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 indices, new Zagreb indices, fourth atom bond connectivity index, fifth geometric arithmetic index, and Sanskruti index. For some literature study and results related to these indices, see [5–13].

In Table 1, the number $S(o)$ represents the sum $\sum_{o\ell \in E(G)} d(\ell)$ and the number $S(\ell)$ represents the sum $\sum_{\ell o \in E(G)} d(o)$, where d_o is the degree of vertex o and d_ℓ represents the degree of vertex ℓ . In 2016, Gutman et al. [26] proved the following theorems for some of the indices in Table 1.

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

$$\overline{M}_1(G) = 2|E(G)|(|V(G) - 1) - M_1(G). \quad (1)$$

Theorem 2 (See [26]). *Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges. Then,*

$$\overline{M}_2(G) = 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G). \quad (2)$$

FIGURE 1: The M-carbon structure $M[3,3,2]$.

TABLE 1: Famous degree-based topological indices.

S. no.	Topological index	Notation	Formula	Authors
1	Randić index	$R_{-(1/2)}(G)$	$\sum_{o\ell \in E(G)} 1/\sqrt{d_o d_\ell}$	Randić [14] in 1975
2	General Randić index	$R_\alpha(G)$	$\sum_{o\ell \in E(G)} (d_o d_\ell)^\alpha$	Bollobás and Erdős [15] and Amic et al. [16] in 1988
3	Atom bond connectivity index	$ABC(G)$	$\sum_{o\ell \in E(G)} \sqrt{d_o + d_\ell - 2/d_o d_\ell}$	Estrada et al. [17]
4	Geometric arithmetic index	$GA(G)$	$\sum_{o\ell \in E(G)} 2\sqrt{d_o d_\ell / (d_o + d_\ell)}$	Vukićević and Furtula. [18]
5	First Zagreb	$M_1(G)$	$\sum_{o\ell \in E(G)} (d_o + d_\ell)$	Gutman and Trinajstić in 1972[19]
6	Second Zagreb	$M_2(G)$	$\sum_{o\ell \in E(G)} (d_o \times d_\ell)$	Gutman and Das in 2004 [20]
7	New degree-based Zagreb index	$HM(G)$	$\sum_{o\ell \in E(G)} (d_o + d_\ell)^2$	Shirdel et al. [21] in 2013
8	First Zagreb coindex	$\overline{M}_1(G)$	$\sum_{o\ell \notin E(G)} [d_o + d_\ell]$	In 2008, Došlić [22]
9	Second Zagreb coindex	$\overline{M}_2(G)$	$\sum_{o\ell \notin E(G)} d_o d_\ell$	Same as above
10	Fourth atom bond connectivity index	$ABC_4(G)$	$\sum_{o\ell \in E(G)} \sqrt{S(o) + S(\ell) - 2/S(o)S(\ell)}$	Ghorbani and Hosseinzadeh [23]
11	Fifth version of geometric arithmetic index	GA_5	$\sum_{o\ell \in E(G)} 2\sqrt{S(o)S(\ell)/S(o) + S(\ell)}$	Graovac et al. [24]
12	Sanskriti index	$S(G)$	$\sum_{o\ell \in E(G)} (S(o) \times S(\ell)/S(o) + S(\ell) - 2)^3$	In 2016, Hosamani [25]

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 $t = 1, 3, 5, \dots$ and even layers for $t = 2, 4, 6, \dots$, both are generated by different unit cells. The one depicted in Figure 3 is the odd layer (that is for $t = 1, 3, 5, \dots$) which was generated by the unit of Figure $t = 2, 4, 6, \dots$). 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 colour. 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

$$R_\alpha(M[r, s, t]) = 2 \times 4^a - 7 \times 16^a + 2 \times 2^a t + 8 \times 6^a r + 2 \times 6^a s + 2 \times 6^a t - 4 \times 8^a s - 6 \times 8^a t - 4 \times 9^a r - 2 \times 9^a s - 3 \times 9^a t - 2 \times 12^a s - 4 \times 12^a t - 4 \times 16^a r + 7 \times 16^a s + 10 \times 16^a t - 8 \times 6^a - 2 \times 3^a + 2 \times 2^a + 2 \times 3^a st + 4 \times 8^a st + 2 \times 9^a rs + 6 \times 9^a rt + 4 \times 12^a rs + 4 \times 12^a rt - 8 \times 16^a rs - 14 \times 16^a rt - 11 \times 16^a st + 5 \times 9^a + 16 \times 16^a rst + 6 \times 8^a + 2 \times 12^a. \quad (3)$$

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 $R_\alpha(G)$ of $M[r, s, t]$ is computed as follows:

$$\begin{aligned} R_\alpha(M[r, s, t]) &= \sum_{o\ell \in E(G)} (d_o \times d_\ell)^\alpha \\ &= (2t + 2)(1 \times 2)^\alpha + (2st - 2)(1 \times 3)^\alpha + (2)(2 \times 2)^\alpha + (8r + 2s + 2t - 8)(2 \times 3)^\alpha \\ &\quad + (4st - 4s - 6t + 6)(2 \times 4)^\alpha + (6rt + 2rs - 4r - 2s - 3t + 5)(3 \times 3)^\alpha + (4rs + 4rt - 2s - 4t + 2)(3 \times 4)^\alpha \\ &\quad + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7)(4 \times 4)^\alpha. \end{aligned} \quad (4)$$

The result follows after some simple computations from this equation.

It is very simple and clear to see that from the above Theorem 3, the following Corollary is true. $\square$

Corollary 1

$$R_\alpha(M[r, s, t]) = \begin{cases} 256rst - 62rs - 122rt - 138st - 52r + 50s + 53t - 37 & \text{if } \alpha = 1 \\ \frac{23r}{36} - \frac{17s}{144} + \frac{23st}{48} + \frac{13t}{24} + \frac{rt}{8} + \frac{rs}{18} + rst + \frac{77}{144} & \text{if } \alpha = -1 \\ 2\sqrt{3}st + 4\sqrt{8}st + 2\sqrt{9}rs + 16\sqrt{16}rst - 2\sqrt{3} + 2\sqrt{2} + 2\sqrt{2}t + 8\sqrt{6}r + 2\sqrt{6}s + 2\sqrt{6}t - 4\sqrt{8}s - 6\sqrt{8}t - 4\sqrt{9}r - 2\sqrt{9}s - 3\sqrt{9}t - 2\sqrt{12}s - 4\sqrt{12}t - 4\sqrt{16}r + 7\sqrt{16}s + 10\sqrt{16}t + 2\sqrt{4} - 8\sqrt{6} + 6\sqrt{8} + 5\sqrt{9} + 2\sqrt{12} - 7\sqrt{16} + 6\sqrt{9}rt + 4\sqrt{12}rs + 4\sqrt{12}rt - 11\sqrt{16}st - 14\sqrt{16}rt - 8\sqrt{16}rs & \text{if } \alpha = \frac{1}{2} \\ \frac{2\sqrt{3}st}{3} + \frac{\sqrt{8}st}{2} + \frac{2\sqrt{9}rs}{9} + \sqrt{16}rst - \frac{2\sqrt{3}}{3} + \sqrt{2} + \sqrt{2}t + \frac{4\sqrt{6}r}{3} + \frac{\sqrt{6}s}{3} + \frac{\sqrt{6}t}{3} - \frac{\sqrt{8}s}{2} - \frac{3\sqrt{8}t}{4} - \frac{4\sqrt{9}r}{9} - \frac{2\sqrt{9}s}{9} - \frac{\sqrt{9}t}{3} - \frac{\sqrt{12}s}{6} - \frac{\sqrt{12}t}{3} - \frac{\sqrt{16}r}{4} + \frac{7\sqrt{16}s}{16} + \frac{5\sqrt{16}t}{8} + \frac{\sqrt{4}}{2} - \frac{4\sqrt{6}}{3} + \frac{3\sqrt{8}}{4} + \frac{5\sqrt{9}}{9} + \frac{\sqrt{12}}{6} - \frac{7\sqrt{16}}{16} + \frac{2\sqrt{9}rt}{3} + \frac{\sqrt{12}rs}{3} + \frac{\sqrt{12}rt}{3} - \frac{11\sqrt{16}st}{16} - \frac{7\sqrt{16}rt}{8} - \frac{\sqrt{16}rs}{2} & \text{if } \alpha = \frac{-1}{2} \end{cases}. \quad (5)$$

FIGURE 2: (a) The M-carbon unit cell. (b) Chain of three units and units connected by blue edges.

FIGURE 3: The odd layer (for $t = 1$) of three chains and bonding of chains is shown by blue edges.

FIGURE 4: Even layer construction. (a) The unit cell. (b) Chain of three units. (c) The layer of three chains.

FIGURE 5: The structure $M[3, 3, 2]$. The connection of two layers. Bonding is shown in red color.

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

TABLE 2: Degree-based edge partition of $M[r, s, t]$ for $r, s, t \geq 2$.

(d_u, d_v)	Frequency
(1, 2)	$2t + 2$
(1, 3)	$2st - 2$
(2, 2)	2
(2, 3)	$8r + 2s + 2t - 8$
(2, 4)	$4st - 4s - 6t + 6$
(3, 3)	$6rt + 2sr - 4r - 2s - 3t + 5$
(3, 4)	$4rs + 4rt - 2s - 4t + 2$
(4, 4)	$16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7$

$$M_1(M[r, s, t]) = 128rst - 24rs - 48rt - 56st - 16r + 16s + 14t - 10. \quad (6)$$

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:

TABLE 3: Sum degree-based edge partition of $M[r, s, t]$ for $r, s, t \geq 3$.

$(S(o), S(\ell))$	Frequency	$(S(o), S(\ell))$	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)	$2t$
(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)	$16rst-24rt-20rs-21st+38t+23s+24r-40$

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	$\overline{M}_1$	$\overline{M}_2$	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	143 434	2245544	16724
(4, 4, 4)	11399	79	1157.6	250	6190	868642	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	383	18796	1339	1347	37720	2.72×10^7	290756
(8, 8, 8)	110835	563	28636	2013	57446	6.14×10^7	1.1×10^8	445144
(9, 9, 9)	160964	792	41418	2871	83060	1.2×10^8	2.3×10^8	646172
(10, 10, 10)	224273	1077	57525	3943	115330	2.3×10^8	4.4×10^8	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_5	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	1.4595×10^6
(7, 7, 7)	3110	4936	1813	4914	2.46×10^6
(8, 8, 8)	4688	7469	2720	7440	3.8×10^6
(9, 9, 9)	6725	10747	3887	10711	5.6×10^6
(10, 10, 10)	9282	14865	5348	14820	7.9×10^6

$$\begin{aligned}
M_1(M[r, s, t]) &= \sum_{o\ell \in E(G)} (d_o + d_\ell) \\
&= (2t + 2)(1 + 2) + (2st - 2)(1 + 3) + (2)(2 + 2) + (8r + 2s + 2t - 8)(2 + 3) \\
&\quad + (4st - 4s - 6t + 6)(2 + 4) + (6rt + 2rs - 4r - 2s - 3t + 5)(3 + 3) + (4rs + 4rt - 2s - 4t + 2)(3 + 4) \\
&\quad + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7)(4 + 4).
\end{aligned} \tag{7}$$

Thus, the result follows by simple calculations.

The next theorem gives us the new degree-based Zagreb index as defined in [21]. $\square$

Theorem 5. *The new degree-based Zagreb index $HM(M[r, s, t])$ of M -carbon structure is given by*

$$\begin{aligned}
HM(M[r, s, t]) &= 1024rst - 244rs - 484rt - 528st \\
&\quad - 200r + 184s + 188t - 136.
\end{aligned} \tag{8}$$

Proof. Let G be the chemical structural graph of M -carbon $M[r, s, t]$; then, by using serial number 7 of Table 1 and edge partition given in Table 2, the new degree-based Zagreb index HM of $M[r, s, t]$ is computed as follows:

$$\begin{aligned}
HM(M[r, s, t]) &= \sum_{o\ell \in E(G)} (d_o + d_\ell)^2 \\
&= (2t + 2)(1 + 2)^2 + (2st - 2)(1 + 3)^2 + (2)(2 + 2)^2 + (8r + 2s + 2t - 8)(2 + 3)^2 \\
&\quad + (4st - 4s - 6t + 6)(2 + 4)^2 + (6rt + 2rs - 4r - 2s - 3t + 5)(3 + 3)^2 + (4rs + 4rt - 2s - 4t + 2)(3 + 4)^2 \\
&\quad + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7)(4 + 4)^2.
\end{aligned} \tag{9}$$

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. $\square$

Theorem 6. *The first Zagreb coindex index $\overline{M}_1(M[r, s, t])$ of M -carbon structure is given by*

$$\begin{aligned}
\overline{M}_1(M[r, s, t]) &= 256r^2s^2t^2 - 32r^2s^2t - 64r^2st^2 - 80s^2t^2r + 16s^2rt + 16t^2rs - 160rst + 28rs \\
&\quad + 56rt + 66st + 16r - 18s - 16t + 10.
\end{aligned} \tag{10}$$

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:

$$\begin{aligned}
\overline{M}_1(M[r, s, t]) &= 2|E(M[r, s, t])|(|V(M[r, s, t]) - 1) - M_1(M[r, s, t]) \\
&= 2(16rst - 4rt - 5st - 2rs + t + s)(8rst - 1) - 128rst - 24rs - 48rt - 56st \\
&\quad - 16r + 16s + 14t - 10.
\end{aligned} \tag{11}$$

Thus, the result follows by simple calculations. $\square$

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

$$\begin{aligned}\overline{M}_2(M[r, s, t]) = & 512r^2s^2t^2 - 128r^2s^2t - 256r^2st^2 - 320s^2t^2r + 8r^2s^2 + 32r^2st + 32r^2t^2 \\ & + 104s^2rt + 144t^2rs + 50s^2t^2 - 8s^2r - 344rst - 16rt^2 - 20s^2t - 20st^2 + 74rs \\ & + 146rt + 2s^2 + 170st + 2t^2 + 60r - 58s - 60t + 42.\end{aligned}\quad (12)$$

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:

$$\begin{aligned}\overline{M}_2(M[r, s, t]) = & 2|E(M[r, s, t])|^2 - \frac{1}{2}M_1(M[r, s, t]) - M_2(M[r, s, t]) \\ = & 2(16rst - 4rt - 5st - 2rs + t + s)^2 - (1/2)(128rst - 24rs - 48rt - 56st - 16r + 16s + 14t - 10) \\ & - (256rst - 62rs - 122rt - 138st - 52r + 50s + 53t - 37).\end{aligned}\quad (13)$$

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. $\square$

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

$$\begin{aligned}ABC(M[r, s, t]) = & +\frac{2rs\sqrt{15}}{3} + \frac{2rt\sqrt{15}}{3} - 2rs\sqrt{6} - \frac{7rt\sqrt{6}}{2} - \frac{25st\sqrt{6}}{12} + 4rt + \frac{4rs}{3} - \frac{s\sqrt{15}}{3} \\ & - \frac{2t\sqrt{15}}{3} + 4rst\sqrt{6} - \frac{29\sqrt{6}}{12} - \sqrt{2}t - \sqrt{2}s + \frac{10}{3} + \frac{\sqrt{15}}{3} + 2\sqrt{2}st - \sqrt{6}r \\ & + \frac{7\sqrt{6}s}{4} + \frac{5\sqrt{6}t}{2} + \sqrt{2} + 4\sqrt{2}r - \frac{8r}{3} - \frac{4s}{3} - 2t.\end{aligned}\quad (14)$$

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:

$$\begin{aligned}ABC(M[r, s, t]) = & \sum_{o\ell \in E(G)} \sqrt{\frac{d_o + d_\ell - 2}{d_o d_\ell}} \\ = & (2t + 2) \left(\sqrt{\frac{1 + 2 - 2}{1 \times 2}} \right) + (2st - 2) \left(\sqrt{\frac{1 + 3 - 2}{1 \times 3}} \right) + (2) \left(\sqrt{\frac{2 + 2 - 2}{2 \times 2}} \right) + (8r + 2s + 2t - 8) \\ & + \left(\sqrt{\frac{2 + 3 - 2}{2 \times 3}} \right) + (4st - 4s - 6t + 6) \left(\sqrt{\frac{2 + 4 - 2}{2 \times 4}} \right) + (6rt + 2rs - 4r - 2s - 3t + 5) \\ & \cdot \left(\sqrt{\frac{3 + 3 - 2}{3 \times 3}} \right) + (4rs + 4rt - 2s - 4t + 2) \left(\sqrt{\frac{3 + 4 - 2}{3 \times 4}} \right) \\ & + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7) \left(\sqrt{\frac{4 + 4 - 2}{4 \times 4}} \right).\end{aligned}\quad (15)$$

The results now follow after some simple computations of above expression. $\square$

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

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

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:

$$\begin{aligned}
 GA(M[r, s, t]) = & \sum_{o\ell \in E(G)} \frac{2\sqrt{d_o \times d_\ell}}{d_o + d_\ell}, \\
 & \cdot (2t + 2) \left(\frac{2\sqrt{1 \times 2}}{1 + 2} \right) + (2st - 2) \left(\frac{2\sqrt{1 \times 3}}{1 + 3} \right) + (2) \left(\frac{2\sqrt{2 \times 2}}{2 + 2} \right) + (8r + 2s + 2t - 8) \left(\frac{2\sqrt{2 \times 3}}{2 + 3} \right) \\
 & + (4st - 4s - 6t + 6) \left(\frac{2\sqrt{2 \times 4}}{2 + 4} \right) + (6rt + 2rs - 4r - 2s - 3t + 5) \left(\frac{2\sqrt{3 \times 3}}{3 + 3} \right) \\
 & + (4rs + 4rt - 2s - 4t + 2) \left(\frac{2\sqrt{3 \times 4}}{3 + 4} \right) \\
 & + (16rst - 8rs - 14rt - 11st - 4r + 7s + 10t - 7) \left(\frac{2\sqrt{4 \times 4}}{4 + 4} \right).
 \end{aligned} \tag{17}$$

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 Ghorbani 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 $G \cong M[r, s, t]$. $\square$

Theorem 10. The ABC_4 index of the graph $G \cong M[r, s, t]$ of M -carbon with $r \geq 3, s \geq 3, t \geq 3$ is given by

$$\begin{aligned}
 ABC_4(G) = & 3 + \sqrt{3}st + \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{2}s}{5} - \frac{5\sqrt{3}t}{2} + \frac{\sqrt{57}}{18} - \frac{\sqrt{357}}{21} + \frac{5\sqrt{11}}{22} + \frac{\sqrt{14}}{28} - \frac{12\sqrt{2}t}{5} + \frac{\sqrt{6}r}{3} + \frac{t\sqrt{14}}{4} + \frac{t\sqrt{77}}{11} \\
 & + \frac{4r\sqrt{330}}{45} - \frac{4\sqrt{7}r}{15} - \frac{14\sqrt{7}t}{15} + \frac{2r\sqrt{770}}{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{4t\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} + rst\sqrt{30} + \frac{37\sqrt{42}}{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{2}rs}{5} + \frac{9\sqrt{2}rt}{5} \\
 & + \frac{4\sqrt{7}rt}{5} - \frac{4\sqrt{170}}{15} + \frac{4\sqrt{21}}{21} + \frac{2\sqrt{195}}{13} + \frac{2\sqrt{138}}{5} + \frac{\sqrt{77}}{77} + \frac{3\sqrt{110}}{110} - \frac{11\sqrt{30}}{6} + \frac{\sqrt{35}}{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{2\sqrt{897}}{39} - \frac{19\sqrt{2}r}{5} - \frac{2\sqrt{330}}{15}.
 \end{aligned} \tag{18}$$

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:

$$\begin{aligned}
 ABC_4(M[r, s, t]) &= \sum_{o\ell \in E(G)} \sqrt{\frac{S(o) + S(\ell) - 2}{S(o)S(\ell)}} \\
 &= (4) \left(\sqrt{\frac{3+7-2}{3 \times 7}} \right) + (2) \left(\sqrt{\frac{3+8-2}{3 \times 8}} \right) + (2t) \left(\sqrt{\frac{4+11-2}{4 \times 11}} \right) + (2st - 2s - 4t + 6) \\
 &\quad \cdot \left(\sqrt{\frac{4+12-2}{4 \times 12}} \right) + (2st - 2s - 4t + 4) \left(\sqrt{\frac{4+13-2}{4 \times 13}} \right) \\
 &\quad + (2) \left(\sqrt{\frac{5+5-2}{5 \times 5}} \right) + (2) \left(\sqrt{\frac{5+7-2}{5 \times 7}} \right) + (2) \left(\sqrt{\frac{5+8-2}{5 \times 8}} \right) + (2) \left(\sqrt{\frac{6+7-2}{6 \times 7}} \right) + (2) \left(\sqrt{\frac{6+8-2}{6 \times 8}} \right) \\
 &\quad + (8r - 8) \left(\sqrt{\frac{6+9-2}{6 \times 9}} \right) + (2t - 2) \left(\sqrt{\frac{7+8-2}{7 \times 8}} \right) + (2) \left(\sqrt{\frac{7+11-2}{7 \times 11}} \right) + (2t - 2) \left(\sqrt{\frac{7+12-2}{7 \times 12}} \right)
 \end{aligned}$$

$$\begin{aligned}
& + (2) \left(\sqrt{\frac{7+15-2}{7 \times 15}} \right) + (2t-2) \left(\sqrt{\frac{8+8-2}{8 \times 8}} \right) + (2t-2) \left(\sqrt{\frac{8+10-2}{8 \times 10}} \right) + (2t-2) \left(\sqrt{\frac{8+11-2}{8 \times 11}} \right) \\
& + (4st-10t+6) \left(\sqrt{\frac{8+12-2}{8 \times 12}} \right) + (2) \left(\sqrt{\frac{8+14-2}{8 \times 14}} \right) + (2t-4) \left(\sqrt{\frac{8+15-2}{8 \times 15}} \right) + (8r-8) \left(\sqrt{\frac{9+10-2}{9 \times 10}} \right) \\
& + (2) \left(\sqrt{\frac{9+12-2}{9 \times 12}} \right) + (2r-2) \left(\sqrt{\frac{9+14-2}{9 \times 14}} \right) + (4r-6) \left(\sqrt{\frac{9+15-2}{9 \times 15}} \right) \\
& + (4rs+6rt-16r-4s-8t+18) \left(\sqrt{\frac{10+10-2}{10 \times 10}} \right) + (2) \left(\sqrt{\frac{10+11-2}{10 \times 11}} \right) + (4r-6) \left(\sqrt{\frac{10+14-2}{10 \times 14}} \right) \\
& + (4rs+4rt-12r-4s-4t+12) \left(\sqrt{\frac{10+15-2}{10 \times 15}} \right) + (2t-2) \left(\sqrt{\frac{11+12-2}{11 \times 12}} \right) + (2t-2) \left(\sqrt{\frac{11+15-2}{11 \times 15}} \right) \\
& + (2) \left(\sqrt{\frac{11+16-2}{11 \times 16}} \right) + (2st-2s-4t+4) \left(\sqrt{\frac{12+13-2}{12 \times 13}} \right) + (2t) \left(\sqrt{\frac{12+15-2}{12 \times 15}} \right) + (2st+2s-4t-6) \\
& \cdot \left(\sqrt{\frac{12+16-2}{12 \times 16}} \right) + (2t-2) \left(\sqrt{\frac{13+14-2}{13 \times 14}} \right) + (4st-4s-10t+10) \times \left(\sqrt{\frac{13+15-2}{13 \times 15}} \right) \\
& + (4r-4) \left(\sqrt{\frac{14+15-2}{14 \times 15}} \right) + (4r-6) \left(\sqrt{\frac{14+16-2}{14 \times 16}} \right) + (6rt-2r-7t+1) \left(\sqrt{\frac{15+15-2}{15 \times 15}} \right) \\
& + (10rs-28r-10s+4rt-4t+30) \left(\sqrt{\frac{15+16-2}{15 \times 16}} \right) + (16rst-24rt-20rs-21st+38t+23s+24r-40) \\
& \cdot \left(\sqrt{\frac{16+16-2}{16 \times 16}} \right).
\end{aligned} \tag{19}$$

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

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

$$\begin{aligned}
GA_5(G) = & -21 + 6r + 19s + \frac{15\sqrt{3}st}{7} + \frac{16t\sqrt{5}}{9} - 21st - \frac{8\sqrt{5}}{9} + \frac{13\sqrt{3}}{7} + 25t + \frac{4\sqrt{19}}{5} \\
& + \frac{16\sqrt{13}}{17} + \frac{\sqrt{3}s}{7} - \frac{30\sqrt{3}t}{7} + \frac{16\sqrt{11}}{27} - \frac{916\sqrt{14}}{345} + \frac{548r\sqrt{14}}{345} + \frac{2r\sqrt{35}}{3} + \frac{8t\sqrt{21}}{19} + \frac{48r\sqrt{10}}{19} \\
& + \frac{8t\sqrt{22}}{19} - \frac{80s\sqrt{15}}{31} - \frac{32t\sqrt{15}}{31} - \frac{8\sqrt{6}r}{5} - \frac{8\sqrt{6}s}{5} - \frac{28\sqrt{6}t}{5} - 12rt - 16rs + \frac{8t\sqrt{14}}{15} - \frac{8\sqrt{210}}{29} \\
& - \frac{2\sqrt{165}}{13} + \frac{4t\sqrt{182}}{27} + \frac{8t\sqrt{30}}{23} - \frac{2s\sqrt{195}}{7} - \frac{5t\sqrt{195}}{7} + \frac{52\sqrt{6}}{11} + \frac{8st\sqrt{39}}{25} \\
& + \frac{8\sqrt{13}st}{17} + \frac{4\sqrt{42}}{13} + \frac{2st\sqrt{195}}{7} + 16rst + \frac{2\sqrt{105}}{11} + \frac{8t\sqrt{11}}{15} + \frac{2t\sqrt{165}}{13} - \frac{8\sqrt{21}}{19} + \frac{5\sqrt{195}}{7} \\
& - \frac{8\sqrt{13}s}{17} - \frac{16\sqrt{13}t}{17} + \frac{387\sqrt{15}}{62} - \frac{8\sqrt{22}}{19} - \frac{472\sqrt{10}}{247} + \frac{2\sqrt{77}}{9} + \frac{4\sqrt{110}}{21} \\
& - \frac{16\sqrt{30}}{23} - \frac{2\sqrt{35}}{3} + \frac{8\sqrt{7}}{11} - \frac{4\sqrt{182}}{27} + \frac{8r\sqrt{210}}{29} + \frac{16\sqrt{39}}{25} - \frac{8\sqrt{33}}{23} + \frac{8t\sqrt{33}}{23} \\
& - \frac{8s\sqrt{39}}{25} - \frac{16t\sqrt{39}}{25} - \frac{193r\sqrt{15}}{31} + \frac{80rs\sqrt{15}}{31} + \frac{32rt\sqrt{15}}{31} + \frac{8rs\sqrt{6}}{5} + \frac{8rt\sqrt{6}}{5} + \frac{8st\sqrt{6}}{5}.
\end{aligned} \tag{20}$$

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:

$$\begin{aligned}
 GA_5(M[r, s, t]) &= \sum_{o\ell \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) \\
 &\quad \cdot \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) \\
 &\quad + (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) \\
 &\quad + (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) \\
 &\quad \cdot \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) \\
 &\quad \cdot \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) \\
 &\quad + (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) \\
 &\quad + (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) \\
 &\quad + (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) \\
 &\quad \cdot \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) \\
 &\quad \cdot \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) \\
 &\quad \cdot \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) \\
 &\quad \cdot \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) \\
 &\quad \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) \\
 &\quad \cdot \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) \\
 &\quad + (16rst - 24rt - 20rs - 21st + 38t + 23s + 24r - 40)\left(\frac{2\sqrt{16 \times 16}}{16+16}\right).
 \end{aligned} \tag{21}$$

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

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

$$S(G) = c_1 r + c_2 s - c_0 - c_4 st + c_2 t - c_5 rt - c_6 rs + c_7 rst, \quad (22)$$

where $c_0 = (177434147265976313012358335881357 \ 65065 \ 63/ \ 233972495845970544399543494688000000)$, $c_1 = (384 \ 10 \ 15904100770126879995213/ \ 3876335270 \ 2814242 \ 799$

$6964000)$, $c_2 = (42042269311169825975177/81507807551 \ 42420850)$, $c_3 = (33779105325980576848378857231211/ \ 3203582868001177090884000000)$, $c_4 = (56697 \ 7749527 \ 70 \ 1739/61888713909750)$, $c_5 = (731518633569104009441/98 \ 93 \ 2250100348000)$, $c_6 = (26845875203 \ 03660 \ 8/5408 \ 104050675)$ 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{aligned} GA_5(M[r, s, t]) &= \sum_{o\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 + (2t) \left(\frac{4 \times 11}{4+11-2} \right)^3 + (2st - 2s - 4t + 6) \\ &\quad \cdot \left(\frac{4 \times 12}{4+12-2} \right)^3 + (2st - 2s - 4t + 4) \left(\frac{4 \times 13}{4+13-2} \right)^3 + (2) \left(\frac{5 \times 5}{5+5-2} \right)^3 \\ &\quad + (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 \\ &\quad + (8r - 8) \left(\frac{6 \times 9}{6+9-2} \right)^3 + (2t - 2) \left(\frac{7 \times 8}{7+8-2} \right)^3 + (2) \left(\frac{7 \times 11}{7+11-2} \right)^3 + (2t - 2) \\ &\quad \cdot \left(\frac{7 \times 12}{7+12-2} \right)^3 + (2) \left(\frac{8 \times 15}{8+15-2} \right)^3 + (2t - 2) \left(\frac{8 \times 8}{8+8-2} \right)^3 + (2t - 2) \\ &\quad \cdot \left(\frac{8 \times 10}{8+10-2} \right)^3 + (2t - 2) \left(\frac{8 \times 11}{8+11-2} \right)^3 + (4st - 10t + 6) \left(\frac{8 \times 12}{8+12-2} \right)^3 \\ &\quad + (2) \left(\frac{8 \times 14}{8+14-2} \right)^3 + (2t - 4) \left(\frac{8 \times 15}{8+15-2} \right)^3 + (8r - 8) \left(\frac{9 \times 10}{9+10-2} \right)^3 \\ &\quad + (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 \\ &\quad + (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) \\ &\quad \cdot \left(\frac{10 \times 14}{10+14-2} \right)^3 + (4rs + 4rt - 12r - 4s - 4t + 12) \left(\frac{10 \times 15}{10+15-2} \right)^3 + (2t - 2) \\ &\quad \cdot \left(\frac{11 \times 12}{11+12-2} \right)^3 + (2t - 2) \left(\frac{11 \times 15}{11+15-2} \right)^3 + (2) \left(\frac{11 \times 16}{11+16-2} \right)^3 + (2st - 2s - 4t + 4) \\ &\quad \cdot \left(\frac{12 \times 13}{12+13-2} \right)^3 + (2t) \left(\frac{12 \times 15}{12+15-2} \right)^3 + (2st + 2s - 4t - 6) \\ &\quad \cdot \left(\frac{12 \times 16}{12+16-2} \right)^3 + (2t - 2) \left(\frac{13 \times 14}{13+14-2} \right)^3 + (4st - 4s - 10t + 10) \\ &\quad \times \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) \\ &\quad \cdot \left(\frac{15 \times 15}{15+15-2} \right)^3 + (10rs - 28r - 10s + 4rt - 4t + 30) \left(\frac{15 \times 16}{15+16-2} \right)^3 \\ &\quad + (16rst - 24rt - 20rs - 21st + 38t + 23s + 24r - 40) \left(\frac{16 \times 16}{16+16} \right)^3. \end{aligned} \quad (23)$$

FIGURE 6: Comparison of GA index and GA_5 index of $M[r, s, t]$ for fix $t = 1$. Red color represents GA, and green color represents GA_5 .

FIGURE 7: Comparison of R_{-1} , $R_{-1/2}$, ABC_4 , $R_{1/2}$, ABC , and GA indices of $M[r, s, t]$ for fix $t = 1$. Niagara azure, green, cyan, blue, purple, and red represents R_{-1} , $R_{-1/2}$, ABC_4 , $R_{1/2}$, ABC , and GA indices, respectively.

The results now follow after some simple calculations. $\square$

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

FIGURE 8: Comparison of first Zagreb coindex index $\overline{M}_1$ and second Zagreb coindex $\overline{M}_2$ of $M[r, s, t]$. Purple and blue represents $\overline{M}_1$ and $\overline{M}_2$, respectively.

FIGURE 9: Comparison of $\overline{M}_1$ and $\overline{M}_2$ indices of $M[r, s, t]$, where purple color represents $\overline{M}_1$ and blue color represents $\overline{M}_2$.

related values of R_{-1} , $R_{-1/2}$, ABC_4 , $R_{1/2}$, ABC , 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 , HM , S , $\overline{M}_1$, and $\overline{M}_2$ 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_{-1} , $R_{-1/2}$, ABC_4 , $R_{1/2}$, ABC , GA , GA_5M_1 , R_1 , HM , S , M_1 , and M_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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