Computation of Topological Indices of Double and Strong Double Graphs of Chain Silicate(CS_n)

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Abstract
Topological indices are very useful to assume certain physiochemical properties of the chemical compound. A molecular descriptor which changes the molecular structures into certain real numbers is said to be a topological index. In this paper we compute the topological indices of the double and strong double graphs of the chain silicate(CS_n), $n \geq 2$. In addition, we also present a numerical and graphical comparison of topological indices of the double and strong double graphs of the chain silicate(CS_n), $n \geq 2$.

Keywords : Topological index, Double graphs, Strong double graphs, Chain Silicate.

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1. Introduction

Let G be a simple, finite connected graph. $V(G)$ and $E(G)$ are the vertex and edge sets of graph G, respectively. The number of elements in $V(G)$ and $E(G)$ represents the order and size of graph G. Vertex degree is the number of edges joining to a vertex in a graph G. The number of connected vertices to a fixed vertex is known as neighbourhood. The degree of a vertex is denoted by d_u where $u \in V(G)$. Hand–shaking Lemma is very useful for calculating thetotal number of edges in a graph G. For undefined terms and notations, we refer[1].

Topological indices are the mathematical measures which correspond to the structures of any simple finite graph. They are invariant under the graph isomorphism. The interest of study of topological indices is mainly associated with its applications in QSAR/QSPR. Topological indices analyse the physicalcharacteristics such as molar volume, melting point, surfacetension, boiling point, molar refraction, and heats ofvaporization.Topological indices also represent the biological behaviorof compounds such as pH regulation, stimulation ofcell growth and nutrition. Hence,these topological indices may be helpful to know thechemical and physical characteristics and biologicalbehaviors.

Silicates are obtained by fusing metal oxides or metal carbonates with sand. Essentially all the silicates contain SiO4 tetrahedron. In chemistry, the corner vertices of SiO4 tetrahedron represent oxygen ions and the centre vertex represents the silicon ion. In graph theory, we call the corner vertices as oxygen nodesand the centre vertex as silicon node. The different types of silicate structure arise from the ways in which these tetrahedron are arranged.While tetrahedron are arranged linearly, chain silicates are obtained[14]. See Figure1.The number of vertices in (CS_n) are $3n+1$ and the number of edges are $6n$.

Lemma 1. [2] If G is a graph of size m then

$$\sum_{u\in V(G)} deg(u) = 2m \qquad \text{.................(1)}$$

The topological index concept comes from the work of Wiener, who introduced the Wiener index.The wiener index is defined in [3] as follows

$$w(G) = \frac{1}{2}\sum_{(u,v)} \mathrm{d}(u,v) \qquad \text{.................(2)}$$

Where $d(u,v)$ is the distance among vertices u and v of a graph G.

The geometric – arithmetic index (GA) of graph G is defined [4] as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{\mathrm{d_u} d_v}}{\mathrm{d_u}+d_v} \qquad \text{.................(3)}$$

The atomic bond connectivity index (ABC) of graph G is defined [5] as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{\mathrm{d_u}+d_v-2}{\mathrm{d_u} d_v}} \qquad \text{.................(4)}$$

The forgotten index (F) of graph G is defined [6] as

$$F(G) = \sum_{uv\in E(G)} (d_u^2 + d_v^2) \qquad \text{.................(5)}$$

The inverse sum indeg index (ISI) is define [7] as

$$ISI(G) = \sum_{uv\in E(G)} \frac{1}{\frac{1}{d_u}+\frac{1}{d_v}} \qquad \text{.................(6)}$$

The first multiplicative –Zagreb (PM_1) and second multiplicative – Zagreb index (PM_2) are defined [8] as

$$PM_1(G) = \prod_{uv\in E(G)} (d_u)^2 \qquad \text{.................(7)}$$

$$PM_2(G) = \prod_{uv\in E(G)} (\mathrm{d_u}.d_v) \qquad \text{.................(8)}$$

The first multiplicative Zagreb Index (PM_1) can also be written in the sum of the edges [9] of G

$$PM_1(G) = \prod_{uv \in E(G)} (d_u + d_v) \qquad \text{................(9)}$$

For more details about topological indices and molecular graphs [10-13]

Definition 1:[15]The double graph of graph G is represented by $D(G)$. Assume two copies of a graph and join each vertex in one copy to its neighbour in the other copy in order to produce the double graph of the graph. For example, the graph(CS_2) and itsdouble graph D(CS_2) is shown in Figure 2.

Definition 2:[16]The strong double graph $SD(G)$ of the graph G is obtained by taking two graphs and joining the closed neighbourhoods of each vertex in one graph to the adjacent vertex in the other graph. For example, the graph(CS_2) and its strong double graph $SD(CS_2)$ is shown in Figure 3.

Motivated by the results of [17], we computed some degree- based topological indices of double graphs and strong double graphs of chain silicate(CS_n) in sections 2 and 4 respectively. The comparison is given in sections 3 and 5. In section 6, we provide conclusion for the whole study.

2. Degree–Based Topological Indices of Double Graph of Chain Silicate(CS_n)

This section we will compute the degree–based topological indices of the double graph of chain silicate(CS_n)

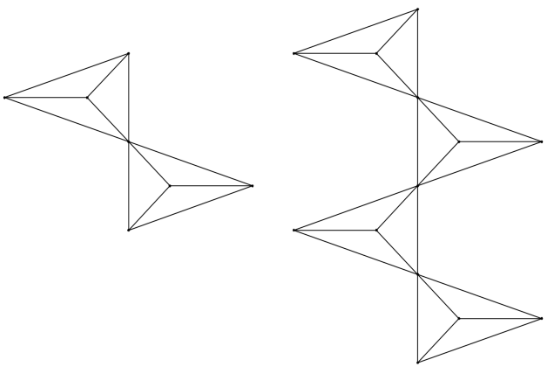

Figure 1: Graph of chain silicate$(CS_2 \; and \; CS_4)$

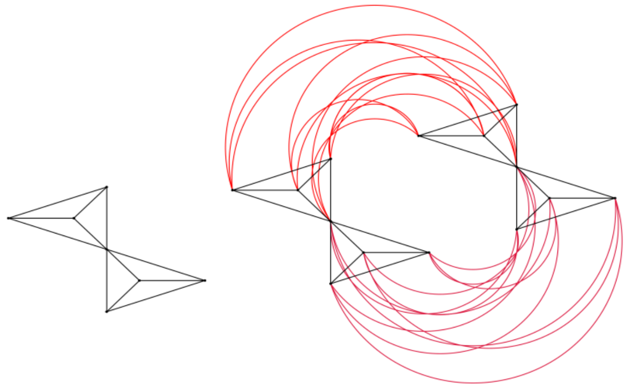

Figure 2:Chain silicate $(CS_2)$and its double graph$D(CS_2)$

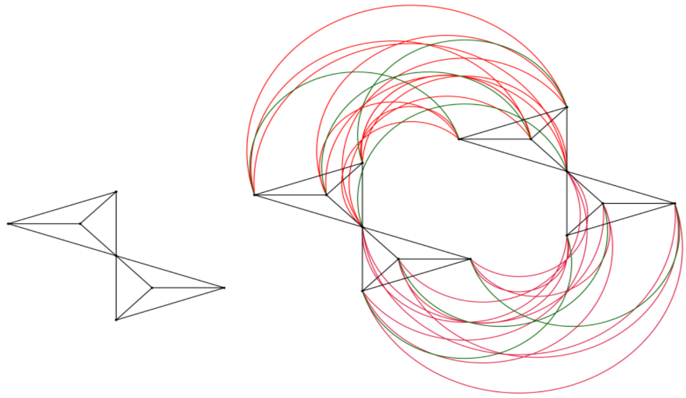

Figure 3: Chain silicate$(CS_2)$and its strong double graph$SD(CS_2)$

Table 1: Edge partition of$D(CS_n)$

$E[d_u, d_u]$	$E_{(6,6)}$	$E_{(6,12)}$	$E_{(12,12)}$
Number of edges	4n+16	16n-8	4n-8

Theorem 1: Let $D(CS_n)$ be the double graph of chain silicate(CS_n) ; then the geometric arithmetic index of $D(CS_n)$ is $GA[D(CS_n)] = \left(\frac{24+32\sqrt{2}}{3}\right)n + \left(\frac{24-16\sqrt{2}}{3}\right)$

Proof: In the double graph of chain silicate,there are $6n + 2$ vertices and $24n$ edges. In $D(CS_n)$, we have $4(n + 1)$ vertices of degree 6 and $2(n - 1)$ vertices of degree 12.

We split the edges of $[D(CS_n)]$ into the edges of the type $E[d_u, d_v]$, where uv is an edge. InD (CS_n), contains the edges of type $E_{(6,6)}$,$E_{(6,12)}$and $E_{(12,12)}$. A list of their edges are given in Table 1.

By applying equation (3) and Table 1, we obtain the result.

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$GA[D(CS_n)] = |E_{(6,6)}| \sum_{uv\in E[D(CS_n)]} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + |E_{(6,12)}| \sum_{uv\in E[D(CS_n)]} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$+|E_{(12,12)}| \sum_{uv\in E[D(CS_n)]} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$= 4(n+4)\left[\frac{2\sqrt{36}}{12}\right] + 8(2n-1)\left[\frac{2\sqrt{72}}{18}\right] + 4(n-2)\left[\frac{2\sqrt{144}}{24}\right]$$

$$GA[D(CS_n)] = \left(\frac{24+32\sqrt{2}}{3}\right)n + \left(\frac{24-16\sqrt{2}}{3}\right)$$

Theorem 2: The ABC index of the double graph $D(CS_n)$ of chain silicateis

$$ABC[D(CS_n)] = \left(\frac{2\sqrt{10}+16\sqrt{2}+\sqrt{22}}{3}\right)n + \left(\frac{8\sqrt{10}-8\sqrt{2}-2\sqrt{22}}{3}\right)$$

Proof : By applying equation (4) and Table 1, we obtain the result.

$$ABC[D(CS_n)] = |E_{(6,6)}| \sum_{uv\in E[D(CS_n)]} \frac{\sqrt{d_u+d_v-2}}{d_u d_v} + |E_{(6,12)}| \sum_{uv\in E[D(CS_n)]} \frac{\sqrt{d_u+d_v-2}}{d_u d_v}$$

$$+|E_{(12,12)}| \sum_{uv\in E[D(CS_n)]} \frac{\sqrt{d_u+d_v-2}}{d_u d_v}$$

$$= 4(n+4)\left[\frac{\sqrt{10}}{6}\right] + 8(2n-1)\sqrt{\frac{16}{72}} + 4(n-2)\left[\frac{\sqrt{22}}{12}\right]$$

$$ABC[D(CS_n)] = \left(\frac{2\sqrt{10}+16\sqrt{2}+\sqrt{22}}{3}\right)n + \left(\frac{8\sqrt{10}-8\sqrt{2}-2\sqrt{22}}{3}\right)$$

Theorem 3: The forgotten index of the double graph $D(CS_n)$ of chain silicateis

$$F[D(CS_n)] = 4320n - 2592$$

Proof: By applying equation (5) and Table 1, we obtain the result

$$F[D(CS_n)] = |E_{(6,6)}| \sum_{uv\in E[D(CS_n)]} (d_u^2+d_v^2) + |E_{(6,12)}| \sum_{uv\in E[D(CS_n)]} (d_u^2+d_v^2)$$

$$+|E_{(12,12)}| \sum_{uv\in E[D(CS_n)]} (d_u^2+d_v^2)$$

$$= 4(n+4)(6^2+6^2) + 8(2n-1)(6^2+12^2) + 4(n-2)(12^2+12^2)$$

$$F[D(CS_n)] = 4320n - 2592$$

Theorem 4: The inverse sum indeg index ofthe double graph$D(CS_n)$ of chain silicateis

$$ISI[D(CS_n)] = 100n - 32$$

Proof: By applying equation (6) and Table 1, we obtain the result

$$ISI[D(CS_n)] = |E_{(6,6)}| \sum_{uv\in E[D(CS_n)]} \frac{d_u d_v}{(d_u+d_v)} + |E_{(6,12)}| \sum_{uv\in E[D(CS_n)]} \frac{d_u d_v}{(d_u+d_v)}$$

$$+|E_{(12,12)}| \sum_{uv\in E[D(CS_n)]} \frac{d_u d_v}{(d_u+d_v)}$$

$$= 4(n+4)\left(\frac{36}{12}\right) + 8(2n-1)\left(\frac{72}{18}\right) + 4(n-2)\left(\frac{144}{24}\right)$$

$$ISI[D(CS_n)] = 100n - 32$$

Theorem 5: The first multiplicative-Zagreb index of the double graph $D(CS_n)$ of chain silicateis $PM_1[D(CS_n)] = 3981312n^3 + 5971968n^2 - 35831808\text{n} + 15925248$

Proof: By applying equation (9) and table 1, we obtain the result,

$$PM_1[D(CS_n)] = |E_{(6,6)}| \prod_{uv\in E[D(CS_n)]} (d_u+d_v) \times |E_{(6,12)}| \prod_{uv\in E[D(CS_n)]} (d_u+d_v)$$

$$\times |E_{(12,12)}| \prod_{uv\in E[D(CS_n)]} (d_u+d_v)$$

$$= 4(n+4)(6+6) \times 8(2n-1)(6+12) \times 4(n-2)(12+12)$$

$$PM_1[D(CS_n)] = 3981312n^3 + 5971968n^2 - 35831808\text{n} + 15925248$$

Theorem 6 : The second multiplicative – Zagreb index of the double graph $D(CS_n)$ of chain silicateis $PM_2[D(CS_n)] = 955551488n^3 + 143327232n^2 - 859963392\text{n} + 382205952$.

Proof : By applying equation (8) and Table 1, We obtain the result.

$$PM_2[D(CS_n)] = |E_{(6,6)}| \prod_{uv\in E[D(CS_n)]} (d_u . d_v) \times |E_{(6,12)}| \prod_{uv\in E[D(CS_n)]} (d_u . d_v)$$

$$\times |E_{(12,12)}| \prod_{uv\in E[D(CS_n)]} (d_u . d_v)$$

$$= 4(n+4)(6\times 6) \times 8(2n-1)(6\times 12) \times 4(n-2)(12\times 12)$$

$$PM_2[D(CS_n)] = 955551488n^3 + 143327232n^2 - 859963392\text{n} + 382205952$$

Table 2: Computation of topological indices of double graph of chain silicate$D(CS_n)$

n	$GA(D(CS_n))$	$ABC\left((D(CS_n))\right)$	$F(D(CS_n))$	$ISI\left((D(CS_n))\right)$	$PM_1\left((D(CS_n))\right)$	$PM_2\left((D(CS_n))\right)$
2	46.6274	23.9628	6048	188	0	6.8800×10^9

3	69.7123	35.1769	10368	298	6.9672×10^{7}	2.4892×10^{10}
4	92.7973	46.3910	14688	408	2.2295×10^{8}	6.0390×10^{10}
5	115.8822	57.6052	19008	518	4.8372×10^{8}	1.1910×10^{11}
6	138.9671	68.8193	23328	628	8.7588×10^{8}	2.0678×10^{11}
7	162.521	80.0334	27648	738	1.4233×10^{9}	3.2913×10^{11}
8	185.1370	91.2475	31968	848	2.1499×10^{9}	4.9191×10^{11}
9	208.2220	102.4617	36288	958	3.0795×10^{9}	7.0084×10^{11}
10	231.3069	113.6758	40608	968	4.2361×10^{9}	9.6166×10^{11}

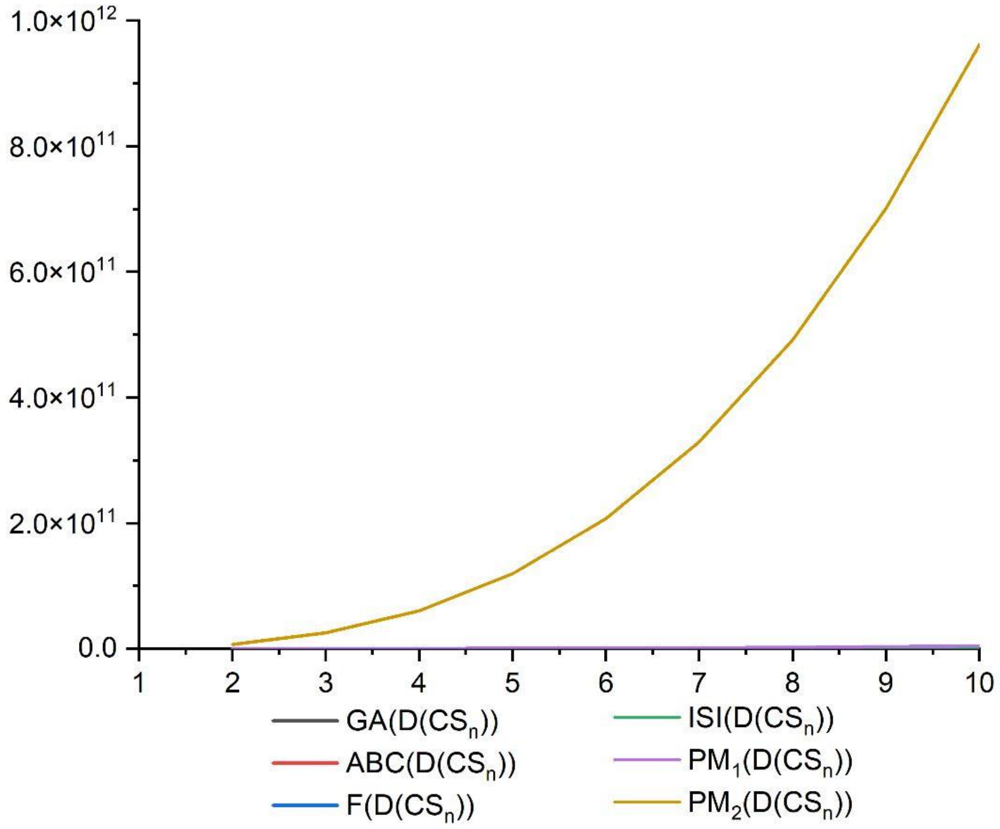

Figure 4: Graphical representation of topological indices of double graph of oxide network $(D(CS_n))$

3. Comparison

In this section, we present a numerical and graphical comparison of topological indices that included the geometric arithmetic index (GA), Atom bond connectivity index (ABC),forgotten index (F), inverse sum indeg index (ISI), first multiplicative–Zagreb index (PM_1) and second multiplicative–Zagreb index (PM_2) for $n = 1,2,3,\ldots,10$ for the double graph of chain silicate$D(CS_n)$, as given in Table 2 and Figure 4. 2756

4. Degree– Based Topological Indices of Strong Double Graphs of Chain Silicate(CS_n)

This section we will compute the degree based topological indices of strong double graph of chain silicate(CS_n).

Table 3: Edge partition of$SD(CS_n)$

$E[d_u, d_u]$	$E_{(7,7)}$	$E_{(7,13)}$	$E_{(13,13)}$
Number of edges	6n+18	16n-8	5n-9

Theorem 7: Let $SD(CS_n)$ be the strong double graph of chain silicate(CS_n); then the geometric arithmetic index of $SD(CS_n)$ is $GA(SD(CS_n)) = \left(\frac{55+8\sqrt{91}}{5}\right)n + \left(\frac{45-4\sqrt{91}}{5}\right)$.

Proof: In the strong double graph of chain silicatethere are $6n + 2$ vertices and $27n + 1$ edges. There are $4(n + 1)$ vertices in$SD(CS_n)$ of degree 7 and $2(n - 1)$vertices of degree1313.

We split the edges of $[SD(CS_n)]$ into the edges of type $E(d_u, d_v)$, where uv is an edge. In $SD(CS_n)$ contains the edges of type $E_{(7,7)}, E_{(7,13)}$ and $E_{(13,13)}$. A list of their edges are given in table 3. By applying equation (3) and Table 3, we obtain the result

$$GA(G) = \sum_{uv\in E[G]} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$GA(SD(CS_n)) = |E_{(7,7)}| \sum_{uv\in E[SD(CS_n)]} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$+ |E_{(7,13)}| \sum_{uv\in E[SD(CS_n)]} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + |E_{(13,13)}| \sum_{uv\in E[SD(CS_n)]} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

$$= 6(n+3)\left[\frac{2\sqrt{49}}{14}\right] + 8(2n-1)\left[\frac{2\sqrt{91}}{20}\right] + (5n-9)\left[\frac{2\sqrt{169}}{26}\right]$$

$$GA(SD(CS_n)) = \left(\frac{55+8\sqrt{91}}{5}\right)n + \left(\frac{45-4\sqrt{91}}{5}\right)$$

Theorem 8: The ABC index of the strong double graph $SD(CS_n)$ of chain silicateis

$$ABC(SD(CS_n)) = \left(\frac{12\sqrt{3}}{7} + \frac{16\sqrt{18}}{\sqrt{91}} + \frac{10\sqrt{6}}{13}\right)n + \left(\frac{36\sqrt{3}}{7} - \frac{8\sqrt{18}}{\sqrt{91}} - \frac{18\sqrt{6}}{13}\right)$$

Proof : By applying equation (4) and Table 3, we obtain the result.

$$ABC[SD(CS_n)] = |E_{(7,7)}| \sum_{uv\in E[SD(CS_n)]} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$+|E_{(7,13)}| \sum_{uv\in E[SD(CS_n)]} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} + |E_{(13,13)}| \sum_{uv\in E[SD(CS_n)]} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$= 6(n+3)\left(\frac{\sqrt{12}}{7}\right) + 8(2n-1)\left(\sqrt{\frac{18}{91}}\right) + (5n-9)\left(\frac{\sqrt{24}}{13}\right)$$

$$ABC(SD(CS_n)) = \left(\frac{12\sqrt{3}}{7} + \frac{16\sqrt{18}}{\sqrt{91}} + \frac{10\sqrt{6}}{13}\right)n + \left(\frac{36\sqrt{3}}{7} - \frac{8\sqrt{18}}{\sqrt{91}} - \frac{18\sqrt{6}}{13}\right)$$

Theorem 9: The forgotton index of the strong double graph $SD(CS_n)$ of chain silicateis

$$F[SD(CS_n)] = 5766\text{n} - 3022$$

Proof : By applying equation (5) and table 3, we obtain the result

$$F[SD(CS_n)] = |E_{(7,7)}| \sum_{uv\in E[SD(CS_n)]} (d_u^2 + d_v^2)$$

$$+|E_{(7,13)}| \sum_{uv\in E[SD(CS_n)]} (d_u^2 + d_v^2) + |E_{(13,13)}| \sum_{uv\in E[SD(CS_n)]} (d_u^2 + d_v^2)$$

$$= 6(n+3)(7^2+7^2) + 8(2n-1)(7^2 + 13^2) + (5n-9)(13^2 + 13^2)$$

$$F[SD(CS_n)] = 5766\text{n} - 3022.$$

Theorem 10: The inverse sum indeg index ofthe strong graph$SD(CS_n)$ of chain silicateis

$$ISI[SD(CS_n)] = \left(\frac{1263}{10}\right)n - \left(\frac{319}{10}\right)$$

Proof: By applying equation (6) and Table 3, we obtain the result.

$$ISI[SD(CS_n)] = |E_{(7,7)}| \sum_{uv\in E[SD(CS_n)]} \frac{(d_u d_v)}{(d_u+d_v)}$$

$$+|E_{(7,13)}| \sum_{uv\in E[SD(CS_n)]} \frac{(d_u d_v)}{(d_u+d_v)} + |E_{(13,13)}| \sum_{uv\in E[SD(CS_n)]} \frac{(d_u d_v)}{(d_u+d_v)}$$

$$= 6(n+3)\left(\frac{49}{14}\right) + 8(2n-1)\left(\frac{91}{20}\right) + (5n-9)\left(\frac{169}{26}\right)$$

$$ISI[SD(CS_n)] = \left(\frac{1263}{10}\right)n - \left(\frac{319}{10}\right)$$

Table 4: Computation of topological indices of strong double graph of chain silicate$(SD(CS_n))$

n	$GA(SD(CS_n))$	$ABC(SD(CS_n))$	$F(SD(CS_n))$	$ISI(SD(CS_n))$	$PM_1(SD(CS_n))$	$PM_2(SD(CS_n))$
2	53.8945	25.8969	8510	220.7	5.2416×10^6	5.4257×10^8
3	80.1575	37.8664	14276	347	6.2899×10^7	6.5108×10^9
4	106.4205	49.8358	20042	473.3	1.8834×10^8	1.9496×10^{10}
5	132.6836	61.8053	25808	599.6	4.0255×10^8	4.1669×10^{10}
6	158.9466	73.7747	31576	725.9	7.2648×10^8	7.5200×10^{10}
7	185.2096	85.7442	37340	852.2	1.1811×10^9	1.2225×10^{11}
8	211.4727	97.7136	43106	978.5	1.7873×10^9	1.8501×10^{11}
9	237.7357	109.6831	48872	1104.8	2.5662×10^9	2.6564×10^{11}
10	263.9987	121.6525	54638	1231.1	3.5387×10^9	3.6630×10^{11}

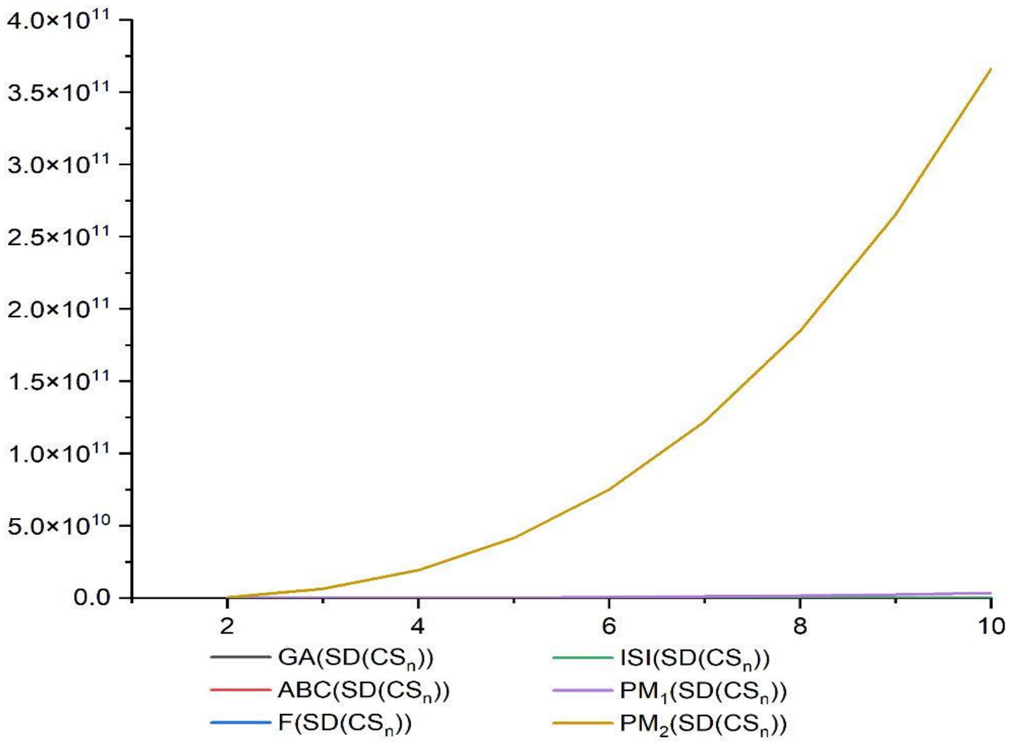

Figure 5: Graphical representation of topological indices of strong double graph of chain silicate$(SD(CS_n))$

Theorem 11: The first multiplicative –Zagreb index of the strong double graph $SD(CS_n)$ of chain silicateis $PM_1[SD(CS_n)] = 3494400n^3 + 2446080n^2 - 20966400n + 9434880$

Proof: By applying equation (9) and table 3, we obtain the result,

$$PM_1[SD(CS_n)] = |E_{(7,7)}| \prod_{uv\in E[SD(CS_n)]} (d_u+d_v) \times |E_{(7,13)}| \prod_{uv\in E[SD(CS_n)]} (d_u+d_v) \times |E_{(13,13)}| \prod_{uv\in E[SD(CS_n)]} (d_u+d_v)$$

$$= 6(n+3)\,(7+7) \times 8(2n-1)(7+13) \times (5n-9)(13+13)$$

$$PM_1[SD(CS_n)] = 3494400n^3 + 2446080n^2 - 20966400\text{n} + 9434880$$

Theorem 12 : The second multiplicative – Zagreb index of the double graph $SD(CS_n)$ of chain silicateis $PM_2[SD(CS_n)] = 361714080n^3 + 253199856n^2 - 2170284480\text{n} + 976628016$

Proof : By applying equation (8) and Table 3, We obtain the result.

$$PM_2[SD(CS_n)] = |E_{(7,7)}| \prod_{uv\in E[SD(CS_n)]} (d_u.d_v) \times |E_{(7,13)}| \prod_{uv\in E[SD(CS_n)]} (d_u.d_v) \times |E_{(13,13)}| \prod_{uv\in E[SD(CS_n)]} (d_u.d_v)$$

$$= 6(n+3)(7\times 7) \times 8(2n-1)(7\times 13) \times (5n-9)(13\times 13)$$

$$PM_2[SD(CS_n)] = 361714080n^3 + 253199856n^2 - 2170284480\text{n} + 976628016$$

5. Comparison

In this section, we present a numerical and graphical comparison of topological indices that included the geometric arithmetic index (GA), Atom bond connectivity index (ABC), forgotton index (F), inverse sum indeg index (ISI), first multiplicative–zagreb index (PM_1) and second multiplicative–zagreb index (PM_2) for $n = 1,2,3,\ldots,10$ for the strong double graph of chain silicate $SD(CS_n)$, as given in Table 4 and Figure 5.

6. Conclusion

We have computed the closed formulae of topological indicessuch as the geometricarithmetic index (GA), atom bondconnectivity index (ABC), forgotten index (F),inverse sum indeg index (ISI),first multiplicative-Zagreb index (PM_1),second multiplicative-Zagreb index(PM_2) of double and strong double graphs of chain silicate(CS_n). Thegeometric structure and comparison of obtained results areshown graphically and numerically.

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