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# Some Results on Contra Harmonic Index of Some Molecular Graphs

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**Abstract:** Topological index is a mathematical coding of the molecular graphs that predicts the physiochemical, biological, toxicological and structural properties of chemical compounds that are directly associated with molecular graphs. In this paper, we find the Contra Harmonic index of some graphs which are also the chemical structures of certain alkanes.

***Keywords***: *Graphs, Contra Harmonic Mean graphs, Contra Harmonic index, Path, Cycle, Triangular chain, Corona product*

## 1. Introduction

Chemical graph theory is a pivotal branch of mathematical chemistry where molecular structures are modelled as graphs called molecular graphs, with atoms represented as vertices and chemical bonds as edges. A primary tool in this field is the topological index which is a numerical descriptor derived from a graph's structure that correlates with the physicochemical properties of the corresponding molecule. These indices play a crucial role in Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) studies, enabling the prediction of properties like boiling point, stability and biological activity without resorting to expensive lab experiments.

The pioneering Wiener index introduced by Harold Wiener in the year 1947, conceived for modeling alkane boiling points, remains historically significant for its focus on distance sums [8]. Subsequent development emphasized degree-based indices. The Zagreb indices [1] linked to molecular $\pi$-electron energy and the highly successful Randić index generated extensive research. Each index provides a unique lens on molecular structure, prompting the exploration of related mathematical means. The Contra Harmonic index is a more recent addition defined via the Contra Harmonic mean of vertex degrees [4 ]. Here, initially we identify the Contra Harmonic index of fundamental molecular graphs. A simple graph can be moulded into a chemical structure by using some graph operations. So, many chemical graphs can be generated by applying graphical operations on simple graphs, for instance, alkane ($C_3H_6$) is the corona product of $P_3$ and $K_{1,2}$.

**Definition 1.2:** 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 $G$.

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

## 2. Results

**Theorem 2.1:** Contra Harmonic index of Cycle $C_n$ is 2n

**Proof**

Let $C_n$ be a Cycle with n vertices and n edges

Let $u_1, u_2, \dots, u_n$ be vertices of $C_n$ such that $u_1$ is adjacent to $u_2, u_2$ is adjacent to $u_3$, …, $u_{n-1}$ is adjacent to $u_n$ and $u_n$ is adjacent to $u_1$

Then $|E(G)| = n$ and $d(u_i) = 2$, for all $i$

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

$$= \frac{d(u_1)^2 + d(u_2)^2}{d(u_1) + d(u_2)} + \dots + \frac{d(u_{n-1})^2 + d(u_n)^2}{d(u_{n-1}) + d(u_n)} + \frac{d(u_n)^2 + d(u_1)^2}{d(u_n) + d(u_1)}$$

$$= \frac{2^2 + 2^2}{2 + 2} + \dots + \frac{2^2 + 2^2}{2 + 2} \ (n \ times)$$

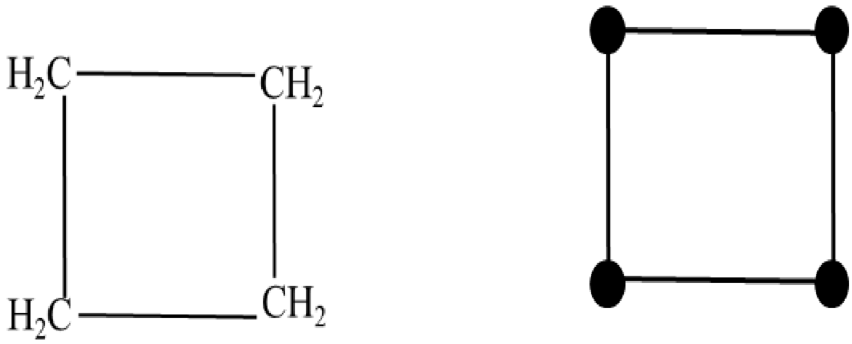
$$= n\left(\frac{2^2 + 2^2}{2 + 2}\right)$$

$$= 2n$$

Therefore, $CH(C_n) = 2n$

**Example 2.1**

The following example shows the Contra Harmonic index of cyclobutane using simple graph (hydrogen depleted graph) $C_4$. Here, $CH(C_4)$ is 8




a) Lewis structure of cyclobutane

b) simple graph $C_4$ (hydrogen depleted graph) of cyclobutane

**Figure 1**

**Theorem 2.2:** Contra Harmonic index of Path $P_n$ is $2(n-3) + \frac{10}{3}, n \geq 3$

**Proof**

Let $P_n$ be a Path

Let $u_1, u_2, \dots, u_n$ be vertices of $P_n$ such that $u_i$ is adjacent to $u_{i+1}$, for all $2 \leq i \leq n-1$

Then $|E(G)| = n - 1$ and $d(u_1) = 1, d(u_n) = 1$, $d(u_i) = 2$, for all $2 \leq i \leq n-1$

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

$$= \sum_{\substack{u_iu_{i+1} \in E(G) \\ i=1,n-1}} \frac{d(u_i)^2 + d(u_{i+1})^2}{d(u_i) + d(u_{i+1})} + \sum_{\substack{u_iu_{i+1} \in E(G) \\ i \neq 1,n-1}} \frac{d(u_i)^2 + d(u_{i+1})^2}{d(u_i) + d(u_{i+1})}$$

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

$$= 2 \times \frac{5}{3} + (n-3)\left(\frac{2^2 + 2^2}{2 + 2}\right)$$

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

Therefore, $CH(P_n) = 2(n-3) + \frac{10}{3}, n \geq 3$

**Example 2.2:**

The following example shows the Contra Harmonic index of alkane using simple graph (hydrogen depleted graph) $P_4$. Here, $CH(P_4)$ is $\frac{16}{3}$.


a) Lewis structure of alkane

b) simple graph $P_4$ of alkane (hydrogen depleted graph)

**Figure 2**

**Theorem 2.3:** Contra Harmonic index of $C_n \odot K_{1,2}$ is $\frac{54n}{5}$.

**Proof**

Let $C_n$ be a cycle with vertices $u_1, u_2, \dots, u_n$ and let $v_i, w_i$ be the pendant vertices adjacent to $u_i$, $1 \leq i \leq n$

Then $d(u_i) = 4$ and $d(v_i) = d(w_i) = 1$

$$CH(C_n \odot K_{1,2}) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

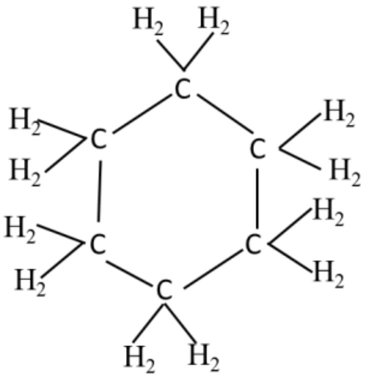
$$= \sum_{u_iw_i \in E(G)} \frac{d(u_i)^2 + d(w_i)^2}{d(u_i) + d(w_i)} + \sum_{u_iv_i \in E(G)} \frac{d(u_i)^2 + d(v_i)^2}{d(u_i) + d(v_i)} + \sum_{u_iu_j \in E(G)} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

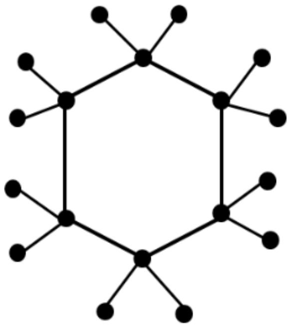
$$= n\left(\frac{4^2 + 1^2}{4 + 1}\right) + n\left(\frac{4^2 + 1^2}{4 + 1}\right) + n\left(\frac{4^2 + 4^2}{4 + 4}\right)$$

Therefore, $CH(C_n \odot K_{1,2}) = \frac{54n}{5}$

**Example 2.3:**

The following example shows the Contra Harmonic index of cyclohexane $C_6H_{12}$ using molecular graph $C_6 \odot K_{1,2}$. Here, $CH(C_6 \odot K_{1,2}) = CH(C_6H_{12})$ is $\frac{324}{5}$.



a) Lewis structure of cyclohexane $C_6H_{12}$ Molecular graph of cyclohexane $C_6H_{12}$ ($C_6 \odot K_{1,2}$)

**Figure 3**

**Theorem 2.4:** Contra Harmonic index of $P_n \odot K_{1,2}$ is

$$\frac{54(n-3)}{5}+\frac{120}{7}, n \geq 3$$

**Proof**

Let $P_n$ be a path with vertices $u_1, u_2, \dots, u_n$ and let $v_i, w_i$ be the pendant vertices adjacent to $u_i$, $1 \leq i \leq n$

Then $d(u_1)=d(u_n)=3$, $d(u_i)=4, 2 \leq i \leq n-1$ and $d(v_i)=d(w_i)=1$

$$CH(P_n \odot K_{1,2}) = \sum_{uv \in E(G)} \frac{d(u)^2+d(v)^2}{d(u)+d(v)}$$

$$= \sum_{\substack{u_iw_i \in E(G) \\ i \neq 1,n}} \frac{d(u_i)^2+d(w_i)^2}{d(u_i)+d(w_i)} + \sum_{\substack{u_iv_i \in E(G) \\ i \neq 1,n}} \frac{d(u_i)^2+d(v_i)^2}{d(u_i)+d(v_i)} + \sum_{\substack{u_iw_i \in E(G) \\ i = 1,n}} \frac{d(u_i)^2+d(w_i)^2}{d(u_i)+d(w_i)}$$
$$+ \sum_{\substack{u_iv_i \in E(G) \\ i = 1,n}} \frac{d(u_i)^2+d(v_i)^2}{d(u_i)+d(v_i)} + \sum_{\substack{u_iu_{i+1} \in E(G) \\ i = 1,n-1}} \frac{d(u_i)^2+d(u_{i+1})^2}{d(u_i)+d(u_{i+1})}$$
$$+ \sum_{\substack{u_iu_{i+1} \in E(G) \\ 2 \leq i \leq n-2}} \frac{d(u_i)^2+d(u_{i+1})^2}{d(u_i)+d(u_{i+1})}$$

$$= (n-3)\left(\frac{4^2+1^2}{4+1}\right) + (n-3)\left(\frac{4^2+1^2}{4+1}\right) + 2\left(\frac{3^2+1^2}{3+1}\right) + 2\left(\frac{3^2+1^2}{3+1}\right) + 2\left(\frac{3^2+4^2}{3+4}\right) + (n-3)\left(\frac{4^2+4^2}{4+4}\right)$$

$$= (n-3)\left(\frac{17}{5}+\frac{17}{5}+4\right) + 2\left(\frac{10}{4}+\frac{10}{4}+\frac{25}{7}\right)$$

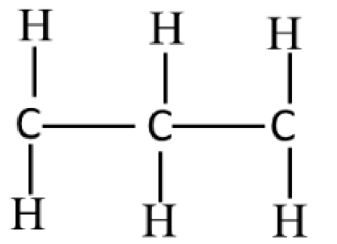
$$= \frac{54(n-3)}{5}+\frac{120}{7}$$

Therefore, $CH(P_n \odot K_{1,2}) = \frac{54(n-3)}{5}+\frac{120}{7}, n \geq 3$

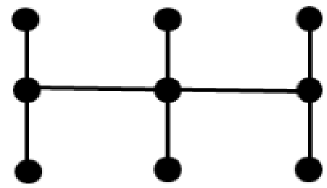
**Example 2.4:**

The following example shows the Contra Harmonic index of cyclohexane $C_3H_6$ using

molecular graph $P_3 \odot K_{1,2}$. Here,
$CH(P_3 \odot K_{1,2}) = CH(C_3H_6)$ is $\frac{120}{7}$.




a) Lewis structure of alkane $C_3H_6$



b) Molecular graph of alkane $C_3H_6$

**Figure 4**

**Theorem 2.5:** Contra Harmonic index of $T_1(n)$ is $\frac{32n}{3} - 4$

**Proof**

Let $u_1, u_2, \dots, u_n$ be vertices in base of the triangles of $T_1(n)$ and let $v_1, v_2, \dots, v_{n-1}$ be the vertices in the peak of the triangles of $T_1(n)$

Then $d(u_1) = d(u_n) = 2$, $d(v_i) = 2, 1 \le i \le n-1$ and $d(u_i) = 4, 2 \le i \le n-1$

$$CH(T_1(n)) = \sum_{uv \in E(G)} \frac{d(u)^2 + d(v)^2}{d(u) + d(v)}$$

$$= \sum_{\substack{u_i v_j \in E(G) \\ i=1,n}} \frac{d(u_i)^2 + d(v_j)^2}{d(u_i) + d(v_j)} + \sum_{\substack{u_i v_j \in E(G) \\ i \neq 1,n}} \frac{d(u_i)^2 + d(v_j)^2}{d(u_i) + d(v_j)} + \sum_{\substack{u_i u_j \in E(G) \\ i=1,n}} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$+ \sum_{\substack{u_i u_j \in E(G) \\ i \neq 1,n}} \frac{d(u_i)^2 + d(u_j)^2}{d(u_i) + d(u_j)}$$

$$= 2 \times \left(\frac{2^2+2^2}{2+2}\right) + 2(n-1)\left(\frac{4^2+2^2}{4+2}\right) + 2\left(\frac{4^2+2^2}{4+2}\right) + (n-2)\left(\frac{4^2+4^2}{4+4}\right)$$

$$= (2 \times 2) + 2n\left(\frac{20}{6}\right) + 4(n-2)$$

Therefore, $CH(T_1(n)) = \frac{32n}{3} - 4$

**Example 2.5:**

The following example shows the Contra Harmonic index of $T_1(4)$. Taking several layers of $T_1(n)$ forms a boron nanotube. Here, $CH(T_1(4))$ is $\frac{116}{3}$

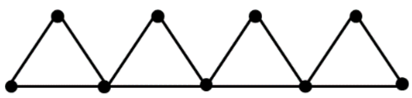


**Figure 5:** $T_1(4)$

## 3. Conclusion

In this paper, we present some applications of obtained results for particular chemical structures such as alkanes and cycloalkanes. Identifying the indices of simple graph structures simplify the identification of complex chemical compounds.

## References


[1] Cao, J, Ali, U, Javaid, M & Huang, C, ‘Zagreb Connection Indices of Molecular Graphs Based on Operations’, *Complexity*, (2020) vol. 2020, no. 1, 7385682.

[2] Groavak, A & Pisanski, T, ‘On the Weiner Index of a Graph’, *Journal of Mathematical Chemistry*, (1991) vol. 8, no. 1, pp. 53-62.

[3] Harary, F, *Graph Theory*, Narosa Publishing House, New Delhi, (1988).

[4] Ragavi, S & Sridevi, R, ‘Contra Harmonic Index of Graphs’, *International Journal of Mathematics Trends and Technology*, (2020) vol. 66, no. 12, pp: 116-121.

[5] Rajeshni Golda, J 2019, Contra harmonic mean labeling of graphs, Ph. D. Thesis submitted to Manonmaniam Sundaranar University (2019).

[6] Sandhya, SS, Somasundaram, S, & Ponraj, R, ‘Some More Results on Harmonic Mean Graphs’, *Journal of Mathematics Research*, (2012) vol. 4, no. 1, pp: 21-29.

[7] Ullah, A, Zaman, S & Harmaz, A, ‘Zagreb Connection Topological Descriptors and Structural Property of the Triangular Snake Structures’, *Physica Scripta*, (2023) vol. 98, no. 2, 025009.

[8] Wiener, H, ‘Structural Determination of Paraffin Boiling Points’, *Journal of the American Chemical Society*, (1947) vol. 69, no. 1, pp: 17-20.