Hindawi
Journal of Chemistry
Volume 2020, Article ID 9805829, 12 pages
https://doi.org/10.1155/2020/9805829

Research Article

Reverse Zagreb and Reverse Hyper-Zagreb Indices for Crystallographic Structure of Molecules

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Received 9 October 2019; Accepted 8 February 2020; Published 13 March 2020

Academic Editor: Jia-Bao Liu

In the fields of chemical graph theory, topological index is a type of a molecular descriptor that is calculated based on the graph of a chemical compound. Topological indices help us collect information about algebraic graphs and give us mathematical approach to understand the properties of algebraic structures. With the help of topological indices, we can guess the properties of chemical compounds without performing experiments in wet lab. There are more than 148 topological indices in the literature, but none of them completely give all properties of under study compounds. Together, they do it to some extent; hence, there is always room to introduce new indices. In this paper, we present first and second reserve Zagreb indices and first reverse hyper-Zagreb indices, reverse GA index, and reverse atomic bond connectivity index for the crystallographic structure of molecules. We also present first and second reverse Zagreb polynomials and first and second reverse hyper-Zagreb polynomials for the crystallographic structure of molecules.

1. Introduction

Topological indices enable us to collect information about algebraic structures and give us a mathematical approach to understand the properties of algebraic structures. Here, we will discuss some newly introduced first and second reverse Zagreb indices, hyper-Zagreb indices, and their polynomials for the crystallographic structure of molecules [1–9].

A graph having no loop or multiple edges is known as simple graph. A molecular graph is a simple graph in which atoms and bonds are represented by vertex and edge sets, respectively. The vertex degree is the number of edges attached to that vertex [10–16]. The maximum degree of vertex among the vertices of a graph is denoted by $\Delta(G)$. Kulli et al. [17] introduce the concept of reverse vertex degree C_y, defined as $C_y = \Delta(G) - d_g(v) + 1$.

In discrete mathematics, graph theory in general is not only the study of different properties of objects but it also tells us about objects having same properties as investigating object. These properties of different objects are of main interest. In particular, graph polynomials related to graph are rich in information. Mathematical tools like polynomials and topological-based numbers have significant importance to collect information about the properties of chemical compounds. We can find out many hidden information about compounds through these tools. Multifold graph polynomials are present in the literature. Actually, topological indices are numeric quantities that tell us about the whole structure of graph. There are many topological indices [18, 19] that help us to study physical, chemical reactivities, and biological properties. Wiener, in 1947 [20], firstly introduce the concept of topological index while working on boiling point. In particular, Hosoya polynomial [21] plays an important in the area of distance-based topological indices; we can find out Wiener index, hyper-Wiener index, and Tratch–Stankevich–Zefirov index by Hosoya polynomial [22, 23]. Other well-established polynomials are Zagreb and hyper-Zagreb polynomials introduced by Gao.

The first and second reverse Zagreb indices are as follows:

$$\begin{aligned} CM_1(G) &= \sum_{uv \in E(G)} (c_u + c_v), \\ CM_2(G) &= \sum_{uv \in E(G)} (c_u . c_v). \end{aligned} \quad (1)$$

Now, the first and second reverse hyper-Zagreb indices are given by

$$\begin{aligned} HCM_1(G) &= \sum_{uv \in E(G)} (c_u + c_v)^2, \\ HCM_2(G) &= \sum_{uv \in E(G)} (c_u . c_v)^2. \end{aligned} \quad (2)$$

Atom-bond connectivity index can be abbreviated as ABC index. It is defined as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u(G) + d_v(G) - 2}{d_u(G).d_v(G)}}. \quad (3)$$

Another degree-based topological index that utilizes the difference between the geometric and arithmetic means was invented by Vukicevic and Furtula, namely, geometric-arithmetic index and is defined as follows:

$$GA(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u(G).d_v(G)}}{(1/2)[d_u(G) + d_v(G)]}. \quad (4)$$

With the help of reverse Zagreb and hyper-Zagreb indices, we are now able to write the reverse Zagreb and hyper Zagreb polynomials:

$$\begin{aligned} CM_1(G,x) &= \sum_{uv \in E(G)} x^{(c_u + c_v)}, \\ CM_2(G,x) &= \sum_{uv \in E(G)} x^{(c_u . c_v)}, \\ HCM_1(G,x) &= \sum_{uv \in E(G)} x^{(c_u + c_v)^2}, \\ HCM_2(G,x) &= \sum_{uv \in E(G)} x^{(c_u . c_v)^2}. \end{aligned} \quad (5)$$

We introduce the idea of reverse atom-bond connectivity index and reverse geometric-arithmetic index, and it is defined as follows:

$$\begin{aligned} CABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{c_u(G) + c_v(G) - 2}{c_u(G).c_v(G)}}, \\ CGA(G) &= \sum_{uv \in E(G)} \frac{\sqrt{c_u(G).c_v(G)}}{(1/2)[c_u(G) + c_v(G)]}. \end{aligned} \quad (6)$$

2. Main Results

Here, we will compute reverse Zagreb and reverse hyper-Zagreb indices for the crystallographic structure of molecules.

2.1. Crystallographic Structure of the Molecule Cu_2O. The unit cell of the crystallographic structure of the molecule Cu_2O is given in Figure 1 and the crystal structure of Cu_2O [3, 3, 3] is given in Figure 2.

Theorem 1. *Let G be the chemical graph of Cu_2O, with m, α, $t \geq 1$. The first and second reverse Zagreb indices are as follows:*

(1) $CM_1(Cu_2O) = 32m\alpha t + 20m\alpha + 20mt + 20\alpha t + 36 - 28m - 28\alpha - 28t$

(2) $CM_2(Cu_2O) = 24m\alpha t + 24m\alpha + 24mt + 24\alpha t - 12m - 12\alpha - 12t$

Proof. From Figure 2, we can say that there are 3 types of edges in Cu_2O:

$$\begin{aligned} E_1(Cu_2O) &= \{uv \in E(Cu_2O); d_u = 1, d_v = 2\}, \\ E_2(Cu_2O) &= \{uv \in E(Cu_2O); d_u = 2, d_v = 2\}, \\ E_3(Cu_2O) &= \{uv \in E(Cu_2O); d_u = 2, d_v = 4\}. \end{aligned} \quad (7)$$

We have $|E_1(Cu_2O)| = 4\alpha + 4m + 4t - 8$, $|E_2(Cu_2O)| = 4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12$, and $|E_3(Cu_2O)| = 4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)$. In this structure, the maximum edge degree is 4, and then, the reverse edges are given as follows:

$$c_u = \Delta(G) - d_G(u) + 1 = 5 - d_G(u). \quad (8)$$

The reverse edge set of Cu_2O is given as follows:

$$\begin{aligned} CE_1(Cu_2O) &= \{uv \in E(Cu_2O); c_u = 4, c_v = 3\}, \\ CE_2(Cu_2O) &= \{uv \in E(Cu_2O); c_u = 3, c_v = 3\}, \\ CE_3(Cu_2O) &= \{uv \in E(Cu_2O); c_u = 3, c_v = 1\}. \end{aligned} \quad (9)$$

We have $|CE_1(Cu_2O)| = 4\alpha + 4m + 4t - 8$, $|CE_2(Cu_2O)| = 4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12$, and $|CE_3(Cu_2O)| = 4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)$.

(i) The first reverse ZI for Cu_2O is given by

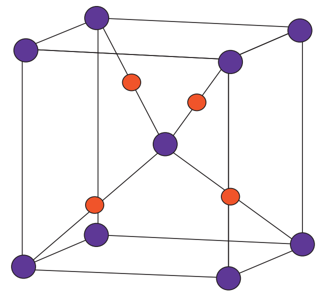

FIGURE 1: Unit cell of Cu_2O [1, 1, 1].

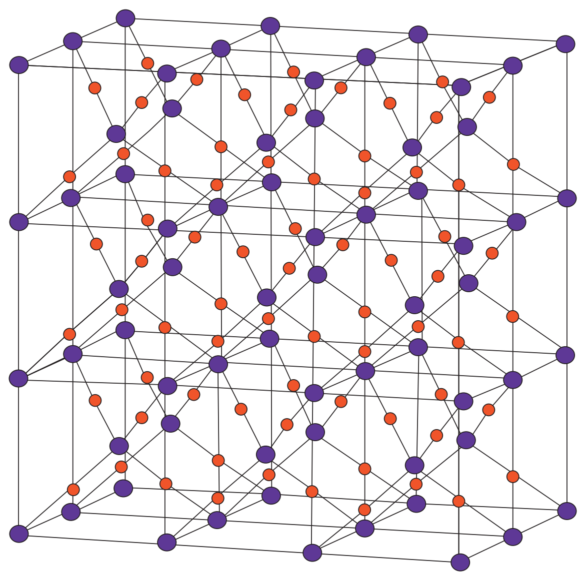

FIGURE 2: Crystal structure of Cu_2O [3, 3, 3].

$$\begin{aligned}
\mathrm{CM}_1(\mathrm{Cu_2O}) &= \sum_{uv\epsilon E(G)} (c_u + c_v) \\
&= (4+3)(4\alpha + 4m + 4t - 8) + (3+3)(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) + (3+1) \\
&\quad \cdot (4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)) \\
&= 32m\alpha t + 20m\alpha + 20mt + 20\alpha t + 36 - 28m - 28\alpha - 28t.
\end{aligned} \tag{10}$$

(ii) The second reverse ZI for Cu_2O is given by

$$\begin{aligned}
\mathrm{CM}_2(\mathrm{Cu_2O}) &= \sum_{uv\epsilon E(G)} (c_u . c_v) \\
&= (4\times 3)(4\alpha + 4m + 4t - 8) + (3\times 3)(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) \\
&\quad + (3\times 1)(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)) \\
&= 24m\alpha t + 24m\alpha + 24mt + 24\alpha t - 12m - 12\alpha - 12t.
\end{aligned} \tag{11}$$

□

Theorem 2. *The first and second reverse Zagreb polynomials for Cu_2O with m, n, $t \geq 1$ are as follows:*

$$\begin{aligned}
1.\mathrm{CM}_1(\mathrm{Cu_2O}, x) &= x^7(4\alpha + 4m + 4t - 8) + x^6(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) \\
&\quad + x^4(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1), \\
2.\mathrm{CM}_2(\mathrm{Cu_2O}, x) &= x^{12}(4\alpha + 4m + 4t - 8) + x^9(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) \\
&\quad + x^3(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1).
\end{aligned} \tag{12}$$

Proof. Now, by the reverse edge partitions of Cu_2O, we have the following results:

(i) The first reverse Zagreb polynomial for Cu_2O is given as follows:

$$\begin{aligned}
\mathrm{CM}_1(\mathrm{Cu_2O}, x) &= \sum_{uv\epsilon E(G)} x^{(c_u + c_v)} \\
&= (4\alpha + 4m + 4t - 8)x^{(3+4)} + (4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12)x^{(3+3)} \\
&\quad + \big(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)x^{(3+1)} \\
&= x^7(4\alpha + 4m + 4t - 8) + x^6(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) \\
&\quad + x^4(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1).
\end{aligned} \tag{13}$$

(ii) The second reverse Zagreb polynomial for Cu_2O, with m, α, $t \geq 1$, is given as follows:

$$\begin{aligned}
\mathrm{CM}_2(\mathrm{Cu_2O}, x) &= \sum_{uv\epsilon E(G)} x^{(c_u . c_v)} \\
&= (4\alpha + 4m + 4t - 8)x^{(3\times4)} + (4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12)x^{(3\times3)} \\
&\quad + \big(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)x^{(3\times1)} \\
&= x^{12}(4\alpha + 4m + 4t - 8) + x^9(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) \\
&\quad + x^3(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1).
\end{aligned} \tag{14}$$

□

Theorem 3. *The first and second reverse hyper-Zagreb indices of silicon-carbon Cu_2O with m, α, $t \geq 1$ are as follows:*

(1) $HCM_1(Cu_2O) = 32m\alpha t + 128m\alpha + 128mt + 128\alpha t - 76m - 76\alpha - 76t + 24$

(2) $HCM_2(Cu_2O) = 18m\alpha t + 315m\alpha + 315mt + 315\alpha t - 63m - 63\alpha - 63t - 189$

Proof. Let G be a graph of Cu_2O. Then, by reverse edge partition and definition of reverse hyper-Zagreb indices, we have the following results:

(i) The first reverse hyper-ZI for Cu_2O is given by

$$\begin{aligned}
\mathrm{CM}_1(\mathrm{Cu_2O}) &= \sum_{uv\epsilon E(G)} (c_u + c_v)^2 \\
&= (4+3)^2(4\alpha + 4m + 4t - 8) + (3+3)^2(4\alpha m + 4\alpha t + 4mt - 8\alpha - 8m - 8t + 12) \\
&\quad + (3+1)^2(4(2\alpha mt - \alpha m - \alpha t - mt + \alpha + m + t - 1)) \\
&= 32m\alpha t + 128m\alpha + 128mt + 128\alpha t - 76m - 76\alpha - 76t + 24.
\end{aligned} \tag{15}$$

(ii) The second reverse hyper-ZI for Cu_2O is given by

$$\begin{aligned}
CM_2(Cu_2O) &= \sum_{uv\epsilon E(G)} (c_u.c_v)^2 \\
&= (4\times 3)^2(4\alpha+4m+4t-8)+(3\times 3)^2(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12) \\
&\quad +(3\times 1)^2(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1)) \\
&= 18m\alpha t+315m\alpha+315mt+315\alpha t-63m-63\alpha-63t-189.
\end{aligned} \tag{16}$$

□

Theorem 4. *The first and second reverse hyper-Zagreb polynomials of Cu_2O with m, α, $t \geq 1$ are as follows:*

$$\begin{aligned}
1.HCM_1(Cu_2O,x) &= x^{144}(4\alpha+4m+4t-8)+x^{81}(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12) \\
&\quad +x^{9}(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1), \\
2.HCM_1(Cu_2O,x) &= x^{144}(4\alpha+4m+4t-8)+x^{81}(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12) \\
&\quad +x^{9}(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1).
\end{aligned} \tag{17}$$

Proof. Now, by the reverse edge partitions for Cu_2O, we have the following results:

(i) The first reverse Zagreb polynomial for Cu_2O is given as follows:

$$\begin{aligned}
HCM_1(Cu_2O,x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2} \\
&= (4\alpha+4m+4t-8)x^{(3+4)^2}+(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12)x^{(3+3)^2} \\
&\quad +(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1)x^{(3+1)^2} \\
&= x^{49}(4\alpha+4m+4t-8)+x^{36}(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12) \\
&\quad +x^{16}(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1).
\end{aligned} \tag{18}$$

(ii) The second reverse Zagreb polynomial for Cu_2O is given as follows:

$$\begin{aligned}
HCM_2(Cu_2O,x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)^2} \\
&= (4\alpha+4m+4t-8)x^{(3\times 4)^2}+(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12)x^{(3\times 3)^2} \\
&\quad +(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1)x^{(3\times 1)^2} \\
&= x^{144}(4\alpha+4m+4t-8)+x^{81}(4\alpha m+4\alpha t+4mt-8\alpha-8m-8t+12) \\
&\quad +x^{9}(4(2\alpha mt-\alpha m-\alpha t-mt+\alpha+m+t-1).
\end{aligned} \tag{19}$$

□

Theorem 5. *Let G be the graph of Cu_2O with $m, \alpha, t \geq 1$. The reverse atom-bond connectivity index and reverse geometric-arithmetic index for Cu_2O with $m, \alpha, t \geq 1$ are as follows:*

$$1.\mathrm{CABC}(\mathrm{Cu_2O}) = \frac{1}{3}[(8\sqrt{6})m\alpha t + (8-32\sqrt{6})(m\alpha + mt + \alpha t) + (2\sqrt{15} - 16 + 32\sqrt{6})(m+\alpha+t) + (24 - 16\sqrt{15} - 32\sqrt{6})],$$
$$2.\mathrm{CGA}(\mathrm{Cu_2O}) = \frac{1}{14}[(56\sqrt{3})m\alpha t + (56-28\sqrt{3})(m\alpha + \alpha t + mt) + (-112+39\sqrt{3})(m+\alpha+t) + (168-71\sqrt{3})]. \tag{20}$$

Proof. By the reverse edge partition, we have the following results:

(i) The reverse atom-bond connectivity index for Cu_2O is given by

$$\begin{aligned}\mathrm{CABC}(\mathrm{Cu_2O}) &= \sum_{uv\epsilon E(G)} \sqrt{\frac{c_u(G)+c_v(G)-2}{c_u(G).c_v(G)}}\\ &= [4m+4\alpha+4t-8]\left[\sqrt{\frac{4+3-2}{4\times 3}}\right] + [4m\alpha + 4\alpha t + 4mt - 8m - 8\alpha - 8t + 12]\left[\sqrt{\frac{3+3-2}{3\times 3}}\right]\\ &\quad + [4(2m\alpha t - m\alpha - mt - \alpha t + m + \alpha + t - 1)]\left[\sqrt{\frac{3+1-2}{3\times 1}}\right]\\ &= \frac{1}{3}[(8\sqrt{6})m\alpha t + (8-32\sqrt{6})(m\alpha + mt + \alpha t) + (2\sqrt{15} - 16 + 32\sqrt{6})(m+\alpha+t) + (24-16\sqrt{15}-32\sqrt{6})].\end{aligned} \tag{21}$$

(ii) The reverse geometric-arithmetic index for Cu_2O is given by

$$\begin{aligned}\mathrm{CGA}(\mathrm{Cu_2O}) &= \sum_{uv\epsilon E(G)} \frac{\sqrt{c_u(G).c_v(G)}}{(1/2)[c_u(G)+c_v(G)]}\\ &= [4m+4\alpha+4t-8]\left[\frac{\sqrt{4\times 3}}{(1/2)[4+3]}\right] + [4m\alpha + 4\alpha t + 4mt - 8m - 8\alpha - 8t + 12]\left[\frac{\sqrt{3\times 3}}{(1/2)[3+3]}\right]\\ &\quad + [4(2m\alpha t - m\alpha - mt - \alpha t + m + \alpha + t - 1)]\left[\frac{\sqrt{3\times 1}}{(1/2)[3+1]}\right]\\ &= \frac{1}{14}[(56\sqrt{3})m\alpha t + (56-28\sqrt{3})(m\alpha + \alpha t + mt) + (-112+39\sqrt{3})(m+\alpha+t) + (168-71\sqrt{3})].\end{aligned} \tag{22}$$

□

The values of calculated topological indices of Cu_2O at different levels are given in Table 1.

2.2. Titanium Difluoride $TiF_2[m, \alpha, t]$. The unit cell of crystallographic structure of titanium difluoride $TiF_2[m, \alpha, t]$ is given in Figure 3 and the crystal structure of TiF_2 [1, 2, 4] is given in Figure 4.

Theorem 6. *Let G be the graph of titanium difluoride $TiF_2[m, \alpha, t]$, with $m, \alpha, t \geq 1$. The first and second reverse Zagreb indices are as follows:*

(1) $CM_1(TiF_2[m, \alpha, t]) = 192m\alpha t + 64m\alpha + 64mt + 64\alpha t - 16m - 16\alpha - 16t + 8$

(2) $CM_2(TiF_2[m, \alpha, t]) = 160m\alpha t + 320m\alpha + 320mt + 320\alpha t - 80m - 80\alpha - 80t + 40$

Table 1: Values of calculated topological indices of Cu_2O at different levels.

	m = 1 α = 1 t = 1	m = 2 α = 2 t = 2	m = 3 α = 3 t = 3	m = 1 α = 2 t = 3	m = 3 α = 2 t = 1	m = 3 α = 4 m = 5	m = 2 α = 4 t = 6
First reverse ZI	44	364	1188	280	280	2560	2116
Second reverse ZI	60	408	1188	336	336	2424	2064
First reverse hyper-ZI	212	1360	3660	1168	1168	7048	6280
Second reverse hyper-ZI	585	3357	8235	3006	3006	14940	13779
Reverse ABC index	−252.9	−117.5	−285.5	−117.4	−117.4	−469.1	−430.1
Reverse GA index	222	46.02	176.17	31.63	31.63	405.96	321.24

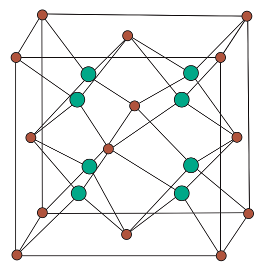

Figure 3: Unit cell of $TiF_2[m, \alpha, t]$.

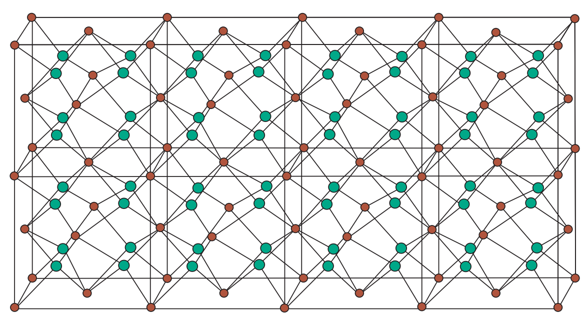

Figure 4: Crystal structure of TiF_2 [1, 2, 4].

Proof. Let G be a graph of titanium difluoride $TiF_2[m, \alpha, t]$. The vertex and edge sets of titanium difluoride $TiF_2[m, \alpha, t]$ are $|V(TiF_2[m, \alpha, t])| = 12m\alpha t + 2m\alpha + 2mt + 2\alpha t + m + \alpha + t + 1$ and $|E(TiF_2[m, \alpha, t])| = 32m\alpha t$, respectively. From Figure 4, we can say that there are five type of edges in $TiF_2[m, \alpha, t]$. The edge set of $|TiF_2[m, \alpha, t]| = 32m\alpha t$ is portioned into four edge sets:

$$\begin{aligned} E_1(TiF_2[m,\alpha,t]) &= \{uv\epsilon E(TiF_2[m,\alpha,t]); d_u = 1, d_v = 4\},\\ E_2(TiF_2[m,\alpha,t]) &= \{uv\epsilon E(TiF_2[m,\alpha,t]); d_u = 2, d_v = 4\},\\ E_3(TiF_2[m,\alpha,t]) &= \{uv\epsilon E(TiF_2[m,\alpha,t]); d_u = 4, d_v = 4\},\\ E_4(TiF_2[m,\alpha,t]) &= \{uv\epsilon E(TiF_2[m,\alpha,t]); d_u = 4, d_v = 8\}. \end{aligned} \tag{23}$$

We have $|E_1(TiF_2[m, \alpha, t])| = 8$, $|E_2(TiF_2[m, \alpha, t])| = 8(m + \alpha + t - 3)$, $|E_3(TiF_2[m, \alpha, t])| = 16(m\alpha + \alpha t + mt) - 16(m + \alpha + t) + 24$, and $|E_4(TiF_2[m, \alpha, t])| = 32m\alpha t - 16(mt + m\alpha + \alpha t) + 8(m + \alpha + t) - 8$. The maximum edge degree is 8; then, the reverse edges are given as follows:

$$c_u = \Delta(G) - d_G(u) + 1 = 9 - d_G(u). \tag{24}$$

The reverse edge set of $TiF_2[m, \alpha, t]$ is given as follows:

$$\begin{aligned} CE_1(TiF_2[m,\alpha,t]) &= \{uv\varepsilon E(TiF_2[m,\alpha,t]); c_u = 8, c_v = 5\},\\ CE_2(TiF_2[m,\alpha,t]) &= \{uv\varepsilon E(TiF_2[m,\alpha,t]); c_u = 7, c_v = 5\},\\ CE_3(TiF_2[m,\alpha,t]) &= \{uv\varepsilon E(TiF_2[m,\alpha,t]); c_u = 5, c_v = 5\},\\ CE_4(TiF_2[m,\alpha,t]) &= \{uv\varepsilon E(TiF_2[m,\alpha,t]); c_u = 5, c_v = 1\}. \end{aligned} \tag{25}$$

We have $|E_1(\mathrm{TiF}_2[m, \alpha, t])| = 8$, $|E_2(\mathrm{TiF}_2[m, \alpha, t])| = 8(m + \alpha + t - 3)$, $|E_3(\mathrm{TiF}_2[m, \alpha, t])| = 16(m\alpha + \alpha t + mt) - 16(m + \alpha + t) + 24$, and $|E_4(\mathrm{TiF}_2[m, \alpha, t])| = 32m\alpha t - 16(mt + m\alpha + \alpha t) + 8(m + \alpha + t) - 8$.

(i) The first reverse ZI for $\mathrm{TiF}_2[m, \alpha, t]$ is given by

$$\begin{aligned} \mathrm{CM}_1(\mathrm{TiF}_2[m,\alpha,t]) &= \sum_{uv \epsilon E(G)} (c_u + c_v) \\ &= (8+5)(8) + (7+5)[8(m+\alpha+t-3)] + (5+5)[16(mn+\alpha t+mt) - 16(m+\alpha+t) + 24] \\ &\quad + (5+1)[32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8] \\ &= 192m\alpha t + 64m\alpha + 64mt + 64\alpha t - 16m - 16\alpha - 16t + 8. \end{aligned} \tag{26}$$

(ii) The second reverse ZI for $\mathrm{TiF}_2[m, \alpha, t]$ is given by

$$\begin{aligned} \mathrm{CM}_2(\mathrm{TiF}_2[m,\alpha,t]) &= \sum_{uv \epsilon E(G)} (c_u . c_v) \\ &= (8\times 5)(8) + (7\times 5)[8(m+\alpha+t-3)] + (5\times 5)[16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24] \\ &\quad + (5\times 1)[32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8] \\ &= 160m\alpha t + 320m\alpha + 320mt + 320\alpha t - 80m - 80\alpha - 80t + 40. \end{aligned} \tag{27}$$

□

Theorem 7. *The first and second reverse Zagreb polynomials for* $\mathrm{TiF}_2[m, \alpha, t]$ *are as follows:*

(1) $CM_1(\mathrm{TiF}_2[m, \alpha, t], x) = 8x^{13} + [8(m + \alpha + t - 3)]x^{12} + [16(m\alpha + \alpha t + mt) - 16(m + \alpha + t) + 24]x^{10} + [32m\alpha t - 16(mt + m\alpha + \alpha t) + 8(m + \alpha + t) - 8]x^6$

(2) $CM_2(\mathrm{TiF}_2[m, \alpha, t], x) = 8x^{40} + [8(m + \alpha + t - 3)]x^{35} + [16(m\alpha + \alpha t + mt) - 16(m + \alpha + t) + 24]x^{25} + [32m\alpha t - 16(mt + m\alpha + \alpha t) + 8(m + \alpha + t) - 8]x^5$

Proof. Now, by the reverse edge partitions for $\mathrm{TiF}_2[m, \alpha, t]$, we have the following results:

(i) The first reverse Zagreb polynomial for $\mathrm{TiF}_2[m, \alpha, t]$ is given as follows:

$$\begin{aligned} \mathrm{CM}_1(\mathrm{TiF}_2[m,\alpha,t],x) &= \sum_{uv \epsilon E(G)} x^{(c_u+c_v)} \\ &= (8)x^{(8+5)} + [8(m+\alpha+t-3)]x^{(7+5)} + [16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24]x^{(5+5)} \\ &\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{(5+1)} \\ &= 8x^{13} + [8(m+\alpha+t-3)]x^{12} + [16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24]x^{10} \\ &\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{6}. \end{aligned} \tag{28}$$

(ii) The second reverse Zagreb polynomial for $\mathrm{TiF}_2[m, \alpha, t]$ is given as follows:

$$\begin{aligned} \mathrm{CM}_2(\mathrm{TiF}_2[m,\alpha,t],x) &= \sum_{uv \epsilon E(G)} x^{(c_u . c_v)} \\ &= (8)x^{(8\times 5)} + [8(m+\alpha+t-3)]x^{(7\times 5)} + [16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24]x^{(5\times 5)} \\ &\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{(5\times 1)} \\ &= 8x^{40} + [8(m+\alpha+t-3)]x^{35} + [16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24]x^{25} \\ &\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{5}. \end{aligned} \tag{29}$$

□

Theorem 8. *The first and second reverse hyper-Zagreb indices of $TiF_2[m, \alpha, t]$ are as follows:*

(1) $HCM_1(TiF_2[m, \alpha, t]) = 1152m\alpha t - 160(m + \alpha + t) + 1024(m\alpha + \alpha t + mt) - 2152$

(2) $HCM_2(TiF_2[m, \alpha, t]) = 800m\alpha t + 9600(m\alpha + \alpha t + mt) - 14600$

Proof. Let G be a graph of silicon-carbon $TiF_2[m, \alpha, t]$. Then, by reverse edge partition and definition of reverse hyper-Zagreb indices, we have the following results:

(i) The first reverse hyper-ZI for $TiF_2[m, \alpha, t]$ is given by

$$\begin{aligned} CM_1(TiF_2[m,\alpha,t]) &= \sum_{uv\epsilon E(G)} (c_u + c_v)^2 \\ &= (8+5)^2(8) + (7+5)^2[8(m+\alpha+t-3)] + (5+5)^2[16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24] \\ &\quad + (5+1)^2[32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8] \\ &= 1152m\alpha t - 160(m+\alpha+t) + 1024(m\alpha+\alpha t+mt) - 2152. \end{aligned} \tag{30}$$

(ii) The second reverse hyper-ZI for $TiF_2[m, \alpha, t]$ is given by

$$\begin{aligned} CM_2(TiF_2[m,\alpha,t]) &= \sum_{uv\epsilon E(G)} (c_u . c_v)^2 \\ &= (8\times5)^2(8) + (7\times5)^2[8(m+\alpha+t-3)] + (5\times5)^2[16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24] \\ &\quad + (5\times1)^2[32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8] \\ &= 800m\alpha t + 9600(m\alpha+\alpha t+mt) - 14600. \end{aligned} \tag{31}$$

□

Theorem 9. *The first and second reverse hyper-Zagreb polynomials of $TiF_2[m, \alpha, t]$ are as follows:*

(1) $HCM_1(TiF_2[m, \alpha, t], x) = 8x^{169} + [8(m + \alpha + t - 3)]x^{144} + [16(m\alpha + \alpha t + mt) - 16(m + \alpha + t) + 24]x^{100} + [32m\alpha t - 16(mt + m\alpha + \alpha t) + 8(m + \alpha + t) - 8]x^{36}$

(2) $HCM_1(TiF_2[m, \alpha, t], x) = 8x^{1600} + [8(m + \alpha + t - 3)]x^{1225} + [16(m\alpha + \alpha t + mt) - 16(m + \alpha + t) + 24]x^{625} + [32m\alpha t - 16(mt + m\alpha + \alpha t) + 8(m + \alpha + t) - 8]x^{25}$

Proof. Now, by the reverse edge partitions for $TiF_2[m, \alpha, t]$, we have the following results:

(i) The first reverse Zagreb polynomial for $TiF_2[m, \alpha, t]$ is given as follows:

$$\begin{aligned} CM_1(TiF_2[m,\alpha,t],x) &= \sum_{uv\epsilon E(G)} x^{(c_u+c_v)^2} \\ &= (8)x^{(8+5)^2} + [8(m+\alpha+t-3)]x^{(7+5)^2} + [16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24]x^{(5+5)^2} \\ &\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{(5+1)^2} \\ &= 8x^{169} + [8(m+\alpha+t-3)]x^{144} + [16(m\alpha+\alpha t+mt) - 16(m+\alpha+t) + 24]x^{100} \\ &\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{36}. \end{aligned} \tag{32}$$

(ii) The second reverse Zagreb polynomial for $TiF_2[m, \alpha, t]$ is given as follows:

$$\begin{aligned}
CM_2(TiF_2[m,\alpha,t],x) &= \sum_{uv\epsilon E(G)} x^{(c_u.c_v)^2} \\
&= (8)x^{(8\times5)^2} + [8(m+\alpha+t-3)]x^{(7\times5)^2} + [16(m\alpha+\alpha t+mt)-16(m+\alpha+t)+24]x^{(5\times5)^2} \\
&\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{(5\times1)^2} \\
&= 8x^{1600} + [8(m+\alpha+t-3)]x^{1225} + [16(m\alpha+\alpha t+mt)-16(m+\alpha+t)+24]x^{625} \\
&\quad + [32m\alpha t - 16(mt+m\alpha+\alpha t) + 8(m+\alpha+t) - 8]x^{25}.
\end{aligned} \tag{33}$$

□

Theorem 10. *Let G be the graph of Cu_2O with m, α, t ≥ 1. The reverse atom-bond connectivity index and reverse geometric-arithmetic index for Cu_2O with m, α, t ≥ 1 are given by*

$$\begin{aligned}
&(1)\mathrm{CABC}(TiF_2[m,\alpha,t]) = \frac{1}{175}[(2240\sqrt{5})m\alpha t + (1225\sqrt{2} - 1225\sqrt{5})(m\alpha+mt+\alpha t) + (40\sqrt{350} - 224\sqrt{50} \\
&\quad + 560\sqrt{5})(m+\alpha+t) + (70\sqrt{110} - 6000\sqrt{14} + 1680\sqrt{2} - 2800\sqrt{5})], \\
&(2)\mathrm{CGA}(TiF_2[m,\alpha,t]) = \frac{1}{3}[(32\sqrt{5})m\alpha t + (48 - 16\sqrt{5})(m\alpha+mt+\alpha t) + (4\sqrt{35} + 8\sqrt{5} - 48)(m+\alpha+t)] \\
&\quad + \frac{1}{39}(96\sqrt{10} - 104\sqrt{5} + 156\sqrt{35} + 936).
\end{aligned} \tag{34}$$

Proof. By the reverse edge partition, we have the following results:

(i) The reverse atom-bond connectivity index for $TiF_2[m, \alpha, t]$ is given by

$$\begin{aligned}
\mathrm{CABC}(TiF_2[m,\alpha,t]) &= \sum_{uv\epsilon E(G)} \sqrt{\frac{c_u(G)+c_v(G)-2}{c_u(G).c_v(G)}} \\
&= [8]\left[\sqrt{\frac{8+5-2}{8\times5}}\right] + [8(m+\alpha+t-3)]\left[\sqrt{\frac{7+5-2}{7\times5}}\right] + [16(m\alpha+\alpha t+mt)-16(m+\alpha+t)+24] \\
&\quad \cdot \left[\sqrt{\frac{5+5-2}{5\times5}}\right] + [32m\alpha t - 16(m\alpha+mt+\alpha t) + 8(m+\alpha+t) - 8]\left[\sqrt{\frac{5+1-2}{5\times1}}\right] \\
&= \frac{1}{175}[(2240\sqrt{5})m\alpha t + (1225\sqrt{2} - 1225\sqrt{5})(m\alpha+mt+\alpha t) + (40\sqrt{350} - 224\sqrt{50} + 560\sqrt{5}) \\
&\quad \cdot (m+\alpha+t) + (70\sqrt{110} - 6000\sqrt{14} + 1680\sqrt{2} - 2800\sqrt{5})].
\end{aligned} \tag{35}$$

Table 2: Values of calculated topological indices of $TiF_2[m, \alpha, t]$ at different levels.

	m = 1, α = 1, t = 1	m = 2, α = 2, t = 2	m = 3, α = 3, t = 3	m = 1, α = 2, t = 3	m = 3, α = 2, t = 1	m = 3, α = 4, m = 5	m = 2, α = 4, t = 6
First reverse ZI	344	2216	6776	1768	1768	14344	11848
Second reverse ZI	920	4680	12280	4040	4040	23720	20840
First reverse hyper-ZI	1592	18392	55160	15064	15064	113176	96280
Second reverse hyper-ZI	15000	107000	266200	95800	95800	484600	446200
Reverse ABC index	-127.8	27.9	492.6	-23.57	-23.6	1346.4	860.3
Reverse GA index	79.1	276.3	784.1	224.5	224.5	1634.1	1241.3

(ii) The reverse geometric-arithmetic index for $TiF_2[m, \alpha, t]$ is given by

$$
\begin{aligned}
\mathrm{CGA}\left(\mathrm{TiF}_2[m,\alpha,t]\right) &= \sum_{uv\epsilon E(G)} \frac{\sqrt{c_u(G).c_v(G)}}{(1/2)\left[c_u(G)+c_v(G)\right]} \\
&= [8]\left[\frac{\sqrt{8\times 5}}{(1/2)[8+5]}\right] + [8(m+\alpha+t-3)]\left[\frac{\sqrt{7\times 5}}{(1/2)[7+5]}\right] + [16(m\alpha+\alpha t+mt)-16(m+\alpha+t)+24] \\
&\quad \cdot \left[\frac{\sqrt{5\times 5}}{(1/2)[5+5]}\right] + [32m\alpha t-16(m\alpha+mt+\alpha t)+8(m+\alpha+t)-8]\left[\frac{\sqrt{5\times 1}}{(1/2)[5+1]}\right] \\
&= \frac{1}{3}\left[(32\sqrt{5})m\alpha t+(48-16\sqrt{5})(m\alpha+mt+\alpha t)+(4\sqrt{35}+8\sqrt{5}-48)(m+\alpha+t)\right] \\
&\quad + \frac{1}{39}(96\sqrt{10}-104\sqrt{5}+156\sqrt{35}+936).
\end{aligned}
\tag{36}
$$

□

The values of calculated topological indices at different levels are given in Table 2.

3. Conclusion

In this paper, we computed first and second reverse Zagreb indices, first and second reverse hyper-Zagreb indices, reverse GA index, reverse atomic bond connectivity index, first and second reverse Zagreb polynomials, and first and second reverse hyper-Zagreb polynomials for the crystallographic structure of molecules [24, 25]. Our results are important to guess the properties [26–28] and study the topology of the crystallographic structure of molecules and can be used in drug delivery [29–31].

Data Availability

All data required for this paper are included within this paper.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

All authors contributed equally to this paper.

Acknowledgments

This research was supported by the Natural Science Fund of Anhui Wenda University of Information Engineering (Grant no. XZR2019A10).

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