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CONTRA HARMONIC INDEX OF SOME CHEMICAL STRUCTURES

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Abstract

Topological indices are numbers connected to the compounds structural formula. There exist various kinds of topological indices. One such degree based topological index is Contra Harmonic Index (CH). CH index of a graph G which is defined as $CH(G) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$. In this article, the CH Index of Rectangular Silicate, Dominating Silicate, Chain Oxide and Double Chain Oxide networks are calculated.

Keywords: Contra Harmonic Index, Molecular graph

AMS Classification: 05C76, 05C09

Introduction

Chemical graph theory is a hybrid of graph theory and chemistry that models and analyzes chemical reactions and molecular structures using graph theory. In the chemical graph theory, atoms and bonds are depicted as vertices and edges in a graph respectively. Chemical graph theory focuses on examining the relationships between chemical structures and their graph representations. Graph features to understand the traits and actions of molecules

Topological indices are numbers connected to the compounds structural formula. It was useful in determining the atom connectivity or molecular makeup of the compounds, even if not many uses were initially understood. The growing interest in topological indices primarily stems from their application in non-empirical QSPR and QSAR. The primary goal of QSAR/QSPR/QSTR[2] is to compute molecular structures in order to create a correlation model between chemical structures and their corresponding physico-chemical properties.

A silicate network is a three-dimensional structure made up of silicon and oxygen atoms, resulting in the formation of SiO_4 tetrahedra. These networks play a crucial role in various applications, including construction materials, glass manufacturing, ceramics, soil enhancement, electronics, and water treatment. In chemical terms, a central silicon atom is joined to four oxygen atoms at each tetrahedron's corners. Minerals are formed when the oxygen atoms of adjacent tetrahedra in distinct silicates connect, creating a continuous network. Removing silicon ions from silicate networks results in oxide networks. The most

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popular topological indexes are Zagreb indices. Gutman and Trinajstic introduced the first and second Zagreb indices $M_1(G)$ and $M_2(G)$[10]. They are defined as $M_1(G) = \sum_{v \in V(G)} d^2(v)$, $M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$.

After that the forgotten topological index was invented by Furtula and Gutman [5], which was defined as $F(G) = \sum_{v \in V(G)} d^3(v)$.

Randic number was invented in 1976 by Milan Randic. For any real α, the generalized randic number $R_\alpha(G)$ is defined $R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^2$.

The inverse sum indeg index (ISI index) is defined in [20] as follows

$$ISI(G) = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}$$

In 1980, Siemion Fajtlowicz [4] introduces harmonic index, which is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$$

For connected graph, the Symmetric division deg index is defined in [7] as

$$SDD(G) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u)d(v)}$$

The Contra Harmonic Index was introduced by S. Ragavi and R. Sridevi in [15] as

$$CH(G) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

The Contra Harmonic Index of Benzenoid networks, Silicate networks and Oxide networks were studied in [16],[17],[18]. In this paper, the CH Index of Dominating Silicate, Regular Triangular Silicate, Chain Oxide and Double Chain Oxide networks were calculated.

Dominating Silicate Network

Drawing algorithm for Dominating Silicate network from Honeycomb network were studied in [20]. Let HC(n) be a n dimensional honeycomb network. Each edge of HC(n) should be divided once. Apply oxygen ions to the newly created vertices. If there are four units between the new nodes in each hexagon cell, join them with an edge. At the new edge crossings, install oxygen ions. After removing the HC(n) nodes and edges, insert a silicon node at the centroid of each regular subgraph K_3 of the dominating oxide network and connect it to another oxide node in the same K_3. Thus we get Dominating Silicate network.

The figure depicts DS_2

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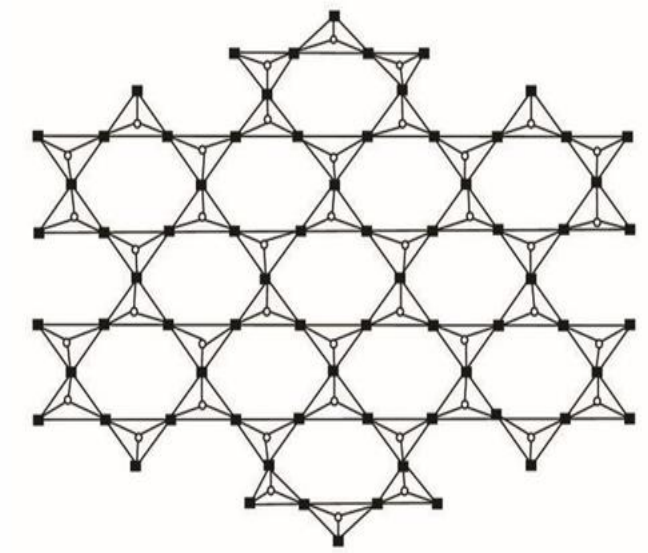

Theorem 1

For Dominating Silicate Network DS_n, $CH(DS_n) = 2(297n^2 - 321n + 111)$.

Proof

DS_n has $45n^2 - 39n + 12$ vertices and $108n^2 - 108n + 36$ edges.

The edge set's partition of DS_n are as follows,

$$E_{(3,3)} = \{e = uv \in E(DS_n) | d_{DS_n}(u) = 3, d_{DS_n}(v) = 3\},$$

$$E_{(3,6)} = \{e = uv \in E(DS_n) | d_{DS_n}(u) = 3, d_{DS_n}(v) = 6\},$$

$$E_{(6,6)} = \{e = uv \in E(DS_n) | d_{DS_n}(u) = 6, d_{DS_n}(v) = 6\},$$

Then $|E_{(3,3)}| = 12n - 6$, $|E_{(3,6)}| = 54n^2 - 42n + 12$ and $|E_{(6,6)}| = 54n^2 - 78n + 30$

$$CH(DS_n) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

$$= \sum_{uv \in E_{(3,3)}} \frac{3^2 + 3^2}{3 + 3} + \sum_{uv \in E_{(3,6)}} \frac{3^2 + 6^2}{3 + 6} + \sum_{uv \in E_{(6,6)}} \frac{6^2 + 6^2}{6 + 6}$$

$$= (12n - 6)\left(\frac{18}{6}\right) + (54n^2 - 42n + 12)\left(\frac{45}{9}\right) + (54n^2 - 78n + 30)\left(\frac{72}{12}\right)$$

$$= 2(297n^2 - 321n + 111).$$

Regular Triangular Silicate Network

Regular Triangular Silicate Network is denoted by RTS_n. According to methodology outlines in [20], RTS_n have $\frac{5n^2+13n+2}{2}$ vertices and $6n^2 + 12n$ edges. RTS_5 is depicted in the figure below.

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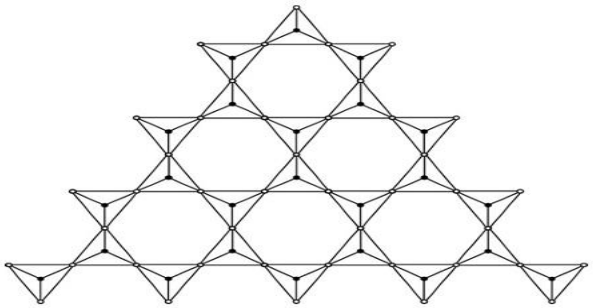


Theorem 2

For RTS_n, $CH(RTS_n) = 33n^2 + 54n - 10$.

Proof

RTS_n has $\frac{5n^2+13n+2}{2}$ vertices and $6n^2 + 12n$ edges.

The edge set's partition of RTS_n are as follows,

$$E_{(3,3)} = \{e = uv \in E(RTS_n) | d_{RTS_n}(u) = 3, d_{RTS_n}(v) = 3\},$$

$$E_{(3,6)} = \{e = uv \in E(RTS_n) | d_{RTS_n}(u) = 3, d_{RTS_n}(v) = 6\},$$

$$E_{(6,6)} = \{e = uv \in E(RTS_n) | d_{RTS_n}(u) = 6, d_{RTS_n}(v) = 6\},$$

Then $|E_{(3,3)}| = 3n + 4$, $|E_{(3,6)}| = 3n^2 + 9n - 2$ and $|E_{(6,6)}| = 3n^2 - 2$.

$$CH(RTS_n) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

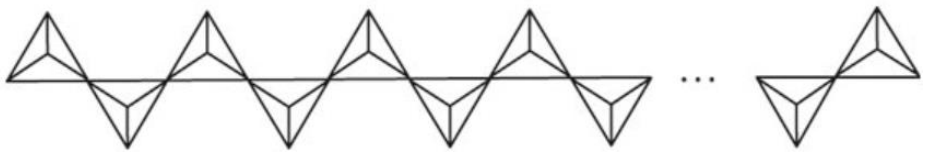
$$= \sum_{uv \in E_{(3,3)}} \frac{3^2 + 3^2}{3 + 3} + \sum_{uv \in E_{(3,6)}} \frac{3^2 + 6^2}{3 + 6} + \sum_{uv \in E_{(6,6)}} \frac{6^2 + 6^2}{6 + 6}$$

$$= (3n + 4)\left(\frac{18}{6}\right) + (3n^2 + 9n - 2)\left(\frac{45}{9}\right) + (3n^2 - 2)\left(\frac{72}{12}\right)$$

$$= 33n^2 + 54n - 10.$$

Chain Oxide Network

Arranging n tetrahedral linearly yields a n dimensional chain silicate network which is represented as CS_n. When all silicon ions are removed from the CS_n, the chain oxide network is created. The formation of an oxide chain occurs when an oxide network linearly shares oxygen with another oxide network. The CS_n and COX_n are depicted in the figure below respectively.



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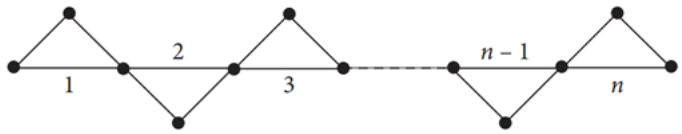


Theorem 3

For COX_n, $CH(COX_n) = 4\left(\frac{8n-3.}{3}\right)$.

Proof:

COX_n has $2n + 1$ vertices and $3n$ edges.

The edge set's partition of COX_n are as follows,

$$E_{(2,2)} = \{e = uv \in E(COX_n) | d_{COX_n}(u) = 2, d_{COX_n}(v) = 2\},$$

$$E_{(2,4)} = \{e = uv \in E(COX_n) | d_{COX_n}(u) = 2, d_{COX_n}(v) = 4\},$$

$$E_{(4,4)} = \{e = uv \in E(COX_n) | d_{COX_n}(u) = 4, d_{COX_n}(v) = 4\},$$

Then $|E_{(2,2)}| = 2$, $|E_{(2,4)}| = 2n$ and $|E_{(4,4)}| = n - 2$

$$CH((COX_n)) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

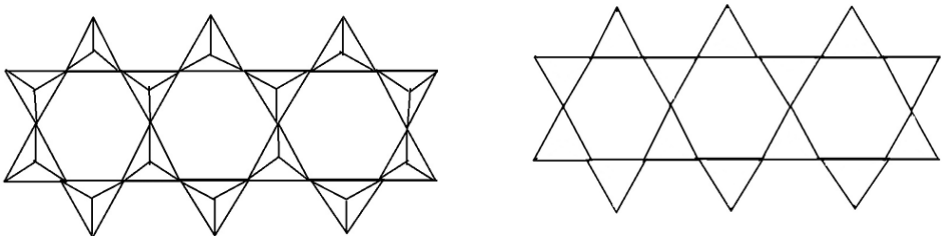
$$= \sum_{uv \in E_{(2,2)}} \frac{2^2 + 2^2}{2 + 2} + \sum_{uv \in E_{(2,4)}} \frac{2^2 + 4^2}{2 + 4} + \sum_{uv \in E_{(4,4)}} \frac{4^2 + 4^2}{4 + 4}$$

$$= 4 + 2n\left(\frac{10}{3}\right) + (n - 2)(4)$$

$$= 4\left(\frac{8n - 3.}{3}\right).$$

Double Chain Oxide Network

Double Chain Silicates are formed when two chain Silicates are joined together by shares Oxygens. When all Silicon ions are removed from Double Chain Silicate Network, Double Chain Oxide Network is formed which consists of three oxygen atoms. DCS_3 and $DCOX_3$ are shown in the following figure respectively.



Theorem 4

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For $DCOX_n$, $CH(DCOX_n) = \frac{208n-16}{3}$.

Proof:

$DCOX_n$ has $10n + 2$ vertices and $18n$ edges.

The edge set's partition of $DCOX_n$ are as follows,

$$E_{(2,4)} = \{e = uv \in E(DCOX_n) | d_{DCOX_n}(u) = 2, d_{DCOX_n}(v) = 4\},$$

$$E_{(4,4)} = \{e = uv \in E(DCOX_n) | d_{DCOX_n}(u) = 4, d_{DCOX_n}(v) = 4\},$$

Then $|E_{(2,4)}| = 4n + 8$ and $|E_{(4,4)}| = 14n - 8$,

$$CH((DCOX_n)) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

$$= \sum_{uv \in E_{(2,4)}} \frac{2^2 + 4^2}{2 + 4} + \sum_{uv \in E_{(4,4)}} \frac{4^2 + 4^2}{4 + 4}$$

$$= (4n + 8)\left(\frac{10}{3}\right) + (14n - 8)(4)$$

$$= \frac{208n - 16}{3}.$$

Conclusion

Pharmaceutical professionals can better understand the biological and chemical properties of new drugs by using recent developments on the application of topological index in treating viral illness. In this paper, the Contra Harmonic Index of Dominating Silicate, Rectangular Silicate, Chain Oxide, Double Chain Oxide network were calculated. Continuous research work has been conducted to determine topological properties using CH index.

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