz et al. [38], Berrocal and Mora [39], and Alaeiyan et al. [40].

Although there have been great contributions in distance-based and degree-based indices of molecular graphs, the studies of special indices for particular molecular structures are still largely limited. For this reason, we discuss some distance-based indices of commonly used biological structures for biological characteristic measuring.

We arrange the rest context as follows: Nordhaus-Gaddum-type inequalities for several distance-based indices are manifested first; then, the reverse eccentric connectivity index of haphthylenic lattice is computed.

2. Main Results and Proofs

The purpose of this section shows the main result of the paper.

2.1 Nordhaus-Gaddum-type inequalities for bipartite molecular graph

The bipartite (molecular) graph G is a graph whose vertex set can be divided into two parts X and Y, where each edge $xy \in E(G)$ satisfies $x \in X$ and $y \in Y$. It implies that for each edge in bipartite molecular graph, one end is in X and the other end is in Y. For any molecular graph G, the $\bar{G}$ is defined as follows: $V(G) = V(\bar{G})$ and $xy \in E(\bar{G})$ if and only if $xy \notin E(G)$.

Theorem 1. Let $G=(X,Y,E)$ be a bipartite molecular graph with $|X| = p$ and $|Y| = q$. Then, we have

$$W_\lambda(G) + W_\lambda(\bar{G}) \geq (1+3^\lambda)pq + 2^{\lambda+1}(\binom{p}{2}+\binom{q}{2}) \qquad \text{if } \lambda > 0,$$

$$W_\lambda(G) + W_\lambda(\bar{G}) \leq (1+3^\lambda)pq + 2^{\lambda+1}(\binom{p}{2}+\binom{q}{2}) \qquad \text{if } \lambda < 0,$$

$$WW(G) + WW(\bar{G}) \geq 7pq + 6(\binom{p}{2}+\binom{q}{2}),$$

$$WW_\lambda(G) + WW_\lambda(\bar{G}) \geq (1+\frac{3^\lambda+9^\lambda}{2})pq + (2^\lambda+4^\lambda)(\binom{p}{2}+\binom{q}{2}) \quad \text{if } \lambda > 0,$$

$$WW_\lambda(G) + WW_\lambda(\bar{G}) \leq (1+\frac{3^\lambda+9^\lambda}{2})pq + (2^\lambda+4^\lambda)(\binom{p}{2}+\binom{q}{2}) \quad \text{if } \lambda < 0,$$

$$\pi(G) + \pi(\bar{G}) \geq 3^{pq}2^{2(\binom{p}{2}+\binom{q}{2})},$$

$$\Pi(G) + \Pi(\bar{G}) \geq \ln(\sqrt{3^{pq}2^{2(\binom{p}{2}+\binom{q}{2})+1}}),$$

$$H_t(G) + H_t(\bar{G}) \leq (\frac{1}{1+t}+\frac{1}{3+t})pq + \frac{2}{2+t}(\binom{p}{2}+\binom{q}{2}).$$

Proof. Set $\bar{d}(u,v)$ as the distance between u and v in molecular graph $\bar{G}$. Clearly, $\bar{G}$

is also a bipartite molecular graph. Next, we only present the proof of $W_\lambda(G)+W_\lambda(\bar{G})$ part for $\lambda > 0$, and other parts can be deduced in the similar way.

Let $x \in X, y \in Y, x, x' \in X$ and $y, y' \in Y$. By the definition of $W_\lambda(G)$ and bipartite structure, we infer

$$W_\lambda(G) = \sum_{x\in X, y\in Y} d^\lambda(x,y) + \sum_{x,x'\in X} d^\lambda(x,x') + \sum_{y,y'\in X} d^\lambda(y,y'),$$
$$W_\lambda(\bar{G}) = \sum_{x\in X, y\in Y} \bar{d}^\lambda(x,y) + \sum_{x,x'\in X} \bar{d}^\lambda(x,x') + \sum_{y,y'\in X} \bar{d}^\lambda(y,y'),$$

By the definition of $\bar{G}$, we verify that $d(x,y)=1$ and $\bar{d}(x,y)\geq 3$ if $xy\in E(G)$ (i.e., $xy \notin E(\bar{G})$). Analogously, we yield $d(x,y)\geq 3$ and $d(x,y)=1$ if $xy\notin E(G)$ (i.e., $xy\in E(\bar{G})$). It implies that each pair of vertices from different partitions of molecular graph *G* contribution at least $1+3^\lambda$ to $W_\lambda(G)+W_\lambda(\bar{G})$, and the total contribution of all pairs is at least $(1+3^\lambda)pq$. For $x, x'\in X$, we get $d(x,x')\geq 2$, $\bar{d}(x,x')\geq 2$, and thus contribution at least $2^\lambda+2^\lambda$ to $W_\lambda(G)+W_\lambda(\bar{G})$. Therefore, for $\lambda>0$, we obtain

$$W_\lambda(G)+W_\lambda(\bar{G}) \geq (1+3^\lambda)pq + 2^{\lambda+1}(\binom{p}{2}+\binom{q}{2}). \qquad \square$$

Now, let's show the sharpness of the bounds presented in Theorem 1 by constructing a family of graphs. In fact, all the bounds shown in Theorem 1 are tight for this kind of graph, but we only explain $W_\lambda(G)$ part for $\lambda>0$. Let G_k be a $(k+1)$-regular (the degree of each vertex is $k+1$) balanced (it means $|X|=|Y|$) bipartite molecular graph of order $2k^2+2k+2$ and diameter 3. If x and y from the same partition, then we derive $d(x,y)=2$ and there are $\binom{k^2+k+1}{2}$ such vertex pairs. If x and y from the different partitions, then for given *x*, there are $k+1$ vertices *y* satisfy $d(x,y)=1$ and k^2 vertices y' satisfy $d(x,y')=3$. Therefore,

$$W_\lambda(G_k) = 2^\lambda \cdot 2\binom{k^2+k+1}{2} + (k+1)(k^2+k+1) + 3^\lambda k^2(k^2+k+1).$$

On the other hand, $\bar{G}_k$ is also a balanced bipartite molecular graph of order $2k^2+2k+2$ and diameter 3, while it is k^2-regular. If x and y from the same partition of G_k, then we derive $\bar{d}(x,y)=2$ and there are $\binom{k^2+k+1}{2}$ such vertex pairs. If x and y from the different partitions of G_k, then for given x, there are $k+1$ vertices y satisfy $\bar{d}(x,y)=3$ and k^2 vertices y' satisfy $\bar{d}(x,y')=1$. Therefore,

$$W_\lambda(\bar{G}_k) = 2^\lambda \cdot 2\binom{k^2+k+1}{2} + 3^\lambda (k+1)(k^2+k+1) + k^2(k^2+k+1).$$

Finally, we get

$$W_\lambda(G) + W_\lambda(\bar{G}) = (1+3^\lambda)pq + 2^{\lambda+1}(\binom{p}{2} + \binom{q}{2})$$

since $p = q = k^2+k+1$ in this example.

Our next result in this subsection is stated as follows.

Theorem 2. Let *G* be a uniquely (each of its *k*-coloring induces the same vertex partition) *k*-colorable graph of order *n*, and *X* be a partition which divides the vertex set into *k* parts corresponding to *k* colors (i.e., $V(G) = V_1 \cup V_2 \cup \cdots \cup V_k$, and $V_i \cap V_j = \varnothing$ for $1 \le i, j \le k$ and $i \ne j$). Let $\bar{G}_X$ be a graph defined as follows: $V(\bar{G}_X) = V(G)$; for $v_i \in V_i$ and $v_j \in V_j$ with $i \ne j$, $v_i v_j \in E(\bar{G}_X)$ if and only if $v_i v_j \notin E(G)$. Assume that $n = pk + q$ where *p*, *q* are the nonnegative integers satisfy $0 \le p \le k-1$. Then, we have

$$W_\lambda(G) + W_\lambda(\bar{G}_X) \ge (1+2^\lambda)\binom{n}{2} + (2^\lambda - 1)((k-q)\binom{p}{2} + q\binom{p+1}{2}) \qquad \text{if } \lambda > 0,$$

$$W_\lambda(G) + W_\lambda(\bar{G}_X) \le (1+2^\lambda)\binom{n}{2} + (2^\lambda - 1)((k-q)\binom{p}{2} + q\binom{p+1}{2}) \qquad \text{if } \lambda < 0,$$

$$WW(G)+WW(\bar{G}_X)\geq 4\binom{n}{2}+2((k-q)\binom{p}{2}+q\binom{p+1}{2}),$$

$$WW_\lambda(G)+WW_\lambda(\bar{G}_X)\geq (1+\frac{2^\lambda+4^\lambda}{2})\binom{n}{2}+(\frac{2^\lambda+4^\lambda}{2}-1)((k-q)\binom{p}{2}+q\binom{p+1}{2}) \quad \text{if } \lambda>0,$$

$$WW_\lambda(G)+WW_\lambda(\bar{G}_X)\leq (1+\frac{2^\lambda+4^\lambda}{2})\binom{n}{2}+(\frac{2^\lambda+4^\lambda}{2}-1)((k-q)\binom{p}{2}+q\binom{p+1}{2}) \quad \text{if } \lambda<0,$$

$$\pi(G)+\pi(\bar{G}_X)\geq 2^{\binom{n}{2}+(k-q)\binom{p}{2}+q\binom{p+1}{2}},$$

$$\prod(G)+\prod(\bar{G}_X)\geq \ln(\sqrt{2^{\binom{n}{2}+(k-q)\binom{p}{2}+q\binom{p+1}{2}+1}}),$$

$$H_t(G)+H_t(\bar{G}_X)\leq (\frac{1}{1+t}+\frac{1}{2+t})\binom{n}{2}+(\frac{1}{2+t}-\frac{1}{1+t})((k-q)\binom{p}{2}+q\binom{p+1}{2}).$$

Proof. Let $n_i=|V_i|$ for $i\in\{1,\cdots,k\}$. Next, we only present the proof of $W_\lambda(G)+W_\lambda(\bar{G})$ part for $\lambda>0$, and other parts can be deduced in the similar way.

If vertices *x*, *y* from the same color class of *G*, then $d_G(x,y)\geq 2$ and $d_G(x,y)\geq 2$. Hence, the total contribution of such vertex pairs are at least $2^{\lambda+1}\sum_{i=1}^{k}\binom{n_i}{2}$. If vertices *x*, *y* from the different color class of *G*, then the contribution of such vertex pair is at least $1+2^\lambda$. Therefore, for $\lambda>0$, we get

$$W_\lambda(G)+W_\lambda(\bar{G}_X)\geq 2^{\lambda+1}\sum_{i=1}^{k}\binom{n_i}{2}+(1+2^\lambda)(\binom{n}{2}-\sum_{i=1}^{k}\binom{n_i}{2})=(1+2^\lambda)\binom{n}{2}+(2^\lambda-1)\sum_{i=1}^{k}\binom{n_i}{2}.$$

At last, our result on $W_\lambda(G)+W_\lambda(\bar{G}_X)$ with $\lambda>0$ is followed from the fact that $\sum_{i=1}^{k}\binom{n_i}{2}$ $\geq (k-q)\binom{p}{2}+q\binom{p+1}{2}$. □

2.2. The reverse eccentric connectivity index of haphthylenic lattices

The naphthylenic net is discussed first in Diudea [41] which contain the sequence: $C_6,C_6,C_4,C_6,C_6,\cdots,C_6,C_6,C_4,C_6,C_6$. As an example, the structure of $NP[n,n]$ is described in Figure 1.

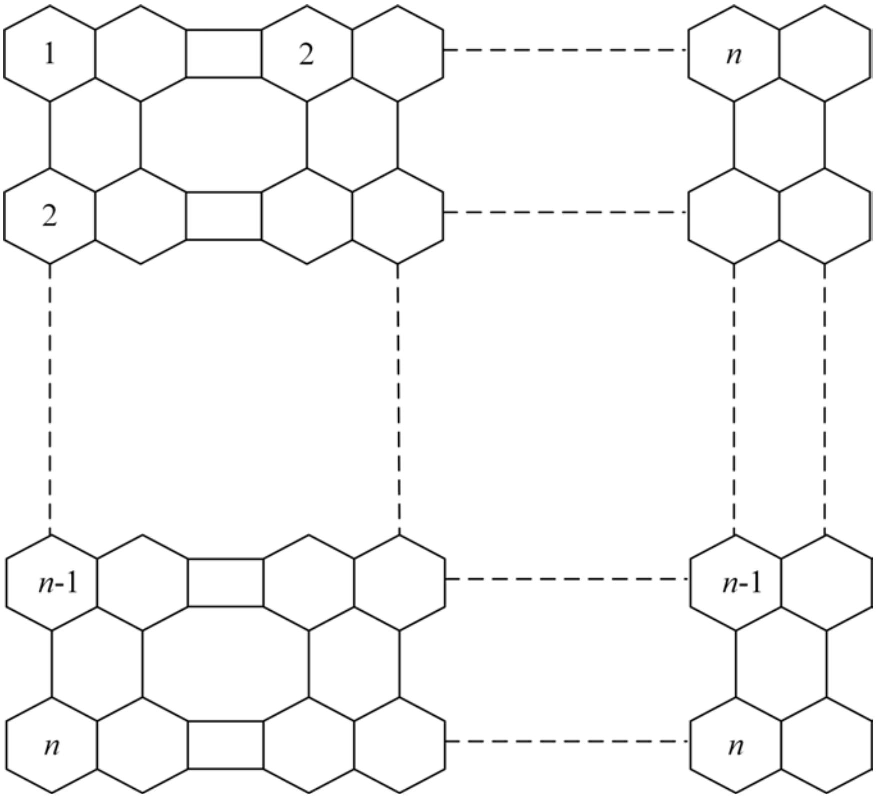

Figure 1. The molecular structure of $NP[n,n]$

By graph structure analysis, we see that $\max\limits_{v\in V(NP[n,n])} ec(v)=7n-2$ and $\min\limits_{v\in V(NP[n,n])} ec(v)=\begin{cases}\frac{7n}{2}, & \text{if } n\equiv 0(\text{mod}2)\\ \frac{7n-1}{2}, & \text{if } n\equiv 1(\text{mod}2)\end{cases}$. The main result in this subsection is stated as follows.

Theorem 3. The reverse eccentric connectivity index of haphthylenic lattices $NP[n,n]$ is:

- If $n\equiv 0(\text{mod}2)$, then

$$
\begin{aligned}
{}^{RE}\xi^{c}(NP[n,n]) &= 2(2\frac{7n-2}{4}+4\frac{7n-3}{5}+2\frac{7n-4}{8}+2\frac{7n-4}{7}+2\frac{7n-4}{5}+2\frac{7n-5}{9}+2\frac{7n-5}{8}+2\frac{7n-5}{6}\\
&+2\frac{7n-5}{5}+4\frac{7n-6}{9}+4\frac{7n-6}{8}+2\frac{7n-6}{5}+6\frac{7n-7}{9}+4\frac{7n-7}{8}+2\frac{7n-7}{5}+8\frac{7n-8}{9}+2\frac{7n-8}{8}+2\frac{7n-8}{6}\\
&+(n-6)\frac{7n-8}{5}+10\frac{7n-9}{9}+(n-6)\frac{7n-9}{8}+2\frac{7n-9}{7}+(n-6)\frac{7n-9}{5}+(n+4)\frac{7n-10}{9}+(n-4)\frac{7n-10}{8}\\
&+2\frac{7n-10}{6}+(2n-2)\frac{7n-11}{9}+2\frac{7n-11}{8}+\cdots)+((n-1)\frac{9n-4}{9}+(n-2)\frac{9n-6}{9}+\cdots+\frac{7n+4}{3}+2\frac{7n+2}{9}+\frac{7n}{9}).
\end{aligned}
$$

• If $n \equiv 1(\mathrm{mod}2)$, then

$$
{}^{RE}\xi^{c}(NP[n,n]) = 2(2\frac{7n-2}{4} + 4\frac{7n-3}{5} + 2\frac{7n-4}{8} + 2\frac{7n-4}{7} + 2\frac{7n-4}{5} + 2\frac{7n-5}{9} + 2\frac{7n-5}{8} + 2\frac{7n-5}{6}
+2\frac{7n-5}{5} + 4\frac{7n-6}{9} + 4\frac{7n-6}{8} + 2\frac{7n-6}{5} + 6\frac{7n-7}{9} + 4\frac{7n-7}{8} + 2\frac{7n-7}{5} + 8\frac{7n-8}{9} + 2\frac{7n-8}{8} + 2\frac{7n-8}{6}
+2\frac{7n-8}{5} + (n-6)\frac{7n-8}{5} + 10\frac{7n-9}{9} + 2\frac{7n-9}{8} + 2\frac{7n-9}{7} + (n-7)\frac{7n-9}{5} + 12\frac{7n-10}{9} + (n-7)\frac{7n-10}{8}
+2\frac{7n-10}{6} + (n-7)\frac{7n-10}{5} + (n+5)\frac{7n-11}{9} + (n-7)\frac{7n-11}{8} + (2n-2)\frac{7n-12}{9} + 2\frac{7n-12}{8} + \cdots)
+((2n-3)\frac{9n-5}{18} + (2n-5)\frac{9n-7}{18} + \cdots + 5\frac{7n+3}{18} + 3\frac{7n+1}{18} + \frac{7n-1}{18}).
$$

Proof. We discuss the reverse eccentric connectivity index according to the parity of n. As we see in Figure 2 and Figure 3, there are different vertex types for even n and odd n. We only analyze the half of $NP[n,n]$ by its symmetry structure.

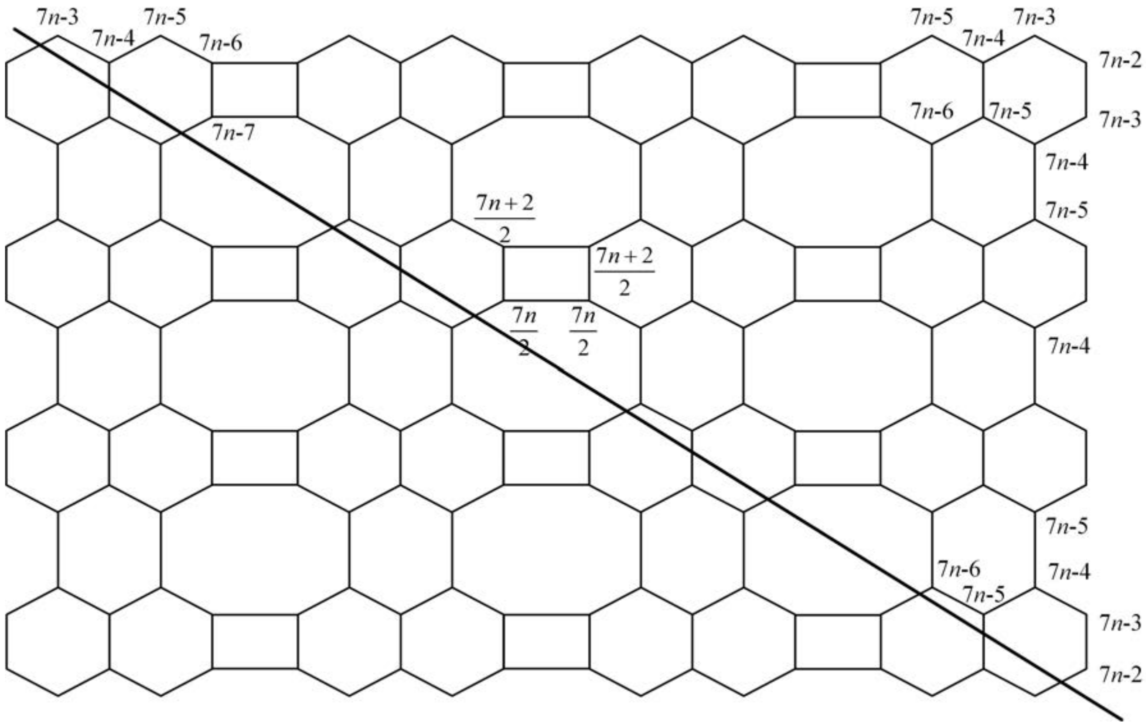

Figure 2. The eccentricity computing of $NP[n,n]$ with $n \equiv 0(\mathrm{mod}2)$

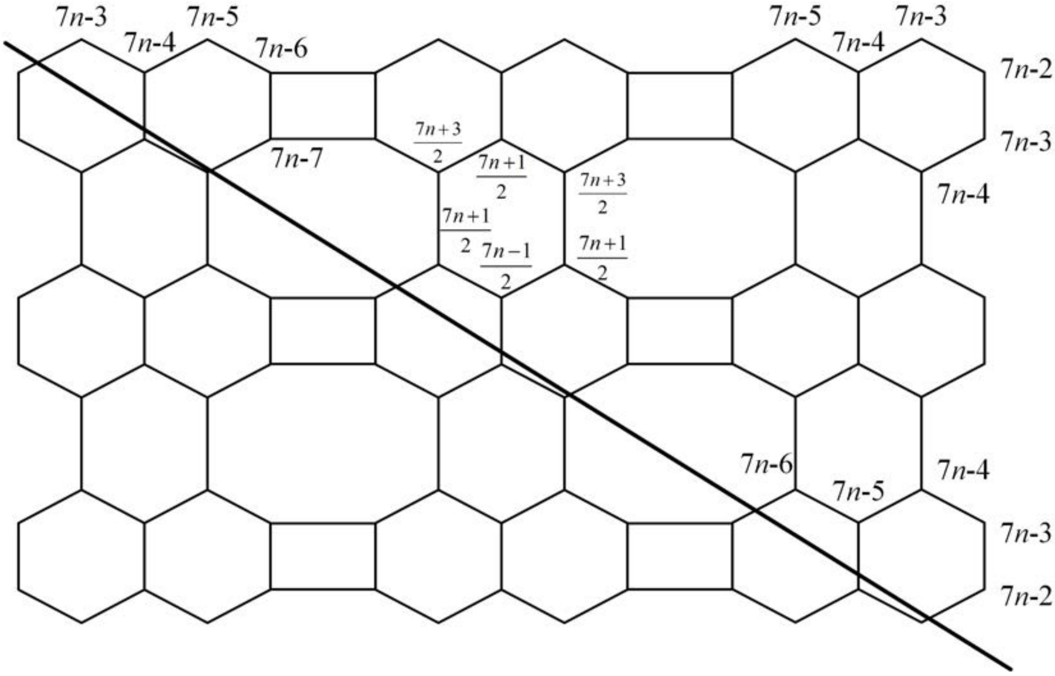

Figure 3. The eccentricity computing of $NP[n,n]$ with $n \equiv 1(\bmod 2)$

For $n \equiv 0(\bmod 2)$, the classes of vertices can be summarized as follows:

- $ec(v) = 7n-2$, $S(v) = 4$ and there are 2 such vertices;
- $ec(v) = 7n-3$, $S(v) = 5$ and there are 4 such vertices;
- $ec(v) = 7n-4$, $S(v) = 8$ and there are 2 such vertices;
- $ec(v) = 7n-4$, $S(v) = 7$ and there are 2 such vertices;
- $ec(v) = 7n-4$, $S(v) = 5$ and there are 2 such vertices;
- $ec(v) = 7n-5$, $S(v) = 9$ and there are 2 such vertices;
- $ec(v) = 7n-5$, $S(v) = 8$ and there are 2 such vertices;
- $ec(v) = 7n-5$, $S(v) = 6$ and there are 2 such vertices;
- $ec(v) = 7n-5$, $S(v) = 5$ and there are 2 such vertices;
- $ec(v) = 7n-6$, $S(v) = 9$ and there are 4 such vertices;
- $ec(v) = 7n-6$, $S(v) = 8$ and there are 4 such vertices;
- $ec(v) = 7n-6$, $S(v) = 5$ and there are 2 such vertices;
- $ec(v) = 7n-7$, $S(v) = 9$ and there are 6 such vertices;

- $ec(v)=7n-7$, $S(v)=8$ and there are 4 such vertices;
- $ec(v)=7n-7$, $S(v)=5$ and there are 2 such vertices;
- $ec(v)=7n-8$, $S(v)=9$ and there are 8 such vertices;
- $ec(v)=7n-8$, $S(v)=8$ and there are 2 such vertices;
- $ec(v)=7n-8$, $S(v)=6$ and there are 2 such vertices;
- $ec(v)=7n-8$, $S(v)=5$ and there are $n-6$ such vertices;
- $ec(v)=7n-9$, $S(v)=9$ and there are 10 such vertices;
- $ec(v)=7n-9$, $S(v)=8$ and there are $n-6$ such vertices;
- $ec(v)=7n-9$, $S(v)=7$ and there are 2 such vertices;
- $ec(v)=7n-9$, $S(v)=5$ and there are $n-6$ such vertices;
- $ec(v)=7n-10$, $S(v)=9$ and there are $n+4$ such vertices;
- $ec(v)=7n-10$, $S(v)=8$ and there are $n-4$ such vertices;
- $ec(v)=7n-10$, $S(v)=6$ and there are 2 such vertices;
- $ec(v)=7n-11$, $S(v)=9$ and there are $2n-2$ such vertices;
- $ec(v)=7n-11$, $S(v)=8$ and there are 2 such vertices;
- $\cdots$
- $ec(v)=\frac{9n-4}{2}$, $S(v)=9$ and there are $2n-2$ such vertices;
- $ec(v)=\frac{9n-6}{2}$, $S(v)=9$ and there are $2n-4$ such vertices;
- $\cdots$
- $ec(v)=\frac{7n+4}{2}$, $S(v)=9$ and there are 6 such vertices;
- $ec(v)=\frac{7n+2}{2}$, $S(v)=9$ and there are 4 such vertices;
- $ec(v)=\frac{7n}{2}$, $S(v)=9$ and there are 2 such vertices.

For $n\equiv 1(\mathrm{mod}2)$, the classes of vertices can be summarized as follows:

- $ec(v)=7n-2$, $S(v)=4$ and there are 2 such vertices;
- $ec(v)=7n-3$, $S(v)=5$ and there are 4 such vertices;
- $ec(v)=7n-4$, $S(v)=8$ and there are 2 such vertices;
- $ec(v)=7n-4$, $S(v)=7$ and there are 2 such vertices;
- $ec(v)=7n-4$, $S(v)=5$ and there are 2 such vertices;
- $ec(v)=7n-5$, $S(v)=9$ and there are 2 such vertices;
- $ec(v)=7n-5$, $S(v)=8$ and there are 2 such vertices;
- $ec(v)=7n-5$, $S(v)=6$ and there are 2 such vertices;
- $ec(v)=7n-5$, $S(v)=5$ and there are 2 such vertices;
- $ec(v)=7n-6$, $S(v)=9$ and there are 4 such vertices;
- $ec(v)=7n-6$, $S(v)=8$ and there are 4 such vertices;
- $ec(v)=7n-6$, $S(v)=5$ and there are 2 such vertices;
- $ec(v)=7n-7$, $S(v)=9$ and there are 6 such vertices;
- $ec(v)=7n-7$, $S(v)=8$ and there are 4 such vertices;
- $ec(v)=7n-7$, $S(v)=5$ and there are 2 such vertices;
- $ec(v)=7n-8$, $S(v)=9$ and there are 8 such vertices;
- $ec(v)=7n-8$, $S(v)=8$ and there are 2 such vertices;
- $ec(v)=7n-8$, $S(v)=6$ and there are 2 such vertices;
- $ec(v)=7n-8$, $S(v)=5$ and there are 2 such vertices;
- $ec(v)=7n-9$, $S(v)=9$ and there are 10 such vertices;
- $ec(v)=7n-9$, $S(v)=8$ and there are 2 such vertices;
- $ec(v)=7n-9$, $S(v)=7$ and there are 2 such vertices;
- $ec(v)=7n-9$, $S(v)=5$ and there are $n-7$ such vertices;

- $ec(v)=7n-10$, $S(v)=9$ and there are 12 such vertices;
- $ec(v)=7n-10$, $S(v)=8$ and there are $n-7$ such vertices;
- $ec(v)=7n-10$, $S(v)=6$ and there are 2 such vertices;
- $ec(v)=7n-10$, $S(v)=5$ and there are $n-7$ such vertices;
- $ec(v)=7n-11$, $S(v)=9$ and there are $n+5$ such vertices;
- $ec(v)=7n-11$, $S(v)=8$ and there are $n-7$ such vertices;
- $ec(v)=7n-12$, $S(v)=9$ and there are $2n-2$ such vertices;
- $ec(v)=7n-12$, $S(v)=8$ and there are 2 such vertices;
- $\cdots$
- $ec(v)=\frac{9n-5}{2}$, $S(v)=9$ and there are $2n-3$ such vertices;
- $ec(v)=\frac{9n-7}{2}$, $S(v)=9$ and there are $2n-5$ such vertices;
- $\cdots$
- $ec(v)=\frac{7n+3}{2}$, $S(v)=9$ and there are 5 such vertices;
- $ec(v)=\frac{7n+1}{2}$, $S(v)=9$ and there are 3 such vertices;
- $ec(v)=\frac{7n-1}{2}$, $S(v)=9$ and there are 1 such vertices.

Finally, the expected result is obtained according to the above vertex classification, the symmetry of molecular graph, and the definition of reverse eccentric connectivity index. □

3. Conclusion

In this paper, by means of molecular graph structure analysis and distance calculation, we report the Nordhaus-Gaddum-type inequalities for bipartite molecular structure and the reverse eccentric connectivity index of haphthylenic lattice. These theoretical conclusions obtained in our paper reveal the biological characteristic of these molecular structures and possess the promising prospects of biology, material and pharmaceuticals engineering applications.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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References

[1] I. Gutman, Total π- Electron Energy of Conjugated Molecules with Non-bonding Molecular Orbitals, Zeitschrift für Naturforschung A-A Journal of Physical Sciences, 2016, 71(2): 161-164.

[2] I. Gutman, G. Indulal, R. Todeschini, Generalizing the McClelland bounds for total π-electron energy, Zeitschrift für Naturforschung A-A Journal of Physical Sciences, 2008, 63(5-6):280-282.

[3] I. Gutman, S. Gojak, B. Furtula, S. Radenkovic, A. Vodopivec, Relating total π-electron energy and resonance energy of benzenoid molecules with

Kekule- and Clar-structure-based parameters, Monatshefte Fur Chemie, 2006, 137(9): 1127-1138.

[4] I. Gutman, N. Cmiljanovic, S. Milosavljevic, S. Radenkovic, Effect of non-bonding molecular orbitals on total π -electron energy, Chemical Physics Letters, 2004, 383(1-2): 171-175.

[5] I. Gutman, K. C. Das, Estimating the total π-electron energy, Journal of the Serbian Chemical Society, 2013, 78(12): 1925-1933.

[6] E. L. Angelina, D. J. R. Duarte, N. M. Peruchena, Is the decrease of the total electron energy density a covalence indicator in hydrogen and halogen bonds?, Journal of Molecular Modeling, 2013, 19(5): 2097-2106.

[7] N. C. Jones, D. Field, J. P. Ziesel, Low-energy total electron scattering in the methyl halides CH3Cl, CH3Br and CH3I, International Journal of Mass Spectrometry, 2008, 277(1-3): 91-95.

[8] M. Peric, I. Gutman, J. Radic-Peric, The Huckel total π-electron energy puzzle, Journal of the Serbian Chemical Society, 2006, 71(7): 771-783.

[9] D. A. Morales, The total π-electron energy as a problem of moments: application of the Backus-Gilbert method, Journal of Mathematical Chemistry, 2005, 38(3): 389-397.

[10] S. Markovic, Approximating total π-electron energy of phenylenes in terms of spectral moments, Indian Journal of Chemistry Section A-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry, 2003, 42(6): 1304-1308.

[11] W. Gao, Y. Q. Wang, W. F. Wang, L. Shi, The first multiplication atom-bond connectivity index of molecular structures in drugs, Saudi Pharmaceutical Journal, 2017, 25(4): 548-555.

[12] W. Gao, M. K. Siddiqui, M. Imran, M. K. Jamil, M. R. Farahani, Forgotten topological index of chemical structure in drugs, Saudi Pharmaceutical Journal, 2016, 24(3): 258-264.

[13] W. Gao, M. R. Farahani, L. Shi, Forgotten topological index of some drug structures, Acta Medica Mediterranea, 2016, 32: 579-585.

[14] W. Gao, W. F. Wang, M. K. Jamil, M. R. Farahani, Electron energy studying of molecular structures via forgotten topological index computation, Journal of Chemistry, Volume 2016, Article ID 1053183, 7 pages, http://dx.doi.org/10.1155/2016/1053183.

[15] W. Gao, W. F. Wang, M. R. Farahani, Topological indices study of molecular structure in anticancer drugs, Journal of Chemistry, Volume 2016, Article ID 3216327, 8 pages, http://dx.doi.org/10.1155/2016/3216327.

[16] W. Gao, W. F. Wang, The eccentric connectivity polynomial of two classes of nanotubes, Chaos, Solitons and Fractals, 2016, 89: 290–294.

[17] W. Gao, W. F. Wang, The fifth geometric arithmetic index of bridge graph and carbon nanocones, Journal of Difference Equations and Applications, 2017, 23(1-2): 100-109.

[18] W. Gao, W. F. Wang, New isolated toughness condition for fractional (g,f,n)-critical graphs, Colloquium Mathematicum, 2017, 147(1): 55-66.

[19] W. Gao, Y. Q. Wang, B. Basavanagoud, M. K. Jamil, Characteristics studies of molecular structures in drugs, Saudi Pharmaceutical Journal, 2017, 25(4): 580-586.

[20] S. M. Hosamani, Correlation of domination parameters with physicochemical properties of octane isomers, Applied Mathematics and Nonlinear Sciences, 2016, 1(2): 345-352.

[21] J. A. Bondy, U. S. R. Mutry, Graph Theory, Spring, Berlin, 2008.

[22] M. Knor, R. Skrekovski, A. Tepeh, Digraphs with large maximum Wiener index, Applied Mathematics and Computation, 2016, 284: 260-267.

[23] H. Mujahed, B. Nagy, Wiener index on rows of unit cells of the face-centred cubic lattice, ACTA Crystallographica A-Foundation and Advances, 2016, 72: 243-249.

[24] J. Quadras, K. Balasubramanian, K. A. Christy, Analytical expressions for Wiener indices of n-circumscribed peri-condensed benzenoid graphs, Journal of Mathematical Chemistry, 2016, 54(3): 823-843.

[25] M. Ghorbani, S. Klavzar, Modified Wiener index via canonical metric representation, and some fullerene patches, Ars Mathematica Contemporanea, 2016, 11(2): 247-254.

[26] J. Sedlar, Extermal unicyclic graphs with respect to additively weighted Harary index, Miskolc Mathematical Notes, 2015, 16(2): 1163-1180.

[27] K. Pattabiraman, P. Paulraja, Harary index of product graphs, Discussions Mathematicae Graph Theory, 2015, 35(1): 17-33.

[28] H. R. Fazlollahi, H. Shabani, A group theoretical method for Computing Harary index, Studia Universitatis Babes-Bolyal Chemia, 2014, 59(1): 23-28.

[29] A. Ilic, G. H. Yu, L. H. Feng, The Harary index of trees, Utilitas Mathematica, 2012, 87: 21-31.

[30] A. Heydari, Harary index of regular dendrimers, Optoelectronics and Advanced Materials-Rapid Communications, 2010, 4(12): 2206-2208.

[31] M. Eliasi, Harary index of zigzag polyhex nanotorus, Digest Journal of Nanomaterials and Biostructures, 2009, 4(4): 757-762.

[32] B. Lucic, A. Milicevic, S. Nikolic, N. Trinajstic, Harary index-twelve years later, Croatica Chemica ACTA, 2002, 75(4): 847-868.

[33] S. Ediz, Reverse eccentric connectivity index, Optoelectron. Adv. Mat., 2012, 6, 664-667.

[34] A. Nejati, A. Mehdi, On reverse eccentric connectivity index of one tetragonal carbon nanocones, Journal of Theoretical and Computational Science, 2014, http://dx.doi.org/10.4172/jtco.1000115.

[35] S. Abraham, C. G. Weismann, Left ventricular end-systolic eccentricity index for assessment of pulmonary hypertension in infants, Echocardiography-A Journal of Cardiovascular Ultrasound and Applied Techniques, 2016, 33(6): 910-915.

[36] A. W. McCrary, J. R. Malowitz, C. P. Hornick, K. D. Hill, C. M. Cotten, G. H. Tatum, P. C. Barker, Differences in Eccentricity Index and Systolic-Diastolic Ratio in Extremely Low-Birth-Weight Infants with Bronchopulmonary Dysplasia at Risk of Pulmonary Hypertension, American Journal of Perinatology, 2016, 33(1): 57-62.

[37] R. Farooq, N. Nazir, M. A. Malik, M. Arfan, Eccentricity based topological indices of a hetrofunctional dendrimer, Journal of Optoelectronics and Advanced Materials, 2015, 17(11-12): 1799-1807.

[38] M. V. Putz, M. A. Tudoran, O. Ori, Topological Organic Chemistry: From Distance Matrix to Timisoara Eccentricity, Current Organic Chemistry, 2015, 19(3): 249-273.

[39] I. Berrocal, I. Mora, Eccentricity index: comparison cardiac phantom and patients with and without cardiac conditions in a high resolution CZT gammacamera, European Journal of Nuclear Medicine and Molecular Imaging, 2014, 41(2): 615-615.

[40] M. Alaeiyan, J. Asadpour, R. Mojarad, A Study of an Infinite Family of Carbon

Nanocones by the Eccentricity Connectivity Polynomial, Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21(10): 849-860.

[41] M.V. Diudea, Phenylenic and Naphthylenic tori, Nanotubes Carbon Nanostruct., 2002, 10(4): 273-292.