Research Article

Topological Descriptors of M-Carbon \( M[r, s, t] \)

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We have studied topological indices of the one the hardest crystal structures in a given chemical system, namely, M-carbon. These structures are based and obtained by the famous algorithm USPEX. The computations and applications of topological indices in the study of chemical structures is growing exponentially. Our aim in this article is to compare and compute some well-known topological indices based on degree and sum of degrees, namely, general Randić indices, Zagreb indices, atom bond connectivity index, geometric arithmetic index, new Zagreb indices, fourth atom bond connectivity index, fifth geometric arithmetic index, and Sanskruti index of the M-carbon \( M[r, s, t] \). Moreover, we have also computed closed formulas for these indices.

1. Introduction

One of the hardest structures of carbon is diamond. In 2011, Andriy and Artem searches 9500 structures of different system sizes, and they produced a large number of superhard allotropes; these allotropes being as hard as diamonds [1]. One of the superhard carbon allotropes that they studied was M-carbon (Figure 1). Scientists also believe that the synthesis and practical applications of some of these structures may be possible. Some studies also exist giving indications that these types of carbon allotropes such as M-carbon have been obtained by applying cold compression on graphite [2, 3].

In this study, we intend to study and compute the degree-based topological indices of M-carbon structures. One of the first and very old topological indices is the Wiener index [4], and this index is also known as the path number. After that, the scientists of various field started exploring this new technique to study chemical and physical properties of chemical structure, compounds, and molecules. A list of topological indices that we shall discuss in this study is given in Table 1, which includes Randić index, general Randić indices, Zagreb indices, atom bond connectivity index, geometric arithmetic index, new Zagreb indices, fourth atom bond connectivity index, fifth geometric arithmetic index, and Sanskruti index of the M-carbon \( M[r, s, t] \). Moreover, we have also computed closed formulas for these indices.

\[ M_1(G) = 2|E(G)|(|V(G)| - 1) - M_1(G). \] (1)

Theorem 1 (See [26]). Let \( G \) be a graph with \(|V(G)|\) vertices and \(|E(G)|\) edges. Then,

\[ M_2(G) = 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G). \] (2)

Theorem 2 (See [26]). Let \( G \) be a graph with \(|V(G)|\) vertices and \(|E(G)|\) edges. Then,
2. Construction of $M[r, s, t]$ for Topological Study

In this section, we shall present our main results about the $M$-carbon structure denoted as $M[r, s, t]$. First, we need to give a brief explanation of the variables $r, s, t$ in the notation $M[r, s, t]$. To find and compute the topological indices of the $M$-carbon structure, we have introduced a way of constructing its structure by the means of these three variables, where $r$ represents the unit as shown in Figures 2(a) and 2(b) represents a chain containing three units, where the connection (bond) is shown in blue color. The variable $s$ represents the number of connected chains with each having $r$ numbers of units (Figure 3). The variable $t$ represents the number of connected layers. There are two types of layers odd layer for $t = 1, 3, 5, \ldots$ and even layers for $t = 2, 4, 6, \ldots$, both are generated by different unit cells. The one depicted in Figure 3 is the odd layer (that is for $t = 1, 3, 5, \ldots$) which was generated by the unit of Figure $t = 2, 4, 6, \ldots$). The unit cell of an even layer is shown in Figure 4(a), the chain in even layer is shown in Figure 4(b), and Figure 4(c) depicts an even layer. Then, finally, the $M$-carbon structure $M[r, s, t]$ is shown in Figure 5, which also depicts how two layers, an even and odd, are connecting. In Figure 5, these connections (bonds) between two layers are shown in red color. So, in this way, we get structure of $M$-carbon (Figure 1). By our construction, the graph of $M$-carbon $M[r, s, t], r \geq 2, s \geq 2, t \geq 2$ consists of $8rst$ number vertices and $16rst - 4rt - 5st - 2rs + t + s$ number of edges.

3. Main Results

The graph $M[r, s, t]$ has $2(s + 1)t, 4r - 2 + 2(s - 1)t, 2rst + 2rs + 6rt - st - 6r - s - 3t + 3$, and $6rst - 2rs - 6rt - 3st + 2r + s + 3t - 1$ vertices of degrees $1, 2, 3$, and $4$, respectively. The degree-based edge partition of $M[r, s, t]$ is given in Table 2.

In all the theorems in the following, we used Maple for the computations of mathematical expression and graphical comparisons.
Theorem 3. Let $G$ be the chemical structural graph of $M$-carbon $M[r, s, t]$, and the general Randić index of $M[r, s, t]$ is given by

$$R_{α}(M[r, s, t]) = 2 \times 4^a - 7 \times 16^a + 2 \times 2^a r + 2 \times 4^a r - 4 \times 8^a r + 4 \times 8^a t - 4 \times 8^a t - 6 \times 8^a t - 6 \times 8^a t - 4 \times 9^a r - 2 \times 9^a s - 3 \times 9^a t - 2 \times 12^a s - 4 \times 12^a t - 4 \times 12^a t - 4 \times 16^a r + 7 \times 16^a s + 10 \times 16^a r - 8 \times 6^a s - 2 \times 3^a + 2 \times 2^a + 2 \times 3^a s + 4 \times 8^a s + 2 \times 9^a r s + 6 \times 9^a r + 4 \times 12^a r s + 4 \times 12^a r s - 8 \times 16^a r s - 14 \times 16^a r r - 11 \times 16^a s r + 5 \times 9^a + 16 \times 16^a s t + 6 \times 8^a + 2 \times 12^a t.$$

Proof. Let $G$ be the chemical structural graph of $M$-carbon $M[r, s, t]$; then, by using serial number 2 of Table 1 and edge partition given in Table 2, the general Randić index $R_{α}(G)$ of $M[r, s, t]$ is computed as follows:

$$R_{α}(M[r, s, t]) = \sum_{α \in E(G)} (d_{\alpha} \times d_{\ell})^α$$

$$= (2t + 2)(1 \times 2)^a + (2st - 2)(1 \times 3)^a + (2t)(2 \times 2)^a + (8r + 2s + 2t - 8)(2 \times 3)^a$$

$$+ (4st + 4s - 6t + 6)(2 \times 4)^a + (6rt + 2s - 4r - 2s - 3t + 5)(3 \times 3)^a + (4rs + 4rt - 2s - 4t + 2)(3 \times 4)^a$$

$$+ (16rst - 8rs - 14rt - 11st - 4rt + 14s + 7s + 10r - 7)(4 \times 4)^a.$$
Corollary 2. The second Zagreb index $M_2(M[r,s,t])$ is the same as $R_\alpha(M[r,s,t])$ for $\alpha = 1$, so $M_2([M[r,s,t]])$ can be obtained from Corollary 1.

Theorem 4. The first Zagreb index $M_1(M[r,s,t])$ of $M$-carbon structure is given by

$$M_1(M[r,s,t]) = 128rst - 24rs - 48rt - 56st - 16r + 16s + 14t - 10.$$  

Proof. Let $G$ be the chemical structural graph of $M$-carbon $M[r,s,t]$; then, by using serial number 5 of Table 1 and edge partition given in Table 2, the first Zagreb index $R_\alpha(G)$ of $M[r,s,t]$ is computed as follows:

\begin{table}[h]
\centering
\begin{tabular}{ |c|c| }
\hline
$(d_u, d_v)$ & Frequency \\
\hline
$(1, 2)$ & $2t + 2$ \\
$(1, 3)$ & $2st - 2$ \\
$(2, 2)$ & $2$ \\
$(2, 3)$ & $8t + 2s + 2t - 8$ \\
$(2, 4)$ & $4st - 4s - 6t + 6$ \\
$(3, 3)$ & $6rst + 2sr - 2s - 3t + 5$ \\
$(3, 4)$ & $4rs + 4rt - 2s - 4t + 2$ \\
$(4, 4)$ & $16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7$ \\
\hline
\end{tabular}
\caption{Degree-based edge partition of $M[r,s,t]$ for $r, s, t \geq 2$.}
\end{table}
Table 3: Sum degree-based edge partition of $M_{r,s,t}$ for $r,s,t \geq 3$.

| $(S(o), S(t))$ | Frequency | $(S(o), S(t))$ | Frequency |
|----------------|-----------|----------------|-----------|
| (3, 7)         | 4         | (3, 8)         | 2         |
| (4, 11)        | $2t$      | (4, 12)        | $2st−2s−4t+6$ |
| (4, 13)        | $2st−2s−4t+4$ | (5, 5)      | 2         |
| (5, 7)         | 2         | (5, 8)         | 2         |
| (6, 7)         | 2         | (6, 8)         | 4s−10     |
| (6, 9)         | $8r−8$    | (7, 8)         | 2t−2      |
| (7, 11)        | 2         | (7, 12)        | 2t−2      |
| (7, 15)        | 2         | (8, 8)         | 2t−2      |
| (8, 10)        | $2t−2$    | (8, 11)        | 2t−2      |
| (8, 12)        | $4st−10t+6$ | (8, 14)      | 2         |
| (8, 15)        | $2t−4$    | (9, 10)        | 8r−8      |
| (9, 12)        | 2         | (9, 14)        | 2r−2      |
| (9, 15)        | $4r−6$    | (10, 10)       | $4rs+6rt−16r−4s−8t+18$ |
| (10, 11)       | 2         | (10, 14)       | 4r−6      |
| (10, 15)       | $4rs+4rt−12r−4s−4t+12$ | (11, 12)     | 2t−2    |
| (11, 15)       | $2t−2$    | (11, 16)       | 2         |
| (12, 13)       | $2st−2s−4t+4$ | (12, 15)     | 2r        |
| (12, 16)       | $2st+2s−4t−6$ | (13, 14)     | 2t−2      |
| (13, 15)       | $4st−4s−10t+10$ | (14, 15)    | 4r−4      |
| (14, 16)       | $4r−6$    | (15, 15)       | $6rt−2r−7t+1$ |
| (15, 16)       | $10rs−28r−10s+4rt−4t+30$ | (16, 16)   | $16rs−24rt−20rs−21st+38t+23s+24r−40$ |

Table 4: Numerical comparison of indices of $M_{r,s,t}$ for some initial values of $r,s,t \geq 2$.

| $(r,s,t)$ | $R_1$ | $R_{-1}$ | $R_{1/2}$ | $R_{-1/2}$ | $M_1$ | $M_1^T$ | $M_2^T$ | $HM$ |
|-----------|-------|----------|-----------|------------|-------|---------|---------|------|
| (2, 2, 2) | 825   | 13.3     | 260.9     | 32.4       | 530   | 10558   | 14398   | 3376 |
| (3, 3, 3) | 4130  | 36.7     | 1157.6    | 106.2      | 2336  | 14343   | 224544  | 16724|
| (4, 4, 4) | 11399 | 79       | 1157.6    | 250        | 6190  | 86864   | 1450978 | 45992|
| (5, 5, 5) | 24168 | 147.3    | 6397.8    | 489.6      | 12860 | 3453670 | 5989852 | 97324|
| (6, 6, 6) | 43973 | 246.6    | 11510     | 847        | 23114 | 10587574| 18818838| 176864|
| (7, 7, 7) | 72350 | 283      | 18796     | 1339       | 1347  | 37720   | 2.72 $\times 10^7$ | 290756|
| (8, 8, 8) | 110835| 563      | 28636     | 2013       | 57446 | 6.14 $\times 10^7$ | 1.1 $\times 10^8$ | 445144|
| (9, 9, 9) | 160964| 792      | 41418     | 2871       | 83060 | 1.2 $\times 10^8$ | 2.3 $\times 10^8$ | 646172|
| (10, 10, 10)| 224273| 1077     | 57525     | 3943       | 115330| 2.3 $\times 10^8$ | 4.4 $\times 10^8$ | 899984|

Table 5: Numerical comparison of indices of $M_{r,s,t}$ for some initial values of $r,s,t \geq 2$.

| $(r,s,t)$ | ABC | GA | ABC$_4$ | GA$_4$ | $S$ |
|-----------|-----|----|---------|--------|-----|
| (2, 2, 2) | 59.3| 86.2| —       | —      | —   |
| (3, 3, 3) | 220 | 334.6| 138.8   | 334.7  | 114310|
| (4, 4, 4) | 546.8| 847.8| 330.6   | 843.3  | 347250|
| (5, 5, 5) | 1098| 1721| 651.8   | 1712.2 | 775750|
| (6, 6, 6) | 1933| 3052| 1135    | 3037   | 1.4595 $\times 10^6$ |
| (7, 7, 7) | 3110| 4936| 1813    | 4914   | 2.46 $\times 10^6$ |
| (8, 8, 8) | 4688| 7469| 2720    | 7440   | 3.8 $\times 10^6$ |
| (9, 9, 9) | 6725| 10747| 3887    | 10711  | 5.6 $\times 10^6$ |
| (10, 10, 10)| 9282| 14865| 5348    | 14820  | 7.9 $\times 10^6$ |
\[ M_1(M[r, s, t]) = \sum_{o \in E(G)} (d_o + d_t) \]
\[ = (2t + 2)(1 + 2) + (2st - 2)(1 + 3) + (2)(2 + 2) + (8r + 2s + 2t - 8)(2 + 3) \]
\[ + (4st - 4s - 6t + 6)(2 + 4) + (6rt + 2rs - 4r - 2s - 3t + 5)(3 + 3) + (4rs + 4rt - 2s - 4t + 2)(3 + 4) \]
\[ + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7)(4 + 4). \]

Thus, the result follows by simple calculations.

Theorem 5. The new degree-based Zagreb index \( HM(M[r, s, t]) \) of M-carbon structure is given by
\[
HM(M[r, s, t]) = 1024rst - 244rs - 484rt - 528st - 200r + 184s + 188t - 136.
\]

Thus, the result follows by simple calculations.

In the next two theorems, we shall compute the newly defined Zagreb coindex indices which are defined in the form of nonedges of a chemical graph.

\[
HM(M[r, s, t]) = \sum_{o \in E(G)} (d_o + d_t)^2
\]
\[ = (2t + 2)(1 + 2)^2 + (2st - 2)(1 + 3)^2 + (2)(2 + 2)^2 + (8r + 2s + 2t - 8)(2 + 3)^2 \]
\[ + (4st - 4s - 6t + 6)(2 + 4)^2 + (6rt + 2rs - 4r - 2s - 3t + 5)(3 + 3)^2 + (4rs + 4rt - 2s - 4t + 2)(3 + 4)^2 \]
\[ + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7)(4 + 4)^2. \]

Thus, the result follows by simple calculations.

Theorem 6. The first Zagreb coindex index \( \overline{M}_1(M[r, s, t]) \) of M-carbon structure is given by
\[
\overline{M}_1(M[r, s, t]) = 256r^2s^2t^2 - 32r^2s^2t - 64r^2st^2 - 80s^2t^2r + 16s^2rt + 16t^2rs - 160rst + 28rs + 56rt + 66st + 16r - 18s - 16t + 10.
\]

Proof. The first Zagreb coindex index of chemical structural graph of M-carbon \( M[r, s, t] \) can be computed by using both serial number 8 of Table 1 and Theorem 1. It is explained and calculated as follows:
\[
\overline{M}_1(M[r, s, t]) = 2|E(M[r, s, t])|(|V(M[r, s, t])| - 1) - M_1(M[r, s, t])
\]
\[ = 2(16rst - 4rt - 5st - 2rs + t + s)(8rst - 1) - 128rst - 24rs - 48rt - 56st - 16r + 16s + 14t - 10. \]
Thus, the result follows by simple calculations. □

**Theorem 7.** The second Zagreb coindex index $\overline{M}_2(M[r,s,t])$ of M-carbon structure is given by

$$\overline{M}_2(M[r,s,t]) = 512r^2s^2t^2 - 128r^2s^2t - 256r^2st^2 - 320s^2r^2 + 8r^2s^2 + 32r^2st + 32r^2t^2$$

$$+ 104s^2rt + 144rts^2 + 50s^2t^2 - 8s^2r - 344rst - 16rt^2 - 20s^2t - 20st^2 + 74rs$$

$$+ 146rt + 2s^2 + 170st + 2t^2 + 60r - 58s - 60t + 42.$$  

(12)

**Proof.** The second Zagreb coindex index of chemical structural graph of M-carbon $M[r,s,t]$ can be computed by using both serial number 9 of Table 1 and Theorem 2. It is explained and calculated as follows:

$$\overline{M}_2(M[r,s,t]) = 2|E(M[r,s,t])|^2 - \frac{1}{2}M_1(M[r,s,t]) - M_2(M[r,s,t])$$

$$= 2(16rst - 4rt - 5st - 2rs + t + s)^2 - (1/2)(128rst - 24rs - 48rt - 56st - 16r + 16s + 14t - 10)$$

$$- (256rst - 62rs - 122rt - 138st - 52r + 50s + 53t - 37).$$

(13)

Thus, the result follows by simple calculations.

In the coming two theorems, we shall find closed formulas for the ABC and GA indices of $M[r,s,t]$ M-carbon structure.

**Theorem 8.** Consider the graph $G \equiv M[r,s,t]$ of M-carbon with $r \geq 2, s \geq 2, t \geq 2$; then, its ABC index is equal to

$$ABC(M[r,s,t]) = \frac{2rs\sqrt{15}}{3} + \frac{2rt\sqrt{15}}{3} - 2rs\sqrt{6} - \frac{7rt\sqrt{6}}{2} - \frac{25st\sqrt{6}}{12} + 4rt + \frac{4rs}{3} - \frac{s\sqrt{15}}{3}$$

$$- \frac{2t\sqrt{15}}{3} + 4rst\sqrt{6} - \frac{29\sqrt{6}}{12} - \sqrt{2t} - \sqrt{2s} + \frac{10}{3} + \frac{\sqrt{15}}{3} + 2\sqrt{2st} - \sqrt{6r}$$

$$+ \frac{7\sqrt{6}s}{4} + \frac{5\sqrt{6}t}{2} + \sqrt{2} + 4\sqrt{2r} - \frac{8r}{3} - \frac{4s}{3} - 2t.$$  

(14)

**Proof.** Let $G$ be the chemical structural graph of M-carbon $M[r,s,t]$; then, by using serial number 3 of Table 1 and edge partition given in Table 2, the ABC index of $M[r,s,t]$ is computed as follows:

$$ABC(M[r,s,t]) = \sum_{e \in E(G)} \sqrt{\frac{d_o + d_e - 2}{d_o d_e}}$$

$$= (2t + 2)\left(\frac{1 + 2 - 2}{1 \times 2}\right) + (2st - 2)\left(\frac{1 + 3 - 2}{1 \times 3}\right) + (2)\left(\frac{2 + 2 - 2}{2 \times 2}\right) + (8r + 2s + 2t - 8)$$

$$+ \left(\frac{2 + 3 - 2}{2 \times 3}\right) + (4st - 4s - 6t + 6)\left(\frac{2 + 4 - 2}{2 \times 4}\right) + (6rt + 2rs - 4r - 2s - 3t + 5)$$

$$\cdot \left(\frac{3 + 3 - 2}{3 \times 3}\right) + (4rs + 4rt - 2s - 4t + 2)\left(\frac{3 + 4 - 2}{3 \times 4}\right)$$

$$+ (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7)\left(\frac{4 + 4 - 2}{4 \times 4}\right).$$  

(15)
Theorem 9. Consider the graph $G = M[r, s, t]$ of $M$-carbon with $r \geq 2, s \geq 2, t \geq 2$; then, its GA index is equal to

$$GA(M[r, s, t]) = 16rst - 11st - \frac{8\sqrt{2}t}{3} + \frac{16\sqrt{3}}{3} + \frac{\sqrt{3}}{7} + \frac{16\sqrt{6}r}{5} + \frac{4\sqrt{6}t}{5} + \frac{4\sqrt{6}t}{5} - \frac{16\sqrt{6}}{5} + \frac{8\sqrt{2}st}{3} - \frac{8\sqrt{2}s}{3} - 6rs - 8rt - 8r + 5s + 7t + \frac{16\sqrt{3}rs}{7} + \frac{16\sqrt{3}rt}{7} \quad (16)$$

Proof. Let $G$ be the chemical structural graph of $M$-carbon $M[r, s, t]$; then, by using serial number 4 of Table 1 and edge partition given in Table 2, the GA index of $M[r, s, t]$ is computed as follows:

$$GA(M[r, s, t]) = \sum_{e \in E(G)} \frac{2d_o \times d_e}{d_o + d_e} \cdot (2t + 2) \left( \frac{2\sqrt{1} \times \frac{2}{1 + 2}}{1 + 2} \right) + (2st - 2) \left( \frac{2\sqrt{1} \times \frac{3}{1 + 3}}{1 + 3} \right) + (2) \left( \frac{2\sqrt{2} \times 2}{2 + 2} \right) + (8r + 2s + 2t - 8) \left( \frac{2\sqrt{3} \times 3}{2 + 3} \right)$$

$$+ (4st - 4s - 6t + 6) \left( \frac{2\sqrt{2} \times 4}{2 + 4} \right) + (6rt + 2rs - 4r - 2s - 3t + 5) \left( \frac{2\sqrt{3} \times 3}{3 + 3} \right) \quad (17)$$

$$+ (4rs + 4rt - 2s - 4t + 2) \left( \frac{2\sqrt{3} \times 4}{3 + 4} \right)$$

$$+ (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7) \left( \frac{2\sqrt{4} \times 4}{4 + 4} \right).$$

The results now follow after some simple computations of the above expression.

Table 3 provides the edge partition of the $M$-carbon structure $M[r, s, t]$ on the bases of sum of the degrees in the open neighbourhood of the end vertices of each an edge for each edge of $M[r, s, t]$. The first of such type of indices were introduced by Ghorbhani and Hosseinzadeh [23], and then, another one was introduced by Hosamani [25]. These are defined in Table 1.

In the following three theorems, we gave closed formula for the three indices, namely, fourth atom bond connectivity index $ABC_4(G)$, fifth version of geometric arithmetic index $GA_5(G)$, and Sanskruti index $S(G)$ for the graph of $G = M[r, s, t]$. □
Theorem 10. The $ABC_4$ index of the graph $G \equiv M[r, s, t]$ of $M$-carbon with $r \geq 3, s \geq 3, t \geq 3$ is given by

$$ABC_4(G) = 3 + \sqrt{3st} + \frac{\sqrt{462}}{21} + \frac{11t\sqrt{5}}{15} + \frac{t\sqrt{143}}{11} - \frac{3\sqrt{770}}{35} + \frac{\sqrt{2090}}{55} + \frac{2\sqrt{5}}{5} + \frac{3\sqrt{3}}{2} + \frac{47\sqrt{2}}{10}$$

$$- \frac{6\sqrt{2s}}{5} - \frac{5\sqrt{5r}}{2} + \frac{\sqrt{57}}{18} - \frac{\sqrt{357}}{21} + \frac{5\sqrt{11}}{22} + \frac{\sqrt{14}}{28} - \frac{12\sqrt{2t}}{5} + \frac{\sqrt{6r}}{3} + \frac{t\sqrt{14}}{4} + \frac{t\sqrt{77}}{11}$$

$$+ \frac{4\sqrt{138}}{45} - \frac{4\sqrt{7r}}{15} + \frac{14\sqrt{7t}}{35} + \frac{6r\sqrt{70}}{35} + \frac{t\sqrt{70}}{10} + \frac{s\sqrt{42}}{6} - \frac{t\sqrt{42}}{3}$$

$$+ \frac{23t\sqrt{182}}{182} + \frac{3r\sqrt{30}}{2} + \frac{281s\sqrt{30}}{240} + \frac{41t\sqrt{30}}{24} + \frac{4r\sqrt{110}}{55} + \frac{4r\sqrt{170}}{15} - \frac{2r\sqrt{138}}{5}$$

$$- \frac{2s\sqrt{138}}{15} - \frac{2t\sqrt{138}}{15} + \frac{4r\sqrt{78}}{9} + \frac{s\sqrt{78}}{12} - \frac{t\sqrt{78}}{6} - \frac{t\sqrt{374}}{22} + \frac{t\sqrt{357}}{21} - \frac{7r\sqrt{435}}{15}$$

$$- \frac{s\sqrt{435}}{6} - \frac{t\sqrt{435}}{15}$$

$$- \frac{s\sqrt{195}}{13} - \frac{2t\sqrt{195}}{13} - \frac{s\sqrt{897}}{39} - \frac{2t\sqrt{897}}{39} - \frac{5rs\sqrt{30}}{4} - \frac{3rt\sqrt{30}}{2} - \frac{251st\sqrt{30}}{240}$$

$$+ \frac{2rs\sqrt{138}}{15} + \frac{2rt\sqrt{138}}{15} + \frac{st\sqrt{78}}{12} + \frac{\sqrt{6}}{6} + \frac{rst\sqrt{30}}{6} + \frac{37\sqrt{342}}{42} - \frac{\sqrt{374}}{22}$$

$$+ \frac{rs\sqrt{435}}{6} + \frac{rt\sqrt{435}}{15} + \frac{st\sqrt{195}}{13} + \frac{st\sqrt{897}}{39} + \frac{st\sqrt{42}}{6} + \frac{6\sqrt{2rs}}{5} + \frac{9\sqrt{2rt}}{5}$$

$$+ \frac{4\sqrt{7rt}}{5} + \frac{4\sqrt{170}}{15} + \frac{4\sqrt{21}}{21} + \frac{2\sqrt{195}}{13} + \frac{2\sqrt{138}}{5} + \frac{\sqrt{77}}{7} + \frac{3\sqrt{110}}{110} - \frac{11\sqrt{30}}{6} + \frac{35\sqrt{7}}{7}$$

$$+ \frac{\sqrt{435}}{2} + \frac{2\sqrt{7}}{15} + \frac{13\sqrt{70}}{35} + \frac{23\sqrt{182}}{182} + \frac{25\sqrt{78}}{36} + \frac{28\sqrt{97}}{39} - \frac{19\sqrt{2r}}{5} - \frac{2\sqrt{330}}{15}.$$

Proof. Let $G$ be the chemical structural graph of $M$-carbon $M[r, s, t]$; then, by using serial number 10 of Table 1 and edge partition given in Table 3, the $ABC$ index of $M[r, s, t]$ is computed as follows:

$$ABC_4(M[r, s, t]) = \sum_{a \in E(G)} \sqrt{S(a) + S(\ell)} - \sqrt{S(a)S(\ell)}$$

$$= (4)\left(\frac{3 + 7 - 2}{3 \times 7}\right) + (2)\left(\frac{3 + 8 - 2}{3 \times 8}\right) + (2t)\left(\frac{4 + 11 - 2}{4 \times 11}\right) + (2st - 2s - 4t + 6)$$

$$\cdot \left(\frac{4 + 12 - 2}{4 \times 12}\right) + (2st - 2s - 4t + 4)\left(\frac{4 + 13 - 2}{4 \times 13}\right)$$

$$+ (2)\left(\frac{5 + 5 - 2}{5 \times 5}\right) + (2)\left(\frac{5 + 7 - 2}{5 \times 7}\right) + (2)\left(\frac{5 + 8 - 2}{5 \times 8}\right) + (2)\left(\frac{6 + 7 - 2}{6 \times 7}\right) + (2)\left(\frac{6 + 8 - 2}{6 \times 8}\right)$$

$$+ (8r - 8)\left(\frac{6 + 9 - 2}{6 \times 9}\right) + (2t - 2)\left(\frac{7 + 8 - 2}{7 \times 8}\right) + (2)\left(\frac{7 + 11 - 2}{7 \times 11}\right) + (2t - 2)\left(\frac{7 + 12 - 2}{7 \times 12}\right)$$
\[ + (2) \left( \frac{7 + 15 - 2}{7 \times 15} \right) + (2t - 2) \left( \frac{8 + 8 - 2}{8 \times 8} \right) + (2t - 2) \left( \frac{8 + 10 - 2}{8 \times 10} \right) + (2t - 2) \left( \frac{8 + 11 - 2}{8 \times 11} \right) \]
\[ + (4s - 10t + 6) \left( \frac{8 + 12 - 2}{8 \times 12} \right) + (2t - 4) \left( \frac{8 + 15 - 2}{8 \times 15} \right) + (8r - 8) \left( \frac{9 + 10 - 2}{9 \times 10} \right) \]
\[ + (2) \left( \frac{9 + 12 - 2}{9 \times 12} \right) + (2r - 2) \left( \frac{9 + 14 - 2}{9 \times 14} \right) + (4r - 6) \left( \frac{9 + 15 - 2}{9 \times 15} \right) \]
\[ + (4s + 6rt - 16r - 4s - 8t + 18) \left( \frac{10 + 10 - 2}{10 \times 10} \right) + (2t - 4) \left( \frac{10 + 11 - 2}{10 \times 11} \right) + (4r - 6) \left( \frac{10 + 14 - 2}{10 \times 14} \right) \]
\[ + (4s + 4rt - 12r - 4s - 4t + 12) \left( \frac{10 + 15 - 2}{10 \times 15} \right) + (2r - 2) \left( \frac{11 + 12 - 2}{11 \times 12} \right) + (2t - 2) \left( \frac{11 + 15 - 2}{11 \times 15} \right) \]
\[ + (4r - 4) \left( \frac{12 + 16 - 2}{12 \times 16} \right) + (2st - 2s - 4t + 4) \left( \frac{13 + 14 - 2}{13 \times 14} \right) + (4r - 6) \left( \frac{13 + 15 - 2}{13 \times 15} \right) \]
\[ + (4r - 4) \left( \frac{14 + 15 - 2}{14 \times 15} \right) + (4r - 6) \left( \frac{14 + 16 - 2}{14 \times 16} \right) + (6rt - 2r - 7t + 1) \left( \frac{15 + 15 - 2}{15 \times 15} \right) \]
\[ + (10rs - 28r - 10s + 4rt - 4t + 30) \left( \frac{15 + 16 - 2}{15 \times 16} \right) + (16rst - 24rt - 20rs - 21st + 38t + 23s + 24r - 40) \]
\[ \times \left( \frac{16 + 16 - 2}{16 \times 16} \right). \]

The results now follow after some simple computation of the above expression.

**Theorem 11.** Consider the graph \( G \equiv M [r, s, t] \) of \( M \)-carbon with \( r, s, t \geq 3 \); then, its \( GA_5 \) index is given by

\[ GA_5 (G) = -21 + 6r + 19s + \frac{15 \sqrt{3} + 5t}{7} + \frac{16t \sqrt{5}}{9} - 21st - \frac{8 \sqrt{5}}{9} + \frac{13 \sqrt{3}}{7} + 25t + \frac{4 \sqrt{19}}{5} \]
\[ + \frac{16 \sqrt{13}}{17} + \frac{\sqrt{3} + 5t}{7} - \frac{8 \sqrt{22}}{31} - \frac{30 \sqrt{3} + 1t}{11} \frac{1}{27} + \frac{916 \sqrt{14}}{345} + \frac{548 \sqrt{14}}{345} + \frac{2r \sqrt{35}}{3} + \frac{8 \sqrt{21}}{19} + \frac{48 \sqrt{10}}{19} \]
\[ + \frac{8 \sqrt{22}}{31} + \frac{8 \sqrt{6r}}{5} + \frac{8 \sqrt{6s}}{5} + \frac{28 \sqrt{6t}}{5} - \frac{12rt - 16rs + 8 \sqrt{14}}{15} + \frac{- 2 \sqrt{165}}{23} + \frac{13 \sqrt{39}}{11} + \frac{8st \sqrt{39}}{25} \]
\[ + \frac{8 \sqrt{13} st}{17} + \frac{4 \sqrt{42}}{7} + \frac{2st \sqrt{195}}{11} \frac{1}{7} + \frac{2 \sqrt{105}}{13} + \frac{8 \sqrt{7}}{19} + \frac{2 \sqrt{77}}{9} + \frac{4 \sqrt{110}}{21} \]
\[ + \frac{8 \sqrt{13} s}{17} + \frac{16 \sqrt{13} t}{17} + \frac{38t \sqrt{15}}{19} - \frac{8 \sqrt{22}}{19} + \frac{472 \sqrt{10}}{247} + \frac{2 \sqrt{77}}{9} + \frac{4 \sqrt{110}}{21} \]
\[ - \frac{16 \sqrt{30}}{23} + \frac{2 \sqrt{35}}{3} + \frac{8 \sqrt{7}}{11} - \frac{4 \sqrt{182}}{29} + \frac{8 \sqrt{210}}{29} + \frac{6 \sqrt{39}}{25} + \frac{8 \sqrt{33}}{23} + \frac{8 \sqrt{33}}{23} \]
\[ - \frac{8 \sqrt{39}}{25} + \frac{16 \sqrt{39}}{25} - \frac{193 \sqrt{15}}{31} + \frac{80rs \sqrt{15}}{31} + \frac{32rt \sqrt{15}}{31} + \frac{8rs \sqrt{6}}{5} + \frac{8rt \sqrt{6}}{5} + \frac{8st \sqrt{6}}{5}. \]
Proof. Let $G$ be the chemical structural graph of $M$-carbon $M[r,s,t]$, then, by using serial number 11 of Table 1 and edge partition given in Table 3, the GA index of $M[r,s,t]$ is computed as follows:

$$GA_5(M[r,s,t]) = \sum_{e \in E(G)} \frac{2\sqrt{S(o) \times S(\ell)}}{S(o) + S(\ell)}$$

$$= (4) \left(\frac{2\sqrt{3 \times 7}}{3 + 7}\right) + (2) \left(\frac{2\sqrt{3 \times 8}}{3 + 8}\right) + (2t) \left(\frac{2\sqrt{4 \times 11}}{4 + 11}\right) + (2st - 2s - 4t + 6)$$

$$- \left(\frac{2\sqrt{4 \times 12}}{4 + 12}\right) + (2st - 2s - 4t + 4) \left(\frac{2\sqrt{4 \times 13}}{4 + 13}\right) + (2) \left(\frac{2\sqrt{5 \times 5}}{5 + 5}\right)$$

$$+ (2) \left(\frac{2\sqrt{5 \times 7}}{5 + 7}\right) + (2) \left(\frac{2\sqrt{5 \times 8}}{5 + 8}\right) + (2) \left(\frac{2\sqrt{6 \times 7}}{6 + 7}\right) + (2) \left(\frac{2\sqrt{6 \times 8}}{6 + 8}\right)$$

$$+ (8r - 8) \left(\frac{2\sqrt{6 \times 9}}{6 + 9}\right) + (2t - 2) \left(\frac{2\sqrt{7 \times 8}}{7 + 8}\right) + (2) \left(\frac{2\sqrt{7 \times 11}}{7 + 11}\right) + (2t - 2)$$

$$- \left(\frac{2\sqrt{7 \times 12}}{7 + 12}\right) + (2) \left(\frac{2\sqrt{7 \times 15}}{7 + 15}\right) + (2t - 2) \left(\frac{2\sqrt{8 \times 8}}{8 + 8}\right) + (2t - 2)$$

$$- \left(\frac{2\sqrt{8 \times 10}}{8 + 10}\right) + (2t - 2) \left(\frac{2\sqrt{8 \times 11}}{8 + 11}\right) + (4st - 10t + 6) \left(\frac{2\sqrt{8 \times 12}}{8 + 12}\right)$$

$$+ (2) \left(\frac{2\sqrt{8 \times 14}}{8 + 14}\right) + (2t - 4) \left(\frac{2\sqrt{8 \times 15}}{8 + 15}\right) + (8r - 8) \left(\frac{2\sqrt{9 \times 10}}{9 + 10}\right)$$

$$+ (2) \left(\frac{2\sqrt{9 \times 12}}{9 + 12}\right) + (2r - 2) \left(\frac{2\sqrt{9 \times 14}}{9 + 14}\right) + (4r - 6) \left(\frac{2\sqrt{9 \times 15}}{9 + 15}\right)$$

$$+ (4rs + 6rt - 16r - 4s - 8t + 18) \left(\frac{2\sqrt{10 \times 10}}{10 + 10}\right) + (2) \left(\frac{2\sqrt{10 \times 11}}{10 + 11}\right) + (4r - 6)$$

$$- \left(\frac{2\sqrt{10 \times 14}}{10 + 14}\right) + (4rs + 4rt - 12r - 4s - 4t + 12) \left(\frac{2\sqrt{10 \times 15}}{10 + 15}\right) + (2t - 2)$$

$$- \left(\frac{2\sqrt{11 \times 12}}{11 + 12}\right) + (2t - 2) \left(\frac{2\sqrt{11 \times 15}}{11 + 15}\right) + (2) \left(\frac{2\sqrt{11 \times 16}}{11 + 16}\right) + (2st - 2s - 4t + 4)$$

$$- \left(\frac{2\sqrt{12 \times 13}}{12 + 13}\right) + (2t) \left(\frac{2\sqrt{12 \times 15}}{12 + 15}\right) + (2st + 2s - 4t - 6)$$

$$- \left(\frac{2\sqrt{12 \times 16}}{12 + 16}\right) + (2t - 2) \left(\frac{2\sqrt{13 \times 14}}{13 + 14}\right) + (4st - 4s - 10t + 10)$$

$$\times \left(\frac{2\sqrt{13 \times 15}}{13 + 15}\right) + (4r - 4) \left(\frac{2\sqrt{14 \times 15}}{14 + 15}\right) + (4r - 6) \left(\frac{2\sqrt{14 \times 16}}{14 + 16}\right) + (6rt - 2r - 7t + 1)$$

$$- \left(\frac{2\sqrt{15 \times 15}}{15 + 15}\right) + (10rs - 28r - 10s + 4rt - 4t + 30) \left(\frac{2\sqrt{15 \times 16}}{15 + 16}\right)$$

$$+ (16rst - 24rt - 20rs - 21st + 38t + 23s + 24r - 40) \left(\frac{2\sqrt{16 \times 16}}{16 + 16}\right)$$. 
The results now follow after some simple computation of the above expression. □

Theorem 12. Consider the graph \( G = M[r, s, t] \) of M-carbon with \( r, s, t \geq 3 \); then, its Sanskruti index \( S(G) \) is given by

\[
S(G) = c_1 r + c_2 s - c_0 - c_4 st + c_3 tr - c_9 r s + c_7 r s t,
\]

where \( c_0 = (17743414726597313012358335881357 \ 6506563/ \ 233972495845970544399543494688000000) \), \( c_1 = (38410 \ 1590410077012687995213/ \ 3876335270 \ 28142422799694000) \), \( c_2 = (4204226931169825975177/8150780755142420850) \), \( c_3 = (3377910532598057684378857231211/32035828680011770908840000000) \), \( c_4 = (56697774952770 \ 173936888713909750) \), \( c_5 = (731518633569104009441/9893 \ 2250100348000) \), \( c_6 = (26845875203 \ 03660 \ 85408 \ 104050675) \) and, \( c_7 = (33554432/3375) \).

Proof. Let \( G \) be the chemical structural graph of M-carbon \( M[r, s, t] \); then, by using serial number 12 of Table 1 and edge partition given in Table 3, the Sanskruti index \( S(M[r, s, t]) \) of \( M[r, s, t] \) is computed as follows:

\[
\begin{align*}
\text{GA}_S(M[r, s, t]) &= \sum_{\ell \in E(G)} \left( \frac{S(o) \times S(\ell)}{S(o) + S(\ell) - 2} \right)^3 \\
&= (4) \left( \frac{3 \times 7}{3 + 7 - 2} \right)^3 + (2) \left( \frac{3 \times 8}{3 + 8 - 2} \right)^3 + (2r) \left( \frac{4 \times 11}{4 + 11 - 2} \right)^3 + (2st - 2s - 4t + 6) \\
&+ (2) \left( \frac{5 \times 7}{5 + 7 - 2} \right)^3 + (2) \left( \frac{5 \times 8}{5 + 8 - 2} \right)^3 + (2) \left( \frac{6 \times 7}{6 + 7 - 2} \right)^3 + (2) \left( \frac{6 \times 8}{6 + 8 - 2} \right)^3 \\
&+ (8r - 8) \left( \frac{6 \times 9}{6 + 9 - 2} \right)^3 + (2t - 2r) \left( \frac{7 \times 8}{7 + 8 - 2} \right)^3 + (2) \left( \frac{7 \times 11}{7 + 11 - 2} \right)^3 + (2t - 2) \\
&+ (2) \left( \frac{7 \times 12}{7 + 12 - 2} \right)^3 + (2) \left( \frac{15 \times 7}{15 + 7 - 2} \right)^3 + (2t - 2) \left( \frac{8 \times 8}{8 + 8 - 2} \right)^3 + (2t - 2) \\
&+ (2) \left( \frac{8 \times 10}{8 + 10 - 2} \right)^3 + (2t - 2) \left( \frac{8 \times 11}{8 + 11 - 2} \right)^3 + (4st - 10r + 6) \left( \frac{8 \times 12}{8 + 12 - 2} \right)^3 \\
&+ (2) \left( \frac{9 \times 12}{9 + 12 - 2} \right)^3 + (2r - 2) \left( \frac{9 \times 14}{9 + 14 - 2} \right)^3 + (4r - 6) \left( \frac{9 \times 15}{9 + 15 - 2} \right)^3 \\
&+ (4rs + 6rt - 16r - 4s - 8t + 18) \left( \frac{10 \times 10}{10 + 10 - 2} \right)^3 + (2) \left( \frac{10 \times 11}{10 + 11 - 2} \right)^3 + (4r - 6) \\
&+ (4rs + 4rt - 12r - 4s - 4t + 12) \left( \frac{10 \times 15}{10 + 15 - 2} \right)^3 + (2t - 2) \\
&+ (2) \left( \frac{11 \times 12}{11 + 12 - 2} \right)^3 + (2r - 2) \left( \frac{11 \times 15}{11 + 15 - 2} \right)^3 + (2t - 2) \left( \frac{11 \times 16}{11 + 16 - 2} \right)^3 + (2st - 2s - 4t + 4) \\
&+ (2t) \left( \frac{12 \times 15}{12 + 15 - 2} \right)^3 + (2st + 2s - 4t - 6) \\
&+ (2t) \left( \frac{13 \times 14}{13 + 14 - 2} \right)^3 + (4st - 4s - 10r + 10) \\
&+ (2t - 2) \left( \frac{13 \times 15}{13 + 15 - 2} \right)^3 + (4r - 4) \left( \frac{14 \times 15}{14 + 15 - 2} \right)^3 + (4r - 6) \left( \frac{14 \times 16}{14 + 16 - 2} \right)^3 + (6rt - 2r - 7t + 1) \\
&+ (2t) \left( \frac{15 \times 15}{15 + 15 - 2} \right)^3 + (16rs - 24rt - 20rs - 21st + 38t + 23s + 24r - 40) \left( \frac{16 \times 16}{16 + 16} \right)^3.
\end{align*}
\]
The results now follow after some simple calculations.

4. Comparison and Discussion

In this section, we shall discuss and compare all the computed indices (degree based and sum degree based) from Theorems 3–12 both graphically and numerically (by a tables).

Tables 4 and 5 provide us a numerical comparison. From these two tables and computations, we can analyse that which type of indices are closed related and can be used to study the same type of chemical, biochemical, physical, and biophysical properties of the structure of M[r, s, t]. We can see that the values of GA and GA_5 are very close and almost similar, so we can purpose that any one of them can be used in place of each other for the study of chemical structure M[r, s, t]. They also show the same kind of behaviour in graphical analysis (Figure 6). On the same pattern, we can also see the closely related values of R_{-1}, R_{-1/2}, ABC_4, R_{1/2}, ABC, and GA, and GA_5, and these values are also produced in an increasing order, respectively. So, we can purpose to use those indices which give smaller values for the study of respective properties of structure M[r, s, t] giving smaller values after the experimental study and the graphical comparison in Figure 7 which also shows the same type of patterns. Similarly, the indices M_1, R_1, H_M, S, M_1, and M_2 give us larger values even for such small initial inputs of r, s, t. Such behaviour shows that (and we purpose that) they cannot be used as closely related to the previous mentioned indices to study the same type of properties of M[r, s, t]. We can also see the behaviour of these indices in Figures 8 and 9. It is purposed to use these indices in the study of such properties of M[r, s, t] which gives higher experimental values.

5. Conclusion

In this article, we have studied the structure M[r, s, t] of M-carbon in the form of its degree and sum degree-based
indices. The indices that we computed and discussed in the article are $R_{r,s,t}$, $R_{r,s,t,1/2}$, $ABC_{4r}$, $R_{1/2,ABC}$, $GA$, $GA_{3,1}$, $R_{1,ABC}$, $HM$, $S$, $MT_1$, and $MT_2$. We also compared these indices numerically and graphically to show which type of indices behaved in different and same patterns (or values). We have found exact formulas for these indices for the structure of $M[r,s,t]$ of M-carbon.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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