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. 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 \( d_G(v) \) as the number of the non-neighbors of the vertex \( v \in V(G) \) where \( d_G(v) = n - 1 - d_G(v) \). Hence

The Non-Neighbor First Zagreb Index is defined as

\[
M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))
\]

The Non-Neighbor Second Zagreb Index is defined as

\[
M_2(G) = \sum_{uv \in E(G)} (d_G(u)d_G(v))
\]

The Non-Neighbor Harmonic Index is defined as

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

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.
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 $P_4$ respectively. Hence the hydrogen depleted molecular graphs of alkanes corresponds to the path $P_n$.

\[ M_1(G) = 2(n-2)^2 \]

The Non-Neighbor Second Zagreb Index of a path, $P_n (n \geq 3) = 2\left(\frac{2(n-3)}{(n-3) + 2(n-3)}\right) + (n-3)\left(\frac{2(n-3)}{(n-3) + (n-3)}\right) = 2(n-2) + (n-3)^3$

Hence $M_2(G) = (n-3)(n^2 - 4n + 5)$

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

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.
The molecular graph $G$ of alkenes with one multiple edge represents the multigraph 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

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

$$= 3[2n-5] + (n-3)[2n-6]$$

Hence $M_1(G) = 2n^2 - 6n + 3$

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

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

$$= 3(n-2)(n-3) + (n-3)^3$$

Hence $M_2(G) = (n-3)(n^2 - 3n + 3)$

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

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

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

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

**Proof:** A path $P_n$ with two multiple edges 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 neighbors of the interior vertex is $(n-3)$. There are $(n-1)$ edges in $P_n$, of which two are interior 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 two multiple edges

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

$$= 4[2n-5] + (n-3)[2n-6]$$

Hence $M_1(G) = 2(n^2 - 2n - 1)$.

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

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

$$= 4(n-2)(n-3) + (n-3)^3$$
Hence \( M_2(G) = (n-3)(n^2 - 2n + 1) \).

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

**Remark 2.1:** For the molecular graph \( G \) with \( n = 3 \) vertices, 

\( H(G) = 4 \) for alkanes

\( H(G) = 6 \) for alkenes

\( H(G) = 8 \) 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 exist.

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>
<thead>
<tr>
<th>Topological Index</th>
<th>Ethane</th>
<th>Propane</th>
<th>Butane</th>
<th>Pentane</th>
<th>Hexane</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_1(G) )</td>
<td>0</td>
<td>2</td>
<td>8</td>
<td>18</td>
<td>32</td>
</tr>
<tr>
<td>( M_2(G) )</td>
<td>0</td>
<td>0</td>
<td>5</td>
<td>20</td>
<td>51</td>
</tr>
<tr>
<td>( H(G) )</td>
<td>-</td>
<td>4</td>
<td>2.33</td>
<td>1.8</td>
<td>1.57</td>
</tr>
</tbody>
</table>

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>
<thead>
<tr>
<th>Topological Index</th>
<th>Ethene</th>
<th>Proene</th>
<th>Butene</th>
<th>Pentene</th>
<th>Hexene</th>
</tr>
</thead>
<tbody>
<tr>
<td>( M_1(G) )</td>
<td>0</td>
<td>3</td>
<td>11</td>
<td>23</td>
<td>39</td>
</tr>
<tr>
<td>( M_2(G) )</td>
<td>0</td>
<td>0</td>
<td>7</td>
<td>26</td>
<td>63</td>
</tr>
<tr>
<td>( H(G) )</td>
<td>-</td>
<td>6</td>
<td>3</td>
<td>2.2</td>
<td>1.86</td>
</tr>
</tbody>
</table>

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 alkenes, alkynes show a gradual increase as the number of carbon atoms increases. We also infer that the Non-Neighbor Harmonic index of alkenes, alkynes show a gradual decreases as the number of carbon atoms increases.

### REFERENCES