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Some topological indices of pentagonal double chains

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Abstract. In graph theory, lattices are used when some structural part of the graph repeats itself finitely or infinitely many times. They have applications in complex analysis and geometry in mathematics, and also natural applications in chemical graph theory. As a lattice can be taken as a graph, it is also possible to use them in the study of large networks. Recently, some topological graph indices of pentagonal chains is studied and here, we study some topological graph indices of pentagonal double chains similarly to that work. We make use of the vertex and edge partitions of these graphs and calculate their indices by means of these partitions and combinatorial methods.

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1 Introduction

Pentagonal chains are important tools in network theory and some chemical applications. A topological graph index is a mathematical formula which is invariant for all isomorphic graphs. Topological graph indices have been defined and studied in the last eight decades. The most important applications of topological graph indices are in Chemical Graph Theory. Any molecule can be modeled by a graph constructed so that each vertex corresponds to an atom and each edge corresponds to a chemical bond between the corresponding atoms. By studying the obtained graph mathematically by means of a topological graph index, we can save time and money as we get information on some physico-chemical property of the graph without any use of laboratory experiments. There are many papers on topological graph

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indices of several molecular structures. In [4], the Zagreb indices which form the largest class of topological graph indices have been defined and studied. In [1], some Zagreb indices are calculated. In [6], one of the most well-known indices called Randić index was studied. In a recent paper, some topological indices of pentagonal chains are calculated [5]. An important and useful variant of pentagonal chains is pentagonal double chains. A pentagonal double chain consisting of k units of pentagons is denoted by $C_{5,k}^2$ and illustrated in Fig. 1:

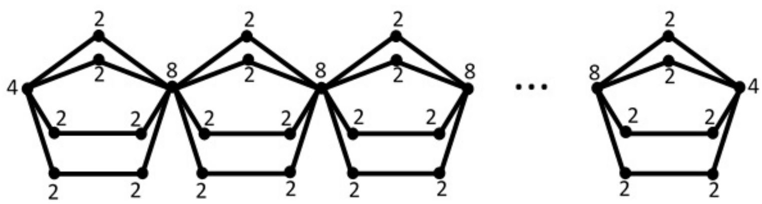

Figure 1 Pentagonal double chain $C_{5,k}^2$

It is easy to see that the degree sequence of $C_{5,k}^2$ consisting of the vertex degrees is

$$D(C_{5,k}^2) = \{2^{(6k)}, 4^{(2)}, 8^{(k-1)}\}.$$

Similarly, the edge partition table of $C_{5,k}^2$ is as in Table 1.

(d_i, d_j)	$\sharp\,(v_i, v_j)$
(2,2)	$2k$
(2,4)	8
(2,8)	$8k-8$

Table 1. The edge partition table of $C_{5,k}^2$

The omega invariant, [3], of the connected graph $C_{5,k}^2$ is

$$\Omega(C_{5,k}^2) = 2 \cdot 2 + 6 \cdot (k-1) = 6k - 2.$$

Hence the number of faces of $C_{5,k}^2$ would be $\Omega(C_{5,k}^2)/2 + 1 = 3k$, see [2, 3].

In the coming sections, we shall make our proofs by means of this degree sequence and edge partition table.

2 Main additive topological indices of $C_{5,k}^2$

Most of the topological graph indices are defined in terms of vertex degrees. Each such degree based index consists of some mathematical formula. This formula frequently contains a sum or product over the vertices or edges of the graph. In this section, we calculate some additive topological indices of the pentagonal double chain $C_{5,k}^2$. These indices are listed below:

The inverse sum index is defined by

$$ISI(G) = \sum_{uv\in E(G)} \frac{dudv}{du+dv}.$$

Next we recall the sigma index. It is an important irregularity measure defined by

$$\sigma(G) = \sum_{uv\in E(G)} (du-dv)^2.$$

The Bell index is defined as another irregularity measure by

$$B(G) = \sum_{u\in V(G)} (du-\tfrac{2m}{n})^2$$

where the order and size of G are denoted by n and m, respectively.

The first and second generalized Zagreb indices are defined as follows:

$$M_1^\alpha(G) = \sum_{u\in V(G)} du^\alpha$$

and

$$M_2^\alpha(G) = \sum_{uv\in E(G)} (dudv)^\alpha.$$

The total irregularity index is defined as another irregularity index by taking all the vertex degrees into account:

$$Irr_t(G) = \sum_{u\in V(G)} \left|du-\tfrac{2m}{n}\right|.$$

The harmonic index is defined by

$$H(G) = \sum_{uv\in E(G)} \frac{2}{du+dv}.$$

Generalized Harmonic index is similarly defined by taking arbitrary power α as follows:

$$H_\alpha^*(G) = \sum_{uv\in E(G)} \left(\frac{2}{du+dv}\right)^\alpha.$$

One of the famous degree based topological graph indices is the atom bond connectivity index which has molecular applications in terms of atoms and chemical bonds between them which are respectively modeled by vertices and edges of the graph modeling the molecule:

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{du+dv-2}{dudv}}.$$

The geometric-arithmetic index is defined as the ratio of these two means over all the edges of the graph by

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{dudv}}{du+dv}.$$

The augmented Zagreb index is defined by

$$AZ(G) = \sum_{uv\in E(G)} \left(\frac{dudv}{du+dv-2}\right)^3.$$

Another irregularity index is the Albertson index defined by the sum of absolute values of all the differences between degrees of pairs of vertices forming an edge:

$$Alb(G) = \sum_{uv\in E(G)} |du-dv|.$$

One of the most well-known topological graph indices is known as the Randić index which is defined as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{dudv}}.$$

By taking the α-th power in the Randić index, the generalized Randić index is defined:

$$R_\alpha(G) = \sum_{uv\in E(G)} \frac{1}{(dudv)^\alpha}.$$

The reciprocal Randić index is defined similarly to Randić index and has some advantages in chemical calculations:

$$RR(G) = \sum_{uv\in E(G)} \sqrt{dudv}$$

and finally, we recall the sum connectivity index as

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{du+dv}}.$$

We now present our result:

Theorem 2.1 *Some additive topological indices of $C^2_{5,k}$ are as follows:*

$$\begin{aligned}
ISI(C^2_{5,k}) &= \tfrac{2(111k-16)}{15};\\
\sigma(C^2_{5,k}) &= 32(9k-8);\\
B(C^2_{5,k}) &= \tfrac{8}{(7k+1)^2}\left[9k(21k^2-18k-5)-4\right];\\
M_1^\alpha(C^2_{5,k}) &= 2^\alpha\left[(2^{2\alpha}+6)k+2^\alpha(2-2^\alpha)\right];\\
M_2^\alpha(C^2_{5,k}) &= 2^{2\alpha+1}\left[2^{2\alpha+2}(k-1)+2^{\alpha+2}+k\right];\\
Irr_t(C^2_{5,k}) &= \tfrac{4}{7k+1}(9k^2+15k-10);\\
H(C^2_{5,k}) &= \tfrac{39k+16}{15};\\
H^*_\alpha(C^2_{5,k}) &= 2\left(k\cdot 2^{-\alpha}+4\cdot 3^{-\alpha}+4(k-1)\cdot 5^{-\alpha}\right);\\
ABC(C^2_{5,k}) &= 5\sqrt{2}k;\\
GA(C^2_{5,k}) &= \tfrac{2(63k-8)}{15};\\
AZ(C^2_{5,k}) &= 80k;\\
Alb(C^2_{5,k}) &= 16(3k-2);\\
R(C^2_{5,k}) &= 3k+2(\sqrt{2}-1);\\
RR(C^2_{5,k}) &= 36k+16(\sqrt{2}-2);\\
R_\alpha(C^2_{5,k}) &= 2^{1-2\alpha}\left[k+2^{2-2\alpha}+(k-1)^{2-4\alpha}\right];\\
\chi(C^2_{5,k}) &= \tfrac{3k(5+4\sqrt{10})+4(5\sqrt{6}-3\sqrt{10})}{15}.
\end{aligned}$$

Proof. The indices B, M_1 and Irr_t are calculated only by means of all vertex degrees. So we use the degree sequence of $C^2_{5,k}$ to prove the result for these three indices: We first calculate the Bell index. Using the degree sequence, we get

$$\begin{aligned}
B(C^2_{5,k}) &= 6k\left(2-\tfrac{20k}{7k+1}\right)^2+2\left(4-\tfrac{20k}{7k+1}\right)^2+(k-1)\left(8-\tfrac{20k}{7k+1}\right)^2\\
&= \tfrac{8}{(7k+1)^2}\left[9k(21k^2-18k-5)-4\right].
\end{aligned}$$

Here we use the fact that the order of $C^2_{5,k}$ is $n = 7k + 1$ and the size of $C^2_{5,k}$ is $m = 10k$. Next, using the degree sequence of $C^2_{5,k}$, we obtain

$$\begin{aligned} M_1^\alpha(C^2_{5,k}) &= 6k(2^\alpha) + 2(2^{2\alpha}) + (k-1)\cdot(2^{3\alpha}) \\ &= 2^\alpha\left[(6+2^{2\alpha})k + 2^\alpha(2-2^\alpha)\right]. \end{aligned}$$

Thirdly, we calculate the total irregularity index:

$$\begin{aligned} Irr_t(C^2_{5,k}) &= 6k\left|2 - \tfrac{20k}{7k+1}\right| + 2\left|4 - \tfrac{20k}{7k+1}\right| + (k-1)\left|8 - \tfrac{20k}{7k+1}\right| \\ &= \tfrac{4}{7k+1}(9k^2 + 15k - 10). \end{aligned}$$

For all other indices, we need to use the vertex pairs which are forming an edge in the graph $C^2_{5,k}$. So we use Table 1. We start with the ISI index.

$$\begin{aligned} ISI(C^2_{5,k}) &= 2k\cdot\tfrac{4}{4} + 8\cdot\tfrac{8}{6} + (8k-8)\cdot\tfrac{16}{10} \\ &= \tfrac{2(111k-16)}{15}. \end{aligned}$$

Next we continue with the sigma index. By Table 1, we have

$$\begin{aligned} \sigma(C^2_{5,k}) &= 2k(2-2)^2 + 8(2-4)^2 + (8k-8)(2-8)^2 \\ &= 32(9k-8). \end{aligned}$$

All other indices are calculated in a similar manner:

$$\begin{aligned} M_2^\alpha(C^2_{5,k}) &= 2k\cdot 4^\alpha + 8\cdot 8^\alpha + (8k-8)\cdot 16^\alpha \\ &= 2^{2\alpha+1}\left(k + 4\cdot 2^\alpha + (4k-4)\cdot 2^{2\alpha}\right). \end{aligned}$$

$$\begin{aligned} H(C^2_{5,k}) &= 2k\cdot\tfrac{2}{4} + 8\cdot\tfrac{2}{6} + 8(k-1)\cdot\tfrac{2}{10} \\ &= \tfrac{1}{15}(39k+16). \end{aligned}$$

$$\begin{aligned} H^*_\alpha(C^2_{5,k}) &= 2k(\tfrac{2}{4})^\alpha + 8(\tfrac{2}{6})^\alpha + 8(k-1)(\tfrac{2}{10})^\alpha \\ &= 2\left(k\cdot 2^{-\alpha} + 4\cdot 3^{-\alpha} + 4(k-1)5^{-\alpha}\right). \end{aligned}$$

$$\begin{aligned} ABC(C^2_{5,k}) &= 2k\cdot\sqrt{\tfrac{2}{4}} + 8\cdot\sqrt{\tfrac{4}{8}} + 8(k-1)\cdot\sqrt{\tfrac{8}{16}} \\ &= 5\sqrt{2}k. \end{aligned}$$

$$\begin{aligned} GA(C^2_{5,k}) &= 2k\cdot\tfrac{2\sqrt{4}}{4} + 8\cdot\tfrac{2\sqrt{8}}{6} + 8(k-1)\cdot\tfrac{2\sqrt{16}}{10} \\ &= \tfrac{2}{15}(63k-8). \end{aligned}$$

$$\begin{aligned} AZ(C^2_{5,k}) &= 2k(\tfrac{4}{2})^3 + 8(\tfrac{8}{4})^3 + 8(k-1)(\tfrac{16}{8})^3 \\ &= 80k. \end{aligned}$$

$$\begin{aligned} Alb(C^2_{5,k}) &= 2k|2-2| + 8|2-4| + 8(k-1)|2-8| \\ &= 16(3k-2). \end{aligned}$$

$$\begin{aligned} R(C^2_{5,k}) &= 2k\cdot\tfrac{1}{\sqrt{4}} + 8\cdot\tfrac{1}{\sqrt{8}} + 8(k-1)\cdot\tfrac{1}{\sqrt{16}} \\ &= 3k + 2(\sqrt{2}-1). \end{aligned}$$

$$\begin{aligned} R_\alpha(C^2_{5,k}) &= 2k\tfrac{1}{2^{2\alpha}} + 8\tfrac{1}{2^{3\alpha}} + 8(k-1)\tfrac{1}{2^{4\alpha}} \\ &= 2^{1-2\alpha}\left[k + 2^{2-\alpha} + (k-1)2^{2-4\alpha}\right]. \end{aligned}$$

$$\begin{aligned} RR(C^2_{5,k}) &= 2k\sqrt{4} + 8\sqrt{8} + 8(k-1)\sqrt{16} \\ &= 36k + 16(\sqrt{2}-2). \end{aligned}$$

$$\begin{aligned} \chi(C^2_{5,k}) &= 2k\cdot\tfrac{1}{\sqrt{4}} + 8\cdot\tfrac{1}{\sqrt{6}} + 8(k-1)\cdot\tfrac{1}{\sqrt{10}} \\ &= \tfrac{1}{15}\left[3k(5+4\sqrt{10}) + 4(5\sqrt{6} - 3\sqrt{10})\right]. \end{aligned}$$

3 Multiplicative topological indices of $C^2_{5,k}$

In this section, we calculate some multiplicative topological indices of pentagonal double chain $C^2_{5,k}$. These multiplicative versions of the indices are obtained usually by replacing the sum sign with a product sign. We consider the following ones:

$$\Pi_1(G) \quad = \prod_{uv\in E(G)}(du+dv)$$

and

$$\Pi_2(G) \quad = \prod_{uv\in E(G)} dudv$$

are called the multiplicative first and second Zagreb indices. Similarly the multiplicative forgotten index, sometimes named as the multiplicative third Zagreb index is defined by

$$\Pi_3(G) \quad = \prod_{uv\in E(G)}(du^2+dv^2).$$

Recall that the sum of all vertex degrees is equal to twice the size of the graph. The most easiest and fundamental multiplicative index is the Narumi-Katayama index defined similarly as the product of all vertex degrees:

$$NK(G) \quad = \prod_{u\in V(G)} du.$$

Geometric-arithmetic multiplicative index is defined as

$$GA\Pi(G) \quad = \prod_{uv\in E(G)} \frac{2\sqrt{dudv}}{du+dv}.$$

The first and second multiplicative hyper Zagreb indices are recently defined another variant of Zagreb indices as

$$H\Pi_1(G) \quad = \prod_{uv\in E(G)}(du+dv)^2$$

and

$$H\Pi_2(G) \quad = \prod_{uv\in E(G)}(dudv)^2.$$

General sum connectivity index is given by

$$H_\alpha(G) \quad = \prod_{uv\in E(G)}(du+dv)^\alpha.$$

Multiplicative Randić index is defined by

$$R\Pi(G) \quad = \prod_{uv\in E(G)} \frac{1}{\sqrt{dudv}}.$$

The multiplicative sum connectivity index is defined by

$$\chi\Pi(G) \quad = \prod_{uv\in E(G)} \frac{1}{\sqrt{du+dv}}$$

and finally, the multiplicative atom bond connectivity index is defined by

$$ABC\Pi(G) \quad = \prod_{uv\in E(G)} \sqrt{\frac{du+dv-2}{dudv}}.$$

We then have the following result:

Theorem 3.1 *Some multiplicative topological indices of pentagonal double chain $C^2_{5,k}$ are as follows:*

$$\Pi_1(C^2_{5,k}) \quad = 2^{12k}\cdot 3^8\cdot 5^{8(k-1)};$$

$$\Pi_2(C^2_{5,k}) \quad = 2^{4(9k-2)};$$

$$\begin{aligned}
\Pi_3(C^2_{5,k}) &= 2^{22k} \cdot 5^8 \cdot 17^{8(k-1)};\\
NK(C^2_{5,k}) &= 2^{9k+1};\\
GA\Pi(C^2_{5,k}) &= 2^{8k+4} \cdot 3^{-8} \cdot 5^{8-8k};\\
H\Pi_1(C^2_{5,k}) &= 2^{24k} \cdot 3^{16} \cdot 5^{16(k-1)};\\
H\Pi_2(C^2_{5,k}) &= 2^{4(9k+4)};\\
H_\alpha(C^2_{5,k}) &= 2^{12k\alpha} \cdot 3^{8\alpha} \cdot 5^{8\alpha(k-1)};\\
R\Pi(C^2_{5,k}) &= 2^{2(2-9k)};\\
\chi\Pi(C^2_{5,k}) &= 2^{-6k} \cdot 3^{-4} \cdot 5^{4(1-k)};\\
ABC\Pi(C^2_{5,k}) &= 2^{-5k}.
\end{aligned}$$

Proof. First we start with the first multiplicative Zagreb index of $C^2_{5,k}$. Using the degree sequence, we get

$$\begin{aligned}
\Pi_1(C^2_{5,k}) &= (2+2)^{2k} \cdot (2+4)^8 \cdot (2+8)^{8k-8}\\
&= 2^{12k} \cdot 3^8 \cdot 5^{8(k-1)}.
\end{aligned}$$

Next we calculate the second multiplicative Zagreb index of $C^2_{5,k}$ by using Table 1:

$$\begin{aligned}
\Pi_2(C^2_{5,k}) &= (2^2)^{2k} \cdot (2^3)^8 \cdot (2^4)^{8(k-1)}\\
&= 2^{4(9k-2)}.
\end{aligned}$$

The remaining of the results on multiplicative indices can be proven similarly as below:

$$\begin{aligned}
\Pi_3(C^2_{5,k}) &= (2^2+2^2)^{2k} \cdot (2^2+4^2)^8 \cdot (2^2+8^2)^{8(k-1)}\\
&= 2^{22k} \cdot 5^8 \cdot 17^{8k-8}.
\end{aligned}$$

$$\begin{aligned}
GA\Pi(C^2_{5,k}) &= \left(\frac{2\sqrt{4}}{4}\right)^{2k} \cdot \left(\frac{2\sqrt{8}}{6}\right)^{8} \cdot \left(\frac{2\sqrt{16}}{10}\right)^{8k-8}\\
&= 2^{8k+4} \cdot 3^{-8} \cdot 5^{8-8k}.
\end{aligned}$$

$$\begin{aligned}
H\Pi_1(C^2_{5,k}) &= (2^2)^{4k} \cdot (2\cdot 3)^{16} \cdot (2\cdot 5)^{16k-16}\\
&= 2^{24k} \cdot 3^{16} \cdot 5^{16(k-1)}.
\end{aligned}$$

$$\begin{aligned}
H\Pi_2(C^2_{5,k}) &= 2^{4k} \cdot 2^{24} \cdot 2^{32k-8}\\
&= 2^{4(9k+4)}.
\end{aligned}$$

$$\begin{aligned}
H_\alpha(C^2_{5,k}) &= \left((2^2)^\alpha\right)^{2k} \cdot ((2\cdot 3)^\alpha)^8 \cdot ((2\cdot 5)^\alpha)^{8k-8}\\
&= 2^{12k\alpha} \cdot 3^{8\alpha} \cdot 5^{8\alpha(k-1)}.
\end{aligned}$$

$$\begin{aligned}
R\Pi(C^2_{5,k}) &= \left(\frac{1}{\sqrt{4}}\right)^{2k} \cdot \left(\frac{1}{\sqrt{8}}\right)^{8} \cdot \left(\frac{1}{\sqrt{16}}\right)^{8k-8}\\
&= 2^{2(2-9k)}.
\end{aligned}$$

$$\begin{aligned}
\chi\Pi(C^2_{5,k}) &= \left(\frac{1}{\sqrt{4}}\right)^{2k} \cdot \left(\frac{1}{\sqrt{6}}\right)^{8} \cdot \left(\frac{1}{\sqrt{10}}\right)^{8k-8}\\
&= 2^{-6k} \cdot 3^{-4} \cdot 5^{4(1-k)}.
\end{aligned}$$

$$\begin{aligned}
ABC\Pi(C^2_{5,k}) &= \left(\sqrt{\frac{2}{4}}\right)^{2k} \cdot \left(\sqrt{\frac{4}{8}}\right)^{8} \cdot \left(\sqrt{\frac{8}{16}}\right)^{8k-8}\\
&= 2^{-5k}.
\end{aligned}$$

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