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TOPOLOGICAL INDICES OF PENTAGONAL CHAINS

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ABSTRACT. Lattices are useful in many areas of science when some structure repeats itself finitely or infinitely. They have applications in complex analysis and geometry in mathematics. Naturally, a lattice can also be thought as a graph and in most cases, it is useful in the study of large networks. Here, we study some additive topological graph indices of some interesting lattice structures called as pentagonal chains obtained by k pentagons and denoted by $C_{5,k}^1$. The indices are selected to their application potentials. We make use of the vertex and edge partitions of these chain graphs and calculate their indices by means of these partitions and combinatorial methods. In applications to chemical graph theory and network science, one can choose the convenient value k of the pentagons to get the most convenient result to their aim.

1. INTRODUCTION

Topological graph indices are mathematical formulae which help to determine some properties of graphs. As many social and scientific problems can be modeled by graphs, such information could be very valuable in most cases. For example, we can model a molecule by a graph by modeling atoms by vertices and chemical bonds between the atoms by the edges connecting the corresponding vertices. This way, we can use topological graph indices to find a mathematical value from the graph which can be interpreted to obtain some chemical property of the corresponding molecule without needing money and time consuming laboratory experiments. Topological graph indices have been introduced and studied in the last eight decades. In [2], the first and second Zagreb indices are defined and some chemical applications were presented. In [1], some calculations related to several Zagreb indices are done. In [3], one of the most popular graph indices called the Randić index were introduced and studied.

A pentagonal chain is obtained by joining k pentagons in a chain so that one vertex of each pentagon is identified with a vertex of next pentagon as in Fig. 1:



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

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We denote a pentagonal chain having k pentagons by $C_{5,k}^1$. Clearly there are two types of vertices, those of degree 2 and those of degree 4. The partition table for the vertices is



tition table of $C_{5,k}^1$

where \sharp is used for the statement "the number of". There are two types of edges one type having two end vertices of degree 2 and other type having one end vertex of degree 2 and the other of degree 4. Hence the partition table for edges of $C_{5,k}^1$ is as follows:

(d_i, d_j)	$\ddagger (v_i, v_j)$
(2,2)	k+4
(2,4)	4(k-1)
TABLE 2. The edge	
partition table of C_{5k}^1	

2. Main additive results

In this section, we study some additive topological graph indices of $C_{5,k}^1$. The indices we are interested in here are listed below:

The first and second Zagreb indices are defined in [2] as follows:

$$M_1(G) = \sum_{u \in V(G)} du^2$$

and

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

The forgotten index is introduced by

$$F(G) = \sum_{u \in V(G)} du^3$$

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 redefined first, second and third Zagreb indices of a graph G are respectively defined by

$$ReZG_1(G) = \sum_{u,v \in E(G)} \left[\frac{d(u) + d(v)}{d(u) \cdot d(v)} \right],$$

$$ReZG_2(G) = \sum_{u,v \in E(G)} \left[\frac{d(u) \cdot d(v)}{d(u) + d(v)} \right]$$

and

$$ReZG_3(G) = \sum_{u,v \in E(G)} [d(u) \cdot d(v)] [d(u) + d(v)]$$

For all real values of r and s, the second Gourava index is defined by

$$M_{r,s}(G) = \sum_{u,v \in E(G)} [d(u)^r \cdot d(v)^s + d(u)^s \cdot d(v)^r].$$

The reformulated first and third Zagreb indices of a graph G are respectively defined by

$$RM_1(G) = \sum_{u,v \in E(G)} [d(uv)^2] \\ = \sum_{u,v \in E(G)} [d(u) + d(v) - 2]^2$$

and

$$RM_3(G) = \sum_{u,v \in E(G)} [d(uv)^3].$$

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

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

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

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

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

Another well-known 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:

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

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

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

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

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

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 main result of the section:

Theorem 2.1. Some additive topological graph indices of $C_{5,k}^1$ are

$$\begin{split} M_1(C_{5,k}^1) &= 4(7k-2); \\ M_2(C_{5,k}^1) &= 4(9k-4); \\ F(C_{5,k}^1) &= 8(11k-10); \\ M_1^{\alpha}(C_{5,k}^1) &= 2^{\alpha}k(3+2^{\alpha})+2^{\alpha+1}(1-2^{\alpha-1}); \\ M_2^{\alpha}(C_{5,k}^1) &= 2^{2\alpha}(k(2^{\alpha+2}+1)+4-2^{\alpha+2}); \\ ReZG_1(C_{5,k}^1) &= 4k+1; \\ ReZG_2(C_{5,k}^1) &= 16(13k-8); \\ M_{r,s}(C_{5,k}^1) &= 2^{r+s+1}\left(k(1+2^{r+1}+2^{s+1})+2(1-2^r-2^s)\right); \\ RM_1(C_{5,k}^1) &= 4(17k-12); \\ RM_3(C_{5,k}^1) &= 8(33k-28). \\ ISI(C_{5,k}^1) &= 16(k-1); \\ B(C_{5,k}^1) &= 16(k-1); \\ B(C_{5,k}^1) &= 16(k-1); \\ H_{\alpha}^*(C_{5,k}^1) &= (k+4)2^{-\alpha}+4(k-1)3^{-\alpha}; \\ ABC(C_{5,k}^1) &= \frac{(3+8\sqrt{2})k+12-8\sqrt{2}}{3}; \\ AZ(C_{5,k}^1) &= 40k; \\ R(C_{5,k}^1) &= \frac{1+2\sqrt{2}}{2}k+2-\sqrt{2}; \\ RR(C_{5,k}^1) &= 2\left[(1+4\sqrt{2})k+4(1-\sqrt{2})\right]; \end{split}$$

$$\chi(C_{5,k}^1) = \frac{3+4\sqrt{6}}{+}k + \frac{2(3-\sqrt{6})}{3}.$$

Proof. We start with the first Zagreb index using Table 1 giving the vertex partition of $C_{5,k}^1$. We have

$$M_1(C_{5,k}^1) = \sum_{v \in V(G)} dv^2$$

= 2²(3k + 2) + 4²(k - 1)
= 4(7k - 2).

Secondly, by Table 2, we have

$$M_2(C_{5,k}^1) = \sum_{uv \in E(G)} du dv$$

= 2 \cdot 2 \cdot (k+4) + 2 \cdot 4 \cdot (4k-4)
= 4(9k-4).

Next, we have the forgotten index of $C^1_{5,k}$ by means of Table 1:

$$F(C_{5,k}^1) = 2^3(3k+2) + 4^3(k-1) = 8(11k-10)$$

For other indices, we do similar calculations as below to obtain the result:

$$\begin{split} M_1^{\alpha}(C_{5,k}^1) &= 2^{\alpha}(3k+2) + 4^{\alpha}(k-1) \\ &= 2^{\alpha}k(3+2^{\alpha}) + 2^{\alpha+1}(1-2^{\alpha-1}) \\ M_2^{\alpha}(C_{5,k}^1) &= (2\cdot2)^{\alpha}(k+4) + (2\cdot4)^{\alpha}(4k-4) \\ &= 2^{2\alpha}\left[k+2^{\alpha+2}k+4-2^{\alpha+2}\right] \\ H_{\alpha}(C_{5,k}^1) &= (2+2)^{\alpha}(k+4) + (2+4)^{\alpha}(4k-4) \\ &= 2^{\alpha}\left(k(2^{\alpha}+4\cdot3^{\alpha})+4(2^{\alpha}-3^{\alpha})\right) \\ ReZG_1(C_{5,k}^1) &= \frac{2+2}{2\cdot2}(k+4) + \frac{2+4}{2\cdot4}4(k-1) \\ &= 4k+1 \\ ReZG_2(C_{5,k}^1) &= \frac{2\cdot2}{2+2}(k+4) + \frac{2\cdot4}{2+4}4(k-1) \\ &= \frac{19}{4}k + \frac{4}{3} \\ ReZG_3(C_{5,k}^1) &= 2\cdot2(2+2)(k+4) + 2\cdot4(2+4)4(k-1) \\ &= 16(13k-8) \\ M_{r,s}(C_{5,k}^1) &= (2^{r}2^s+2^{r}2^s)(k+4) + (2^{r}4^s+4^{r}2^s)(4k-4) \\ &= 2^{r+s+1}\left(k(1+2^{r+1}+2^{s+1})+2(1-2^{r}-2^{s})\right) \\ RM_1(C_{5,k}^1) &= (2+2-2)^{2}(k+4) + (2+4-2)^{2}(4k-4) \\ &= 4(17k-12) \\ RM_3(C_{5,k}^1) &= (2+2-2)^{3}(k+4) + (2+4-2)^{3}(4k-4) \\ &= 8(33k-28) \\ ISI(C_{5,k}^1) &= (k+4)\frac{4}{4}+4(k-1)\frac{8}{6} \\ &= \frac{1}{3}(19k-4) \end{split}$$

$$\begin{split} \sigma(C_{5,k}^{1}) &= 4(k-1)(2-4)^{2} \\ &= 16(k-1) \\ B(C_{5,k}^{1}) &= (3k+2)(2-\frac{10k}{4k+1})^{2} + (k-1)(4-\frac{10k}{4k+1})^{2} \\ &= \frac{4(3k+2)(k-1)}{4k+1} \\ H_{\alpha}^{*}(C_{5,k}^{1}) &= (k+4)(\frac{2}{4})^{\alpha} + 4(k+1)(\frac{2}{6})^{\alpha} \\ &= (k+4)2^{-\alpha} + 4(k-1)3^{-\alpha} \\ R_{\alpha}(C_{5,k}^{1}) &= (k+4)\frac{1}{2^{2\alpha}} + 4(k-1)\frac{1}{2^{3\alpha}} \\ &= 2^{-2\alpha}(k+4+4(k-1)2^{-\alpha}) \\ H(C_{5,k}^{1}) &= (k+4)\frac{2}{4} + 4(k-1)\frac{2}{6} \\ &= \frac{1}{6}(11k+4) \\ ABC(C_{5,k}^{1}) &= (k+4)\frac{2\sqrt{4}}{4} + 4(k-1)\frac{2\sqrt{8}}{6} \\ &= \frac{\sqrt{2}}{2} \cdot 5n \\ GA(C_{5,k}^{1}) &= (k+4)\frac{2\sqrt{4}}{4} + 4(k-1)\frac{2\sqrt{8}}{6} \\ &= \frac{1}{3}(12-8\sqrt{2}+k(3+8\sqrt{2})) \\ AZ(C_{5,k}^{1}) &= (k+4)(\frac{4}{2})^{3} + 4(k-1)(\frac{8}{4})^{3} \\ &= 40k \\ Alb(C_{5,k}^{1}) &= (k+4)(2-2|+4(k-1)|2-4| \\ &= 8(k-1) \\ R(C_{5,k}^{1}) &= (k+4)\frac{1}{\sqrt{4}} + 4(k-1)\frac{1}{\sqrt{8}} \\ &= \frac{1}{2}(2(2-\sqrt{2})+(1+2\sqrt{2})k) \\ RR(C_{5,k}^{1}) &= (k+4)\frac{1}{\sqrt{4}} + 4(k-1)\sqrt{8} \\ &= 2\left[4(1-\sqrt{2})+k(1+4\sqrt{2})\right] \\ \chi(C_{5,k}^{1}) &= (k+4)\frac{1}{\sqrt{4}} + 4(k-1)\frac{1}{\sqrt{6}} \\ &= \frac{3+4\sqrt{6}}{6}k + \frac{6-2\sqrt{6}}{3}. \end{split}$$

3. Main multiplicative results

Next, we calculate some multiplicative topological indices of the pentagonal chain $C^1_{5,k}.$ We have our main result:

Theorem 3.1. Some multiplicative topological indices of the pentagonal chain $C_{5,k}^1$ are as follows:

$$\Pi_1(C_{5,k}^1) = 2^{10k};$$

$$\Pi_2(C_{5,k}^1) = 2^{2(7k-2)};$$

$$\Pi_3(C_{5,k}^1) = 2^{15k};$$

$$NK(C_{5,k}^1) = 2^{5k};$$

$$\Pi_1^*(C_{5,k}^1) = 2^{2(3k+2)} \cdot 3^{4(k-1)};$$

$$\begin{aligned} GA\Pi(C_{5,k}^1) &= 2^{6(k-1)} | cdot 3^{2(1-k)}; \\ H\Pi_1(C_{5,k}^1) &= \left(2^{3k+2} \cdot 3^{2k-2}\right)^4; \\ H\Pi_2(C_{5,k}^1) &= (2^{7k-2})^4; \\ H_\alpha(C_{5,k}^1) &= (2^{3k+2} \cdot 3^2k - 2)^{2\alpha}; \\ R\Pi(C_{5,k}^1) &= 2^{2-7k}; \\ \chi\Pi(C_{5,k}^1) &= 2^{-3k-2} \cdot 3^{2(1-k)}; \\ ABC\Pi(C_{5,k}^1) &= \left(\frac{\sqrt{2}}{2}\right)^{5k}. \end{aligned}$$

Proof. By Table 1 and Table 2 for $C_{5,k}^1$, we have

$$\begin{split} \Pi_1(C_{5,k}^1) &= (2^2)^{3k+2} \cdot (2^4)^{k-1} \\ &= 2^{10k}; \\ \Pi_2(C_{5,k}^1) &= (2^2)^{k+4} \cdot (2^3)^{4k-4} \\ &= 2^{2(7k-2)}; \\ \Pi_3(C_{5,k}^1) &= (2^3)^{3k+2} \cdot (2^6)^{k-1} \\ &= 2^{15k}; \\ NK(C_{5,k}^1) &= 2^{3k+2} \cdot 2^{2k-2} \\ &= 2^{5k}; \\ \Pi_1^*(C_{5,k}^1) &= (2^2)^{k+4} \cdot (2 \cdot 3)^{4k-4} \\ &= 2^{2(3k+2)} \cdot 3^{4(k-1)}; \\ GA\Pi(C_{5,k}^1) &= (\frac{2\sqrt{4}}{4})^{k+4} \cdot (\frac{2\sqrt{8}}{6})^{4k-4} \\ &= 2^{6(k-1)} \cdot 3^{4(1-k)}, \\ H\Pi_1(C_{5,k}^1) &= ((2^2)^2)^{k+4} \cdot ((2 \cdot 3)^2)^{4k-4} \\ &= (2^{3k+2} \cdot 3^{2k-2})^4; \\ H\Pi_2(C_{5,k}^1) &= ((2^2)^2)^{k+4} \cdot ((2 \cdot 3)^2)^{4k-4} \\ &= (2^{7k-2})^4; \\ H_{\alpha}(C_{5,k}^1) &= ((2^2)^{\alpha})^{k+4} \cdot ((2 \cdot 3)^{\alpha})^{4k-4} \\ &= (2^{3k+2} \cdot 3^{2k-2})^{2\alpha}; \\ R\Pi(C_{5,k}^1) &= (\frac{1}{\sqrt{4}})^{k+4} \cdot (\frac{1}{\sqrt{8}})^{4k-4} \\ &= 2^{2-7k}; \\ \chi\Pi(C_{5,k}^1) &= (\frac{1}{\sqrt{4}})^{k+4} \cdot (\frac{1}{\sqrt{6}})^{4(k-1)} \\ &= 2^{(-3k-2)} \cdot 3^{2(1-k)}; \end{split}$$

and finally

$$ABC\Pi(C_{5,k}^{1}) = \left(\sqrt{\frac{4-2}{4}}\right)^{k+4} \cdot \left(\sqrt{\frac{6-2}{8}}\right)^{4(k-1)} = \left(\frac{\sqrt{2}}{2}\right)^{5k}.$$

References

- K. C. Das, N. Akgunes, M. Togan, A. Yurttas, I. N. Cangul and A. S. Cevik, On the first Zagreb index and multiplicative Zagreb coindices of graphs, Analele Stiintifice ale Universitatii Ovidius Constanta 24 (2016), 153–176.
- [2] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons, Chemical Physics Letters 17 (1972), 535–538.
- [3] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975), 6609– 6615.

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