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Some Topological Indices of Pentagonal Quadruple Chains

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Abstract:

Some topological graph indices of pentagonal chains, pentagonal double chains, and pentagonal triple chains have been studied previously. In this study, we examine the topological graph indices of pentagonal quadruple chains, following a similar approach. We utilize the vertex and edge partitions of these graphs and calculate their indices using these partitions and combinatorial methods. Most of the indices computed here are based on the degrees of adjacent vertices.

Keywords: Pentagonal quadruple chain, Zagreb index, vertex degrees, graph index.

2010 MSC: 05C07, 05C30, 05C38

1 Introduction

In graph theory, lattices are used when a part of the graph repeats itself either finitely or infinitely many times. They have applications in complex analysis, topology, and geometry in mathematics, as well as in chemical graph theory. Since a lattice can be considered a graph, it is also possible to use them in the study of large networks.

Pentagonal chains are important tools in network theory and have various chemical applications. A topological graph index is a mathematical formula that remains invariant for all isomorphic graphs. Topological graph indices have been defined and studied over the last eight decades. The most significant applications of topological graph indices are in Chemical Graph Theory. Any molecule can be modeled as a graph where each vertex represents an atom, and each edge represents a chemical bond between the corresponding atoms. By studying the resulting graph mathematically through a topological graph index, we can save time and money by obtaining information about certain physico-chemical properties of the graph without the need for laboratory experiments. Many papers have been published on the topological graph indices of various molecular structures. In [6], 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 [9], one of the most well-known indices called Randi´c index was studied.In a recent paper, some topological indices of pentagonal chains are calculated [8]. Similarly, several topological indices of pentagonal double chains are studied in [7]. An important and useful variant of pentagonal chains is pentagonal triple chains. A pentagonal quadruple chain consisting of k units of pentagons is denoted by $C^4_{5,k}$ and illustrated in Figure 1:

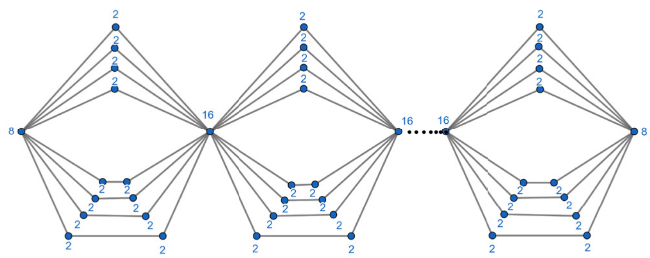

Figure 1: Pentagonal quadruple chain $C^4_{5,k}$

It is easy to see that the degree sequence of $C^4_{5,k}$ consisting of the vertex degrees is

$$D\left(C^4_{5,k}\right) = \left\{2^{(12k)}, 8^2, 16^{(k-1)}\right\}$$

Similarly, the edge partition table of $C^4_{5,k}$ is given in Table 1.

(d_i, d_j)	Number of vertices(v_i, v_j)
(2,2)	4k
(2,8)	16
(2,16)	16k-16

Table 1. The edge partition table of $C^4_{5,k}$

The omega invariant of the connected graph $C^4_{5,k}$ is

$$\Omega\left(C^4_{5,k}\right) = 6.2 + 14(k-1) = 14k - 2$$

Hence the number of faces of $C^4_{5,k}$ would be $\Omega\left(C^4_{5,k}\right)/2 + 1 = 7k$, see [2, 3]. We shall make our proofs by means of degree sequence and edge partition table.

2 Additive topological indices of $C^4_{5,k}$

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 quadruple chain $C^4_{5,k}$. These indices are listed below:

The First and Second Zagreb indices are among the oldest and most famous topological indices. These 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 inverse sum index is defined by

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

The Sigma index is an important irregularity measure defined by

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

The Bell index is defined as irregularity measure defined by

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

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

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

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

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 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 (ABC) is defined by:

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

The Geometric-arithmetic index is defined as:

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

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 is defined as:

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

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 results:

Theorem 2.1. *Some additive topological indices of pentagonal quadruple chain for $C^4_{5,k}$ are as follows*

$M_1(C^4_{5,k}) = 2^{\alpha}[12k + 2^{(2\alpha+1)} + 2^{7\alpha}(k-1)]$

$M_2(C^4_{5,k}) = 4^{(\alpha+1)}[k + 4^{(\alpha+1)}8^{\alpha}(4k-4)]$

$ISI(C^4_{5,k}) = \frac{8}{45}[29 + 160k]$

$\sigma(C^4_{5,k}) = 64[49k - 40]$

$B(C^4_{5,k})) = \frac{8}{(13k+1)^2}[735k^3 - 397k^2 - 42k - 2]$

$Irr_t(C^4_{5,k})) = 0$

$H(C^4_{5,k})) = \frac{170k+64}{45}$

$H^*_{\alpha}(C^4_{5,k})) = 4[2^{-\alpha} + 4.5^{-\alpha} + 4.9^{-\alpha}(k-1)]$

$ABC(C^4_{5,k})) = \frac{1}{\sqrt{2}}(20k)$

$GA(C^4_{5,k})) = \frac{4}{45}[45k + 36\sqrt{10} + 80\sqrt{2}(k-1)]$

$AZ(C^4_{5,k}) = 360k$

$Alb(C^4_{5,k}) = 32[7k - 4]$

$R(C^4_{5,k}) = 2[k + 2 + \sqrt{2}(k-1)]$

$R_{\alpha}(C^4_{5,k}) = 4^{(1-\alpha)}k + 16^{(1-\alpha)} + 16.32^{-\alpha}(k-1)$

$RR(C^4_{5,k}) = 8[k + 8 + 8\sqrt{2}(k-1)]$

$\chi(C^4_{5,k}) = 2[k + \frac{8}{\sqrt{10}} + \frac{8}{\sqrt{18}}(k-1)]$

Proof: *Let $C^4_{5,k}$ be a Pentagonal quadruple chain of order $n = 13k+1$ and the size $m = 20k$. Now we calculate the additive topological indices of $C^4_{5,k}$ by using existing additive topological indices are mentioned above and using the table 1.*

3 Multiplicative topological indices of $C_{5,k}^4$

In this section, we calculate some multiplicative topological indices of pentagonal quadruple chain $C_{5,k}^4$. *These multiplicative versions of the indices are obtained usually by replacing the sum sign with a product sign. We consider the following ones:*

$$\prod_1(G) = \prod_{uv\in E(G)}(du + dv)$$

And

$$\prod_2(G) = \prod_{uv\in E(G)}(dudv)$$

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:

$$\prod_3(G) = \prod_{uv\in E(G)}(du^2 + dv^2)$$

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:

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

Geometric-arithmetic multiplicative index is defined as:

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

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

$$H\prod_1(G) = \prod_{uv\in E(G)}(du + dv)^2$$

and

$H\prod_2(G) = \prod_{uv\in E(G)}(dudv)^2$

General sum connectivity index is given by

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

Multiplicative Randić index is defined by

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

The multiplicative sum connectivity index is defined by

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

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

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

We then have the following result:

Theorem 3.1. *Some multiplicative topological indices of pentagonal quadruple chain for* $C^4_{5,k}$ *are as follows*

$\prod_1(C^{)}_{5,k} = 2^{(24k+16)}.5^{16}.3^{(32k-32)}$

$\prod_2(C^4_{5,k}) = 2^{(88k-16)}$

$\prod_3(C^4_{5,k}) = 2^{44k}.17^{16}.65^{(16k-16)}$

$NK(C^4_{5,k}) = 2^{(16k+2)}$

$GA\prod(C^4_{5,k}) = 2^{(40k-32)}.5^8.3^{(32-32k)}$

$H\prod_1(C^4_{5,k}) = 2^{48k}.5^{32}.3^{(64k-64)}$

$H\prod_\alpha(C^4_{5,k}) = 2^{24\alpha k}.5^{16\alpha}.3^{\alpha(32k-32)}$

$R\prod(C_{5,k}^{4}) = 2^{-(84k+64)}$

$\chi\prod(C_{5,k}^{4}) = 2^{-12k}.5^{-8}.3^{(16-16k)}$

$ABC\prod(C_{5,k}^{4}) = 2^{-10k}$

Proof: *Let* $C_{5,k}^{4}$ *be a Pentagonal quadruple chain of order* $n = 13k + 1$ *and the size* $m = 20k$. *Now we calculate the multiplicative topological indices of* $C_{5,k}^{4}$ *by using existing multiplicative topological indices are mentioned above and using the table 1.*

CONCLUSION

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