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Contra Harmonic Index of Some Networks

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ABSTRACT:

Topological indices are numerical descriptors that are used in the field of mathematical chemistry to characterize the structural, biological, chemical and physical features of chemical compounds based on their molecular graphs. These are imployed in quantitative structure-activity relationship (QSAR) studies. In this paper we find the Contra Harmonic index of some networks which include hexagonal, silicate, oxide and honeycomb network and also the nanostructure $TUC_4C_8(p,q)$.

Keywords: Graphs, Contra Harmonic index, Silicate network, Hexagonal network, Oxide network, Honeycomb network, $TUC_4C_8(p,q)$

1. Introduction

Topological indices are used to predict various molecular properties such as boiling points, critical temperatures and biological activities. Ever since the introduction of Wiener index in 1947 by Harold Wiener [3], several topological indices have been introduced, aiding in predicting different characteristics of chemical compounds.

All graphs in this paper are finite, simple and undirected graphs. For all other standard terminology and notations, we follow Harary [1]. S. S. Sandhya, S. Somasundaram and J. Rajeshni Golda introduced Contra Harmonic Mean labeling of graphs [2]. S. Ragavi and R. Sridevi introduced Contra Harmonic index of graphs in [4]. Topological properties of various networks are being studied recently to understand the properties of several nanostructures [5,6].

A silicate network $SL(n)$ of dimension n, has n hexagons between centre and boundary of $SL(n)$. A hexagonal network $HX(n)$ is said to be of dimension n, when number of vertices on one side of hexagon is n. An oxide network $OX(n)$ of dimension n, when number of vertices on one side of $OX(n)$ is n. A honeycomb network $HC(n)$ is said to be of dimension n, when number of hexagons on one boundary of network is n.

When delving into network studies, the exploration of 2D lattice of $TUC_4C_8(p,q)$ becomes unavoidable, which led us to study the Contra Harmonic index of 2D lattice, nanotube and nanotorus of $TUC_4C_8(p,q)$. p And q denote the number of squares in a row and column of the network respectively. Several topological properties and indices of $TUC_4C_8(p,q)$ have been investigated in [8].

The following definition and notes on the edge partitions of the networks will be used in further study:

Definition 1.1 [2]: A graph $G(V,E)$ with p vertices and q edges is said to be Contra Harmonic Mean graph if it is possible to label the vertices $x \in V$ with distinct labels $f(x)$ from $0,1,2,\ldots\ldots,q$ in such a way that each edge $e = uv$ is labeled with $f(e = uv) = \left\lceil \frac{f(u)^2+f(v)^2}{f(u)+f(v)} \right\rceil$ or $\left\lfloor \frac{f(u)^2+f(v)^2}{f(u)+f(v)} \right\rfloor$. then we get distinct edge labels. In this case f is called Contra Harmonic Mean labeling of G and G is called Contra Harmonic Mean graph.

Definition 1.2 [4]**:** Contra Harmonic index of a graph G is defined as sum of the term $\frac{d(u)^2+d(v)^2}{d(u)+d(v)}$ over all edges uv of graph G.

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

Note 1.3 [7]**:** Number of edges of silicate network with the degree of incident vertices (3,3), (3,6) and (6,6) are $6n, 18n^2 + 6n$ and $18n^2 - 12n$ respectively.

Note 1.4 [7]**:** Number of edges of honeycomb network with the degree of incident vertices (2,2), (2,3) and (3,3) are $6n, 12(n-1)$ and $9n^2 - 15n + 6$ respectively.

Note 1.5 [7]**:** Number of edges of hexagonal network with the degree of incident vertices $(3,4), (3,6), (4,4), (4,6)$ and (6,6) are $12, 6, 6(n-3), 12(n-2)$ and $9n^2 - 33n + 30$ respectively.

Note 1.6 [7]**:** Number of edges of oxide network with the degree of incident vertices (2,4) and (4,4) are $12n$ and $18n^2 - 12$ respectively.

Theorem 1.7: Contra Harmonic index of an m-regular graph G with n edges is mn

2. Results

Theorem 2.1: Contra Harmonic index of $SL(n)$ is $98n^2 - 24n$

Proof

Let $SL(n)$ be a silicate network with dimension n

Let $u_1, u_2, \dots, u_n$ be vertices of $SL(n)$

$$CH(SL(n)) = \sum_{u_i u_j \in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$= 6n\left[\frac{3^2+3^2}{3+3}\right] + (18n^2+6n)\left[\frac{3^2+6^2}{3+6}\right] + (18n^2-12n)\left[\frac{6^2+6^2}{6+6}\right]$$

$$= 98n^2 - 24n$$

Therefore, $CH(SL(n)) = 98n^2 - 24n$

Example 2.1

Figure 1 shows $SL(2)$. Using theorem 2.1, $CH(SL(2))$ is 344

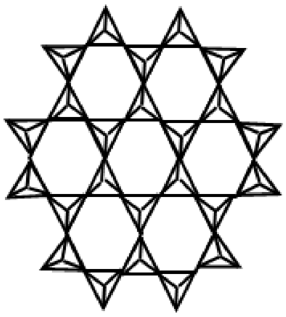

Figure 1: Silicate network of dimension two

Theorem 2.2: Contra Harmonic index of $HX(n)$ is $54n^2 + \frac{558}{5}n + \frac{1962}{35}$

Proof

Let $HX(n)$ be a hexagonal network with dimension n

Let $u_1, u_2, \dots, u_n$ be vertices of $HX(n)$

$$CH(HX(n)) = \sum_{u_i u_j \in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$= 12\left(\frac{3^2+4^2}{3+4}\right) + 6\left(\frac{3^2+6^2}{3+6}\right) + 6(n-3)\left(\frac{4^2+4^2}{4+4}\right) + 12(n-2)\left(\frac{4^2+6^2}{4+6}\right) + (9n^2 - 33n + 30)\left(\frac{6^2+6^2}{6+6}\right)$$

$$= \left(12 \times {}^{25}/_{7}\right) + \left(6 \times {}^{45}/_{9}\right) + 6(n-3)\,{}^{32}/_{8} + 6(n-2)\,{}^{52}/_{10} + (9n^2 - 33n + 30)\,{}^{72}/_{12}$$

$$= 54n^2 + \frac{558}{5}n + \frac{1962}{35}$$

Therefore, $CH(HX(n)) = 54n^2 + \frac{558}{5}n + \frac{1962}{35}$

Example 2.2

Figure 2 shows $HX(4)$. Using theorem 2.2, $CH(HX(4)) = 1366.45$

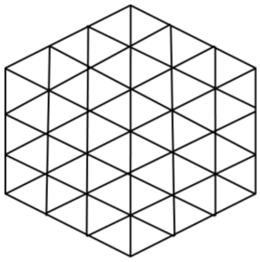

Figure 2: Hexagonal network of dimension four

Theorem 2.3: Contra Harmonic index of $OX(n)$ is $72n^2 - 8n$

Proof

Let $OX(n)$ be an oxide network with dimension n

Let $u_1, u_2, \ldots, u_n$ be vertices of $OX(n)$

$$CH(OX(n)) = \sum_{u_iu_j \in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$= 12n\left(\frac{2^2 + 4^2}{2 + 4}\right) + (18n^2 - 12n)\left(\frac{4^2 + 4^2}{4 + 4}\right)$$

$$= 72n^2 - 8n$$

Therefore, $CH(OX(n)) = 72n^2 - 8n$

Example 2.3

Figure 3 shows $OX(4)$. Using theorem 2.3, $CH(OX(4)) = 1120$

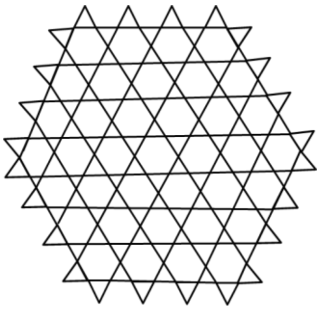

Figure 3: Oxide network of dimension four

Theorem 2.4: Contra Harmonic index $HC(n)$ is $27n^2 - \frac{69}{5}n - \frac{6}{5}$

Proof

Let $HC(n)$ be a honeycomb network with dimension n

Let $u_1, u_2, \ldots, u_n$ be vertices of $HC(n)$

$$CH(HC(n)) = \sum_{u_iu_j \in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$= 6\left(\frac{2^2 + 2^2}{2 + 2}\right) + 12(n - 1)\left(\frac{2^2 + 3^2}{2 + 3}\right) + (9n^2 - 15n + 6)\left(\frac{3^2 + 3^2}{3 + 3}\right)$$

$$= 27n^2 - \frac{69}{5}n - \frac{6}{5}$$

Therefore, $CH(HC(n)) = 27n^2 - \frac{69}{5}n - \frac{6}{5}$

Example 2.4
Figure 4 shows $HC(2)$. Using theorem 2.4, $CH(HC(2)) = 79.2$

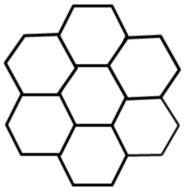

Figure 4: Honeycomb network of dimension two

Note 2.5: Table 1 shows the edge partition of 2D lattice and nanotube of$TUC_4C_8(p,q)$. Let G denote the 2D lattice of$TUC_4C_8(p,q)$ and H denote the nanotube of $TUC_4C_8(p,q)$

(d_u, d_v)	(3,3)	(2,2)	(2,3)
Number of edges uv, $uv \in E(G)$	$6pq - 5p - 5q + 4$	4	$4p + 4q - 8$
Number of edges uv, $uv \in E(H)$	$6pq - 5p$	0	$4p$

Table 1

Theorem 2.6: Contra Harmonic index of 2D lattice of $TUC_4C_8(p,q)$ is $18pq - \frac{23}{5}p - \frac{23}{5}q - \frac{4}{5}$

Proof
Let G denote the 2D lattice of $TUC_4C_8(p,q)$
Let $u_1, u_2, \ldots, u_n$ be vertices of G

$$CH(G) = \sum_{u_iu_j \in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$=(6pq - 5p - 5q + 4)\left(\frac{3^2+3^2}{3+3}\right) + 4 \times \left(\frac{2^2+2^2}{2+2}\right) + (4p + 4q - 8)\left(\frac{3^2+2^2}{3+2}\right)$$
$$= 18pq - \frac{23}{5}p - \frac{23}{5}q - \frac{4}{5}$$

Therefore, $CH(G) = 18pq - \frac{23}{5}p - \frac{23}{5}q - \frac{4}{5}$

Example 2.6
Figure 5 shows $G =$ 2D lattice of $TUC_4C_8(5,4)$. Using theorem 2.6, $CH(G)$ =317.8

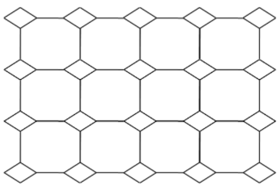

Figure 5: 2D lattice of $TUC_4C_8(5,4)$

Theorem 2.7: Contra Harmonic index of nanotube of $TUC_4C_8(p,q)$ is $18pq - \frac{23}{5}p$

Proof

Let H denote the nanotube of $TUC_4C_8(p,q)$

Let $u_1,u_2,\ldots,u_n$ be vertices of H

$$CH(H) = \sum_{u_iu_j\in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$=(6pq-5p)\left(\frac{3^2+3^2}{3+3}\right) + 4p\left(\frac{3^2+2^2}{3+2}\right)$$

$$= 18pq - \frac{23}{5}p$$

Therefore, $CH(H) = 18pq - \frac{23}{5}p$

Example 2.7

Figure 6 shows $H = TUC_4C_8(5,4)$ nanotube. Using theorem 2.7, $CH(H) = 337$

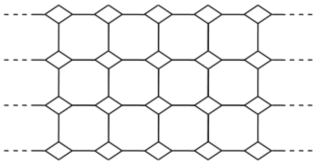

Figure 6: $TUC_4C_8(5,4)$ nanotube

Corollary 2.8: Contra Harmonic index of nanotorus of $TUC_4C_8(p,q)$ is $18pq$

Proof

Let J denote the nanotorus of $TUC_4C_8(p,q)$

$|E(H)| = 6pq$

Since J is a 3-regular graph, by Result 1.6

$CH(G) = 3 \times 6pq = 18pq$

Therefore, $CH(J) = 18pq$

Example 2.8

Figure 7 shows $J = TUC_4C_8(5,4)$ nanotorus. Using corollary 2.8, $CH(J) = 360$

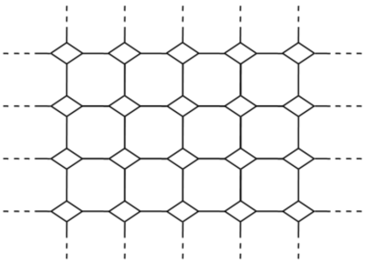

Figure 7: $TUC_4C_8(5,4)$ nanotorus

3. Conclusion

In this paper, we find the Contra Harmonic index of some networks like silicate, hexagonal, honeycomb and oxide networks. Contra Harmonic index of 2D lattice, nanotube and nanotorus of $TUC_4C_8(p,q)$ are also studied. This study aids in understanding various properties of the mentioned compounds. Further study can be done on networks like dendrimers, benzenoid systems and line graphs of the studied compounds.

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