International Journal of Scientific Research in Computer Science, Engineering and Information Technology
ISSN : 2456-3307 (www.ijsrcseit.com)
doi : https://doi.org/10.32628/IJSRCSEIT

Computation of CTI of Certain Graphs

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Article Info
Publication Issue :
Volume 8, Issue 6
November-December-2022
Page Number : 67-71
Article History
Accepted: 01 Nov 2022
Published: 05 Nov 2022

ABSTRACT
Topological indices are real numbers that remain unchanged under graph isomorphism. In the literature, chromatic analogues to topological indices proposed in 2017. Most recently, studies of chromatic Zagreb indices have obtained. In this study, the idea of chromatic topological indices and irregularity indices of cycle graphs, complete graphs and corresponding line graphs were discussed.
Keywords: Chromatic Zagreb Indices, Complete Graph, Cycle Graph, Irregularity Index and Line graph.

I. INTRODUCTION

Chemical graph theory has a wide range of applications in today's world, particularly in the pharmaceutical industry. It is primarily concerned with mathematical modeling of chemical phenomena and acquiring useful insights into chemical behavior. One of the essential conceptions of molecular descriptors in chemical graph theory is a topological index of a graph G, which is a real number retained under isomorphism. The chromatic topological indices of a graph G was recently coined in [6] to identify a novel coloring version of these indices that encompasses both proper coloring and topological indices. The vertex degrees are swapped with minimal coloring in this case, however the additional coloring conditions of proper coloring are maintained. The graphs in this work are finite, non-trivial, undirected, linked and free of loops and multiple edges. See [3,10,11,12] for notation and terminology not expressly described here.

Analogous to the definitions of Zagreb indices of graphs (see [2,4,5,9]), the notions of different chromatic Zagreb indices have been introduced in [6] as follows:

Definition1.1

[6] Let $C=\{c_1,c_2,\ldots,c_l\}$ be the proper coloring of any graph G .Since $|C|=l$, G has $l!$ minimum parameter colorings. Denote these colorings as $\phi_t(G), 1\le t\le l!$.

Let $\phi(v_i)=c_s,\ 1\le i\le n, 1\le s\le l$ .Then for $1\le t\le l!$,

- The first chromatic Zagreb index of G is defined as:

$$M_1^{\phi_t}(G)=\sum_{i=1}^{n} c(v_i)^2$$
$$=\sum_{j=1}^{l}\theta(c_j)\cdot j^2,\ c_j\in C$$

- The second chromatic Zagreb index of G is defined as:

$$M_2^{\phi_t}(G)=\sum_{i=1}^{n-1}\sum_{j=2}^{n}(c(v_i)\cdot c(v_j)),\ v_iv_j\in E(G)$$
$$=\sum_{1\le t,s\le l}^{t<s}(t\cdot s)\eta_{ts}$$

- The chromatic irregularity index of G is defined as:

$$M_3^{\phi_t}(G)=\sum_{i=1}^{n-1}\sum_{j=2}^{n}|c(v_i)-c(v_j)|,v_iv_j\in E(G)$$
$$=\sum_{1\le t,s\le l}^{t<s}|t-s|\eta_{ts}$$

- The chromatic total irregularity index of G is defined as:

$$M_4^{\phi_t}(G)=\frac{1}{2}\sum_{i=1}^{n-1}\sum_{j=2}^{n}|c(v_i)-c(v_j)|,v_i,v_j\in V(G)$$

Here η_{ts} is the number of edges $e(=uv)$ in G such that $c(u)=t$ and $c(v)=s$.

In account of the foresaid considerations, the minimum and maximum chromatic Zagreb indices, as well as the related irregularity indices, are defined as follows:

$$M_i^{\phi^-}(G)=\min\{M_i^{\phi_t(G)}:1\le t\le l!\},1\le i\le 4$$
$$M_i^{\phi^+}(G)=\max\{M_i^{\phi_t(G)}:1\le t\le l!\},1\le i\le 4$$

II. CYCLE GRAPH (C_n)

[6] A graph made up of only one cycle is known as a cycle graph or circular graph and a cycle with n vertices is denoted by C_n.

A. Chromatic Topological Indices of C_n.

Case 1(a): n is odd.

$$M_1^{\phi^-}(C_n)=\frac{5n+3}{2}$$
$$M_2^{\phi^-}(C_n)=2n+5$$
$$M_3^{\phi^-}(C_n)=n+1$$
$$M_4^{\phi^-}(C_n)=\frac{n^2+4n-5}{8}$$

Proof:

The chromatic number of a cycle graph C_n is 3, when n is odd. Let $v_1,v_2,\dots,v_n$ be the vertices of C_n. To calculate the minimum Zagreb indices, we use ϕ^- coloring pattern to C_n as described below.

Two maximum independent sets are $\{v_1,v_3,\dots,v_{n-2}\}$ and $\{v_2,v_4,\dots,v_{n-1}\}$ with same cardinality $\frac{n-1}{2}$. We color them with minimum colors 1 and 2 respectively. The remaining vertex v_n is colored with 3.

(i.e.,) $c(v_{2i-1})=1, c(v_{2i})=2; 1\le i\le\frac{n-1}{2}$ and $c(v_n)=3$. Also $\theta(1)=\theta(2)=\frac{n-1}{2},\theta(3)=1$ and $\eta_{12}=n-2,\eta_{13}=\eta_{23}=1$.

Therefore

$$M_1^{\phi^-}(C_n)=\sum_{j=1}^{l}\theta(c_j)\cdot j^2=\frac{5n+3}{2}$$
$$M_2^{\phi^-}(C_n)=\sum_{1\le t,s\le l}^{t<s}(t\cdot s)\eta_{ts}=2n+5$$
$$M_3^{\phi^-}(C_n)=\sum_{1\le t,s\le l}^{t<s}|t-s|\eta_{ts}=n+1$$
$$M_4^{\phi^-}(C_n)=\frac{1}{2}\sum_{i=1}^{n-1}\sum_{j=2}^{n}|c(v_i)-c(v_j)|=\frac{n^2+4n-5}{8}$$

Case 1(b): n is odd.

$$M_1^{\phi^+}(C_n)=\frac{13n-11}{2}$$
$$M_2^{\phi^+}(C_n)=6n-7$$
$$M_3^{\phi^+}(C_n)=2n-2$$
$$M_4^{\phi^+}(C_n)=\frac{n^2-1}{4}$$

Proof:

The chromatic number of a cycle graph C_n is 3, when n is odd. Let $v_1,v_2,\dots,v_n$ be the vertices of C_n. To calculate the minimum Zagreb indices, we use ϕ^+ coloring pattern to C_n as described below.

Two maximum independent sets are $\{v_1,v_3,\dots,v_{n-2}\}$ and $\{v_2,v_4,\dots,v_{n-1}\}$ with same cardinality $\frac{n-1}{2}$. We color them with maximum colors 3 and 2 respectively. The remaining vertex v_n is colored with 1.

(i.e.,) $c(v_{2i-1})=3, c(v_{2i})=2; 1\le i\le\frac{n-1}{2}$ and $c(v_n)=1$. Also $\theta(1)=1,\theta(2)=\frac{n-1}{2}=\theta(3)$ and $\eta_{12}=\eta_{13}=1,\eta_{23}=n-2$.

Therefore

$$M_1^{\phi^+}(C_n) = \sum_{j=1}^{l} \theta(c_j) \cdot j^2 = \frac{13n-11}{2}$$

$$M_2^{\phi^+}(C_n) = \sum_{1 \le t,s \le l}^{t<s} (t \cdot s)\eta_{ts} = 6n-7$$

To find M_3 and M_4 we make use of another ϕ^+ coloring as; $c(v_{2i-1}) = 1, c(v_{2i}) = 3; 1 \le i \le \frac{n-1}{2}$ and $c(v_n) = 2$. Which results $\theta(1) = \frac{n-1}{2}, \theta(2) = 1, \theta(3) = \frac{n-1}{2}$ and $\eta_{12} = n-2$, $\eta_{13} = \eta_{23} = 1$.

Therefore

$$M_3^{\phi^+}(C_n) = \sum_{1 \le t,s \le l}^{t<s} |t-s| \eta_{ts} = 2n-2$$

$$M_4^{\phi^+}(C_n) = \frac{1}{2}\sum_{i=1}^{n-1}\sum_{j=2}^{n} |c(v_i) - c(v_j)| = \frac{n^2-1}{4}$$

Case 2: n is even.

$$M_1^{\phi^-}(C_n) = M_1^{\phi^+}(C_n) = \frac{5n}{2}$$

$$M_2^{\phi^-}(C_n) = M_2^{\phi^+}(C_n) = 2n$$

$$M_3^{\phi^-}(C_n) = M_3^{\phi^+}(C_n) = n$$

$$M_4^{\phi^-}(C_n) = M_4^{\phi^+}(C_n) = \frac{n^2}{8}$$

Proof:

The chromatic number of a cycle graph C_n is 2, when n is even. Two maximum independent sets are $\{v_1, v_3, \dots, v_{n-1}\}$ and $\{v_2, v_4, \dots, v_n\}$ with same cardinality $\frac{n}{2}$. Also $c(v_{2i-1}) = 1, c(v_{2i}) = 2; 1 \le i \le \frac{n}{2}$. Also $\theta(1) = \theta(2) = \frac{n}{2}$ and $\eta_{12} = n$. Hence the result is obvious.

III. COMPLETE GRAPH (K_n)

[1] A simple graph is said to be complete if every pair of two distinct vertex is connected by an edge and a complete graph with n vertices is denoted by K_n.

A. Chromatic Topological Indices of K_n.

$$M_1^{\phi^-}(K_n) = M_1^{\phi^+}(K_n) = \frac{n(n+1)(2n+1)}{6}$$

$$M_2^{\phi^-}(K_n) = M_2^{\phi^+}(K_n) = \sum_{1 \le i,j \le n}^{i<j} i \cdot j$$

$$= \frac{n^2(n-1)(n+1)}{4} - \sum_{i=1}^{n-1} \frac{i^2(i+1)}{2}$$

$$M_3^{\phi^-}(K_n) = M_3^{\phi^+}(K_n) = \sum_{i=1}^{n-1} \frac{i(i+1)}{2}$$

$$M_4^{\phi^-}(K_n) = M_4^{\phi^+}(K_n) = \sum_{i=1}^{n-1} \frac{i(i+1)}{4}$$

Proof:

The chromatic number of a cycle graph K_n is n. Let $v_1, v_2, \dots, v_n$ be the vertices of K_n. Chromatic number of K_n is n. (i.e) $\theta(i) = 1; 1 \le i \le n$ and $\eta_{ij} = 1; 1 \le i < j \le n$. Hence $M_i^{\phi^-}(K_n) = M_i^{\phi^+}(K_n); 1 \le i \le 4$

$$M_1^{\phi^-}(K_n) = M_1^{\phi^+}(K_n) = \frac{n(n+1)(2n+1)}{6}$$

Therefore $M_2^{\phi^-}(K_n) = M_2^{\phi^+}(K_n) = \sum_{1 \le i,j \le n}^{i<j} i \cdot j$

$$= \frac{n^2(n-1)(n+1)}{4} - \sum_{i=1}^{n-1} \frac{i^2(i+1)}{2}$$

$$M_3^{\phi^-}(K_n) = M_3^{\phi^+}(K_n) = \sum_{i=1}^{n-1} \frac{i(i+1)}{2}$$

$$M_4^{\phi^-}(K_n) = M_4^{\phi^+}(K_n) = \sum_{i=1}^{n-1} \frac{i(i+1)}{4}$$

IV. LINE GRAPH ($L(G)$)

The line graph of a graph G denoted by $L(G)$, is the graph whose vertices are the edges of G, with two vertices of $L(G)$ are adjacent whenever the corresponding edges of G are adjacent.

A. Line Graph of Cycle Graph

[7] For any line graph of a cycle graph, the chromatic Zagreb indices and irregularity indices are equal to the corresponding index of a cycle graph. (i.e.,)

$$M_i^{\phi^-}(L(C_n)) = M_i^{\phi^-}(C_n); 1 \le i \le 4$$

$$M_i^{\phi^+}(L(C_n)) = M_i^{\phi^+}(C_n); 1 \le i \le 4$$

Proof:

From the definition of line graph it is easy to verify that $L(C_n) = C_n$. Hence the result is obvious.

B. Line Graph of Complete Graph

- Order of $L(K_n) =$ Size of $K_n = m = \frac{n(n-1)}{2}$.
- Size of $L(K_n) = \frac{n(n-1)(n-2)}{2}$
- Chromatic number of $L(K_n) = \chi(L(K_n) = \begin{cases} n & if\ n\ is\ odd \\ n-1 & if\ n\ is\ even \end{cases}$.
- $L(K_n)$ is regular. (i.e.,) $d(e_i) = 2(n-1), \forall i$

C. Chromatic Topological Indices of $L(K_n)$

For any line graph of a complete graph, the minimum chromatic Zagreb indices and irregularity indices and the maximum chromatic Zagreb indices and irregularity indices are equal. (i.e.,) $M_i^{\phi^-}(L(K_n)) = M_i^{\phi^+}(L(K_n)); 1 \le i \le 4\ n \ge 3$, and it is defined as;

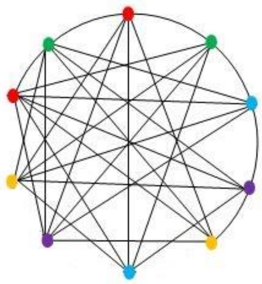
$$M_1^{\phi_t}(L(K_n)) = \begin{cases} \frac{n(n^2-1)(2n+1)}{12}, & if\ n\ is\ odd \\ \frac{n^2(n-1)(2n-1)}{12}, & if\ n\ is\ even \end{cases}$$

$$M_2^{\phi_t}(L(K_n)) = \begin{cases} (n-2)\sum\limits_{1\le i,j\le n}^{i<j} i\cdot j, & if\ n\ is\ odd \\ n = \sum\limits_{1\le i,j\le n}^{i<j} i\cdot j, & if\ n\ is\ even \end{cases}$$

$$= \begin{cases} \frac{n^2(n^2-1)(n-2)}{4} - (n-2)\sum\limits_{i=1}^{n-1}\frac{i^2(i+1)}{2}, & if\ n\ is\ odd \\ \frac{n^3(n^2-1)}{4} - n\sum\limits_{i=1}^{n-2}\frac{i^2(i+1)}{2}, & if\ n\ is\ even \end{cases}$$

$$M_3^{\phi_t}(L(K_n)) = \begin{cases} (n-2)\sum\limits_{i=1}^{n-1}\frac{i(i+1)}{2}, & if\ n\ is\ odd \\ n\sum\limits_{i=1}^{n-2}\frac{i(i+1)}{2}, & if\ n\ is\ even \end{cases}$$

$$M_4^{\phi_t}(L(K_n)) = \begin{cases} \frac{(n-1)^2}{8}\sum\limits_{i=1}^{n-1}\frac{i(i+1)}{2}, & if\ n\ is\ odd \\ \frac{n^2}{8}\sum\limits_{i=1}^{n-2}\frac{i(i+1)}{2}, & if\ n\ is\ even \end{cases}$$



ϕ^- Coloring of $L(K_4)$

Proof:

<u>Case 1: When n is odd.</u>

Consider the minimal coloring of $L(K_n)$, where n is odd. Then $\theta(i) = \frac{n-1}{2}, 1 \le i \le n$ and $\eta_{ij} = n-2, 1 \le i < j \le \frac{n(n-1)}{2}$.

$$M_1^{\phi_t}(L(K_n)) = \frac{n(n^2-1)(2n+1)}{12}$$

$$M_2^{\phi_t}(L(K_n)) = (n-2)\sum_{1\le i,j\le n}^{i<j} i\cdot j$$

$$= \frac{n^2(n^2-1)(n-2)}{4} - (n-2)\sum_{i=1}^{n-1}\frac{i^2(i+1)}{2}$$

$$M_3^{\phi_t}(L(K_n)) = (n-2)\sum_{i=1}^{n-1}\frac{i(i+1)}{2}$$

$$M_4^{\phi_t}(L(K_n)) = \frac{(n-1)^2}{8}\sum_{i=1}^{n-1}\frac{i(i+1)}{2}$$

<u>Case 2: When n is even.</u>

Consider the minimal coloring of $L(K_n)$, where n is even. Then $\theta(i) = \frac{n-1}{2}, 1 \le i \le n$ and $\eta_{ij} = n-2, 1 \le i < j \le \frac{n(n-1)}{2}$.

$$M_1^{\phi_t}(L(K_n)) = \frac{n(n^2-1)(2n+1)}{12}$$

$$M_2^{\phi_t}(L(K_n)) = (n-2)\sum_{1\le i,j\le n}^{i<j} i\cdot j$$

$$= \frac{n^2(n^2-1)(n-2)}{4} - (n-2)\sum_{i=1}^{n-1}\frac{i^2(i+1)}{2}$$

$$M_3^{\phi_t}(L(K_n)) = (n-2)\sum_{i=1}^{n-1}\frac{i(i+1)}{2}$$

$$M_4^{\phi_t}(L(K_n)) = \frac{(n-1)^2}{8}\sum_{i=1}^{n-1}\frac{i(i+1)}{2}$$

V. CONCLUSION

In chemical graph theory and distribution theory, the concept presented in this work has several applications. This document gives an overview of chromatic topological indices for cycle graphs, complete graphs and their line graphs. The study appears to hold promise for future research because these indices can be generated for a wide range of graph classes and derived graph classes. For graph operations, graph products, and graph powers, chromatic topological indices can be calculated. The research on the subject in relation to various forms of graph colorings also seems to be quite promising. The approach can be used to edge colorings and map colorings as well. The subject of this study has a wide range of applications in the chemical industry. If $c(v_i)$ assumes values such as energy, valency, bond strength, and so on, some interesting research using the above-mentioned principles are conceivable in Chemistry. Similar research can be done in a variety of other domains. All these facts show that there is a lot of room for more research in this field. Even the chromatic version of other topological indices opens new study avenues with wide-ranging applicability.

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Cite this article as :

Albina. A, Manonmani. A, "Computation of CTI of Certain Graphs", International Journal of Scientific Research in Computer Science, Engineering and Information Technology (IJSRCSEIT), ISSN : 2456-3307, Volume 8 Issue 6, pp. 67-71, November-December 2022.

Journal URL : https://ijsrcseit.com/CSEIT228579