

Electrochemical Characteristics Analyzing of Molecular Structures via Topological Index Computation

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Abstract: It's revealed from the earlier studies that lots of electrochemical 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 electrochemical properties of chemical materials by means of topological index calculating. In this paper, we study the electrochemical 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 chemistry, electrochemical characteristic, molecular graph, topological index, haphthylenic lattice

1. Introduction

In the past 40 years, a large number of chemical experiments found that there is a closed connection between chemical 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-chemical 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 chemistry, 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 chemical 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

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

and

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

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

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

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 chemical molecular structures are still largely limited. For this reason, we discuss some distance-based indices of commonly used chemical structures for electrochemical 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

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

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

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

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

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

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

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

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

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

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

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

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 $\bar{d}(x, y) = 1$ 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

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

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

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

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., $V(G) = V_1 \cup V_2 \cup \dots \cup V_k$, and $V_i \cap V_j = \emptyset$ for $1 \leq i, j \leq k$ and $i \neq j$). 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 $i \neq j$, $v_i v_j \in E(\bar{G}_X)$ if and only if $v_i v_j \notin E(G)$. Assume that $n = pk + q$ where p, q are the nonnegative integers satisfy $0 \leq p \leq k - 1$. Then, we have

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

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

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

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

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

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

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

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

Proof. Let $n_i = |V_i|$ for $i \in \{1, \dots, k\}$. 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

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

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:

$C_6, C_6, C_4, C_6, C_6, \dots, C_6, C_6, C_4, C_6, C_6$. As an example, the structure of $NP[n, n]$ is described

in Figure 1.

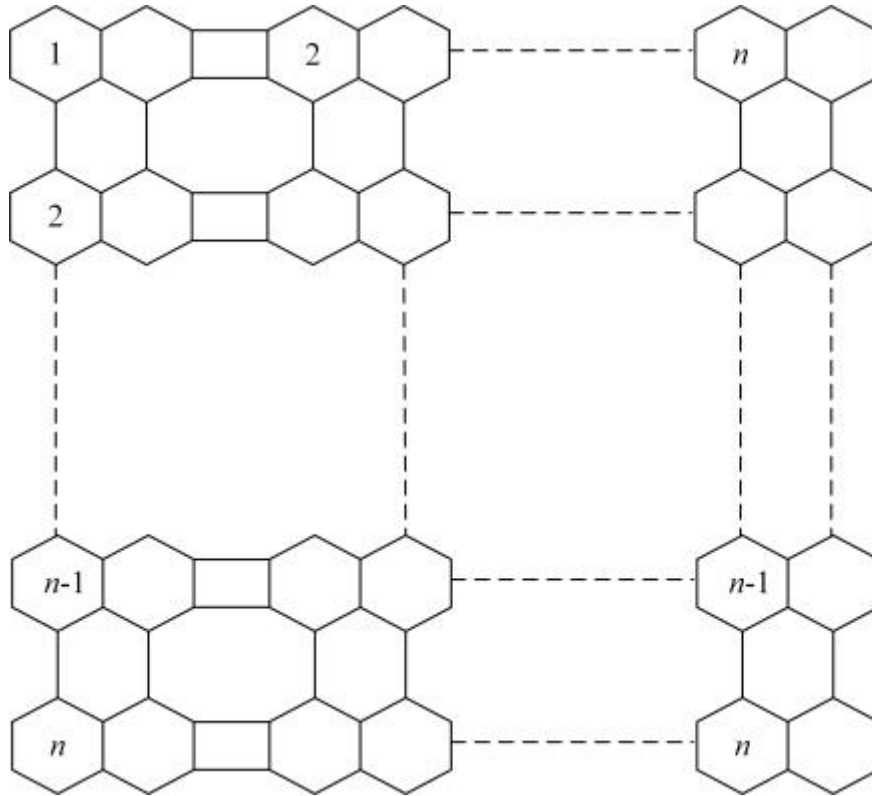


Figure 1. The molecular structure of $NP[n, n]$

By graph structure analysis, we see that $\max_{v \in V(NP[n, n])} ec(v) = 7n - 2$ and

$$\min_{v \in V(NP[n, n])} ec(v) = \begin{cases} \frac{7n}{2}, & \text{if } n \equiv 0 \pmod{2} \\ \frac{7n-1}{2}, & \text{if } n \equiv 1 \pmod{2} \end{cases}. \text{ The main result in this subsection is stated as}$$

follows.

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

is:

• If $n \equiv 0 \pmod{2}$, then

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

• If $n \equiv 1(\text{mod}2)$, then

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

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.

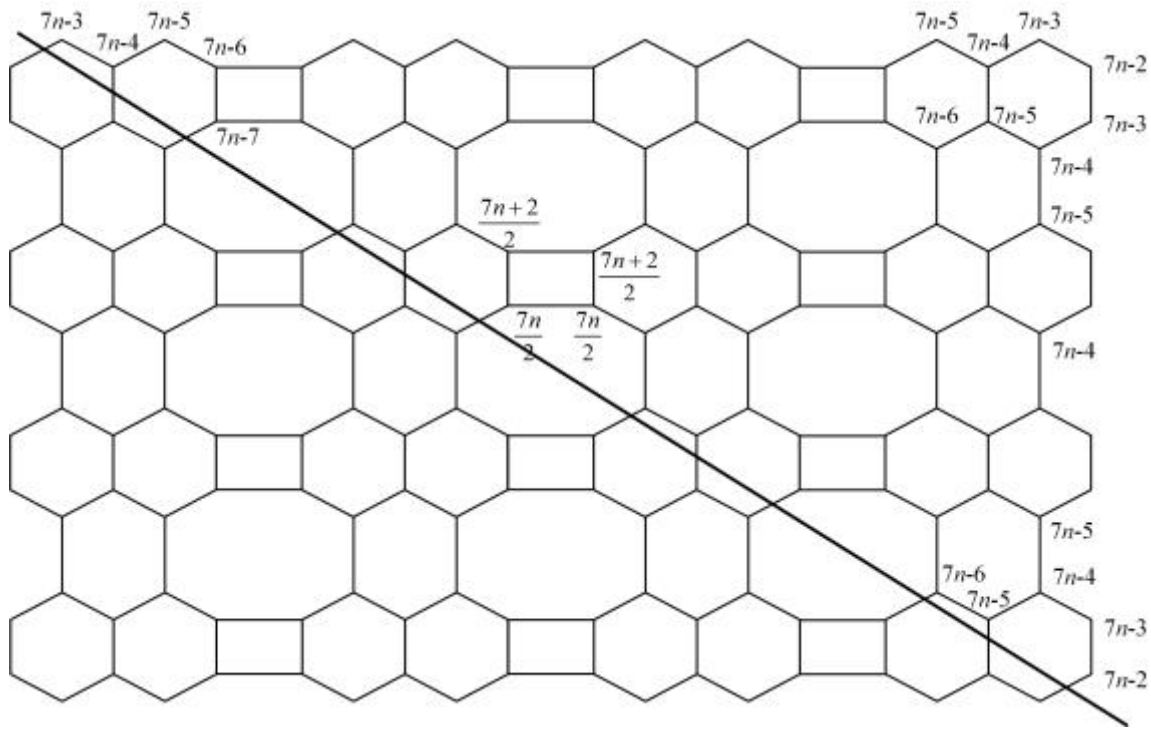


Figure 2. The eccentricity computing of $NP[n,n]$ with $n \equiv 0(\text{mod}2)$

- $ec(v) = 7n - 7$, $S(v) = 8$ 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;
- ...
- $ec(v) = \frac{9n - 4}{2}$, $S(v) = 9$ and there are $2n - 2$ such vertices;
- $ec(v) = \frac{9n - 6}{2}$, $S(v) = 9$ and there are $2n - 4$ such vertices;
- ...
- $ec(v) = \frac{7n + 4}{2}$, $S(v) = 9$ 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 $n \equiv 1 \pmod{2}$, 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;
- ...
- $ec(v) = \frac{9n - 5}{2}$, $S(v) = 9$ and there are $2n - 3$ such vertices;
- $ec(v) = \frac{9n - 7}{2}$, $S(v) = 9$ and there are $2n - 5$ such vertices;
- ...
- $ec(v) = \frac{7n + 3}{2}$, $S(v) = 9$ 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 chemical characteristic of these molecular structures and possess the promising prospects of electrochemical, 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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