Journal of Engineering and Applied Sciences 13 (Special Issue 1): 2266-2273, 2018
ISSN: 1816-949X

Computing the Harmonic Index for Alkanes, Alkenes and Alkynes

[1]Abdul Jalil Manshad Khalaf, [1]Haneen Kareem Aljanabiy and [2]Hussein Abdel Wasi
[1]Faculty of Computer Sciences and Maths, University of Kufa, Kufa, Iraq
[2]College of Information Technology, University of Babylon, Al-Hillah, Iraq

Abstract: Chemical graph theory is one of the branches in mathematical chemistry that uses graph theory as an index for the chemical occurrence. A topological index is a numerical value that describes a chemical structure for many physical and chemical properties. All organic compounds can be considered as hydrocarbons or compounds derived from hydrocarbons. Double bonds as well as atom kinds, i.e., C, N, O, etc. cannot be recognized using simple topological indices which are defined for only unidirectionally connected graphs. Many topological indices have been developed taking into consideration the state of hybridization for each atom included within the molecule. This study is mainly dedicated to collect most of the data obtained for the chemical and mathematical H indices. In this study, general formulas are established and then proved for a particular topological index of some trees which is the harmonic index for alkanes, alkenes and alkynes ISO-alkanes (2-methyl alkanes) and ISO-alkanes (2, 2-methyl alkanes).

Key words: Graph, harmonic index, alkanes, alkenes and alkynes, unidirectionally, hybridization

INTRODUCTION

A Graph G consists of the following sets:

- Non-empty set V whose elements are known as vertices, nodes of G, denoted as V(G)
- Set of Edges E where each edge $e \in E$ is associated with two elements of V, denoted as E(G) the graph G is composed of vertices V and edges E to be defined as G = (V, E) (Mohammed *et al*., 2016a)

Then, the number of edges touching any vertex v on graph G represents the degree of this vertex and it is denoted as d_v (G). Graph invariants employed in chemical graph theory are known as topological indices which are numerical parameters indicating the structural characteristics.

The topology of a molecule is represented in chemistry using a molecular graph through illustrating the way of atoms connection. In such a graph, the atoms are referred as points while the corresponding covalent bonds are represented by edges. Through utilizing such a technique, the properties of such graphs can then be analyzed to conclude the numerical invariants of any graph (Haoer *et al*., 2016).

Through converting the structure of chemical to a numeric number, topological indices can be established, where physicochemical characteristics for a chemical compound including can be correlated such as strain energy, boiling point, stability, etc. Thus, the graphing theory has gained an increasing attention recently, e.g., the study conducted by Hayat and Imran (2014) for some topological characteristics of particular sorts of networks.

Furthermore, molecular graphs topological indices have been extensively employed to correlate relations between the structural and physicochemical properties of molecular compounds (Das *et al*., 2011). The first index topological recognized in chemical graph theory was Hosoya index which is widely known as the topological index. Afterward, various indices have been established, e.g., Balaban's J index, Randiae's molecular connectivity index and TAU indicators. The Wiener index for example was presented by in 1947 for demonstrating the correlations linking the boiling points for kinds of paraffin (Wiener, 1947). On the other hand, the extended topochemical a tom which is abbreviated as ETA was established by refining the TAU indicators.

In the 1980's, S. Fajtlowicz developed a method for expectation in graph theory field by computer program where the relationships were tested among a lot of graphs invariants one of them is the vertex degree based quantity:

$$H(G)=\sum_{u-v}\frac{2}{d_u(G)+d_v(G)} \tag{1}$$

The concept H(G) did not appeal anyone, especially chemists except Zhang's re-formulation of this quantity in 2012 (Zhong, 2012a, b) and it has been called "harmonic index". The chemical applications of harmonic index have been reported till now, besides the current status in mathematical chemistry such studys are very much to be expected and it can also be viewed as a particular case of the general sum-connectivity index (Mohammed *et al*., 2016b; Gupta *et al*., 2002; Gutman, 2013; Haoer *et al*., 2016).

Corresponding Author: Abdul Jalil Manshad Khalaf, Faculty of Computer Sciences and Maths, University of Kufa, Kufa, Iraq

MATERIALS AND METHODS

Harmonic index of alkanes, alkenes and alkynes: In this part, a general formulae is configured for the harmonic index of some classes of chemical trees (alkanes, alkenes and alkynes).

Alkanes: It is one of the organic compounds that have only carbon-carbon single bonds and has got a chemistry formula as: C_nH_{2n+2} where the carbon atoms number is denoted by n Fig. 1 (Haoer *et al*., 2016).

Alkenes: It is another type of hydrocarbon consisting of one or more carbon-carbon double bonds and written as: C_nH_{2n} knowing that n stands for the carbon atoms number (Haoer *et al*., 2016). So, the hydrogen atoms in alkenes are less than in alkanes (Fig. 2).

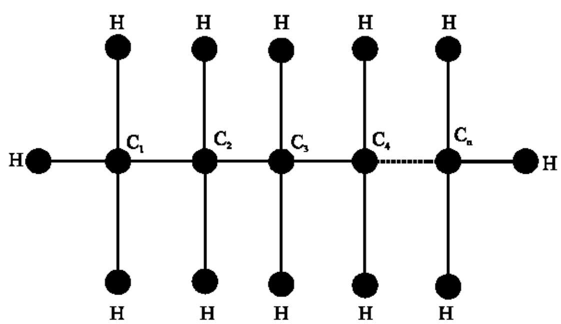

Fig. 1: Classes of alkanes C_nH_{2n+2}

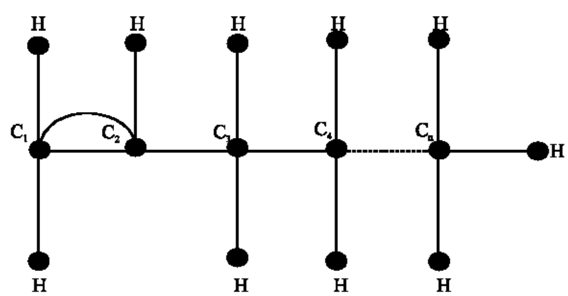

Fig. 2: Classes of alkenes C_nH_{2n}

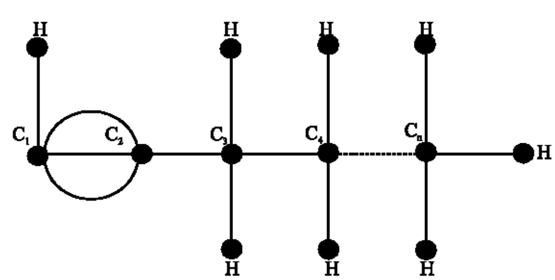

Fig. 3: Classes of alkenes C_nH_{2n-2}

Alkynes: They have one or more carbon-carbon with triple bonds and their molecular formula is: C_nH_{2n-2} where the carbon atoms number is referred as n (Haoer *et al*., 2016). Hence, the hydrogen atoms in Alkynes are less than their counterparts in alkanes and alkenes (Fig. 3).

RESULTS AND DISCUSSION

Theorem 1: Supposing n to be a positive integer number, hence the harmonic index of graph G is:

$$H(G)=\frac{4(n+1)}{5}+\frac{2(n-1)}{8},\ n\geq 1 \tag{2}$$

When G = C_nH_{2n+2} (Fig. 1).

Proof: The following cases are to be proved by mathematical induction:

Case one: When n = 1 then G = CH_4 whose graph is as follows (Fig. 4). Thus:

$$H(CH_4)=\frac{8}{5}$$

Hence, it is true that:

$$H(G)=\frac{4(n+1)}{5}+\frac{2(n-1)}{8}$$

Case two: When n = k and $G_k = C_kH_{2k+2}$ assuming this case true when:

$$k\geq 1,\ H(G)=\frac{4(k+1)}{5}+\frac{2(k-1)}{8}$$

Then, construct the graph $G_{k+1} = C_{k+1}H_{2k+4}$ as follows: The graph G_k has the form Fig. 5. Here, C_i represents the position of Carbon vertex in an ith location and the edge e between C_k vertex in graph G_k and the last vertex of Hydrogen H.

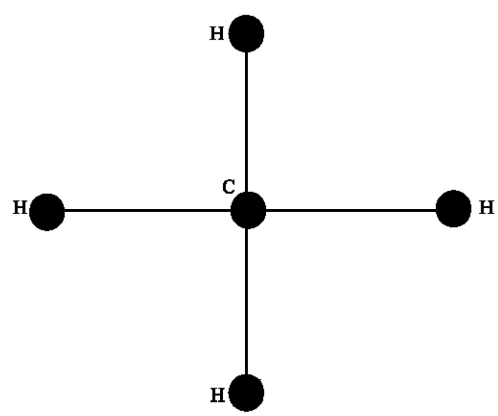

Fig. 4: Methane CH_4

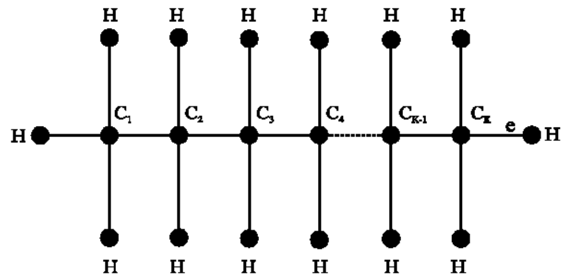

Fig. 5: Graph G_k

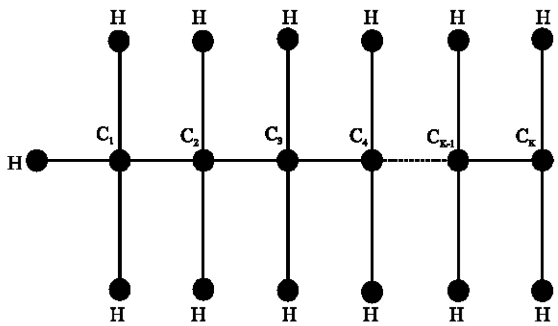

Fig. 6: G^*

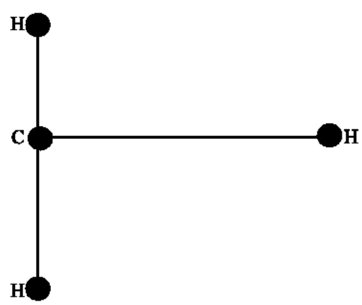

Fig. 7: Graph R

Supposing G* to be a graph obtained by deleting the edge e from G_k Fig. 6. So:

$$
\begin{aligned}
H(G^*) &= H(G)-\frac{2}{1+4} \\
&= \frac{4(k+1)}{5}+\frac{2(k-1)}{8}-\frac{2}{5} \\
&= \frac{4(k+1)-2}{5}+\frac{2k-2}{8} \\
&= \frac{4k+4-2}{5}+\frac{2k-2}{8} \\
&= \frac{4k+2}{5}+\frac{2k-2}{8}
\end{aligned}
$$

Having joined the graph G* with the graph R (Fig. 7). Thus, we have one vertex of carbon adjacent to 3

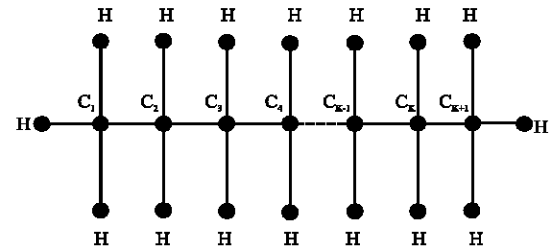

Fig. 8: $C_{k+1}H_{2k+4}$

hydrogen vertices by connecting C_k with C in R to obtain the graph $C_{k+1}H_{2k+4}$ is in the (k+1)th the position of the carbon vertex of this graph (Fig. 8).

In this case, by adding R graph, we get an edge between R and G*. As a matter of fact, adding the degree of vertices of new edges we get three edges connected with (C_{k+1}) vertex and simultaneously they are connected from another side with one vertex. This implies that there are three edges whose vertices degrees equal (4+1) and one edge has got (4+4) degree. Thus, the harmonic index for graphs R and G* assuming R and G* = $C_{k+1}H_{2k+4}$:

$$
\begin{aligned}
H(C_{k+1}H_{2k+4}) &= \frac{4k+2}{5}+\frac{2k-2}{8}+\frac{6}{5}+\frac{2}{8} \\
&= \frac{4k+2+6}{5}+\frac{2k-2+2}{8} \\
&= \frac{4k+8}{5}+\frac{2k}{8} \\
&= \frac{4(k+2)}{5}+\frac{2k}{8} \\
&= \frac{4(k+1+1)}{5}+\frac{2(k+1-1)}{8} \\
&= \frac{4((k+1)+1)}{5}+\frac{2((k+1)-1)}{8}
\end{aligned}
$$

Since, n = k+1, so:

$$H(C_{k+1}H_{2k+4}) = \frac{4(n+1)}{5}+\frac{2(n-1)}{8}$$

Example 2: Let G = C_6H_{14} which is one of alkane formula (Fig. 9). Then, when n = 6, it can be solved following one of the two methods clarified below, first method by definition:

$$H(G_6H_{14}) = \sum_{u-v}\frac{2}{d_u(G)d_v(G)} = \frac{137}{20}$$

Second method by using Theorem 1:

$$
\begin{aligned}
H(G_6H_{14}) &= \frac{4(6+1)}{5}+\frac{2(6-1)}{8} \\
&= \frac{28}{5}+\frac{10}{8} = \frac{137}{20}
\end{aligned}
$$

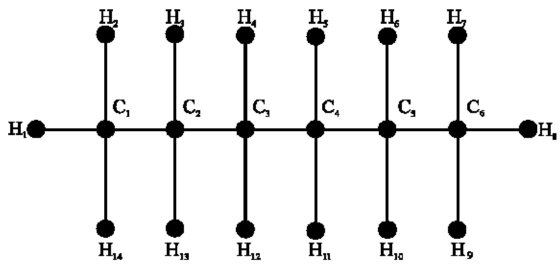

Fig. 9: Hexane C_6H_{14}

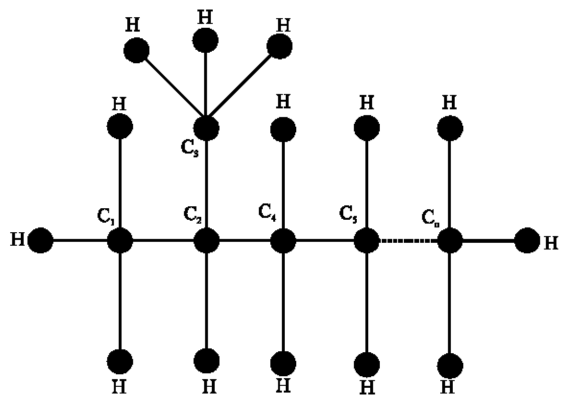

Fig. 10: ISO-alkanes (2-methyl alkanes)

Corollary 3: Assuming n to be a positive integer number. Then, the harmonic index of graph $G = C_nH_{2n+2}$ (Fig. 10) will be:

$$H(G)=\frac{4(n+1)}{5}+\frac{2(n-1)}{8},\ n\geq 4 \tag{3}$$

Proof: This proof is similar in how the theorem has been proven because the graph constructed has the same number of vertices besides it has the same degrees of vertices for each edge and hence, the result of H(G) will be as same as it is for both the alkane and 2-methyl alkanes.

Example 4: Let G = 2-methyl hexane which is one of Alkyne equation (Fig. 11). Then, when n = 7, it can be solved following one of the two methods clarified below. First method by definition:

$$H(C_7H_{16})=\sum_{u-v}\frac{2}{d_u(G)d_v(G)}=\frac{79}{10}$$

Second method by using Corollary 3:

$$H(C_7H_{16})=\frac{4(7+1)}{5}+\frac{2(7-1)}{8}$$
$$=\frac{32}{5}+\frac{10}{8}=\frac{137}{20}$$

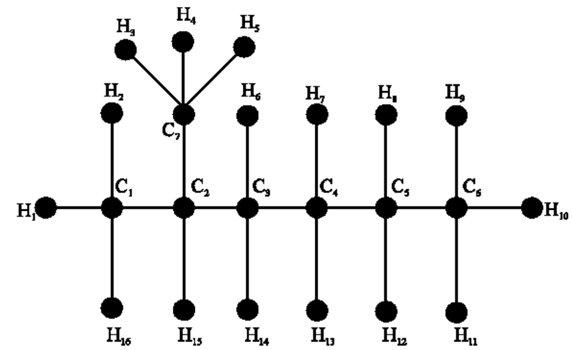

Fig. 11: 2-methyl hexane

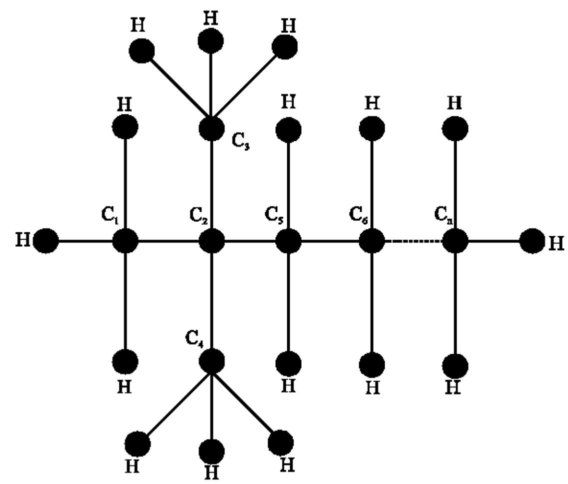

Fig. 12: ISO-alkanes (2,2-methyl alkanes)

Corollary 5: Following the same hypothesis in Corollary the harmonic index of graph $G=C_nH_{2n+2}$ (Fig. 12) is:

$$H(G)=\frac{4(n+1)}{5}+\frac{2(n-1)}{8},n\geq 5 \tag{4}$$

Proof: This proof is similar in how the Theorem 5 has been proven because the graph constructed has the same number of vertices besides it has the same degrees of vertices for each edge and hence, the result of H (G) will be as same as it is for both the alkane and 2, 2-methyl alkanes.

Example 6: Let G = 2, 2-Dimethyl Hexane which is one of alkyne equation (Fig. 13). Then, when n = 8, it can be solved following one of the two methods clarified below: First method by definition:

$$H(C_8H_{18})=\sum_{u-v}\frac{2}{d_u(G)d_v(G)}=\frac{179}{20}$$

Second method by using Corollary 5:

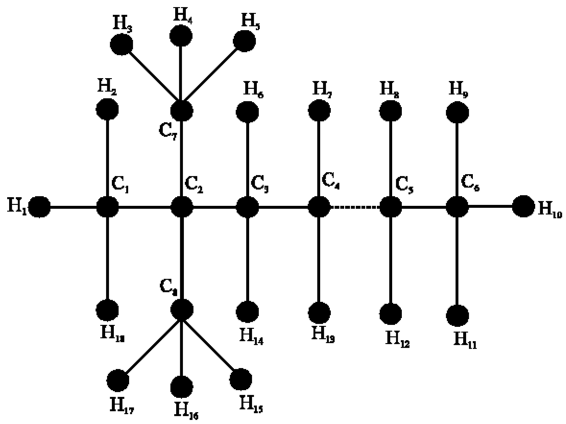

Fig. 13: 2, 2-dimethyl hexane

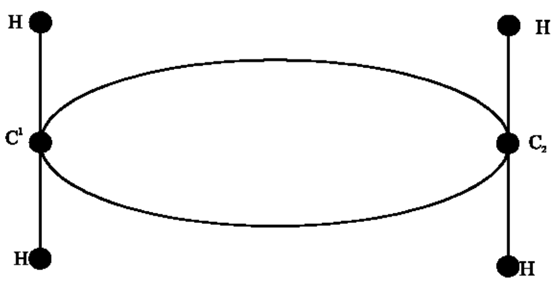

Fig. 14: C_2H_4

$$H(C_8H_{18}) = \frac{4(8+1)}{5}+\frac{2(8-1)}{8}$$
$$= \frac{36}{5}+\frac{14}{8} = \frac{358}{40} = \frac{179}{20}$$

Theorem 6: Assuming to be a positive integer number for the equation $G = C_2H_{2n}$ (Fig. 2). Then, the Harmonic index of graph:

$$H(G)=\frac{4n}{5}+\frac{2n}{8},\ldots,n \geq 2$$

Proof: By means of mathematical induction we will prove the following cases.

Case one: When n = 2 then, $G = C_2H_4$ whose graph will be as Fig. 14. Thus:

$$H(C_2H_4)=\frac{8}{5}+\frac{4}{8}$$

Hence, it is true to say that:

$$H(G)=\frac{4n}{5}+\frac{2n}{8}$$

Case two: When n = k and $G_K = C_KH_{2k+2}$ and assuming this case is true for $k \geq 2$:

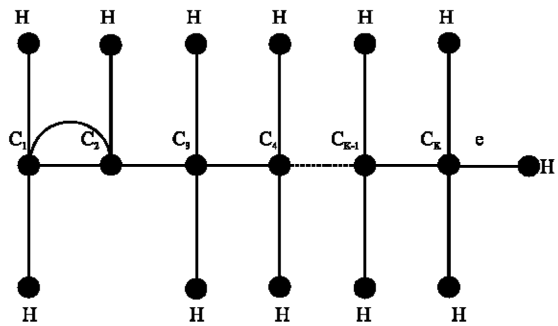

Fig. 15: G_k

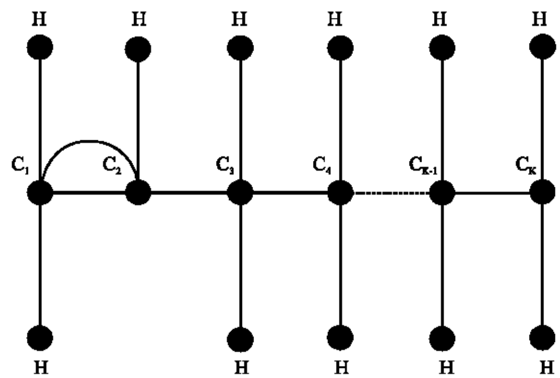

Fig. 16: G^* (case 2)

$$H(G)=\frac{4k}{5}+\frac{2k}{8}$$

Then, constructing the graph of the form $G_{K+1} = C_{K+1}H_{2k+2}$ as follows. The graph G_k has the form (Fig. 15). Here, C_i represents the location of a Carbon vertex in an ith location where the vertex C_K is connected with the end Hydrogen vertex H through the edge e in graph G_k. Now, we suppose to be a graph obtained by deleting the edge from (Fig. 16). So:

$$H(G^*)=H(G)-\frac{2}{1+4}$$
$$=\frac{4k}{5}+\frac{2k}{8}-\frac{2}{5}$$
$$=\frac{4k-2}{5}+\frac{2k}{8}$$

Connecting graph G with graph R (Fig.7). To obtain the graph $C_{k+1}H_{2k+2}$. Thus, we have one vertex of carbon adjacent to 3 hydrogen vertices by connecting C_k with C in R to obtain the graph $C_{k+1}H_{2k+4}$ is in the (k+1)th the position of the carbon vertex of this graph (Fig. 17):

In this case by adding R graph, we get an edge between R and G*. We need to add the degree of vertices

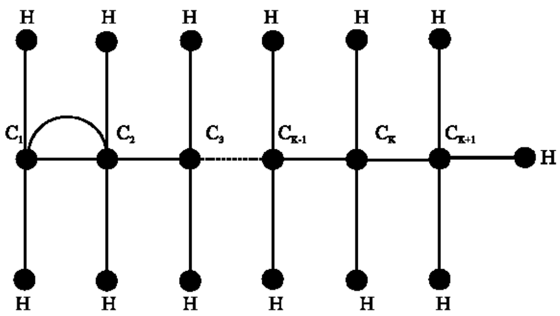

Fig. 17: $G_{k+1}H_{2k+2}$

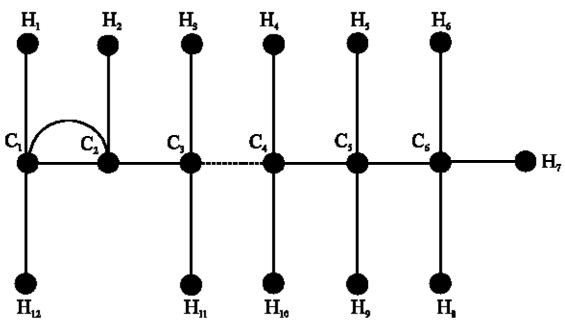

Fig. 18: C_6H_{12}

of new edges; so, we detect three edges connected with (C_{k+1}) vertex and simultaneously they are connected with a one vertex from another side. This implies that there are three edges whose vertices degree equal to (4+1) and one edge has got (4+4) degree, the harmonic index for graphs R and G* assuming R and G* = $C_{k+1}H_{2k+2}$:

$$\begin{aligned}H(C_{k+1}H_{2k+2}) &= \frac{4k\text{-}2}{5}+\frac{2k}{8}+\frac{6}{5}+\frac{2}{8}\\ &= \frac{4k\text{-}2+6}{5}+\frac{2k+2}{8}\\ &= \frac{4k+4}{5}+\frac{2(k+1)}{8}\\ &= \frac{4(k+1)}{5}+\frac{2(k+1)}{8}\end{aligned}$$

Since, n = k+1 so:

$$H(C_nH_{2n})=\frac{4n}{5}+\frac{2n}{8}$$

Example 7: Let G = C_6H_{12} which is one of Alkene equation (Fig. 18). Then, when n = 6, it can be solved following one of the two methods clarified below, first method by definition:

$$H(C_6H_{12})=\sum_{u\sim v}\frac{2}{d_u(G)d_v(G)}=\frac{63}{10} \qquad (5)$$

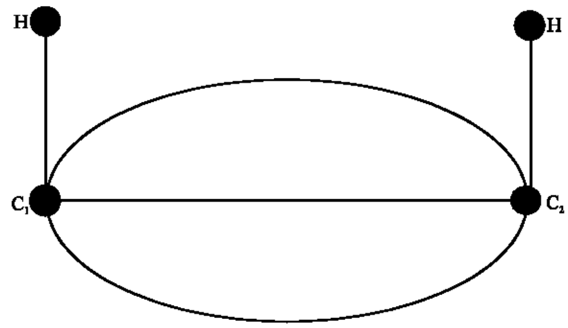

Fig. 19: C_2H_2

Second method by using Theorem 6:

$$\begin{aligned}H(C_6H_{12}) &= 4.\frac{6}{5}+2.\frac{6}{8}\\ &= \frac{24}{5}+\frac{12}{8}=\frac{252}{40}=\frac{63}{10}\end{aligned}$$

Theorem 8: Supposing n to be a positive integer number, then the harmonic index for the graph having the expression G = $C_nH_{2n\text{-}2}$ Fig. 3 is equal to:

$$H(G)=\frac{4n\text{-}4}{5}+\frac{2n+2}{8},\ldots,\ n\geq 2$$

Proof: With the same steps preceded in the proof of theorem in case one when n = 2. Then, C_2H_2 will have the graph (Fig. 19). Thus:

$$H(C_2H_2)=\frac{4}{5}+\frac{6}{8}$$

where it is true to say that:

$$H(G)=\frac{4n\text{-}4}{5}+\frac{2n+2}{8}$$

Case two: When n = k and $G_k = C_kH_{2k\text{-}2}$ whose graph is as follows Fig. 15 where this case can be assumed true for k 2:

$$H(G)=\frac{4k\text{-}4}{5}+\frac{2k+2}{8}$$

Then, the graph can be constructed of the form $G_{k+1} = C_{k+1}\ H_{2k}$ as follows. The graph G_k has the form (Fig. 20). Now, the Carbon vertex position is denoted as C_i in ith location and e is the edge connecting the vertex G_k to the end Hydrogen vertex H in graph Gk. Now, removing edge e from G_k results in a new graph called G^* (Fig. 21):

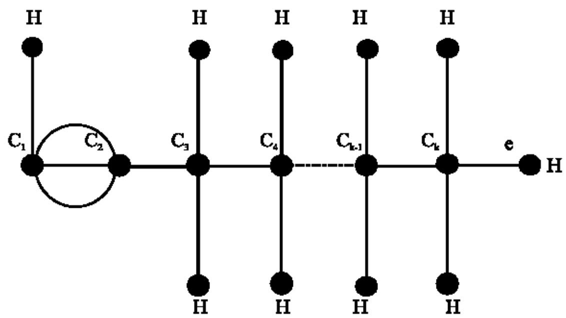

Fig. 20: G_k (case 2)

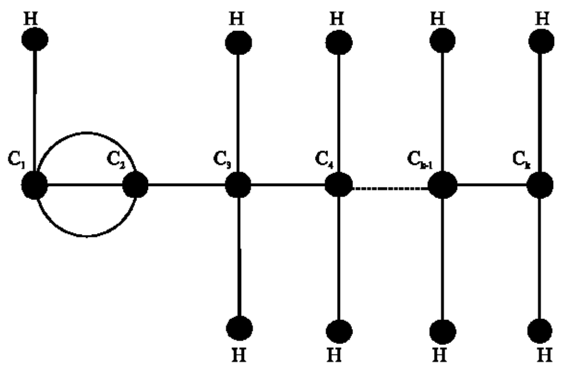

Fig. 21: G^* (Theorem 8)

$$
\begin{aligned}
H(G^*) &= H(G) - \frac{2}{1+4} \\
&= \frac{4k-4}{5} + \frac{2k+2}{8} - \frac{2}{5} \\
&= \frac{4k-4-2}{5} + \frac{2k+2}{8} \\
&= \frac{4k-6}{5} + \frac{2k+2}{8}
\end{aligned}
$$

Now, the graph G* is connected with graph R (Fig. 7). Thus, we have one vertex of carbon adjacent to 3 hydrogen vertices by connecting C_k with C in R, to obtain the graph $C_{k+1}H_{2k+4}$ is in the (k+1)th the position of the carbon vertex of this graph (Fig. 22).

In this case, by adding R graph, we get an edge between R and G*. Adding the degree of vertices of the new edges. In fact, we have three edges connected with (C_{k+1}) vertex and in another side it is connected with one vertex. This implies that there exist three edges, the degree of its vertices is equal to (4+1) and one of edge has (4+4) degree. Then, we obtain the graph C_{k+1} H_{2k} and the harmonic index for graphs R and G* assuming R and $G^* = C_{k+1}H_{2k}$:

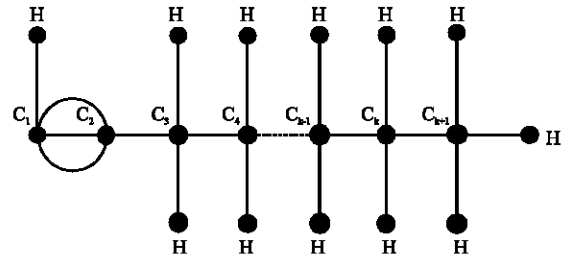

Fig. 22: $C_{k+1}H_{2k}$

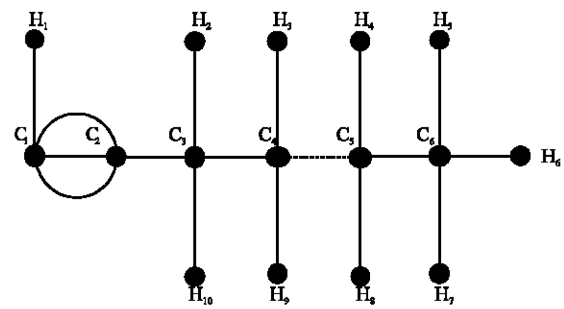

Fig. 23: C_6H_{10}

$$
\begin{aligned}
H(C_{k+1}H_{2k}) &= \frac{4k-6}{5} + \frac{2k+2}{8} + \frac{6}{5} + \frac{2}{8} \\
&= \frac{4k-6+6}{5} + \frac{2k+2+2}{8} \\
&= \frac{4k}{5} + \frac{2k+2+2}{8} \\
&= \frac{4k+4-4}{5} + \frac{2k+2+2}{8} \\
&= \frac{4(k+1)-4}{5} + \frac{2(k+1)+2}{8}
\end{aligned}
$$

Since, n = k+1 so:

$$
H(C_nH_{2n-2}) = \frac{4n-4}{5} + \frac{2n+2}{8}
$$

Example 9: Let G = C_6H_{10} which is Alkyne equation (Fig. 23). Then, when n = 6, it can be solved following one of the two methods clarified below. First method by definition:

$$
H(C_6H_{10}) = \sum_{u-v} \frac{2}{d_u(G)d_v(G)} = \frac{115}{20} \tag{7}
$$

Second method by using Theorem 8:

$$
\begin{aligned}
H(C_6H_{10}) &= \frac{4.6-4}{5} + \frac{2.6+2}{8} \\
&= \frac{20}{5} + \frac{14}{8} = \frac{230}{40} = \frac{115}{20}
\end{aligned}
$$

CONCLUSION

In the current, a general formula is established and proved by mathematical induction for harmonic index of some trees which are alkanes, alkenes, alkynes ISO-alkanes (2-methyl alkanes) and ISO-alkanes (2, 2-methyl alkanes).

In the current research, new methodologies are established and proven through the mathematical induction. For each one of them, a detailed example is presented and solved following two ways, i.e., direct and indirect. The direct method is implemented through using the traditional definition while the other one is based on the new theorems presented in the current study. The comparison conducted between the two aforementioned solutions has led to identical results emphasizing the reliability of the theorems introduced herein.

REFERENCES

Das, K.C., I. Gutman and B. Furtula, 2011. Survey on geometric-arithmetic indices of graphs. Match Commun. Math. Comput. Chem., 65: 595-644.

Gupta, S., M. Singh and A.K. Madan, 2002. Application of graph theory: Relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity. J. Math. Anal. Appl., 266: 259-268.

Gutman, I., 2013. Degree-based topological indices. Croat. Chem. Acta, 86: 351-361.

Haoer, R.S., K.A. Atan, A.M. Khalaf, M. Rushdan and R. Hasni, 2016. Eccentric connectivity index of some chemical trees. Int. J. Pure Appl. Math., 106: 157-170.

Hayat, S. and M. Imran, 2014. Computation of topological indices of certain networks. Applied Math. Comput., 240: 213-228.

Mohammed, M.A., K.A. Atan, A.M. Khalaf, R. Hasni and M.R. Said, 2016b. Atom bond connectivity index of molecular graphs of alkynes and cycloalkynes. J. Comput. Theor. Nanosci., 13: 6698-6706.

Mohammed, M.A., K.A. Attan, A.M. Khalaf, M. Rushdan and R. Hasni, 2016a. The atom bond connectivity index of certain graphs. Int. J. Pure Appl. Math., 106: 415-427.

Wiener, H., 1947. Structural determination of paraffin boiling points. J. Am. Chem. Soc., 69: 17-20.

Zhong, L., 2012b. The harmonic index for graphs. Appl. Math. Lett., 25: 561-566.

Zhong, L., 2012a. The harmonic index on unicyclic graphs. Ars Comb., 104: 261-269.