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Non-Neighbor Topological Indices for Hydrocarbons

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Abstract**—** *A graph can be represented by a unique number, a matrix, a sequence, and a polynomial which represents the whole graph and these representations are uniquely defined for that graph. The representation of the graph by a unique number is called topological index. Depending on vertex degrees, a large number of molecular-graph-based topological indices have been conceived. Based on the non-neighbors of the vertices of a graph G, Non- Neighbor Zagreb Indices and Non-Neighbor Harmonic Index have been introduced. In this paper we summarize the formula of these Non-Neighbor Topological Indices for Hydrocarbons. Also the computation of these topological indices for basic alkanes, alkenes and alkynes are provided.*

Keywords**—** *Topological index, non-neighbor topological index, molecular graphs, hydrocarbons.*

I. INTRODUCTION

Chemical Graph Theory is a branch of Mathematical Chemistry which applies graph theory to the mathematical model of chemical phenomenon. A molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory [7]. In chemical graph, vertices correspond to the atoms of the compound and edges correspond to the covalent bonds. A hydrogen-depleted molecular graph or hydrogen-suppressed molecular graph is the molecular graph with hydrogen vertices deleted. The characterization of a molecule by an associated graph leads to a large number of powerful and useful discriminators called topological indices. In chemical graph theory a topological index is a numerical parameter mathematically derived from hydrogen-suppressed molecular graphs. A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph such as distance based, degree based and both degree and distance based [4]. Topological indices are used in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. Quantitative structure-activity relationship and Quantitative structure-property relationship (QSAR/QSPR) studies are of great importance in modern chemistry and biochemistry. Many descriptors reflect simple molecular properties and thus provide insight into the physicochemical nature of the activity or property under consideration.

Let G be a molecular graph. The sets of vertices and edges of G are denoted by $V=V(G)$ with cardinality n and $E=E(G)$ respectively. Two vertices of G, connected by an edge, are said to be "adjacent". The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex, and will be denoted by $d_v(G)$ or, simply by d_v. The concept of degree in graph theory is closely related (but not identical) to the concept of valence in chemistry.

The vertices that are not adjacent to a vertex $v \in V(G)$ are called non-neighbors [9] of the vertex v. In this paper we define $\overline{d_G(v)}$ as the number of the non-neighbors of the vertex $v \in V(G)$ where $\overline{d_G(v)} = n-1-d_G(v)$ Hence

The Non-Neighbor First Zagreb Index is defined as

$$\overline{M_1(G)} = \sum_{uv \in E(G)} \left(\overline{d_G(u)} + \overline{d_G(v)} \right)$$

The Non-Neighbor Second Zagreb Index is defined as

$$\overline{M_2(G)} = \sum_{uv \in E(G)} \left(\overline{d_G(u)}.\overline{d_G(v)} \right)$$

The Non-Neighbor Harmonic Index is defined as

$$\overline{H(G)} = \sum_{uv \in E(G)} \left(\frac{2}{\overline{d_G(u)} + \overline{d_G(v)}} \right)$$

In this paper non-neighbor topological indices called Non-Neighbor First Zagreb Index, Non-Neighbor Second Zagreb Index and Non-Neighbor Harmonic Index [5, 6] based on the non-neighbors of the vertices of a graph G is computed for Basic Hydrocarbons. In the first section, these non-neighbor topological indices for the molecular graphs of basic alkanes, alkenes and alkynes are provided. In the last section, computed values of these non-neighbor topological indices for basic alkanes, alkenes and alkynes are given. For terms and definition not given in this paper we refer to [1, 2, 3, 7].

II. NON-NEIGHBOR TOPOLOGICAL INDICES FOR BASIC HYDROCARBONS

A. Saturated hydrocarbons

In organic chemistry, a hydrocarbon is an organic compound [8] consisting entirely of hydrogen and carbon atoms. Hydrocarbons which contain only single bond are called alkanes. They are called saturated hydrocarbons with a general formula C_nH_{2n+2}. Illustrative examples of some alkanes are provided in Fig. 1.

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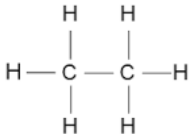
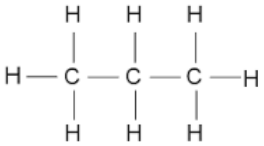
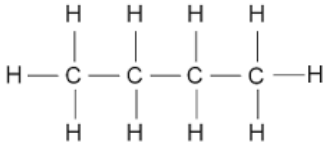


Ethane (C_2H_6)



Propane (C_3H_8)



Butane (C_4H_{10})

Fig. 1.

The hydrogen depleted molecular graphs corresponding to Propane and Butane are shown along with their number of non-neighbors in Fig. 2. They represent the path P_3 and P_4 repectively. Hence the hydrogen depleted molecular graphs of alkanes corresponds to the path P_n.

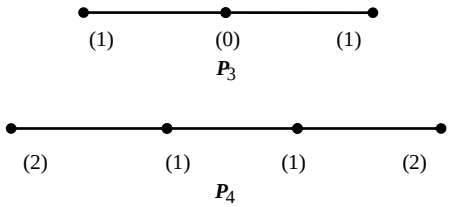


Fig. 2.

Theorem 2.1: *For the molecular graph G of alkanes with* $n \geq 3$ *vertices,* $\overline{M_1(G)} = 2(n-2)^2$, $\overline{M_2(G)} = (n-3)\left(n^2-4n+5\right)$ *and for the molecular graph G of alkanes with* $n \geq 4$ *vertices* $\overline{H(G)} = \frac{4}{2n-5}+1$

Proof: A path P_n represents the molecular graph G of alkanes. A path P_n with n vertices has two pendant vertices and remaining are interior vertices each with degree 2. The number of non-neighbors of the pendant vertex is $(n-2)$. The number of non-neighbors of the interior vertex is $(n-3)$ There are totally $(n-1)$ edges in P_n of which two are corner edges and $(n-3)$ are interior edges. Hence,

The Non-Neighbor First Zagreb Index of a path,

$$P_n(n \geq 3) = 2\left[(n-2)+(n-3)\right]+(n-3)\left[(n-3)+(n-3)\right]$$
$$= 2\left[2n-5\right]+(n-3)[2n-6]$$

Hence $\overline{M_1(G)} = 2(n-2)^2$

The Non-Neighbor Second Zagreb Index of a path,

$$P_n(n \geq 3) = 2\left[(n-2)\times(n-3)\right]+(n-3)\left[(n-3)\times(n-3)\right]$$
$$= 2(n-2)(n-3)+(n-3)^3$$

Hence $\overline{M_2(G)} = (n-3)\left(n^2-4n+5\right)$

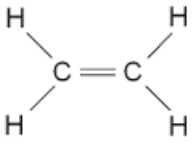
The Non-Neighbor Harmonic Index of a path,

$$P_n(n \geq 4) = 2\left[\frac{2}{(n-2)+(n-3)}\right]+(n-3)\left[\frac{2}{(n-3)+(n-3)}\right]$$

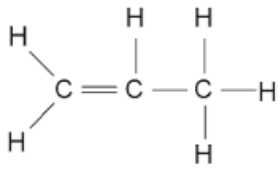
Hence $\overline{H(G)} = \frac{4}{2n-5}+1$

B. Unsaturated Hydrocarbons

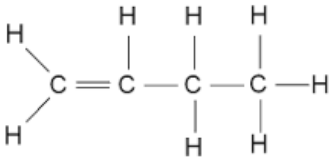
Unsaturated hydrocarbons are organic compounds that have one or more double or triple bonds between carbon atoms. Those with double bonds are called alkenes with general formula C_nH_{2n}. Those with triple bonds are called alkynes with general formula C_nH_{2n-2}. Illustrative examples of some alkenes are provided in Fig. 3.



Ethene (C_2H_4)



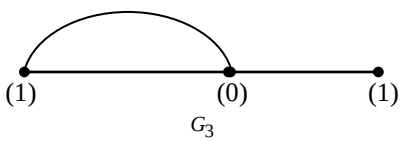
Propene (C_3H_6)



1-Butene (C_4H_8)

Fig. 3.

The hydrogen depleted molecular graphs corresponding to Propene and 1-Butene are shown along with their number of non-neighbors in Fig. 4. Since multiple edges exist they are not simple graphs. They represent the multigraphs G_3, G_4 respectively.



G_3

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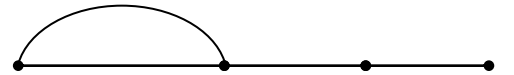
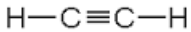


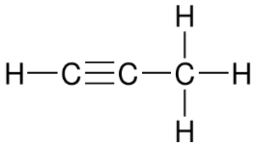
G_4

Fig. 4.

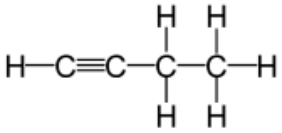
Illustrative examples of some alkynes are provided in Fig. 5.



Ethyne (C_2H_2)



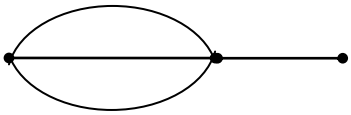
Propyne (C_3H_4)



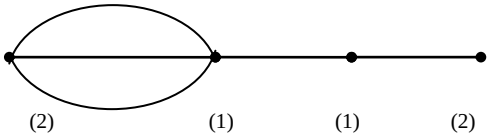
1-Butyne (C_4H_6)

Fig. 5.

The hydrogen depleted molecular graphs corresponding to Propyne and 1-Butyne are shown along with their number of non-neighbors in Fig. 6. Since multiple edges exist they are not simple graphs. They represent the multigraphs $G_3^{'}$,$G_4^{'}$ respectively.



$G_3^{'}$



$G_4^{'}$

Fig. 6.

Theorem 2.2: *For the molecular graph G of alkenes with* $n \geq 3$ *vertices,* $\overline{M_1(G)} = 2n^2 - 6n + 3$, $\overline{M_2(G)} = (n-3)\left(n^2 - 3n + 3\right)$ *and for the molecular graph G of alkenes with* $n \geq 4$ *vertices* $\overline{H(G)} = \frac{6}{2n-5} + 1$.

Proof: A path P_n with one multiple edge represents the molecular graph *G* of alkenes. A path P_n with *n* vertices has two pendant vertices and remaining are interior vertices each with degree 2. The number of non-neighbors of the pendant vertex is $(n-2)$. The number of non-neighbors of the interior vertex is $(n-3)$ There are $(n-1)$ edges in P_n of which two are corner edges and $(n-3)$ are interior edges. Along with these edges there exists one more edge which is a multiple edge. Hence,

The Non-Neighbor First Zagreb Index of a path with one multiple edge

$$P_n(n \geq 3) = 3\left[(n-2)+(n-3)\right] + (n-3)\left[(n-3)+(n-3)\right]$$
$$= 3\left[2n-5\right] + (n-3)\left[2n-6\right]$$

Hence $\overline{M_1(G)} = 2n^2 - 6n + 3$

The Non-Neighbor Second Zagreb Index of a path with one multiple edge

$$P_n(n \geq 3) = 3\left[(n-2)\times(n-3)\right] + (n-3)\left[(n-3)\times(n-3)\right]$$
$$= 3(n-2)(n-3) + (n-3)^3$$

Hence $\overline{M_2(G)} = (n-3)\left(n^2 - 3n + 3\right)$

The Non-Neighbor Harmonic Index of a path with one multiple edge

$$P_n(n \geq 4) = 3\left[\frac{2}{(n-2)+(n-3)}\right] + (n-3)\left[\frac{2}{(n-3)+(n-3)}\right]$$

Hence $\overline{H(G)} = \frac{6}{2n-5} + 1$

Theorem 2.3: *For the molecular graph G of alkynes with* $n \geq 3$ *vertices,* $\overline{M_1(G)} = 2(n^2 - 2n - 1)$, $\overline{M_2(G)} = (n-3)\left(n^2 - 2n + 1\right)$ *and for the molecular graph G of alkynes with* $n \geq 4$ *vertices* $\overline{H(G)} = \frac{8}{2n-5} + 1$.

Proof: A path P_n with two multiple edges represents the molecular graph *G* of alkynes. A path P_n with *n* vertices has two pendant vertices and remaining are interior vertices each with degree 2. The number of non-neighbors of the pendant vertex is $(n-2)$. The number of non-neighbors of the interior vertex is $(n-3)$ There are $(n-1)$ edges in P_n of which two are corner edges and $(n-3)$ are interior edges. Along with these edges there exist two more edges which are multiple edges. Hence,

The Non-Neighbor First Zagreb Index of a path with two multiple edges

$$P_n(n \geq 3) = 4\left[(n-2)+(n-3)\right] + (n-3)\left[(n-3)+(n-3)\right]$$
$$= 4\left[2n-5\right] + (n-3)\left[2n-6\right]$$

Hence $\overline{M_1(G)} = 2(n^2 - 2n - 1)$.

The Non-Neighbor Second Zagreb Index of a path with two multiple edges

$$P_n(n \geq 3) = 4\left[(n-2)\times(n-3)\right] + (n-3)\left[(n-3)\times(n-3)\right]$$
$$= 4(n-2)(n-3) + (n-3)^3$$

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Hence $\overline{M_2(G)} = (n-3)(n^2-2n+1)$.

The Non-Neighbor Harmonic Index of a path with two multiple edges

$$P_n(n \geq 4) = 4\left[\frac{2}{(n-2)+(n-3)}\right] + (n-3)\left[\frac{2}{(n-3)+(n-3)}\right]$$

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

Remark 2.1: *For the molecular graph G with* $n = 3$ *vertices,*

$\overline{H(G)} = 4$ *for alkanes*

$\overline{H(G)} = 6$ *for alkenes*

$\overline{H(G)} = 8$ *for alkynes*

III. Computed values of Non-Neighbor Topological Indices for Basic Hydrocarbons

The topological index of methane, methene and methyne cannot be found as their molecular graph has only one vertex and no edges. The molecular graph of the hydrocarbons ethane, ethene and ethyne has only two vertices in which both are adjacent and the number of non- neighbors of each vertex is zero. Hence the Non-Neighbor First Zagreb index and Non-Neighbor Second Zagreb index of these hydrocarbons are zero while the Non- Neighbor Harmonic index does not exists.

Computed values of Non-Neighbor First Zagreb index, Non-Neighbor Second Zagreb index and Non Neighbor Harmonic index for basic alkanes are given in the table 1.

TABLE 1. Non-Neighbor Harmonic Index of Alkanes.

Topological Index	Ethane	Propane	Butane	Pentane	Hexane
$\overline{M_1(G)}$	0	2	8	18	32
$\overline{M_2(G)}$	0	0	5	20	51
$\overline{H(G)}$	-	4	2.33	1.8	1.57

Computed values of Non-Neighbor First Zagreb index, Non-Neighbor Second Zagreb index and Non Neighbor Harmonic index for basic alkenes are given in the table 2.

TABLE 2. Non-Neighbor Harmonic Index of Alkenes.

Topological Index	Ethene	Proene	Butene	Pentene	Hexene
$\overline{M_1(G)}$	0	3	11	23	39
$\overline{M_2(G)}$	0	0	7	26	63
$\overline{H(G)}$	-	6	3	2.2	1.86

Computed values of Non-Neighbor First Zagreb index, Non-Neighbor Second Zagreb index and Non Neighbor Harmonic index for basic alkynes are given in the table 3.

TABLE 3. Non-Neighbor Harmonic Index of Alkynes.

Topological Index	Ethyne	Propyne	Butyne	Pentyne	Hexyne
$\overline{M_1(G)}$	0	4	14	28	46
$\overline{M_2(G)}$	0	0	9	32	75
$\overline{H(G)}$	-	8	3.67	2.6	2.14

From the computed values obtained in the tables 1, tables 2 and tables 3 we infer that the Non-Neighbor First Zagreb index and Non-Neighbor Second Zagreb index of alkanes, alkenes and alkynes show a gradual increase as the number of carbon atoms increases. We also infer that the Non-Neighbor Harmonic index of alkanes, alkenes and alkynes show a gradual decreases as the number of carbon atoms increases.

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