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On topological indices of double and strong double graph of silicon carbide Si_2C_3-I[p,q]

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Silicon is a semiconductor material with several advantages over the other similar materials, such as its low cost, nontoxicity, and almost limitless availability, as well as many years of expertise in its purification, manufacture, and device development. It is used in practical for all of the most recent electrical products. Graph theory can be used to depict a chemical structure, with vertices representing atoms and edges representing chemical bonds. Molecular descriptors are important in mathematical chemistry, particularly in QSPR/QSAR research. In this research, by using two graph operations, namely; double and strong double graph, we computed the closed formulas for some degree-based topological indices of silicon carbide. Furthermore, we also compare topological indices numerically and graphically.

KEYWORDS

Double graph; topological indices; strong double graph; silicon carbide Si_2C_3-I[p,q].

Introduction

In theoretical chemistry (mostly in QSAR/QSPR research), environmental chemistry, pharmacology, and toxicology, topological indices have numerous applications. Let $\acute{G}$ be an undirected simple graph with $V(\acute{G}) = \{r_1, r_2, r_3, \dots r_n\}$ and $E(\acute{G}) = \{e_1, e_2, e_3, \dots e_m\}$ as the vertex and edge sets. The degree of a vertex r is the number of edges incident to r, and it is symbolized by d_r. For undetermined terminologies and notations, we mention Robin J. Wilson book [1].

Mathematical chemistry provides useful tools like polynomials and functions that rely on information contained in the symmetry of graphs of chemical compounds and very helpful for the prediction of the understudy molecular compound and its characteristics without the usage of quantum mechanics. A topological index is a numerical parameter that describes the topology of a graph. It quantitatively describes the structure of molecules and is utilized in the establishment of qualitative structure activity relationships. Numerous topological indices existing [2,3], but here we investigate the topological indices which based on the degree of vertex [4-6]. Chemical graph theory is a field of mathematical chemistry in which we use graph theory methods to represent chemical activities mathematically.

Topological indices that will be explored in this article are given in Equations (1-7).

In topological indices, Geometric-Arithmetic index is associated with Physico-chemical properties such as entropy and enthalpy of vaporization. Consider a graph G, then geometric-arithmetic index (GA) is defined [7] as:

$$GA(\acute{G}) = \sum_{rs \in E(\acute{G})} \frac{2\sqrt{d_r d_s}}{d_r + d_s}. \quad (1)$$

The atom–bond connectivity index (ABC) is a degree-based graph invariant. It can be used to simulate the thermodynamic properties of organic chemical compounds. Consider a graph G, then atom bond connectivity index (ABC) is defined [8] as follows:

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

The well-known index is forgotten topological index (F), which is very helpful for medical scientists to grasp chemical characteristics of the new drugs and is defined [9] as follows:

$$F(Ǵ) = \sum_{rs\in E(Ǵ)} (d_r^2 + d_s^2). \qquad (3)$$

The Inverse sum index (ISI) is defined [10] as:

$$ISI(Ǵ) = \sum_{rs\in E(Ǵ)} \frac{1}{\frac{1}{d_r} + \frac{1}{d_s}}. \qquad (4)$$

The First and the second multiplicative-Zagreb index multiplicative-Zagreb is used to examine the extreme molecular graphs and is defined [11,12] as follows:

$$PM_1(Ǵ) = \prod_{rs\in E(Ǵ)} (d_r)^2, \qquad (5)$$

$$PM_2(Ǵ) = \prod_{rs\in E(Ǵ)} (d_r . d_s). \qquad (6)$$

We can also write first multiplicative-Zagreb index [13] as:

$$PM_1(Ǵ) = \prod_{rs\in E(Ǵ)} (d_r + d_s). \qquad (7)$$

For more comprehensive and detailed study on indices and graphs, we mention the following articles [14-19, 23-48] for readers.

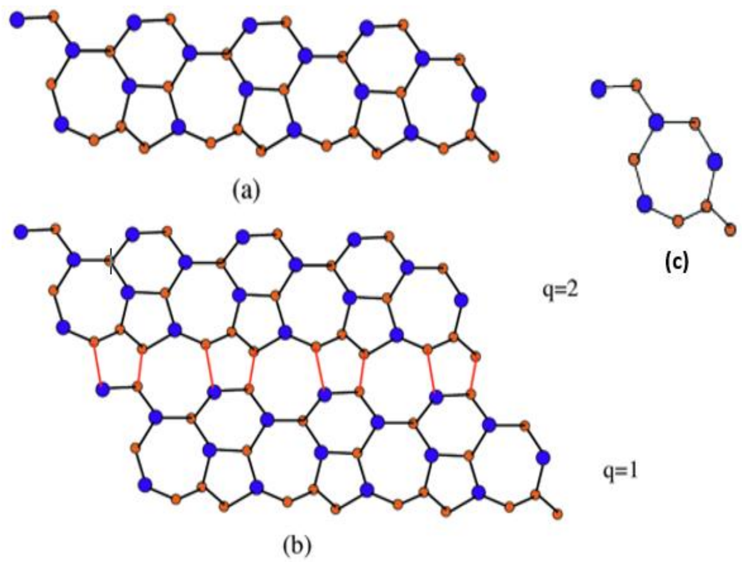

FIGURE 1 Two-dimensional structure of ($Si_2C_3-I[p,q]$)

Silicon Carbide $Si_2C_3 - I[p,q]$ is a molecular graph in two dimensions [20], depicted in Figure 1. We used the following parameters to characterize its molecular graph: We define p as the number of linked unit cells in a row (chain) as in Figure 1(a), and q is the number of linked rows, each having p cells. In Figure 1(b), we showed how the cells in a row (chain) link to each another and how one row relates to another row. Figure 1(c) displays the structure of one-dimensional unit cell.

The double graph of silicon carbide is symbolized by $D[Si_2C_3-I(p,q)]$. Assume two copies of a $Si_2C_3-I(p,q)$, where $(p,q \geq 1)$ and join each vertex in one copy to its neighbor in the other copy to produce the double graph [21] of the silicon carbide $Si_2C_3-I(p,q)$. For example, the double graph of silicon carbide $Si_2C_3-I(1,1)$ is depicted in Figure 2. While for strong double graph $SD[G]$ of the silicon carbide, $Si_2C_3-I(p,q)$ is attained by taking two graphs of $Si_2C_3-I(p,q)$, where $(p,q \geq 1)$ and joining the closed neighborhoods of each vertex in one graph to the adjacent vertex in the other graph [22]. The $SD[Si_2C_3-I(1,1)]$ is depicted in Figure 4.

Main results for double graph of silicon carbide ($Si_2C_3-I(p,q)$)

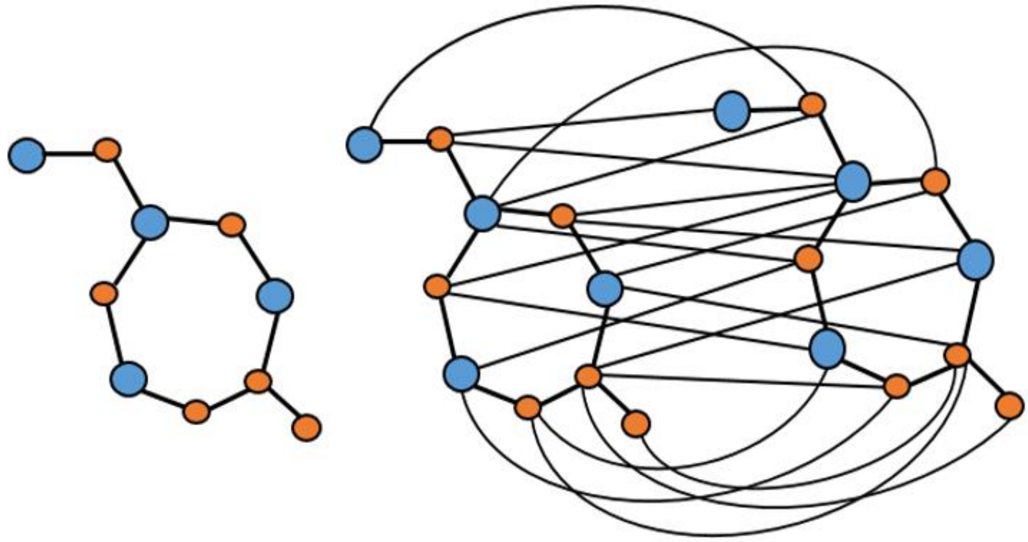

FIGURE 2 Silicon carbide $Si_2C_3-I(1,1)$ and its $D[Si_2C_3-I(1,1)]$

Here, we calculate the indices which base on the degree of vertices, for the double graph of the silicon carbide $Si_2C_3-I(p,q)$. In $D(Si_2C_3-I(p,q))$, we have vertices of degree 2, 4, and 6. Edges of $D(Si_2C_3-I(p,q))$ are split into the edges of type $E[d_r,d_s]$, where rs is represent the edge. Silicon carbide $Si_2C_3-I(p,q)$ contains the edges of the type $E_{(2,4)}$, $E_{(2,6)}$, $E_{(4,4)}$, $E_{(4,6)}$, and $E_{(6,6)}$. Table 1 represents the edges of these types.

TABLE 1 Partitioning of edges

$E[d_r,d_s]$	Number of edges
$E_{(2,4)}$	4
$E_{(2,6)}$	4
$E_{(4,4)}$	$4p+8q$
$E_{(4,6)}$	$24p+32q-36$
$E_{(6,6)}$	$60pq-36p-52q+28$

Theorem 2.1. Let $D(Si_2C_3-I(p,q))$ be the double graph of silicon carbide $Si_2C_3-I(p,q)$. Then,

$$GA[D(Si_2C_3-I(p,q))] = \frac{8\sqrt{2}}{3} + 2\sqrt{3} + (24p+32q-36)\frac{2\sqrt{6}}{5} + 60pq - 32p - 44q + 28.$$

$$ABC[D(Si_2C_3-I(p,q))] = 4\sqrt{2} + (4p+8q)\sqrt{\frac{3}{8}} + (24p + 32q - 36)\sqrt{\frac{1}{3}} + (60pq - 36p - 52q + 28)\frac{\sqrt{10}}{6}.$$

$$F[D(Si_2C_3-I(p,q))] = 384 + 1216p + 1824q + 4320pq.$$

$$ISI[D(Si_2C_3-I(p,q))] = 180pq - 100p - 140q + (24p+32q)\frac{12}{5} + \frac{178}{3}.$$

$$PM_1[D(Si_2C_3-I(p,q))] = 294912(p+2q)(240p+320q-360)(60pq-36p-52q+28).$$

$$PM_2[D(Si_2C_3-I(p,q))] = 679477248(p+2q)(6p+8q-9)(30pq-18p-26q+14).$$

Proof: Consider the double molecular graph of silicon carbide $D(Si_2C_3-I(p,q))$, contains $20\,pq$ vertices and $60\,pq-8p-12q$ edges. By using Equation (1) and Table 1, the GA index calculated as follows:

$$GA[D(Si_2C_3-I(p,q))] = |E_{(2,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s} + |E_{(2,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s} + |E_{(4,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s} + |E_{(4,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s} + |E_{(6,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}.$$

$$GA[D(Si_2C_3-I(p,q))] = 4\left(\frac{2\sqrt{8}}{6}\right) + 4\left(\frac{2\sqrt{12}}{8}\right) + (4p+8q)\frac{2\sqrt{16}}{8} + (24p+32q-36)\frac{2\sqrt{24}}{10} + (60pq-36p-52q+28)\frac{2\sqrt{36}}{12}.$$

$$GA[D(Si_2C_3-I(p,q))] = \frac{8\sqrt{2}}{3} + 2\sqrt{3} + (24p+32q-36)\frac{2\sqrt{6}}{5} + 60pq-32p-44q+28.$$

Via Equation (2) and Table 1, the ABC index is calculated as:

$$ABC[D(Si_2C_3-I(p,q))] = |E_{(2,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}} + |E_{(2,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}} + |E_{(4,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}} + |E_{(4,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}} + |E_{(6,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}.$$

$$ABC[D(Si_2C_3-I(p,q))] = (4)\sqrt{\frac{4}{8}} + (4)\sqrt{\frac{6}{12}} + (4p+8q)\sqrt{\frac{2+4}{16}} + (24p+32q-36)\sqrt{\frac{2+6}{24}} + (60pq-36p-52q+28)\sqrt{\frac{4+6}{36}}.$$

$$ABC[D(Si_2C_3-I(p,q))] = 4\sqrt{2} + (4p+8q)\sqrt{\frac{3}{8}} + (24p+32q-36)\sqrt{\frac{1}{3}} + (60pq-36p-52q+28)\frac{\sqrt{10}}{6}.$$

By applying Equation (3) and Table 1, (F) index is calculated as follows:

$$F[D(Si_2C_3-I(p,q))] = |E_{(2,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r^2+d_s^2)$$

$$+|E_{(2,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r^2+d_s^2) + |E_{(4,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r^2 + d_s^2)$$

$$+|E_{(4,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r^2+d_s^2) + |E_{(6,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r^2 + d_s^2).$$

$$F[D(Si_2C_3-I(p,q))] = (4)(4+16) + (4)(4+36) + (4p+8q)(16+16) + (24p+32q-36)(16+36) + (60pq-36p-52q+28)(36+36).$$

$$F[D(Si_2C_3-I(p,q))] = 384 + 1216p + 1824q + 4320pq.$$

By using Equation (4) and Table 1, *ISI* index is calculated as follows:

$$ISI[D(Si_2C_3-I(p,q))] = |E_{(2,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{(d_r d_s)}{(d_r+d_s)} + |E_{(2,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{(d_r d_s)}{(d_r+d_s)} + |E_{(4,4)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{(d_r d_s)}{(d_r+d_s)} + |E_{(4,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{(d_r d_s)}{(d_r+d_s)} + |E_{(6,6)}| \sum_{rs\in E[D(Si_2C_3-I(p,q))]} \frac{(d_r d_s)}{(d_r+d_s)}.$$

$$ISI[D(Si_2C_3-I(p,q))] = (4)\frac{8}{6} + (4)\frac{12}{8} + (4p+8q)\frac{16}{8} + (24p+32q-36)\frac{24}{10} + (60pq-36p-52q+28)\frac{36}{12}.$$

$$ISI[D(Si_2C_3-I(p,q))] = 180pq - 100p - 140q + (24p+32q)\frac{12}{5} + \frac{178}{3}.$$

By using Equation (7) and Table 1, PM_1 index is calculated as follows:

$$PM_1[D(Si_2C_3-I(p,q))] = |E_{(2,4)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r+d_s) \times |E_{(2,6)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r+d_s) \times |E_{(4,4)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r+d_s) \times |E_{(4,6)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r+d_s) \times |E_{(6,6)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r+d_s).$$

$$PM_1[D(Si_2C_3-I(p,q))] = (4)(6)\times(4)(8) \times (4p+8q)(8) \times (24p+32q-36)(10) \times (60pq-36p-52q+28)(12).$$

$$PM_1[D(Si_2C_3-I(p,q))] = 294912(p+2q)(240p+320q-360)(60pq-36p-52q+28).$$

Via Equation (6) and Table 1, PM_2 index is calculated as:

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

$$PM_2[D(Si_2C_3-I(p,q))] = |E_{(2,4)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r . d_s) \times |E_{(2,6)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r . d_s) \times |E_{(4,4)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r . d_s) \times |E_{(4,6)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r . d_s) \times |E_{(6,6)}| \prod_{rs\in E[D(Si_2C_3-I(p,q))]} (d_r . d_s).$$

$$PM_2[D(Si_2C_3-I(p,q))] = (4)(8)\times(4)(12) \times (4p+8q)(16) \times (24p+32q-36)(24) \times (60pq-36p-52q+28)(36).$$

$$PM_2[D(Si_2C_3-I(p,q))] = 679477248(p+2q)(6p+8q-9)(30pq-18p-26q+14).$$

Comparison

In this section, we compute a numerical and graphical comparison of topological indices based on the degree of the vertex, which are computed above for the double graph of silicon carbide *[D(Si₂C₃-I[p,q])]*, where $p = 1, 2, 3, \ldots, 10$ and $q = 1, 2, 3, \ldots, 10$.

TABLE 2 Computation of indices for double graph of silicon carbide $[D(Si_2C_3\text{-}I[p,q])]$

(p,q)	GA $[D(Si_2C_3-I(p,q))]$	ABC $[D(Si_2C_3-I(p,q))]$	F $[D(Si_2C_3-I(p,q))]$	ISI $[D(Si_2C_3-I(p,q))]$	PM_1 $[D(Si_2C_3-I(p,q))]$	PM_2 $[D(Si_2C_3-I(p,q))]$
(1,1)	38.83125572	24.55232887	1664.00	133.7333333	0	0
(2,2)	197.6998260	183.0039025	11584.0	568.1333333	1.237214×10^{11}	3.563178×10^{12}
(3,3)	476.5683962	496.3748098	30144.0	1362.533333	1.065080×10^{12}	3.067432×10^{13}
(4,4)	875.4369665	964.6650512	57344.0	2516.933333	4.231444×10^{12}	1.218656×10^{14}
(5,5)	1394.305537	1587.874626	93184.0	4031.333333	1.174363×10^{13}	3.382165×10^{14}
(6,6)	2033.174107	2366.003535	1.37664×10^{5}	5905.733333	2.643591×10^{13}	7.613542×10^{14}
(7,7)	2792.042677	3299.051778	1.90784×10^{5}	8140.133333	5.185600×10^{13}	1.493452×10^{15}
(8,8)	3670.911247	4387.019356	2.52544×10^{5}	10734.53333	9.226508×10^{13}	2.657234×10^{15}
(9,9)	4669.779818	5629.906263	3.22944×10^{5}	13688.93333	1.526377×10^{14}	4.395967×10^{15}
(10,10)	5788.648388	7027.712510	4.01984×10^{5}	17003.33333	2.386621×10^{14}	6.873469×10^{15}

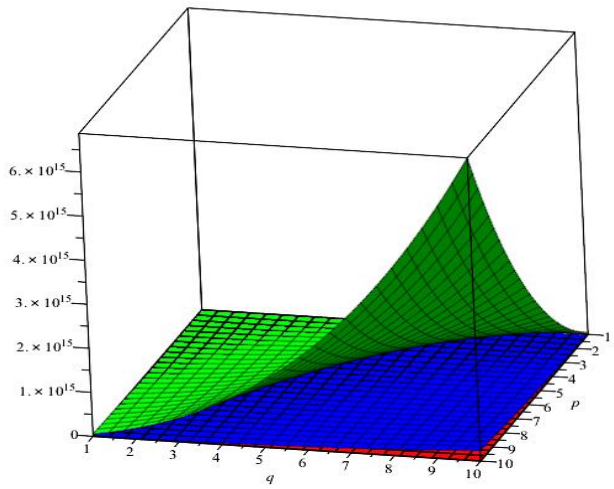

FIGURE 3 Graphical representation of indices for double graph of silicon carbide *$[D(Si_2C_3\text{-}I[p,q])]$*

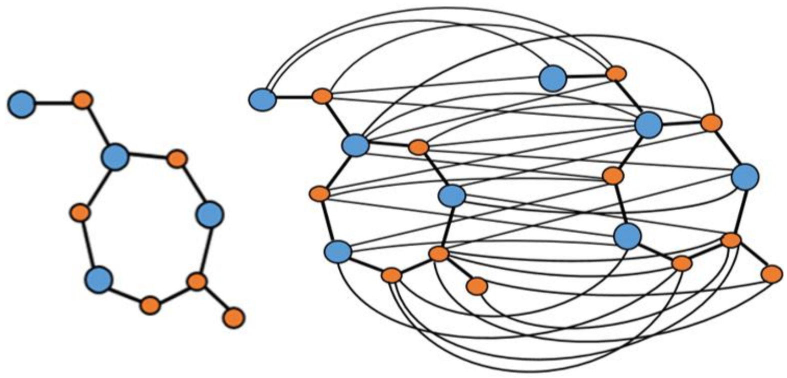

FIGURE 4 Silicon carbide $Si_2C_3-I(1,1)$ and its $SD[Si_2C_3-I(1,1)]$

Main results for strong double graph of silicon carbide $(Si_2C_3-I(p,q))$

We will compute indices which are based on the degree of vertices, for the strong double graph of the silicon carbide $Si_2C_3-I(p,q)$ in this section. In $SD(Si_2C_3-I(p,q))$, we have vertices of degree 3, 5, and 7. Edges of $SD(Si_2C_3-I(p,q))$ were split into the edges of type $E[d_r,d_s]$, where rs is represent the edge. Silicon carbide $Si_2C_3-I(p,q)$ contains edges of the type $E_{(3,3)}$, $E_{(3,5)}$, $E_{(3,7)}$, $E_{(5,5)}$, $E_{(5,7)}$, and $E_{(7,7)}$. Table 3 represents the edges of these types.

TABLE 3 Partitioning of edges

$E[d_r,d_s]$	Number of edges
$E_{(3,3)}$	2
$E_{(3,5)}$	4
$E_{(3,7)}$	4
$E_{(5,5)}$	$4pq+4p+8q+2$
$E_{(5,7)}$	$24p+32q-36$
$E_{(7,7)}$	$66pq-36p-52q+24$

Theorem 4.1. Let $SD(Si_2C_3-I(p,q))$ be the strong double graph of silicon carbide $Si_2C_3-I(p,q)$. Then,

$$GA[SD(Si_2C_3-I(p,q))] = 70pq-32p-44q + \frac{\sqrt{35}}{6}(24p+32q-36) + 28+\sqrt{15}+\frac{4\sqrt{21}}{5}.$$

$$ABC[SD(Si_2C_3-I(p,q))] = (4pq+4p+8q+2)\frac{2\sqrt{2}}{5} + (24p+32q-36)\sqrt{\frac{2}{7}} + (66pq-36p-52q+24)\frac{2\sqrt{3}}{7} + 4\left(\frac{1}{3}+\sqrt{\frac{2}{5}}+\sqrt{\frac{8}{21}}\right).$$

$$F[SD(Si_2C_3-I(p,q))] = 6668pq-1552p-2328q+192.$$

$$ISI[SD(Si_2C_3-I(p,q))] = 241pq-46p-\frac{206}{3}q+\frac{29}{10}.$$

$$PM_1[SD(Si_2C_3-I(p,q))] = 412876800(2pq+2p+4q+1)(6p+8q-9)(33pq-18p-26q+12).$$

$$PM_2[SD(Si_2C_3-I(p,q))] = 31116960000(2pq+2p+4q+1)(6p+8q-9)(33pq-18p-26q+12).$$

Proof: Consider the strong double graph of silicon carbide $SD(Si_2C_3-I(p,q))$, that contains $20pq$ vertices and $70pq-8p-12q$ edges.

By using Equation (1) and Table 3, GA index is calculated as follows:

$$GA[SD(Si_2C_3-I(p,q))] = |E_{(3,3)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}$$

$$+|E_{(3,5)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}$$
$$+|E_{(3,7)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}$$
$$+|E_{(5,5)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}$$
$$+|E_{(5,7)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}$$
$$+|E_{(7,7)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \frac{2\sqrt{d_r d_s}}{d_r+d_s}.$$

$$GA[SD(Si_2C_3-I(p,q))] = (2)\frac{2\sqrt{9}}{3+3} + (4)\frac{2\sqrt{15}}{3+5} + (4)\frac{2\sqrt{21}}{3+7} + (4pq+4p+8q+2)\frac{2\sqrt{25}}{5+5} + (24p+32q-36)\frac{2\sqrt{35}}{5+7} + (66pq-36p-52q+24)\frac{2\sqrt{49}}{7+7}.$$

$$GA[SD(Si_2C_3-I(p,q))] = 70pq-32p-44q + \frac{\sqrt{35}}{6}(24p+32q-36) + 28 + \sqrt{15} + \frac{4\sqrt{21}}{5}.$$

Via Equation (2) and Table 3, ABC index is calculated as:

$$ABC[SD(Si_2C_3-I(p,q))] = |E_{(3,3)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}$$
$$+|E_{(3,5)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}$$
$$+|E_{(3,7)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}$$
$$+|E_{(5,5)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}$$
$$+|E_{(5,7)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}$$
$$+|E_{(7,7)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} \sqrt{\frac{d_r+d_s-2}{d_r d_s}}.$$

$$ABC[SD(Si_2C_3-I(p,q))] = (2)\sqrt{\frac{3+3-2}{9}} + (4)\sqrt{\frac{3+5-2}{15}} + (4)\sqrt{\frac{3+7-2}{21}} + (4pq+4p+8q+2)\sqrt{\frac{5+5-2}{25}} + (24p+32q-36)\sqrt{\frac{5+7-2}{35}} + (66pq-36p-52q+24)\sqrt{\frac{7+7-2}{49}}.$$

$$ABC[SD(Si_2C_3-I(p,q))] = (4pq+4p+8q+2)\frac{2\sqrt{2}}{5} + (24p+32q-36)\sqrt{\frac{2}{7}} + (66pq-36p-52q+24)\frac{2\sqrt{3}}{7} + 4\left(\frac{1}{3}+\sqrt{\frac{2}{5}}+\sqrt{\frac{8}{21}}\right).$$

By Equation (3) and Table 3, (F) index is calculated as follows:

$$F[SD(Si_2C_3-I(p,q))] = |E_{(3,3)}| \sum_{rs\in E[SD(Si_2C_3-I(p,q))]} (d_r^2+d_s^2)$$

$$+|E_{(3,5)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r^2+d_s^2)$$
$$+|E_{(3,7)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r^2+d_s^2)$$
$$+|E_{(5,5)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r^2+d_s^2)$$
$$+|E_{(5,7)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r^2+d_s^2)$$
$$+|E_{(7,7)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r^2+d_s^2).$$

$$F[SD(Si_2C_3-I(p,q))] = (2)(9+9)+(4)(9+25)+(4)(9+49)+(4pq+4p+8q+2)(25+25)+(24p+32q-36)(25+49)+(66pq-36p-52q+24)(49+49).$$

$$F[SD(Si_2C_3-I(p,q))] = 6668pq-1552p-2328q+192.$$

With the help of Equation (4) and the Table 3, ISI index is calculated as:

$$ISI[SD(Si_2C_3-I(p,q))] = |E_{(3,3)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}\frac{(d_rd_s)}{(d_r+d_s)}$$
$$+|E_{(3,5)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}\frac{(d_rd_s)}{(d_r+d_s)}$$
$$+|E_{(3,7)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}\frac{(d_rd_s)}{(d_r+d_s)}$$
$$+|E_{(5,5)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}\frac{(d_rd_s)}{(d_r+d_s)}$$
$$+|E_{(5,7)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}\frac{(d_rd_s)}{(d_r+d_s)}$$
$$+|E_{(7,7)}|\sum_{rs\in E[SD(Si_2C_3-I(p,q))]}\frac{(d_rd_s)}{(d_r+d_s)}.$$

$$ISI[SD(Si_2C_3-I(p,q))] = (2)\frac{9}{6}+(4)\frac{15}{8}+(4)\frac{21}{10}+(4pq+4p+8q+2)\frac{25}{10}+(24p+32q-36)\frac{35}{12}+(66pq-36p-52q+24)\frac{49}{14}.$$

$$= (2pq+2p+4q)5+(6p+8q)\frac{35}{3}+(33pq-18p-26q)7+\frac{29}{10}.$$

$$ISI[SD(Si_2C_3-I(p,q))] = 241pq-46p-\frac{206}{3}q+\frac{29}{10}.$$

By using Equation (7) and Table 3, PM_1 index is calculated as:

$$PM_1[SD(Si_2C_3-I(p,q))] = |E_{(3,3)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r+d_s)$$
$$\times|E_{(3,5)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r+d_s)$$
$$\times|E_{(3,7)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r+d_s)$$
$$\times|E_{(5,5)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r+d_s)$$
$$\times|E_{(5,7)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r+d_s)$$
$$\times|E_{(7,7)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r+d_s).$$

$$PM_1[SD(Si_2C_3-I(p,q))] = (2)(6)\times(4)(8)\times(4)(10)\times(4pq+4p+8q+2)10\times(24p+32q-36)(12)\times(66pq-36p-52q+24)(14).$$

$$PM_1[SD(Si_2C_3-I(p,q))] = 412876800(2pq+2p+4q+1)(6p+8q-9)(33pq-18p-26q+12).$$

Via Equation (6) and Table 3, PM_2 index is calculated as follows:

$$PM_2[SD(Si_2C_3-I(p,q))] = |E_{(3,3)}|\prod_{rs\in E[SD(Si_2C_3-I(p,q))]}(d_r.d_s)$$

$$\times |E_{(3,5)}| \prod_{rs\in E[SD(Si_2C_3-I(p,q))]} (d_r.d_s)$$
$$\times |E_{(3,7)}| \prod_{rs\in E[SD(Si_2C_3-I(p,q))]} (d_r.d_s)$$
$$\times |E_{(5,5)}| \prod_{rs\in E[SD(Si_2C_3-I(p,q))]} (d_r.d_s)$$
$$\times |E_{(5,7)}| \prod_{rs\in E[SD(Si_2C_3-I(p,q))]} (d_r.d_s)$$
$$\times |E_{(7,7)}| \prod_{rs\in E[SD(Si_2C_3-I(p,q))]} (d_r.d_s).$$
$$PM_2[SD(Si_2C_3-I(p,q))] = (2)(9)\times(4)(15)\times(4)(21) \times(4pq+4p+8q+2)25 \times(24p+32q-36)(35)\times(66pq-36p-52q+24)(49).$$
$$PM_2[SD(Si_2C_3-I(p,q))] = 31116960000(2pq+2p+4q+1)(6p+8q-9)(33pq-18p-26q+12).$$

Comparison

In this section, we compute a numerical and graphical comparison of topological indices based on the degree of the vertex (Table 4), which are computed above for the strong double graph of silicon carbide *[SD(Si_2C_3-I[p,q]]*, where $p = 1,2,3,\dots,10$ and $q = 1, 2, 3,\dots, 10$.

TABLE 4 Computation of indices for strong double graph of silicon carbide *[SD(Si_2C_3-I[p,q]]*

(p,q)	GA $[SD(Si_2C_3-I(p,q))]$	ABC $[SD(Si_2C_3-I(p,q))]$	F $[SD(Si_2C_3-I(p,q))]$	ISI $[SD(Si_2C_3-I(p,q))]$	PM_1 $[SD(Si_2C_3-I(p,q))]$	PM_2 $[SD(Si_2C_3-I(p,q))]$
(1,1)	49.25930985	28.19453971	2980.00	129.2333333	1.857945×10^{10}	2.800526×10^{12}
(2,2)	238.4760545	126.1401315	19104.00	737.5666667	9.225319×10^{12}	1.390554×10^{15}
(3,3)	567.6927991	293.9342657	48564.00	1827.900000	8.922969×10^{13}	1.344980×10^{16}
(4,4)	1036.909544	531.5769425	91360.00	3400.233333	4.026192×10^{14}	6.068778×10^{16}
(5,5)	1646.126288	839.0681617	1.47492×10^{5}	5454.566667	1.258694×10^{15}	1.897261×10^{17}
(6,6)	2395.343033	1216.407923	2.16960×10^{5}	7990.900000	3.159250×10^{15}	4.762015×10^{17}
(7,7)	3284.559778	1663.596227	2.99764×10^{5}	11009.23333	6.844353×10^{15}	1.031665×10^{18}
(8,8)	4313.776522	2180.633075	3.95904×10^{5}	14509.56667	1.333812×10^{16}	2.010487×10^{18}
(9,9)	5482.993267	2767.518463	5.05380×10^{5}	18491.90000	2.399450×10^{16}	3.616750×10^{18}
(10,10)	6792.210012	3424.252394	6.28192×10^{5}	22956.23333	4.054307×10^{16}	6.111156×10^{18}

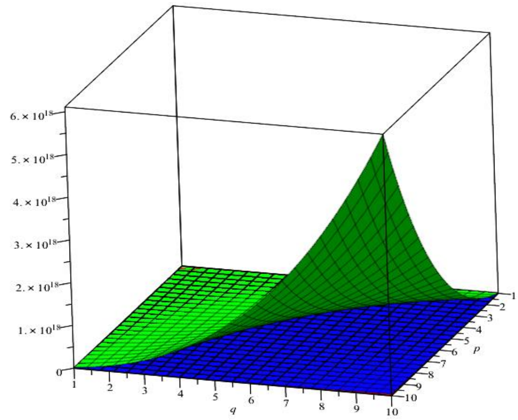

FIGURE 5 Graphical representation of indices for strong double graph of silicon carbide *[SD(Si₂C₃-I[p,q])]*

Conclusion

The findings of this study can help to understand the physical features and biological activities of silicon carbide. In this paper, we investigated the topological indices namely; Inverse sum indeg index (ISI), the first multiplicative-Zagreb index (PM_1), atom bond connectivity index (ABC), forgotten index (F), geometric arithmetic index (GA), the second multiplicative-Zagreb index (PM_2) of strong double and double graph of silicon carbide ($Si_2C_3-I(p,q)$). The comparison and geometric structure of attained results are presented numerically and graphically.

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Conflict of Interest

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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