DEGREE-BASED TOPOLOGICAL INDICES OF ALKANES BY APPLYING SOME GRAPH OPERATIONS

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Abstract

Graph operations play an important role in many application of graph theory because many large graphs can be constructed from small graphs. Here we study two graph-theoretical operations, i.e., the double and the strong double graph. In the organic compounds alkane is least reactive and simplest hydrocarbon that contains hydrogen (H) and carbon (C) atoms and have no any other functional groups. In this paper, we computed the topological indices, namely, Inverse sum indeg index ($ISI$), first multiplicative-Zagreb index ($PM_1$), atom bond connectivity index ($ABC$), forgotten index ($F$), geometric arithmetic index ($GA$), second multiplicative-Zagreb index ($PM_2$) for the double and strong double graph of alkane $C_{1}H_{2t+2}$. In addition, we also give a graphical and numerical comparison of these topological indices.

Keywords: degree-based topological indices; alkanes; strong double graph; double graph.
Mathematics Subject Classification: 05C12, 05C90.

1. Introduction and Preliminaries

Consider that $G$ is an undirected chemical graph having no loops and multiple edges. In chemical graphs, an atom represents the vertex $V$ and the bonding between atoms represents the edge $E$. The order of a graph is the number of vertices in a graph $G$ and the size of a graph is the number of edges in a graph $G$. The degree of a vertex $d_{v}$ is the number of edges connecting it. For undetermined notations and terminologies, R. J. Wilson book is recommended [1]. The Handshaking lemma is very useful for calculating the total number of edges in graph $G$. Lenford Euler discovered it in 1736. The Handshaking lemma is often known as the first theorem of graph theory [2]. Chemical graph theory should be seen not only as equivalent to other fields of
theoretical chemistry but also as complementary and important for a deeper knowledge of the nature of chemical structure and helpful in modeling the molecular structure. One of the most important areas of graph theory is quantitative structural properties (QSPR) and structural activity relationship (QSAR). The topological index can give us information about the shape of the molecule. A chemical structure can be converted into a numerical value using a topological index, which is particularly useful in (QSPR)/(QSAR) investigations. Topological indices shows a significant role in assisting chemists for modelling the molecular structure of chemical compounds and studying their chemical and physical characteristics. Different types of topological indices have been presented, i.e., degree-based [3] [4] [5], distance-based [6], and counting related topological indices etc. [7] [8]. These indices are computed for many graphs and many other new graphs which are constructed by using different graph operations [9]. The idea of topological indices comes from the work of Wiener [10]. Assume the graph $G$, the Wiener index [10] is defined as follows:

$$W(G') = \frac{1}{2} \sum_{(r,s)} d(r,s).$$

(1)

Furtula & Vukicevic [11] introduced the geometric arithmetic index as follows:

$$GA(G') = \sum_{rs \in E(G)} \frac{2\sqrt{d_r d_s}}{d_r + d_s}.$$

(2)

Das, Gutman, & Furtula in [12] introduced the Atom Bond Connectivity index ($ABC$) as follows:

$$ABC(G') = \sum_{rs \in E(G)} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.$$

(3)

Furtula & Gutman [13] introduced the Forgotten index ($F$) as follows:

$$F(G') = \sum_{rs \in E(G)} (d_r^2 + d_s^2).$$

(4)

Pattabiraman [14] introduced the Inverse Sum Indeg index ($ISI$) as follows:

$$ISI(G') = \sum_{rs \in E(G)} \frac{1}{d_r} + \frac{1}{d_s}.$$

(5)

Ali, Kirmani, Rugaie, & Azam [15] introduced the General Inverse Sum indeg index ($ISI_{(\alpha, \beta)}$) as follows:

$$ISI_{(\alpha, \beta)}(G') = \sum_{rs \in E(G)} [d_r d_s]^\alpha [d_r + d_s]^\beta,$$

(6)

where $\alpha$ and $\beta$ are real numbers.

Kazemi [16] introduced the First Multiplicative-Zagreb index ($PM_1$) and second multiplicative-Zagreb index index ($PM_2$) as follows:

$$PM_1(G') = \prod_{rs \in E(G)} (d_r)^2,$$

(7)

$$PM_2(G') = \prod_{rs \in E(G)} (d_r . d_s).$$

(8)
Eliasi, Iranmanesh, & Gutman [17] introduced the another version of First Multiplicative-Zagreb index \((PM_1)\) as follows.

\[
PM_1(G') = \prod_{rs \in E(G')} (d_r + d_s).
\]  

(9)

It is recommended for the readers to study the following research works for more comprehensive information about topological indices ([3, 18-20]).

**Definition 1.1.** Alkanes are completely composed of single-bonded hydrogen and carbon atoms, where carbon and hydrogen are arranged in tree like structures as depicted in Figure 1. The general formula of the alkanes is \(C_mH_{(2m+2)}\) where, \(m \geq 1\). They are commercially very useful because they are the leading component of lubricants and gasoline while the first four alkanes are used primarily for cooking, heating and power generation.

Graph operations plays an important role in many applications of chemical graph theory and some other fields. We use graph operations on alkanes to create a new molecular structure.

**Definition 1.2.** The double graph \(D[G]\) of \(G\) is a graph obtained by taking two copies of \(G\) and joining each vertex in one copy with the neighbors of corresponding vertex in another copy [21]. The double graph of the Alkanes \((C_2H_6)\) is illustrated in Figure 2 and it is represented by \(D(G')\).
Definition 1.3. The strong double graph is represented by $SD[G]$. It is constructed by taking two copies of graph $G$ and linking with closed neighborhood of every vertex in one copy to adjacent vertex in the other copy [22]. Strong double graph $SD(CH_4)$ is illustrated in the following Figure 3.

![Figure 3. Alkane (CH$_4$) and its strong double graph [SD(CH$_4$)].](image)

2. Topological Indices of Double Graph of Alkanes ($C_mH_{2m+2}$)

In this Section, the topological indices for the double graph of alkanes $C_mH_{2m+2}$ will be determined:

**Theorem 2.1.** Suppose that $D(C_mH_{2m+2})$ is the double graph of alkanes $C_mH_{2m+2}$. Then,

- $GA[D(C_mH_{2m+2})] = \frac{1}{5}(52m + 12)$.
- $ABC[D(C_mH_{2m+2})] = \frac{\sqrt{2}}{2}((m - 1)\sqrt{7} + 8m + 8)$.
- $F[D(C_mH_{2m+2})] = 1056m + 32$.
- $ISI[D(C_mH_{2m+2})] = \frac{1}{5}(144m - 16)$.
- $ISI(\alpha, \beta)[D(C_mH_{2m+2})] = 8(m + 1)[16]^\alpha[10]^\beta + 4(m - 1)[64]^\alpha[16]^\beta$.
- $PM_1[D(C_mH_{2m+2})] = 5120(m^2 - 1)$.
- $PM_2[D(C_mH_{2m+2})] = 32768(m^2 - 1)$.

**Proof:** The total number of vertices of the double graph of alkanes is $2(3m + 2)$ and edges are $4(3m + 1)$, respectively. In $D(C_mH_{2m+2})$, we have $4(m + 1)$ vertices having degree 2 and $2m$ vertices having degree 8. We separate edges of the $D(C_mH_{2m+2})$ into the type $E[d_r, d_s]$ in which $rs$ is represents the edges. Edges present in $D(C_mH_{2m+2})$ consists of $E_{(2,8)}$ and $E_{(8,8)}$, and these types of edges are present in Table 1.
Table 1. Separation of edges.

<table>
<thead>
<tr>
<th>$E[d_r, d_s]$</th>
<th>$E_{(2,8)}$</th>
<th>$E_{(8,8)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$8(m + 1)$</td>
<td>$4(m - 1)$</td>
</tr>
</tbody>
</table>

Now by using Equations (2-9) and the

Table 1, we obtain the desired results, i.e.,

$$GA[G] = \sum_{rs \in E(G)} \frac{2\sqrt{d_r d_s}}{d_r + d_s}$$

$$GA[D(C_mH_{2m+2})] = |E_{(2,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s} + |E_{(8,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s}$$

$$GA[D(C_mH_{2m+2})] = 8(m + 1) \left[ \frac{2\sqrt{2(8)}}{10} \right] + 4(m - 1) \left[ \frac{2\sqrt{8(8)}}{16} \right].$$

$$GA[D(C_mH_{2m+2})] = 8(m + 1) \left[ \frac{4}{5} \right] + 4(m - 1).$$

$$GA[D(C_mH_{2m+2})] = \frac{1}{5}(52m + 12).$$

$$ABC[D(C_mH_{2m+2})] = \sum_{rs \in E[D(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}$$

$$= |E_{(2,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}} + |E_{(8,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}$$

$$= 8(m + 1) \sqrt{\frac{8}{16}} + 4(m - 1) \sqrt{\frac{14}{64}}.$$  

$$ABC[D(C_mH_{2m+2})] = \sqrt{2} \left( (m - 1)\sqrt{7} + 8m + 8 \right) \frac{2}{2}.$$  

$$F(G) = \sum_{rs \in E(G)} (d_r^2 + d_s^2).$$

$$F[D(C_mH_{2m+2})] = |E_{(2,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} (d_r^2 + d_s^2) + |E_{(8,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} (d_r^2 + d_s^2).$$

$$= 8(m + 1)(2^2 + 8^2) + 4(m - 1)(8^2 + 8^2).$$

$$= 544(m + 1) + 512(m - 1).$$

$$F[D(C_mH_{2m+2})] = 1056m + 32.$$  

$$ISI[G] = \sum_{rs \in E(G)} \frac{1}{d_r} + \frac{1}{d_s} = \sum_{rs \in E(G)} \frac{(d_r d_s)}{(d_r + d_s)}.$$ 

$$ISI[D(C_mH_{2m+2})] = |E_{(2,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} \frac{(d_r d_s)}{(d_r + d_s)} + |E_{(8,8)}| \sum_{rs \in E[D(C_mH_{2m+2})]} \frac{(d_r d_s)}{(d_r + d_s)}.$$
\[ \text{ISI}[D(C_m H_{2m+2})] = 8(m+1) \left[ \frac{(2)(8)}{(2+8)} \right] + 4(m-1) \left[ \frac{(8)(8)}{(8+8)} \right]. \]

\[ = (m+1) \left[ \frac{64}{5} \right] + 16(m-1). \]

\[ \text{ISI}[D(C_m H_{2m+2})] = \frac{1}{5}(144m - 16). \]

\[ \text{ISI}_{(\alpha, \beta)}(G) = \sum_{rs \in E(G)} [d_u d_v]^\alpha [d_u + d_v]^\beta. \]

\[ = |E_{(2,8)}| \sum_{rs \in E[D(C_{m}H_{2m+2})]} [d_r d_s]^\alpha [d_r + d_s]^\beta + |E_{(8,8)}| \sum_{rs \in E[D(C_{m}H_{2m+2})]} [d_r d_s]^\alpha [d_r + d_s]^\beta. \]

\[ \text{ISI}_{(\alpha, \beta)}[D(C_{m}H_{2m+2})] = 8(m+1)\left[ (2)(8) \right]^\alpha \left[ 2 + 8 \right]^\beta + 4(m-1)\left[ (8)(8) \right]^\alpha \left[ 8 + 8 \right]^\beta. \]

\[ \text{ISI}_{(\alpha, \beta)}[D(C_{m}H_{2m+2})] = 8(m+1)\left[ 16 \right]^\alpha \left[ 10 \right]^\beta + 4(m-1)\left[ 64 \right]^\alpha \left[ 16 \right]^\beta. \]

\[ PM_1[G] = \prod_{rs \in E(G)} (d_r + d_s). \]

\[ PM_1[D(C_{m}H_{2m+2})] = |E_{(2,8)}| \prod_{rs \in E[D(C_{m}H_{2m+2})]} (d_r + d_s) \times |E_{(8,8)}| \prod_{rs \in E[D(C_{m}H_{2m+2})]} (d_r + d_s). \]

\[ PM_1[D(C_{m}H_{2m+2})] = 8(m+1)\left[ 10 \right] \times 4(m-1)\left[ 16 \right]. \]

\[ PM_1[D(C_{m}H_{2m+2})] = 5120(m^2 - 1). \]

\[ PM_2[G] = \prod_{rs \in E(G)} (d_r, d_s). \]

\[ PM_2[D(C_{m}H_{2m+2})] = \prod_{rs \in E[D(C_{m}H_{2m+2})]} (d_r, d_s) \times |E_{(8,8)}| \prod_{rs \in E[D(C_{m}H_{2m+2})]} (d_r, d_s). \]

\[ PM_2[D(C_{m}H_{2m+2})] = 8(m+1)\left[ 16 \right] \times 4(m-1)\left[ 64 \right]. \]

\[ PM_2[D(C_{m}H_{2m+2})] = 32768(m^2 - 1). \]

Comparison

Here, we give a numerically and graphically comparison of the topological indices which based on the degree of the vertices for the double graph of alkanes.

Table 2. Numerical representation of the topological indices double graph of alkanes

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
m & D(C_m H_{2m+2}) & D(C_m H_{2m+2}) & D(C_m H_{2m+2}) & D(C_m H_{2m+2}) & D(C_m H_{2m+2}) & D(C_m H_{2m+2}) \\
\hline
1 & 12.800 & 11.314 & 1088 & 25.600 & 0 & 0 \\
2 & 23.200 & 18.842 & 2144 & 54.400 & 15360 & 98304 \\
3 & 33.600 & 26.369 & 3200 & 83.200 & 40960 & 262144 \\
4 & 44.000 & 33.896 & 4256 & 112.00 & 76800 & 491520 \\
5 & 54.400 & 41.424 & 5312 & 140.80 & 122880 & 786432 \\
6 & 64.800 & 49.952 & 6368 & 169.60 & 179200 & 1146880 \\
7 & 75.200 & 58.480 & 7424 & 198.40 & 245760 & 1572864 \\
8 & 85.600 & 64.005 & 8480 & 227.20 & 322560 & 2064384 \\
9 & 96.000 & 71.535 & 9536 & 256.00 & 409600 & 2621440 \\
10 & 106.40 & 79.060 & 10592 & 284.80 & 506880 & 3244032 \\
\hline
\end{array}
\]
3. Topological Indices of the Strong Double Graph of Alkanes

In this Section, the topological indices for the strong double graph of alkanes will be determined:

**Theorem 3.1.** Suppose that $SD(C_mH_{2m+2})$ is the strong double graph of the alkanes $C_mH_{2m+2}$. Then,

$$GA[SD(C_mH_{2m+2})] = 6m - 3 + 4\sqrt{3}(m + 1).$$

$$ABC[SD(C_mH_{2m+2})] = \frac{1}{9}((8m + 8)\sqrt{30} + 32m - 4).$$

$$F[SD(C_mH_{2m+2})] = 1566m + 108.$$  

$$ISI[SD(C_mH_{2m+2})] = \frac{87m}{2} + 3.$$  

$$ISI_{(\alpha,\beta)}[SD(C_mH_{2m+2})] = 2(m + 1)[9^\alpha][6^\beta] + 8(m + 1)[27^\alpha][12^\beta] + (5m - 4)[81^\alpha][18^\beta].$$

$$PM_1[SD(C_mH_{2m+2})] = 20736(m + 1)^2(5m - 4).$$

$$PM_2[SD(C_mH_{2m+2})] = 314928(m + 1)^2(5m - 4).$$

**Proof:** The number of vertices of the strong double graph of alkanes $SD(C_mH_{2m+2})$ are $2(3m + 2)$ and edges are $3(5m + 2)$, respectively. In $SD(C_mH_{2m+2})$, we have $4(m + 1)$ vertices having degree 3 and $2m$ vertices having degree 9. We separate edges of the $SD(C_mH_{2m+2})$ into the type $E[d_r,d_s]$ in which $rs$ is represents the edges. Edges present in $SD(C_mH_{2m+2})$ consists of $E_{(3,3)}, E_{(3,9)}$ and $E_{(9,9)}$ and these types of edges are present in Table 3.

<table>
<thead>
<tr>
<th>$E[d_r,d_s]$</th>
<th>$E_{(3,3)}$</th>
<th>$E_{(3,9)}$</th>
<th>$E_{(9,9)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$2(m + 1)$</td>
<td>$8(m + 1)$</td>
<td>$5m - 4$</td>
</tr>
</tbody>
</table>

Now by using Equations (2-9) and the
Table 1, we obtain the desired results, i.e.,

\[ GA[G'] = \sum_{rs \in E(G')} \frac{2\sqrt{d_r d_s}}{d_r + d_s}. \]

\[
\begin{align*}
GA[SD(C_mH_{2m+2})] &= |E_{(3,3)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s} + |E_{(3,9)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s} \\
&+ |E_{(9,9)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s}.
\end{align*}
\]

\[= 2(m + 1) \sqrt{9} + 8(m + 1) \frac{2\sqrt{27}}{12} + (5m - 4) \frac{2\sqrt{81}}{18}. \]

\[GA[SD(C_mH_{2m+2})] = 6m - 3 + 4\sqrt{3}(m + 1). \]

\[
\begin{align*}
ABC[G] &= \sum_{rs \in E(G')} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}} \\
&= |E_{(3,3)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}} + |E_{(3,9)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}} \\
&+ |E_{(9,9)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.
\end{align*}
\]

\[ABC[SD(C_mH_{2m+2})] = 2(m + 1) \left(\frac{4}{9} + 8(m + 1) \frac{10}{27} + (5m - 4) \frac{16}{81}\right). \]

\[ABC[SD(C_mH_{2m+2})] = \frac{4}{3} \left((m + 1) + 2(m + 1) \sqrt{\frac{\frac{10}{3} + \frac{1}{3} (5m - 4)}{}}\right). \]

\[ABC[SD(C_mH_{2m+2})] = \frac{1}{9} \left((8m + 8)\sqrt{30} + 32m - 4\right). \]

\[
\begin{align*}
F[G] &= \sum_{rs \in E(G')} (d_r^2 + d_s^2).
\end{align*}
\]

\[
\begin{align*}
F[SD(C_mH_{2m+2})] &= |E_{(3,3)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} (d_r^2 + d_s^2) + |E_{(3,9)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} (d_r^2 + d_s^2) \\
&+ |E_{(9,9)}| \sum_{rs \in E[SD(C_mH_{2m+2})]} (d_r^2 + d_s^2).
\end{align*}
\]

\[= 2(m + 1)(18) + 8(m + 1)(90) + (5m - 4)(162). \]

\[F[SD(C_mH_{2m+2})] = 1566m + 108 \]

\[ISI[G] = \sum_{rs \in E(G)} \frac{1}{d_r + d_s} = \sum_{rs \in E(G)} \frac{(d_r d_s)}{(d_r + d_s)}. \]
Here, we give a numerically and graphically comparison of the topological indices which based on the degree of the vertices for the strong double graph of alkanes \( SD(C_mH_{2m+2}) \).

\[
\text{Comparison}
\]

\[
\begin{align*}
\text{Degree-based Topological Indices of Alkanes by Applying Some Graph Operations} & \quad \text{Section A-Research paper}

\text{Eur. Chem. Bull. 2023.12(Special Issue 5), 39-50} & \quad 47
\end{align*}
\]
Table 4. Numerical representation of the topological indices of strong double graph of alkanes $C_mH_{2m+2}$, for $m = 1, 2, ..., 10$.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$GA$</th>
<th>$ABC$</th>
<th>$F$</th>
<th>$ISI$</th>
<th>$PM_1$</th>
<th>$PM_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SD($C_mH_{2m+2}$)</td>
<td>SD($C_mH_{2m+2}$)</td>
<td>SD($C_mH_{2m+2}$)</td>
<td>SD($C_mH_{2m+2}$)</td>
<td>SD($C_mH_{2m+2}$)</td>
<td>SD($C_mH_{2m+2}$)</td>
</tr>
<tr>
<td>1</td>
<td>16.857</td>
<td>12.848</td>
<td>1674</td>
<td>46.500</td>
<td>82944</td>
<td>1259712</td>
</tr>
<tr>
<td>2</td>
<td>29.785</td>
<td>21.273</td>
<td>3240</td>
<td>90.000</td>
<td>1119744</td>
<td>17006112</td>
</tr>
<tr>
<td>3</td>
<td>42.714</td>
<td>29.697</td>
<td>4806</td>
<td>133.50</td>
<td>3649536</td>
<td>55427328</td>
</tr>
<tr>
<td>4</td>
<td>55.642</td>
<td>38.121</td>
<td>6372</td>
<td>177.00</td>
<td>8294400</td>
<td>125971200</td>
</tr>
<tr>
<td>5</td>
<td>68.570</td>
<td>46.545</td>
<td>7938</td>
<td>220.50</td>
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</tr>
<tr>
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<td>81.499</td>
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<td>264.00</td>
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<tr>
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<tr>
<td>10</td>
<td>133.21</td>
<td>88.666</td>
<td>15768</td>
<td>438.00</td>
<td>115416576</td>
<td>1752889248</td>
</tr>
</tbody>
</table>

Figure 5. Graphically representation of strong double graph of alkanes.

Conclusion
Graph invariants are useful tools for approximating and predicking the characteristics of biological and chemical molecules in the investigation of quantitative structure property relationships (QSPRs) and quantitative structure-activity relationships (QSARs). In this paper, we computed the topological indices, namely, Inverse sum indeg index ($ISI$), first multiplicative-Zagreb index ($PM_1$), atom bond connectivity index ($ABC$), forgotten index ($F$), geometric arithmetic index ($GA$), second multiplicative-Zagreb index ($PM_2$) for the double and strong double graph of alkanes $C_tH_{2t+2}$. We compare our results graphically and numerically at the end.
References


