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Characteristics studies of molecular structures in drugs

Wei Gao [a,*], Yiqiao Wang [b], B. Basavanagoud [c], Muhammad Kamran Jamil [d]

[a] School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China
[b] School of Management, Beijing University of Chinese Medicine, Beijing 100029, China
[c] Department of Mathematics, Karnatak University, Dharwad 580003, India
[d] Department of Mathematics, Riphah Institute of Computing and Applied Sciences, Riphah International University, Lahore, Pakistan

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ABSTRACT

In theoretical medicine, topological indices are defined to test the medicine and pharmacy characteristics, such as melting point, boiling point, toxicity and other biological activities. As basic molecular structures, hexagonal jagged-rectangle and distance-regular structure are widely appeared in medicine, pharmacy and biology engineering. In this paper, we study the chemical properties of hexagonal jagged-rectangle from the mathematical point of view. Several vertex distance-based indices are determined. Furthermore, the Wiener related indices of distance-regular structure are also considered.

1. Introduction

In the chemical and medicine experiment, the scientists found that there is a potential link between the properties of the compound and its molecular structure. As a result, people tend to determine the features of drugs by virtue of mathematical method.

Specifically, let $G = (V(G), E(G))$ be a molecular graph with vertex set $V(G)$ and edge set $E(G)$, then a topological index can be regarded as a positive real function f: $G \to R^+$. Being numerical descriptors of the molecular structure deduced from the corresponding molecular graph, topological indices can be applied in theoretical medicine to test the characteristics of drugs (Tao et al., 2016; Chen et al., 2016; Liu et al., 2016). For example, harmonic index, Wiener index, PI index, Randic index and sum connectivity index can be used to reflect certain structural features and chemical characteristics of organic molecules. In recent years, several articles made contributions to certain distance-based and degree-based indices of special molecular graph (Hosamani (2016), Zhao et al. (2016), Gao et al. (2016a, 2016b, 2016c), Gao and Wang (2015), Gao et al. (2017), Gao and Wang (2016a, 2016b), and Gao and Siddiqui (2017) for more detail). The notations and terminologies used but undefined in this paper can be found in Bondy and Murty (2008).

For any $e = uv \in E(G)$, let

$$n_u(e) = |\{x | x \in V(G), d(u,x) < d(v,x)\}|,$$

$$n_v(e) = |\{x | x \in V(G), d(u,x) > d(v,x)\}|.$$

Graovac and Ghorbani (2010) introduced a distance-based version of the atom-bond connectivity index which was called the second atom bond connectivity index, and it is denoted as

$$ABC_2(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u(e) + n_v(e) - 2}{n_u(e) n_v(e)}}.$$

Tabar et al. (2010) raised a distance-based version of the geometric-arithmetic index, and was called the second geometric-arithmetic index which can be stated as

$$GA_2(G) = \sum_{uv \in E(G)} \frac{2\sqrt{n_u(e) n_v(e)}}{n_u(e) + n_v(e)}.$$

As a traditional topological index, the PI index of molecular graph G was defined as

$$PI_v(G) = \sum_{e=uv} (n_u(e) + n_v(e)).$$

The vertex PI polynomial, as the extension of vertex PI index, was introduced by Ashrafi et al. (2006), which was stated as

* Corresponding author at: School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China.
E-mail address: gaowei@ynnu.edu.cn (W. Gao).

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$$PI_v(G,x) = \sum_{uv\in E(G)} x^{n_u(e)+n_v(e)}.$$

As a distance-based polynomial, the Szeged polynomial is defined as

$$Sz(G,x) = \sum_{e=uv} x^{n_u(e)n_v(e)}.$$

Some results can be referred to Gutman and Ashrafi (2008). For any edge $e = uv$, let

$$n(e) = |\{x|x \in V(G),\ d(u,x) = d(v,x)\}|.$$

Then, the modified version of Szeged index for a molecular graph G was defined as

$$Sz_v^*(G) = \sum_{uv\in E(G)} \left(\left(n_u(e) + \frac{n(e)}{2}\right)\left(n_v(e) + \frac{n(e)}{2}\right)\right).$$

In what follows, let $\lambda \neq 0$ be a real number, t be any non-negative integer number, and $D(G)$ be the diameter of molecular graph G. 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

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

The Harary index is denoted as

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

The corresponding Harary polynomial is denoted by

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

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

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

At last, the reciprocal complementary Wiener (RCW) index is denoted as

$$RCW(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{1 + D(G) - d(u,v)}.$$

The papers on Wiener related indices can refer to Knor et al. (2016), Mujahed and Nagy (2016), Quadras et al. (2016), Ghorbani and Klavzar (2016), Sedlar (2015), Pattabiraman and Paulraja (2015), Fazlollahi and Shabani (2014), Ilic et al. (2012), Heydari (2010), Eliasi (2009) and Lucic et al. (2002).

A hexagonal rectangle is called hexagonal jagged-rectangle, or simply HJR, if the number of hexagonal cells in each row is alternative between n and $n-1$. If the top and bottom rows are longer we call it HIR of type I and its denoted by $I^{n,m}$. Also, $J^{n,m}$ is another type of HJR (see Shiu et al. (1997) and Yousefi-Azari et al. (2007, 2009) for more details on their structures). Several results on hexagonal structure and its application can refer to Aavatsmark (2016), Sharma (2016), Chernatynskiy et al. (2016), Martinez et al. (2016), Das and Roul (2016), Boldrin et al. (2016), and Kroes et al. (2016).

Let $G_i(v) = \{u \in V(G) : d(u,v) = i\}$. The distance-regular molecular graph with diameter $D(G)$ is defined as follows: there are natural numbers $b_0, b_1, \cdots, b_{D(G)-1}$, $c_1 = 1, c_2, \cdots, c_{D(G)}$ such that for each pair of vertices (u,v) with $d(u,v) = j$, we obtain: (1) there are c_j vertices in $G_{j-1}(v)$ adjacent to u $(1 \leqslant j \leqslant D(G))$; (2) there are b_j vertices in $G_{j+1}(v)$ adjacent to u $(0 \leqslant j \leqslant D(G)-1)$. Here $\{b_0, b_1, \cdots, b_{D(G)-1}; c_1 = 1, c_2, \cdots, c_{D(G)}\}$ called the intersection array of molecular graph G. Several result on distance-regular molecular graph can be referred to Deutsch and Rodriguez-Velazquez (2014), Babai and Wilmes (2016), Makhnev and Paduchikh (2015), and Tsiovkina (2015). Furthermore, a k-regular molecular graph with n vertices called the strongly regular with parameter (n,k,θ,μ) if each pair of adjacent vertices has θ common neighbors and each pair of non-adjacent vertices has μ common neighbors.

In the past decades, the computation of distance-based indices for certain special chemical molecular and drugs structure raised many interests among chemists. Although there have been many results in distance-based indices of molecular graphs, the research of indices for special drug structures are still largely limited. In addition, as popular and critical chemical structures, hexagonal jagged-rectangle and distance-regular structure are widely applied in medical science and pharmaceutical engineering. For all these reasons, we give a deep discussion on the computation of the two molecular structures mentioned above.

The main contribution of our work is two-fold. On the one hand, we will manifest certain vertex distance-based indices of hexagonal jagged-rectangle. On the other hand, some Wiener related indices of distance-regular structure will be discussed.

2. Main results and proofs

In this section, we present our main result and proofs. Our tricks are mainly based on the graph theory.

2.1. Distance-based indices of hexagonal jagged-rectangle

It is easy to see that $|V(I^{n,m})| = 2m(2n+1)$ and $|V(J^{n,m})| = 2m(2n+1) + (2n-1)$. The edge set of edge of $I^{n,m}$ or $J^{n,m}$ can be divided into three parts:

- F: the set of all vertical edges;
- L: the set of all oblique edges from left to right;
- R: the set of all oblique edges from right to left.

Our main conclusion is stated as follows.

Theorem 1. *If $n \geqslant m$, then*

$$ABC_2(\mathrm{I}^{n,m}) = \sum_{i=1}^{2m-1}(s(i)+n)\sqrt{\frac{4mn+2m-2}{i(2n+1)(2m-i)(2n+1)}} + \sum_{i=1}^{m-1}4i\sqrt{\frac{4mn+2m-2}{(2m-2i^2-i+4mn)(2i^2+i)}} + \sum_{i=m}^{n-1}4m\sqrt{\frac{4mn+2m-2}{(4nm-4im+2m^2+m)(4im-2m^2+m)}} + \sum_{i=n}^{n+m}4(n+m-i)\sqrt{\frac{4mn+2m-2}{(4mn+2m^2+2n^2+n+m-4im+4in-2i^2+i)(m-2m^2-2n^2-n+4im-4in+2i^2-i)}},$$

$$GA_2(\mathrm{I}^{n,m}) = \sum_{i=1}^{2m-1}(s(i)+n)\frac{\sqrt{i(2n+1)(2m-i)(2n+1)}}{2mn+m} + \sum_{i=1}^{m-1}4i\frac{\sqrt{(2m-2i^2-i+4mn)(2i^2+i)}}{2mn+m} + \sum_{i=m}^{n-1}4m \times \frac{\sqrt{(4nm-4im+2m^2+m)(4im-2m^2+m)}}{2mn+m} + \sum_{i=n}^{n+m}4(n+m-i) \times \frac{\sqrt{(4mn+2m^2+2n^2+n+m-4im+4in-2i^2+i)(m-2m^2-2n^2-n+4im-4in+2i^2-i)}}{2mn+m},$$

$$Sz(\mathrm{I}^{n,m},x) = \sum_{i=1}^{2m-1}(s(i)+n)x^{i(2n+1)(2m-i)(2n+1)} + \sum_{i=1}^{m-1}4ix^{(2m-2i^2-i+4mn)(2i^2+i)} + \sum_{i=m}^{n-1}4mx^{(4nm-4im+2m^2+m)(4im-2m^2+m)} + \sum_{i=n}^{n+m}4(n+m-i) \times x^{(4mn+2m^2+2n^2+n+m-4im+4in-2i^2+i)(m-2m^2-2n^2-n+4im-4in+2i^2-i)},$$

$$Sz_v^*(\mathrm{I}^{n,m}) = 16m^3n^3 + \frac{8}{5}m^5 - \frac{16}{3}m^4n + 24m^3n^2 - \frac{10}{3}m^4 + \frac{7}{5}m + \frac{40}{3}m^3n - \frac{4}{3}mn^3 - 2m^3 + \frac{16}{3}m^2n + \frac{10}{3}m^2 + mn.$$

If $n \leqslant m$, then

$$ABC_2(\mathrm{I}^{n,m}) = \sum_{i=1}^{2m-1}(s(i)+n)\sqrt{\frac{4mn+2m-2}{i(2n+1)(2m-i)(2n+1)}} + \sum_{i=1}^{n-1}4i\sqrt{\frac{4mn+2m-2}{(2m-2i^2-i+4mn)(2i^2+i)}} + \sum_{i=n}^{m-1}4n \times \sqrt{\frac{4mn+2m-2}{(2n^2+4nm-4in+n+2m-2i)(4in-2n^2-n+2i)}} + \sum_{i=m}^{n+m}4(n+m-i) \times \sqrt{\frac{4mn+2m-2}{(4mn+2m^2+2n^2+n+m-4im-4in+2i^2-i)(-2m^2-2n^2-n+4im+4in+m-2i^2+i)}},$$

$$GA_2(\mathrm{I}^{n,m}) = \sum_{i=1}^{2m-1}(s(i)+n)\frac{\sqrt{i(2n+1)(2m-i)(2n+1)}}{2mn+m} + \sum_{i=1}^{n-1}4i\frac{\sqrt{(2m-2i^2-i+4mn)(2i^2+i)}}{2mn+m} + \sum_{i=n}^{m-1}4n \times \frac{\sqrt{(2n^2+4nm-4in+n+2m-2i)(4in-2n^2-n+2i)}}{2mn+m} + \sum_{i=m}^{n+m}4(n+m-i) \times \frac{\sqrt{(4mn+2m^2+2n^2+n+m-4im-4in+2i^2-i)(-2m^2-2n^2-n+4im+4in+m-2i^2+i)}}{2mn+m},$$

$$Sz(\mathrm{I}^{n,m},x) = \sum_{i=1}^{2m-1}(s(i)+n)x^{i(2n+1)(2m-i)(2n+1)} + \sum_{i=1}^{n-1}4ix^{(2m-2i^2-i+4mn)(2i^2+i)} + \sum_{i=n}^{m-1}4nx^{(2n^2+4nm-4in+n+2m-2i)(4in-2n^2-n+2i)} + \sum_{i=m}^{n+m}4(n+m-i) \times x^{(4mn+2m^2+2n^2+n+m-4im-4in+2i^2-i)(-2m^2-2n^2-n+4im+4in+m-2i^2+i)},$$

$$Sz_v^*(\mathrm{I}^{n,m}) = 16m^3n^3 + mn + \frac{56}{3}m^3n^2 + \frac{2}{3}m^3 - \frac{8}{3}mn^2 + \frac{10}{3}n^2 + \frac{8}{3}mn^4 - \frac{16}{15}n^5 + \frac{20}{3}m^3n + \frac{16}{3}mn^3 - \frac{10}{3}n^4 + \frac{m}{3} + \frac{16}{15}n.$$

Proof. Note that there are $2m+1$ rows with vertical edges. Let $s: \mathbb{N} \to \{0,1\}$ be $s(i) = \begin{cases} 1, & \text{if } i \equiv 1(\text{mod } 2) \\ 0, & \text{if } i \equiv 0(\text{mod} 2) \end{cases}$. We get $n_u^i(e) = i(2n+1)$ and $n_v^i(e) = (2m-i)(2n+1)$ where $n_u^i(e)$ is the number of vertices in the i-th row whose distance to u is smaller than the distance to v. Moreover, the number of vertical edges in i-th row is $s(i)+n$.

By the symmetry of $I^{n,m}$, the contributions from L and R to the indices are equal. The following proof is divided into two cases according to the relationship between n and m.

Case 1: $n \geqslant m$. Let Λ_i be the number of oblique edges from left to right in the i-th row. We get

$$\Lambda_i = \begin{cases} 2i, & 1 \leqslant i < m \\ 2m, & m \leqslant i < n \\ 2(n+m-i), & n \leqslant i \leqslant m+n \end{cases},$$

$$n_u^i(e) = \begin{cases} 2m - 2i^2 - i + 4mn, & 1 \leqslant i < m \\ 4nm - 4im + 2m^2 + m, & m \leqslant i < n \\ 4mn + 2m^2 + 2n^2 + n + m - 4im + 4in - 2i^2 + i, & n \leqslant i \leqslant m+n \end{cases},$$

$$n_v^i(e) = \begin{cases} 2i^2 + i, & 1 \leqslant i < m \\ 4im - 2m^2 + m, & m \leqslant i < n \\ m - 2m^2 - 2n^2 - n + 4im - 4in + 2i^2 - i, & n \leqslant i \leqslant m+n \end{cases}.$$

Case 2: $m \geqslant n$. Let Λ_i be the number of oblique edges from left to right in the i-th row. We get

$$\Lambda_i = \begin{cases} 2i, & 1 \leqslant i < n \\ 2n, & n \leqslant i < m \\ 2(n+m-i), & m \leqslant i \leqslant m+n \end{cases},$$

$$n_u^i(e) = \begin{cases} 2m - 2i^2 - i + 4mn, & 1 \leqslant i < n \\ 2n^2 + 4nm - 4in + n + 2m - 2i, & n \leqslant i < m \\ 4mn + 2m^2 + 2n^2 + n + m - 4im - 4in + 2i^2 - i, & m \leqslant i \leqslant m+n \end{cases},$$

$$n_v^i(e) = \begin{cases} 2i^2 + i, & 1 \leqslant i < n \\ 4in - 2n^2 - n + 2i, & n \leqslant i < m \\ -2m^2 - 2n^2 - n + 4im + 4in + m - 2i^2 + i, & m \leqslant i \leqslant m+n \end{cases}.$$

At last, our result is obtained in terms of above computation and the definition of indices. $\square$

Theorem 2. *If $n \geqslant m$, then*

$$ABC_2(J^{n,m}) = \sum_{i=1}^{2m}(s(i)+n)\sqrt{\frac{4mn+2m+2n-3}{i(2n+1)((2m-i)(2n+1)+2n-1)}} + \sum_{i=1}^{m}4i\sqrt{\frac{4mn+2m+2n-3}{(4mn+2m+2n-1-2i^2-i)(2i^2+i)}}(+\sum_{i=m+1}^{n}(4m+2)$$
$$\times\sqrt{\frac{4mn+2m+2n-3}{(-2m^2-m+4im+2i-1)(2m^2+4nm+3m-4im+2n-2i)}} + \sum_{i=n+1}^{n+m}(4(n+m-i)+2)$$
$$\times\sqrt{\frac{4mn+2m+2n-3}{(-2m^2-2n^2+4im+4in-m-n+3i-2i^2-1)(2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i)}},$$

$$GA_2(J^{n,m}) = \sum_{i=1}^{2m}2(s(i)+n)\frac{\sqrt{i(2n+1)((2m-i)(2n+1)+2n-1)}}{4mn+2m+2n-1} + \sum_{i=1}^{m}8i\frac{\sqrt{(4mn+2m+2n-1-2i^2-i)(2i^2+i)}}{4mn+2m+2n-1}$$
$$+\sum_{i=m+1}^{n}(8m+4)\frac{\sqrt{(-2m^2-m+4im+2i-1)(2m^2+4nm+3m-4im+2n-2i)}}{4mn+2m+2n-1} + \sum_{i=n+1}^{n+m}(8(n+m-i)+4)$$
$$\times\frac{\sqrt{(-2m^2-2n^2+4im+4in-m-n+3i-2i^2-1)(2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i)}}{4mn+2m+2n-1},$$

$$Sz(J^{n,m},x) = \sum_{i=1}^{2m}(s(i)+n)x^{i(2n+1)((2m-i)(2n+1)+2n-1)}$$
$$+\sum_{i=1}^{m}4ix^{(4mn+2m+2n-1-2i^2-i)(2i^2+i)}$$
$$+\sum_{i=m+1}^{n}(4m+2)x^{(-2m^2-m+4im+2i-1)(2m^2+4nm+3m-4im+2n-2i)}$$
$$+\sum_{i=n+1}^{n+m}(4(n+m-i)+2)$$
$$\times x^{(-2m^2-2n^2+4im+4in-m-n+3i-2i^2-1)(2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i)},$$

$$Sz_v^*(J^{n,m}) = 16m^3n^3 + 24m^3n^2 + 24m^2n^3 + 12m^2n^2 - 4mn^2 - 2n^2$$
$$+\frac{8}{5}m^5 + \frac{16}{3}m^4n - \frac{4}{3}m^4 + \frac{20}{3}m^3n + \frac{32}{3}mn^3 - \frac{16}{3}m^3$$
$$+\frac{10}{3}m^2n + \frac{4}{3}n^3 - \frac{17}{3}m^2 + \frac{8}{3}mn - \frac{19}{15}m + \frac{2}{3}n.$$

If $n \leqslant m$, then

$$ABC_2(J^{n,m}) = \sum_{i=1}^{2m}(s(i)+n)\sqrt{\frac{4mn+2m+2n-3}{i(2n+1)((2m-i)(2n+1)+2n-1)}} + \sum_{i=1}^{n}4i\sqrt{\frac{4mn+2m+2n-3}{(4mn+2m+2n-1-2i^2-i)(2i^2+i)}} + \sum_{i=n+1}^{m}4n \times \sqrt{\frac{4mn+2m+2n-3}{(2n^2+4nm+3n-4in+2m-2i-1)(4in-2n^2-n+2i)}} + \sum_{i=m+1}^{n+m}(4(n+m-i)+2) \times \sqrt{\frac{4mn+2m+2n-3}{(-2m^2-2n^2+4im+4in-n-m-2i^2+3i-1)(2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i)}},$$

$$GA_2(J^{n,m}) = \sum_{i=1}^{2m}2(s(i)+n)\frac{\sqrt{i(2n+1)((2m-i)(2n+1)+2n-1)}}{4mn+2m+2n-1} + \sum_{i=1}^{n}8i\frac{\sqrt{(4mn+2m+2n-1-2i^2-i)(2i^2+i)}}{4mn+2m+2n-1} + \sum_{i=n+1}^{m}8n \times \frac{\sqrt{(2n^2+4nm+3n-4in+2m-2i-1)(4in-2n^2-n+2i)}}{4mn+2m+2n-1} + \sum_{i=m+1}^{n+m}(8(n+m-i)+4) \times \frac{\sqrt{(-2m^2-2n^2+4im+4in-n-m-2i^2+3i-1)(2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i)}}{4mn+2m+2n-1},$$

$$Sz(J^{n,m},x) = \sum_{i=1}^{2m}(s(i)+n)x^{i(2n+1)((2m-i)(2n+1)+2n-1)} + \sum_{i=1}^{n}4ix^{(4mn+2m+2n-1-2i^2-i)(2i^2+i)} + \sum_{i=n+1}^{m}4nx^{(2n^2+4nm+3n-4in+2m-2i-1)(4in-2n^2-n+2i)} + \sum_{i=m+1}^{n+m}(4(n+m-i)+2) \times x^{(-2m^2-2n^2+4im+4in-n-m-2i^2+3i-1)(2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i)},$$

$$Sz_v^*(J^{n,m}) = 16m^3n^3+24m^2n^3+4m^2n^2-4n^4-6m^2n+4n^3-m^2 - 6mn+2n^2+\frac{56}{3}m^3n^2+\frac{8}{3}mn^4-\frac{16}{15}n^5+\frac{20}{3}m^3n + \frac{64}{3}mn^3+2m^3-\frac{10}{3}mn^2+\frac{m}{3}-\frac{14}{15}n.$$

Proof. Note that there are 2m rows in which 1-th, 3-th, ..., $2m-1$-th rows have exactly $n+1$ vertical edges and other rows have n vertical edges. We get $n_u^i(e) = i(2n+1)$ and $n_v^i(e) = (2m-i)(2n+1)+2n-1$. Furthermore, the number of vertical edges in i-th row is $s(i)+n$.

By the symmetry of $J^{n,m}$, the contributions from L and R to the indices are equal. The following proof is divided into two cases according to the relationship between n and m.

Case 1: $n \geqslant m$. Let Λ_i be the number of oblique edges from left to right in the i-th row. We get

$$\Lambda_i = \begin{cases} 2i, & 1 \leqslant i \leqslant m \\ 2m+1, & m < i \leqslant n \\ 2(n+m-i)+1, & n < i \leqslant m+n \end{cases},$$

$$n_u^i(e) = \begin{cases} 2i^2+i, & 1 \leqslant i \leqslant m \\ -2m^2-m+4im+2i-1, & m < i \leqslant n \\ -2m^2-2n^2+4im+4in-m-n+3i-2i^2-1, & n < i \leqslant m+n \end{cases},$$

$$n_v^i(e) = \begin{cases} 4mn+2m+2n-1-2i^2-i, & 1 \leqslant i \leqslant m \\ 2m^2+4nm+3m-4im+2n-2i, & m < i \leqslant n \\ 2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i, & n < i \leqslant m+n \end{cases}.$$

Case 2: $m \geqslant n$. Let Λ_i be the number of oblique edges from left to right in the i-th row. We get

$$\Lambda_i = \begin{cases} 2i, & 1 \leqslant i \leqslant n \\ 2n, & n < i \leqslant m \\ 2(n+m-i)+1, & m < i \leqslant m+n \end{cases},$$

$$n_u^i(e) = \begin{cases} 2i^2+i, & 1 \leqslant i \leqslant n \\ -2n^2-n+4in+2i, & n < i \leqslant m \\ -2m^2-2n^2+4im+4in-n-m-2i^2+3i-1, & m < i \leqslant m+n \end{cases},$$

$$n_v^i(e) = \begin{cases} 4mn+2m+2n-1-2i^2-i, & 1 \leqslant i \leqslant n \\ 2n^2+4nm+3n-4in+2m-2i-1, & n < i \leqslant m \\ 2m^2+4mn+2n^2-4im+3n+3m-4in+2i^2-3i, & m < i \leqslant m+n \end{cases}.$$

At last, our result is obtained in terms of above computation and the definition of indices. □

2.2. Wiener related indices of distance-regular molecular graph

In this part, we mainly discuss the distance-based indices of distance-regular graphs which is widely appeared in drug molecular structures. The proof of below results mainly follows the tricks presented by Deutsch and Rodriguez-Velazquez (2014). We skip the detail proof here.

Theorem 3. *Let G be a distance-regular molecular graph with intersection array* $\{b_0, b_1, \cdots, b_{D(G)-1}; c_1 = 1, c_2, \cdots, c_{D(G)}\}$. *Then,*

$$W_\lambda(G) = \frac{nb_0}{2} + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}i^\lambda,$$

$$WW(G) = \frac{nb_0}{2} + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}\frac{i+i^2}{2},$$

$$WW_\lambda(G) = \frac{nb_0}{2} + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}\frac{i^\lambda+i^{2\lambda}}{2},$$

$$\pi(G) = \prod_{i=2}^{D} i^{\frac{nb_0}{2}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}},$$

$$\prod(G) = \ln\left(\sqrt{2\prod_{i=2}^{D} i^{\frac{nb_0}{2}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}}}\right),$$

$$H(G) = \frac{nb_0}{2} + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}\frac{1}{i},$$

$$H(G,x) = \frac{nb_0}{2}x + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}\frac{1}{i}x^i$$

$$H_t(G) = \frac{nb_0}{2(1+t)} + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}\frac{1}{i+t},$$

$$RCW(G) = \frac{nb_0}{2D(G)} + \frac{nb_0}{2}\sum_{i=2}^{D}\frac{\prod_{j=1}^{i-1}b_j}{\prod_{j=2}^{i}c_j}\frac{1}{1+D(G)-i}.$$

Theorem 4. *Let G be a strongly regular graph with parameter* (n, k, θ, μ), *then*

$$W_\lambda(G) = \frac{nk}{2} + \frac{(k-\theta-1)nk}{2\mu}2^\lambda,$$

$$WW(G) = \frac{nk}{2} + \frac{3nk(k-\theta-1)}{2\mu},$$

$$WW_\lambda(G) = \frac{nk}{2} + \frac{2^\lambda+4^\lambda}{4}\frac{(k-\theta-1)nk}{\mu},$$

$$\pi(G) = 2^{\frac{(k-\theta-1)nk}{2\mu}},$$

$$\prod(G) = \ln\left(\sqrt{2^{\frac{(\mu+k-\theta-1)nk}{2\mu}}}\right),$$

$$H(G) = \frac{nk}{2} + \frac{(k-\theta-1)nk}{4\mu},$$

$$H(G,x) = \frac{nk}{2}x + \frac{(k-\theta-1)nk}{4\mu}x^2$$

$$H_t(G) = \frac{nk}{2(1+t)} + \frac{(k-\theta-1)nk}{2\mu(2+t)},$$

$$RCW(G) = \frac{nk}{4} + \frac{(k-\theta-1)nk}{2\mu}.$$

3. Conclusion

In our paper, according to the analysis of drug molecular structures, distance calculating and mathematical derivation, we mainly determine the distance-based indices of hexagonal jagged-rectangle (Xie et al., 2016; Peng et al., 2017). As a supplementary conclusion, we report the Wiener related indices of distance-regular molecular graphs. The theoretical formulations obtained in our work illustrate the promising prospects of their application for the pharmacy and chemical engineering.

Conflict of interests

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

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