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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 alkanes are least reactive and simplest hydrocarbon that contains of 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_tH_{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_r 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 $\acute{G}$, the Wiener index [10] is defined as follows:

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

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

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

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

$$ABC(\acute{G}) = \sum_{rs\in E(\acute{G})} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}. \tag{3}$$

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

$$F(\acute{G}) = \sum_{rs\in E(\acute{G})} (d_r^2 + d_s^2). \tag{4}$$

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

$$ISI(\acute{G}) = \sum_{rs\in E(\acute{G})} \frac{1}{\frac{1}{d_r}+\frac{1}{d_s}}. \tag{5}$$

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

$$ISI_{(\boldsymbol{\alpha},\boldsymbol{\beta})}(\acute{G}) = \sum_{rs\in E(\acute{G})} [d_r d_s]^{\alpha}\ [d_r+d_s]^{\beta}, \tag{6}$$

where α and β are real numbers.

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

$$PM_1(\acute{G}) = \prod_{rs\in E(\acute{G})} (d_r)^2, \tag{7}$$

$$PM_2(\acute{G}) = \prod_{rs\in E(\acute{G})} (d_r.\, d_s). \tag{8}$$

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

$$PM_1(G') = \prod_{rs \in E(G')} (d_r + d_s). \tag{9}$$

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

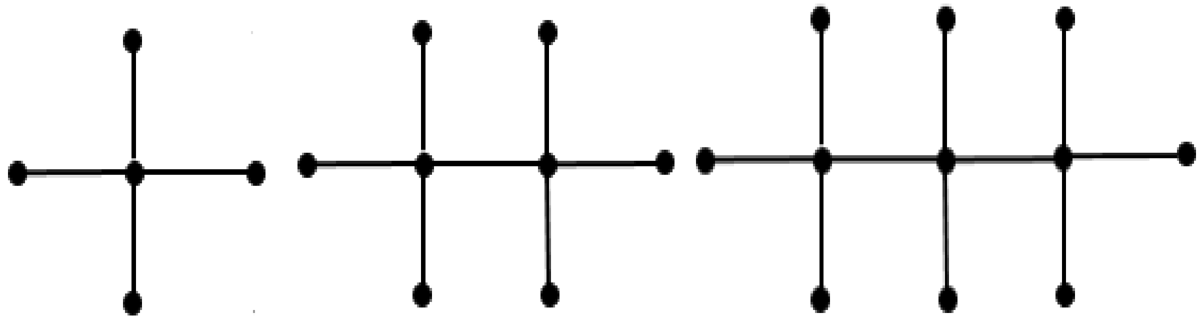

Figure 1. Alkanes (CH_4, C_2H_6 and C_3H_8).

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 $D(G')$.

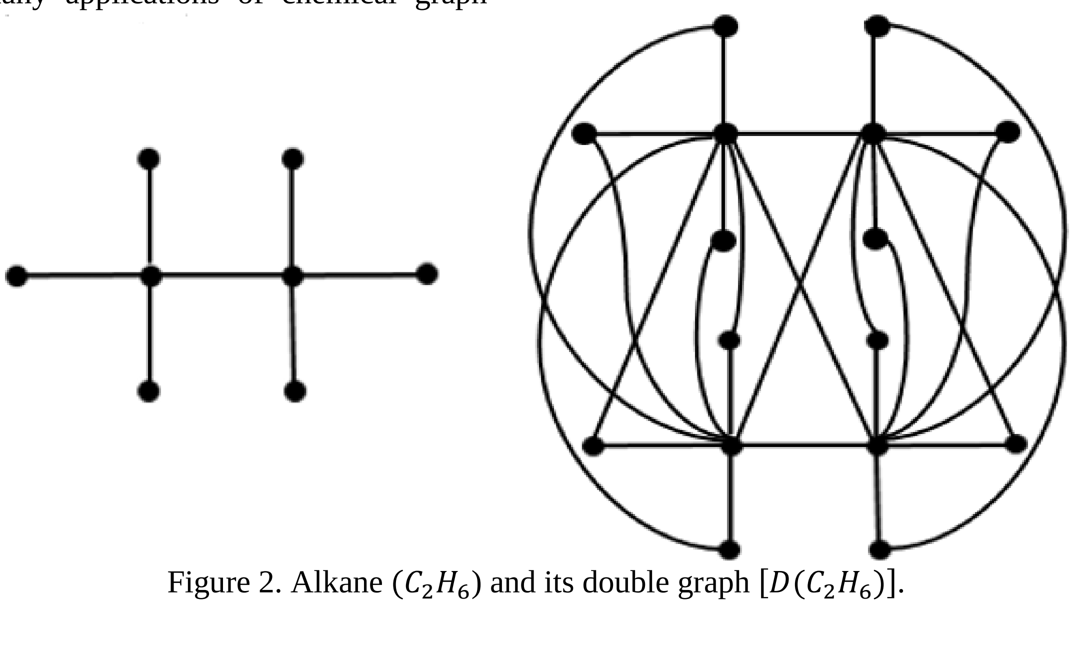

Figure 2. Alkane (C_2H_6) and its double graph [$D(C_2H_6)$].

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.

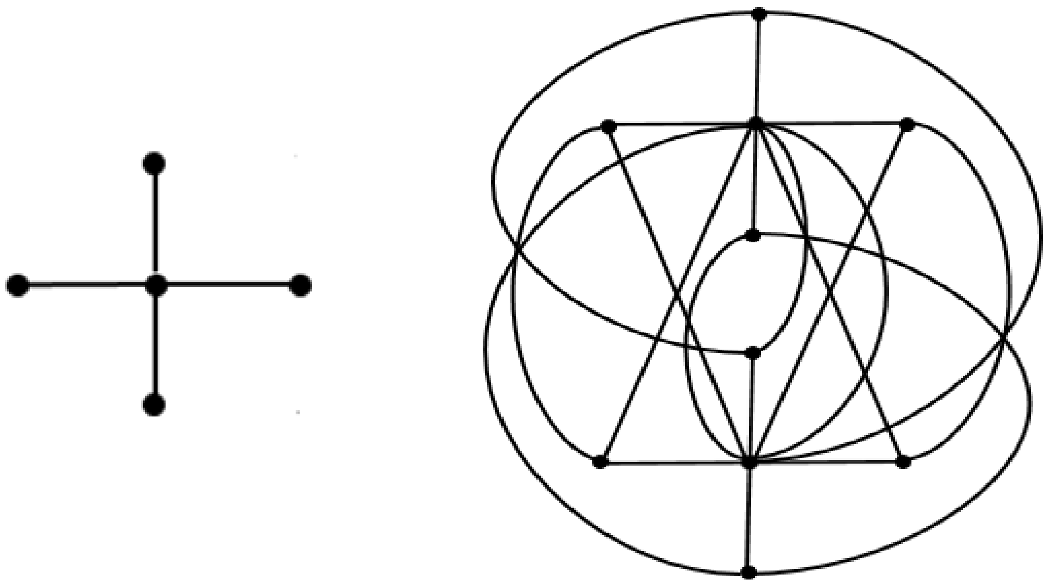

Figure 3. Alkane (CH_4) and its strong double graph $[SD(CH_4)]$.

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,

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

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

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

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

$ISI_{(\alpha,\beta)}[D(C_mH_{2m+2})] = 8(m+1)[16]^{\alpha}\,[10]^{\beta} + 4(m-1)[64]^{\alpha}\,[16]^{\beta}$.

$PM_1[D(C_mH_{2m+2})] = 5120(m^2 - 1)$.

$PM_2[D(C_mH_{2m+2})] = 32768(m^2 - 1)$.

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.

$E[d_r, d_s]$	$E_{(2,8)}$	$E_{(8,8)}$
Number of edges	$8(m+1)$	$4(m-1)$

Now by using *Equations* (2-9) and the

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$ISI[D(C_mH_{2m+2})] = 8(m+1)\left[\frac{(2)(8)}{(2+8)}\right] + 4(m-1)\left[\frac{(8)(8)}{(8+8)}\right].$$
$$= (m+1)\left[\frac{64}{5}\right] + 16(m-1).$$
$$ISI[D(C_mH_{2m+2})] = \frac{1}{5}(144m-16).$$

$$ISI_{(\boldsymbol{\alpha},\boldsymbol{\beta})}(G') = \sum_{rs\in E(G')} [d_u d_v]^{\alpha}\ [d_u+d_v]^{\beta}.$$
$$= |E_{(2,8)}| \sum_{rs\in E[D(C_mH_{2m+2})]} [d_r d_s]^{\alpha}\ [d_r+d_s]^{\beta} + |E_{(8,8)}| \sum_{rs\in E[D(C_mH_{2m+2})]} [d_r d_s]^{\alpha}\ [d_r+d_s]^{\beta}.$$
$$ISI_{(\alpha,\beta)}[D(C_mH_{2m+2})] = 8(m+1)[(2)(8)]^{\alpha}\ [2+8]^{\beta} + 4(m-1)[(8)(8)]^{\alpha}\ [8+8]^{\beta}.$$
$$ISI_{(\alpha,\beta)}[D(C_mH_{2m+2})] = 8(m+1)[16]^{\alpha}\ [10]^{\beta} + 4(m-1)[64]^{\alpha}\ [16]^{\beta}.$$

$$PM_1[G'] = \prod_{rs\in E(G')} (d_r+d_s).$$
$$PM_1[D(C_mH_{2m+2})] = |E_{(2,8)}| \prod_{rs\in E[D(C_mH_{2m+2})]} (d_r+d_s) \times |E_{(8,8)}| \prod_{rs\in E[D(C_mH_{2m+2})]} (d_r+d_s).$$
$$PM_1[D(C_mH_{2m+2})] = 8(m+1)(10) \times 4(m-1)(16).$$
$$PM_1[D(C_mH_{2m+2})] = 5120(m^2-1).$$

$$PM_2[G'] = \prod_{rs\in E(G')} (d_r.d_s).$$
$$PM_2[D(C_mH_{2m+2})] = |E_{(2,8)}| \prod_{rs\in E[D(C_mH_{2m+2})]} (d_r.d_s) \times |E_{(8,8)}| \prod_{rs\in E[D(C_mH_{2m+2})]} (d_r.d_s).$$
$$PM_2[D(C_mH_{2m+2})] = 8(m+1)(16) \times 4(m-1)(64).$$
$$PM_2[D(C_mH_{2m+2})] = 32768(m^2-1).$$

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 C_mH_{2m+2}, for $m = 1, 2 \dots 10$.

m	GA $D(C_mH_{2m+2})$	ABC $D(C_mH_{2m+2})$	F $D(C_mH_{2m+2})$	ISI $D(C_mH_{2m+2})$	PM_1 $D(C_mH_{2m+2})$	PM_2 $D(C_mH_{2m+2})$
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	48.952	6368	169.60	179200	1146880
7	75.200	56.480	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

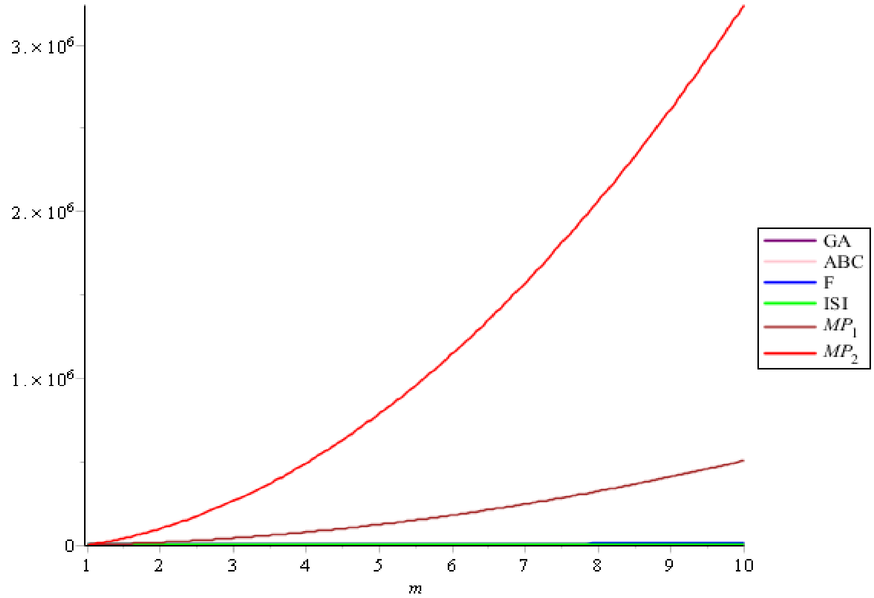

Figure 4. Graphically representation of double graph of alkanes.

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,

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

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

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

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

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

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

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

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 3. Partitioning of edges.

$E[d_r, d_s]$	$E_{(3,3)}$	$E_{(3,9)}$	$E_{(9,9)}$
Number of edges	$2(m+1)$	$8(m+1)$	$5m-4$

Now by using *Equations* (2-9) and the

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

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

$$GA[SD(C_mH_{2m+2})] = |E_{(3,3)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s} + |E_{(3,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s}$$
$$+|E_{(9,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \frac{2\sqrt{d_r d_s}}{d_r + d_s}.$$
$$= 2(m+1)\frac{\sqrt{9}}{6} + 8(m+1)\frac{2\sqrt{27}}{12} + (5m-4)\frac{2\sqrt{81}}{18}.$$
$$GA[SD(C_mH_{2m+2})] = 6m - 3 + 4\sqrt{3}(m+1).$$

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

$$= |\mathrm{E}_{(3,3)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}} + |E_{(3,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}$$
$$+ |E_{(9,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \sqrt{\frac{d_r + d_s - 2}{d_r d_s}}.$$
$$ABC[SD(C_mH_{2m+2})] = 2(m+1)\sqrt{\frac{4}{9}} + 8(m+1)\sqrt{\frac{10}{27}} + (5m-4)\sqrt{\frac{16}{81}}.$$
$$ABC[SD(C_mH_{2m+2})] = \frac{4}{3}\left[(m+1) + 2(m+1)\sqrt{\frac{10}{3}} + \frac{1}{3}(5m-4)\right].$$
$$ABC[SD(C_mH_{2m+2})] = \frac{1}{9}\Big((8m+8)\sqrt{30} + 32m - 4\Big).$$

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

$$F[SD(C_mH_{2m+2})]$$
$$= |E_{(3,3)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} (d_r^2 + d_s^2) + |E_{(3,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} (d_r^2 + d_s^2)$$
$$+|E_{(9,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} (d_r^2 + d_s^2).$$
$$= 2(m+1)(18) + 8(m+1)(90) + (5m-4)(162).$$
$$F[SD(C_mH_{2m+2})] = 1566m + 108$$

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

$$ISI[SD(C_mH_{2m+2})] = |E_{(3,3)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \frac{(d_r d_s)}{(d_r+d_s)} + |E_{(3,9}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \frac{(d_r d_s)}{(d_r+d_s)}$$
$$+|E_{(9,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} \frac{(d_r d_s)}{(d_r+d_s)}.$$
$$ISI[SD(C_mH_{2m+2})] = 2(m+1)\left[\frac{9}{6}\right] + 8(m+1)\left[\frac{27}{12}\right] + (5m-4)\left[\frac{81}{18}\right].$$
$$ISI[SD(C_mH_{2m+2})] = 21(m+1) + (5m-4)\left[\frac{9}{2}\right].$$
$$ISI[SD(C_mH_{2m+2})] = \frac{87m}{2} + 3.$$

$$ISI_{(\boldsymbol{\alpha},\boldsymbol{\beta})}(\,G) = \sum_{rs\in E(\,G)} [d_r d_s]^{\alpha}\ [d_r+d_s]^{\beta}.$$
$$= |E_{(3,3)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} [d_r d_s]^{\alpha}\,[d_r+d_s]^{\beta} + |E_{(3,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} [d_r d_s]^{\alpha}\,[d_r+d_s]^{\beta}$$
$$+ |E_{(9,9)}| \sum_{rs\in E[SD(C_mH_{2m+2})]} [d_r d_s]^{\alpha}\,[d_r+d_s]^{\beta}.$$
$$= 2(m+1)[9]^{\alpha}\,[6]^{\beta} + 8(m+1)[27]^{\alpha}\,[12]^{\beta} + (5m-4)[81]^{\alpha}\,[18]^{\beta}.$$
$$ISI_{(\alpha,\beta)}[SD(C_mH_{2m+2})]$$
$$= 2(m+1)[9]^{\alpha}\,[6]^{\beta} + 8(m+1)[27]^{\alpha}\,[12]^{\beta} + (5m-4)[81]^{\alpha}\,[18]^{\beta}.$$

$$PM_1[G] = \prod_{rs\in E(G)} (d_r+d_s).$$
$$PM_1[SD(C_mH_{2m+2})]$$
$$= |E_{(3,3)}| \prod_{rs\in E[SD(C_mH_{2m+2})]} (d_r+d_s) \times |E_{(3,9)}| \prod_{rs\in E[SD(C_mH_{2m+2})]} (d_r+d_s)$$
$$\times |E_{(9,9)}| \prod_{rs\in E[SD(C_mH_{2m+2})]} (d_r+d_s).$$
$$PM_1[SD(C_mH_{2m+2})] = (m+1)(12) \times (m+1)(96) \times (5m-4)(18).$$
$$PM_1[SD(C_mH_{2m+2})] = \ 20736(m+1)^2(5m-4).$$

$$PM_2[G] = \prod_{rs\in E(G)} (d_r.\,d_s).$$
$$PM_2[SD(C_mH_{2m+2})] = |E_{(3,3)}| \prod_{rs\in E[SD(C_mH_{2m+2})]} (d_r.\,d_s) \times |E_{(3,9)}| \prod_{rs\in E[SD(C_mH_{2m+2})]} (d_r.\,d_s)$$
$$\times |E_{(9,9)}| \prod_{rs\in E[SD(C_mH_{2m+2})]} (d_r.\,d_s).$$
$$PM_2[SD(C_mH_{2m+2})] = 2(m+1)(9) \times 8(m+1)(27) \times\ (5m-4)(81).$$
$$PM_2[SD(C_mH_{2m+2})] = 314928(m+1)^2(5m-4).$$

Comparison

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 $SD(C_mH_{2m+2})$.

Table 4. Numerical representation of the topological indices of strong double graph of alkanes C_mH_{2m+2}, for $m = 1,2, \dots, 10$.

m	GA $SD(C_mH_{2m+}$	ABC $SD(C_mH_{2m+2}$	F $SD(C_mH_{2m+2}$	ISI $SD(C_mH_{2m+2}$	PM_1 $SD(C_mH_{2m+2}$	PM_2 $SD(C_mH_{2m+2}$
1	16.857	12.848	1674	46.500	82944	1259712
2	29.785	21.273	3240	90.000	1119744	17006112
3	42.714	29.697	4806	133.50	3649536	55427328
4	55.642	38.121	6372	177.00	8294400	125971200
5	68.570	46.545	7938	220.50	15676416	238085568
6	81.499	54.969	9504	264.00	26417664	401218272
7	94.427	63.393	11070	307.50	41140224	624817152
8	107.36	71.818	12636	351.00	60466176	918330048
9	120.28	80.242	14202	394.50	85017600	1291204800
10	133.21	88.666	15768	438.00	115416576	1752889248

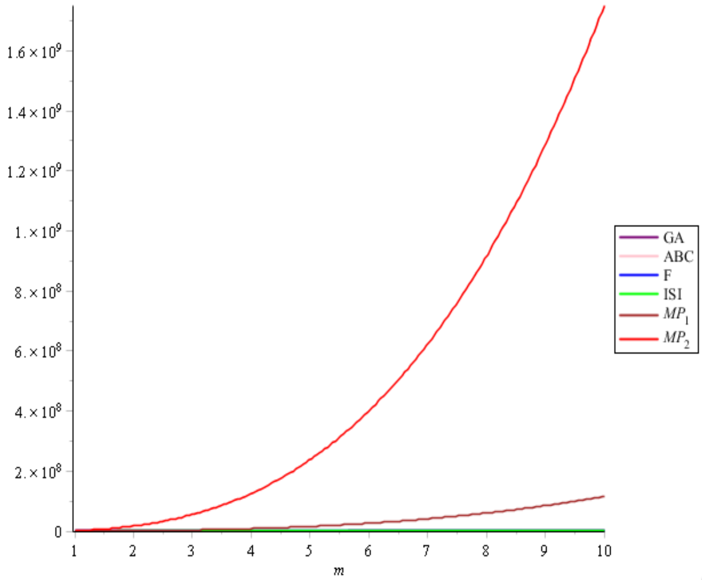

Figure 5. Graphically representation of strong double graph of alkanes.

Conclusion

Graph invariants are useful tools for approximating and predicating 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.

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