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Topological Properties of Crystallographic Structure of Molecules

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Abstract: Chemical graph theory plays an important role in modeling and designing any chemical structure. The molecular topological descriptors are the numerical invariants of a molecular graph and are very useful for predicting their bioactivity. In this paper, we study the chemical graph of the crystal structure of titanium difluoride TiF_2 and the crystallographic structure of cuprite Cu_2O. Furthermore, we compute degree-based topological indices, mainly ABC, GA, ABC_4, GA_5 and general Randić indices. Furthermore, we also give exact results of these indices for the crystal structure of titanium difluoride TiF_2 and the crystallographic structure of cuprite Cu_2O.

Keywords: topological indices; cuprite; atom bond connectivity index; Zagreb indices; geometric arithmetic index; general Randić index; titanium difluoride

1. Introduction

Graph theory is one of the most special and unique branches of mathematics by which the demonstration of any structure is made conceivable. Recently, it has attained much attention among researchers because of its wide range of applications in computer science, electrical networks, interconnected networks, biological networks, chemistry, etc. The chemical graph theory CGT is a fast growing area among researchers. It helps in understanding the structural properties of a molecular graph. There are many chemical compounds that possess a variety of applications in the fields of commercial, industrial, pharmaceutical chemistry and daily life and in the laboratory.

A relationship exists between chemical compounds and their molecular structures. The manipulation and examination of chemical structural information is made conceivable using molecular descriptors. Chemical graph theory is a branch of mathematical chemistry in which the tools of graph theory are applied to model the chemical phenomenon mathematically. Furthermore, it relates to the nontrivial applications of graph theory for solving molecular problems. This theory contributes to a prominent role in the field of chemical sciences; see for details [1–3].

Chem-informatics is a new subject, which is a combination of chemistry, mathematics and information science. It examines the quantitative structure–activity relationship $(QSAR)$ and quantitative structure-property relationship $(QSPR)$, which are utilized to predict the bioactivity and physicochemical properties of chemical compounds [4]. The field of chemical graph theory has attained much attention and consideration among researchers [5,6].

In solid state physics, the electrons of a single, isolated atom occupy atomic orbitals, each of which has a discrete energy level. When two atoms join together to form a molecule, their atomic orbitals overlap [7]. The Pauli exclusion principle dictates that no two electrons can have the same quantum numbers in a molecule. Therefore, if two identical atoms combine to form a diatomic molecule, each atomic orbital splits into two molecular orbitals of different energy, allowing the electrons in the former atomic orbitals to occupy the new orbital structure without any having the same energy. Similarly if a large number N of identical atoms come together to form a solid, such as a crystal lattice, the atoms' atomic orbitals overlap [8]. Since the Pauli exclusion principle dictates that no two electrons in the solid have the same quantum numbers, each atomic orbital splits into N discrete molecular orbitals, each with a different energy.

In chemical graph, the vertices represent atoms, and edges refer to the chemical bonds in the underlying chemical structure. A topological index is a numerical value that is computed mathematically from the molecular graph. It is associated with the chemical constitution indicating the correlation of the chemical structure with many physical, chemical properties and biological activities. The exact formulas of topological indices of certain chemical graphs have been computed and plotted in [9,10].

Let $G = (V, E)$ be a graph where V is the vertex set and E is the edge set of G. The degree $\deg(t)$ (or d_t) of v is the number of edges of G incident with t. The length of the shortest path in a graph G is a distance $d(s,t)$ between s and t. A graph can be represented by a polynomial, a numerical value or by matrix form. There are certain types of topological indices, mainly eccentric-based, degree-based, distance-based indices, etc. In this paper, we deal with degree-based topological indices.

The first and oldest degree-based index was introduced by Milan Randić [11] in 1975 and is defined in the following equation.

$$R_{-\frac{1}{2}}(G) = \sum_{st \in E(G)} \frac{1}{\sqrt{d_s d_t}}$$

In 1988, Bollobás et al. [12] and Amic et al. [13] proposed the general Randić index independently. For more details about the Randić index, its properties and important results, see [14,15]. The general Randić index is defined as:

$$R_\alpha(G) = \sum_{st \in E(G)} (d_s d_t)^\alpha$$

The atom bond connectivity index is of vital importance and was introduced by Estrada et al. [16]. It is defined as:

$$ABC(G) = \sum_{st \in E(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}}$$

The geometric arithmetic index GA of a graph G was introduced by Vukičević et al. [17]. It is defined as:

$$GA(G) = \sum_{st \in E(G)} \frac{2\sqrt{d_s d_t}}{d_s + d_t}$$

The first Zagreb index was introduced in 1972 by [18]. Later on, the second Zagreb index was introduced by [19]. The first and second Zagreb indices are formulated as:

$$M_1(G) = \sum_{st \in E(G)} (d_s + d_t)$$

$$M_2(G) = \sum_{st \in E(G)} (d_s d_t)$$

The fourth version of the atom bond connectivity index ABC_4 of a graph G was introduced by Ghorbhani et al. [20]. It is defined as:

$$ABC_4(G) = \sum_{st \in E(G)} \sqrt{\frac{S_s + S_t - 2}{S_s S_t}}$$

where $S_s = \sum_{st \in E(G)} d_t$ and $S_t = \sum_{st \in E(G)} d_s$.

Another molecular descriptor was the fifth version of the geometric arithmetic index GA_5 of a graph G introduced by Graovac et al. [21]. It is defined as:

$$GA_5(G) = \sum_{st \in E(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t}$$

2. Research Aim

Our aim in this article is to compute the additive topological indices, mainly the atom bond connectivity index, geometric arithmetic index, fourth atom bond connectivity index ABC_4, fifth geometric arithmetic index GA_5 and general Randić index R_α, for $\alpha = \{-1, 1, \frac{1}{2}, -\frac{1}{2}\}$ for $Cu_2O[m,n,t]$ and $TiF_2[m,n,t]$. Moreover, the graphical representation of these exact result is depicted for further explanation of the behavior of these topological indices.

3. Applications of Topological Indices

The atom-bond connectivity (ABC) index provides a very good correlation for the stability of linear alkanes, as well as the branched alkanes and for computing the strain energy of cyclo alkanes [22]. The Randi/'c index is a topological descriptor that has been correlated with many chemical characteristics of molecules and has been found to the parallel to computing the boiling point and Kovats constants of the molecules. To correlate with certain physicochemical properties, the GA index has much better predictive power than the predictive power of the Randić connectivity index [23,24]. The first and second Zagreb index were found to occur for the computation of the total π-electron energy of the molecules within specific approximate expressions [25]. These are among the graph invariants, which were proposed for the measurement of the skeleton of the branching of the carbon-atom [26].

4. Crystallographic Structure of the Molecule Cu_2O

Among various transition metal oxides, Cu_2O has attracted much attention in recent years owing to its distinguished properties and non-toxic nature, low-cost, abundance and simple fabrication process [27]. Nowadays, the promising applications of Cu_2O mainly focus on chemical sensors, solar cells, photocatalysis, lithium-ion batteries and catalysis [28]. The chemical graph of the crystallographic structure of Cu_2O is described in Figures 1 and 2; see details in [29]. Let $G \cong Cu_2O[m,n,t]$ be the chemical graph of Cu_2O with $m \times n$ unit cells in the plane and t layers. We construct this graph first by taking $m \times n$ units in the mn-plane and then storing it up in t layers. The number of vertices and edges of $Cu_2O[m,n,t]$ is $(m+1)(n+1)(t+1) + 5mnt$ and $8mnt$, respectively. In $Cu_2O[m,n,t]$, the number of vertices of degree zero is four; the number of vertices of degree one is $4m + 4n + 4t - 8$; the number of vertices of degree two is $4mnt + 2mn + 2mt + 2nt - 4n - 4m - 4t + 6$; and the number of vertices of degree four is $2nmt - nm - nt - mt + n + m + t - 1$. Furthermore, the edge partition of $Cu_2O[m,n,t]$ based on the degrees of end vertices of each edge is depicted in Table 1.

Table 1. Edge partition of $Cu_2O[m,n,t]$ based on the degrees of end vertices of each edge.

(d_s, d_t)	Frequency	Set of Edges
$(1,2)$	$4n + 4m + 4t - 8$	E_1
$(2,2)$	$4nm + 4nt + 4mt - 8n - 8m - 8t + 12$	E_2
$(2,4)$	$4(2nmt - nm - nt - mt + n + m + t - 1)$	E_3

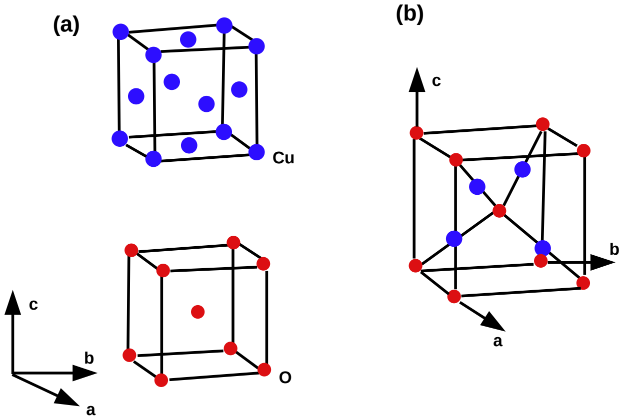

Figure 1. Crystallographic structure of the molecule Cu_2O. (**a**) Structural characteristics of Cu and O atoms in the Cu_2O lattice. The Cu_2O lattice is formed by interpenetrating the Cu and O lattices with each other. (**b**) Unit cell of Cu_2O. Copper atoms are shown as small blue spheres, and oxygen atoms are shown as large red spheres. In the Cu_2O lattice, each Cu atom is coordinated with two O atoms, and each O atom is coordinated with four Cu atoms.

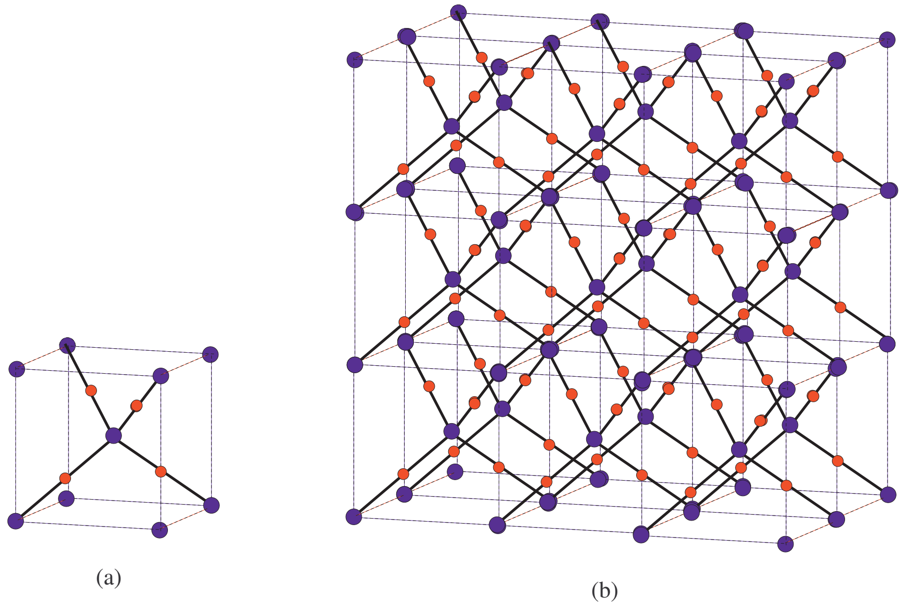

Figure 2. (**a**) Unit cell of $Cu_2O[1,1,1]$ (**b**) Crystallographic structure of $Cu_2O[3,2,3]$.

Theorem 1. *Consider the graph of $G \cong Cu_2O[m,n,t]$ with $m,n,t \geq 1$, then its general Randić index is equal to,*

$$R_\alpha G = \begin{cases} 8\big[8mnt - 2(mn + mt + nt) + m + n + t\big], & \text{if } \alpha = 1, \\ \frac{1}{2}(2mnt + mn + mt + nt + m + n + t - 3), & \text{if } \alpha = -1, \\ 4\big(4\sqrt{2}mnt + 2(1-\sqrt{2})(mn + mt + nt) & \\ +(3\sqrt{2}-4)(m+n+t) - 4\sqrt{2} + 6\big), & \text{if } \alpha = \frac{1}{2}, \\ 2\sqrt{2}mnt + (2-\sqrt{2})(mn + mt + nt) & \\ +(3\sqrt{2}-4)(m+n+t) - 5\sqrt{2} + 6, & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let G be the crystallographic structure of $Cu_2O[m,n,t]$. The general Randić index,

For $\alpha = 1$.

$$\begin{aligned}
R_1(G) &= \sum_{st\in E(G)} (d_s \times d_t) \\
&= \sum_{st\in E_1(G)} (d_s \times d_t) + \sum_{st\in E_2(G)} (d_s \times d_t) + \sum_{st\in E_3(G)} (d_s \times d_t) \\
&= (4m+4n+4t-8)(1\times 2) + (4mn+4mt+4nt-8m-8n-8t+12)(2\times 2) \\
&+ (8mnt-4mn-4mt-4nt+4m+4n+4t-4)(2\times 4) \\
&= 8\big[8mnt - 2(mn+mt+nt) + m+n+t\big]
\end{aligned}$$

For $\alpha = -1$,

$$\begin{aligned}
R_{-1}(G) &= \sum_{st\in E(G)} \frac{1}{(d_s \times d_t)} \\
&= \sum_{st\in E_1(G)} \frac{1}{(d_s \times d_t)} + \sum_{st\in E_2(G)} \frac{1}{(d_s \times d_t)} + \sum_{st\in E_3(G)} \frac{1}{(d_s \times d_t)} \\
&= (4m+4n+4t-8)\frac{1}{(1\times 2)} + (4mn+4mt+4nt-8m-8n-8t+12)\frac{1}{(2\times 2)} \\
&+ (8mnt-4mn-4mt-4nt+4m+4n+4t-4)\frac{1}{(2\times 4)} \\
&= \frac{1}{2}(2mnt+mn+mt+nt+m+n+t-3)
\end{aligned}$$

For $\alpha = \frac{1}{2}$,

$$\begin{aligned}
R_{\frac{1}{2}}(G) &= \sum_{st\in E(G)} \sqrt{(d_s \times d_t)} \\
&= \sum_{st\in E_1(G)} \sqrt{(d_s \times d_t)} + \sum_{st\in E_2(G)} \sqrt{(d_s \times d_t)} + \sum_{st\in E_3(G)} \sqrt{(d_s \times d_t)} \\
&= (4m+4n+4t-8)\sqrt{(1\times 2)} + (4mn+4mt+4nt-8m-8n-8t+12)\sqrt{(2\times 2)} \\
&+ (8mnt-4mn-4mt-4nt+4m+4n+4t-4)\sqrt{(2\times 4)} \\
&= 4\big(4\sqrt{2}mnt + 2(1-\sqrt{2})(mn+mt+nt) + (3\sqrt{2}-4)(m+n+t) - 4\sqrt{2}+6\big)
\end{aligned}$$

For $\alpha = -\frac{1}{2}$,

$$\begin{aligned}
R_{-\frac{1}{2}}(G) &= \sum_{st \in E(G)} \frac{1}{\sqrt{(d_s \times d_t)}} \\
&= \sum_{st \in E_1(G)} \frac{1}{\sqrt{(d_s \times d_t)}} + \sum_{st \in E_2(G)} \frac{1}{\sqrt{(d_s \times d_t)}} + \sum_{st \in E_3(G)} \frac{1}{\sqrt{(d_s \times d_t)}} \\
&= (4m + 4n + 4t - 8)\frac{1}{\sqrt{(1 \times 2)}} + (4mn + 4mt + 4nt - 8m - 8n - 8t + 12)\frac{1}{\sqrt{(2 \times 2)}} \\
&+ (8mnt - 4mn - 4mt - 4nt + 4m + 4n + 4t - 4)\frac{1}{\sqrt{(2 \times 4)}} \\
&= 2\sqrt{2}mnt + (2 - \sqrt{2})(mn + mt + nt) + (3\sqrt{2} - 4)(m + n + t) - 5\sqrt{2} + 6
\end{aligned}$$

□

Theorem 2. *Consider the graph of $G \cong Cu_2O[m, n, t]$ with $m, n, t \geq 1$, then its atom bond connectivity index is equal to,*

$$ABC(G) = 4\sqrt{2}mnt.$$

Proof. Let G be the crystallographic structure of $Cu_2O[m, n, t]$. The result for the atom bond connectivity index is as follows:

$$\begin{aligned}
ABC(G) &= \sum_{st \in E(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}} \\
&= \sum_{st \in E_1(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}} + \sum_{st \in E_2(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}} + \sum_{st \in E_3(G)} \sqrt{\frac{d_s + d_t - 2}{d_s d_t}} \\
&= (4m + 4n + 4t - 8)\sqrt{\frac{1 + 2 - 2}{1 \times 2}} + (4mn + 4mt + 4nt - 8m - 8n - 8t + 12)\sqrt{\frac{2 + 2 - 2}{2 \times 2}} \\
&+ (8mnt - 4mn - 4mt - 4nt + 4m + 4n + 4t - 4)\sqrt{\frac{2 + 4 - 2}{2 \times 4}} \\
&= 4\sqrt{2}mnt.
\end{aligned}$$

□

Theorem 3. *Consider the graph of $G \cong Cu_2O[m, n, t]$ with $m, n, t \geq 1$, then its geometric arithmetic index is equal to,*

$$GA(G) = 4\left[\frac{4\sqrt{2}mnt}{3} - \left(\frac{2\sqrt{2} - 3}{3}\right)(mn + mt + nt - 2m - 2n - 2t) - 2\sqrt{2} + 3\right].$$

Proof. Let G be the crystallographic structure of $Cu_2O[m,n,t]$. The geometric arithmetic index is computed as below:

$$\begin{aligned}
GA(G) &= \sum_{st\in E(G)} \frac{2\sqrt{d_s d_t}}{d_s+d_t} \\
&= \sum_{st\in E_1(G)} \frac{2\sqrt{d_s d_t}}{d_s+d_t} + \sum_{st\in E_2(G)} \frac{2\sqrt{d_s d_t}}{d_s+d_t} + \sum_{st\in E_3(G)} \frac{2\sqrt{d_s d_t}}{d_s+d_t} \\
&= (4m+4n+4t-8)\frac{2\sqrt{1\times 2}}{1+2} + (4mn+4mt+4nt-8m-8n-8t+12)\frac{2\sqrt{2\times 2}}{2+2} \\
&+ (8mnt-4mn-4mt-4nt+4m+4n+4t-4)\frac{2\sqrt{2\times 4}}{2+4} \\
&= 4\left[\frac{4\sqrt{2}mnt}{3} - \Big(\frac{2\sqrt{2}-3}{3}\Big)(mn+mt+nt-2m-2n-2t) - 2\sqrt{2}+3\right]
\end{aligned}$$

□

Theorem 4. *Consider the graph of $G \cong Cu_2O[m,n,t]$ with $m,n,t \geq 1$, then its first and second Zagreb indices are equal to,*

$$\begin{aligned}
M_1(G) &= 4\big(12mnt - 2(mn+mt+nt) + m+n+t\big) \\
M_2(G) &= 8\big(8mnt - 2(mn+mt+nt) + m+n+t\big).
\end{aligned}$$

Proof. Let G be the crystallographic structure of $Cu_2O[m,n,t]$. The first Zagreb index is computed as below:

$$\begin{aligned}
M_1(G) &= \sum_{st\in E(G)} (d_s+d_t) \\
&= \sum_{st\in E_1(G)} (d_s+d_t) + \sum_{st\in E_2(G)} (d_s+d_t) + \sum_{st\in E_3(G)} (d_s+d_t) \\
&= (4m+4n+4t-8)(1+2) + (4mn+4mt+4nt-8m-8n-8t+12)(2+2) \\
&+ (8mnt-4mn-4mt-4nt+4m+4n+4t-4)(2+4) \\
&= 4\big(12mnt - 2(mn+mt+nt) + m+n+t\big)
\end{aligned}$$

The second Zagreb index is computed as below:

$$\begin{aligned}
M_2(G) &= \sum_{st\in E(G)} (d_s d_t) \\
&= \sum_{st\in E_1(G)} (d_s d_t) + \sum_{st\in E_2(G)} (d_s d_t) + \sum_{st\in E_3(G)} (d_s d_t) \\
&= (4m+4n+4t-8)(1\times 2) + (4mn+4mt+4nt-8m-8n-8t+12)(2\times 2) \\
&+ (8mnt-4mn-4mt-4nt+4m+4n+4t-4)(2\times 4) \\
&= 8\big(8mnt - 2(mn+mt+nt) + m+n+t\big)
\end{aligned}$$

□

Table 2 shows the edge partition of the chemical graph $Cu_2O[m,n,t]$ based on the degree sum of end vertices of each edge.

Table 2. Edge partition of $Cu2O[m,n,t]$ with $m,n,t \geq 2$ based on the degree sum of end vertices of each edge.

$(S_s,\ S_t)$	Frequency	Set of Edges
(2, 4)	$4m+4n+4t-8$	E_1
(4, 6)	$4mn+4mt+4nt-8m-8n-8t+12$	E_2
(5, 8)	$4n+4m+4t-8$	E_3
(6, 8)	$4mn+4mt+4nt-8m-8n-8t+12$	E_4
(8, 8)	$8mnt-8mn-8mt-8nt+8m+8n+8t-8$	E_5

Theorem 5. *Consider the graph $G \cong Cu_2O[m,n,t]$ with $m,n,t \geq 2$, then its fourth atom bond connectivity index is equal to,*

$$\begin{aligned} ABC_4(G) &= \sqrt{14}mnt + \Big(\frac{4}{\sqrt{3}} - \sqrt{14} + 2\Big)(mn+mt+nt) - 4\sqrt{2} + 4\sqrt{3} - \sqrt{14} - \frac{2\sqrt{110}}{5} + 6 \\ &+ \Big(2\sqrt{2} - \frac{8}{\sqrt{3}} + \sqrt{14} + \frac{\sqrt{110}}{5} - 4\Big)(m+n+t). \end{aligned}$$

Proof. Let G be the crystallographic structure of $Cu_2O[m,n,t]$. The fourth atom bond connectivity index is computed by using Table 2 in the following equation.

$$\begin{aligned} ABC_4(G) &= \sum_{st \in E(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} \\ &= \sum_{st \in E_1(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st \in E_2(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st \in E_3(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} \\ &+ \sum_{st \in E_4(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st \in E_5(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} \end{aligned}$$

$$\begin{aligned} ABC_4(G) &= (4m+4n+4t-8)\sqrt{\frac{2+4-2}{2\times 4}} + (4mn+4mt+4nt-8m-8n-8t+12)\sqrt{\frac{4+6-2}{4\times 6}} \\ &+ (4m+4n+4t-8)\sqrt{\frac{5+8-2}{5\times 8}} + (4mn+4mt+4nt-8m-8n-8t+12)\sqrt{\frac{6+8-2}{6\times 8}} \\ &+ (8mnt-8mn-8mt-8nt+8m+8n+8t-8)\sqrt{\frac{8+8-2}{8\times 8}} \\ &= \sqrt{14}mnt + \Big(\frac{4}{\sqrt{3}} - \sqrt{14} + 2\Big)(mn+mt+nt) - 4\sqrt{2} + 4\sqrt{3} - \sqrt{14} - \frac{2\sqrt{110}}{5} + 6 \\ &+ \Big(2\sqrt{2} - \frac{8}{\sqrt{3}} + \sqrt{14} + \frac{\sqrt{110}}{5} - 4\Big)(m+n+t) \end{aligned}$$

□

Theorem 6. *Consider the graph $G \cong Cu_2O[m,n,t]$ with $m,n,t \geq 2$, then its fifth geometric arithmetic index is equal to,*

$$
\begin{aligned}
GA_5(G) &= 8mnt + \Big(\frac{16\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} - 8\Big)(mn + mt + nt) - \frac{16\sqrt{2}}{3} + \frac{48\sqrt{3}}{7} + \frac{24\sqrt{6}}{5} - \frac{32\sqrt{10}}{13} - 8 \\
&+ \Big(\frac{8\sqrt{2}}{3} - \frac{32\sqrt{3}}{7} - \frac{16\sqrt{6}}{5} + \frac{16\sqrt{10}}{13} + 8\Big)(m + n + t)
\end{aligned}
$$

Proof. Let G be the crystallographic structure of $Cu_2O[m,n,t]$. The fifth geometric arithmetic index is computed as below:

$$
\begin{aligned}
GA_5(G) &= \sum_{st \in E(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t} \\
&= \sum_{st \in E_1(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t} + \sum_{st \in E_2(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t} + \sum_{st \in E_3(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t} \\
&+ \sum_{st \in E_4(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t} + \sum_{st \in E_5(G)} \frac{2\sqrt{S_s S_t}}{S_s + S_t} \\
&= (4m + 4n + 4t - 8)\frac{2\sqrt{2 \times 4}}{2 + 4} + (4mn + 4mt + 4nt - 8m - 8n - 8t + 12)\frac{2\sqrt{4 \times 6}}{4 + 6} \\
&+ (4m + 4n + 4t - 8)\frac{2\sqrt{5 \times 8}}{5 + 8} + (4mn + 4mt + 4nt - 8m - 8n - 8t + 12)\frac{2\sqrt{6 \times 8}}{6 + 8} \\
&+ (8mnt - 8mn - 8mt - 8nt + 8m + 8n + 8t - 8)\frac{2\sqrt{8 \times 8}}{8 + 8} \\
&= 8mnt + \Big(\frac{16\sqrt{3}}{7} + \frac{8\sqrt{6}}{5} - 8\Big)(mn + mt + nt) - \frac{16\sqrt{2}}{3} + \frac{48\sqrt{3}}{7} + \frac{24\sqrt{6}}{5} - \frac{32\sqrt{10}}{13} - 8 \\
&+ \Big(\frac{8\sqrt{2}}{3} - \frac{32\sqrt{3}}{7} - \frac{16\sqrt{6}}{5} + \frac{16\sqrt{10}}{13} + 8\Big)(m + n + t)
\end{aligned}
$$

□

5. Crystal Structure of Titanium Difluoride

Titanium difluoride is a water-insoluble titanium source for use in oxygen-sensitive applications, such as metal production. Fluoride compounds have diverse applications in current technologies and science, from oil refining and etching to synthetic organic chemistry and the manufacture of pharmaceuticals. The chemical graph of the crystal structure of titanium difluoride $TiF_2[m,n,t]$ is described in Figure 3; for more details, see [30]. Let $G \cong TiF_2[m,n,t]$ be the chemical graph of TiF_2 with $m \times n$ unit cells in the plane and t layers. We construct this graph first by taking $m \times n$ units in the $mn-$plane and then storing it up in t layers. The number of vertices and edges of $TiF_2[m,n,t]$ is $12mnt + 2mn + 2mt + 2nt + m + n + t + 1$ and $32mnt$, respectively.In $TiF_2[m,n,t]$, the number of vertices of degree one is eight; the number of vertices of degree two is $4m + 4n + 4t - 12$; the number of vertices of degree four is $8mnt + 4mn + 4mt + 4nt - 4n - 4m - 4t + 6$; and the number of vertices of degree eight is $4mnt - 2(mn + mt + nt) + m + n + t - 1$. The edge partition of $TiF_2[m,n,t]$ based on the degrees of end vertices of each edge is depicted in Table 3.

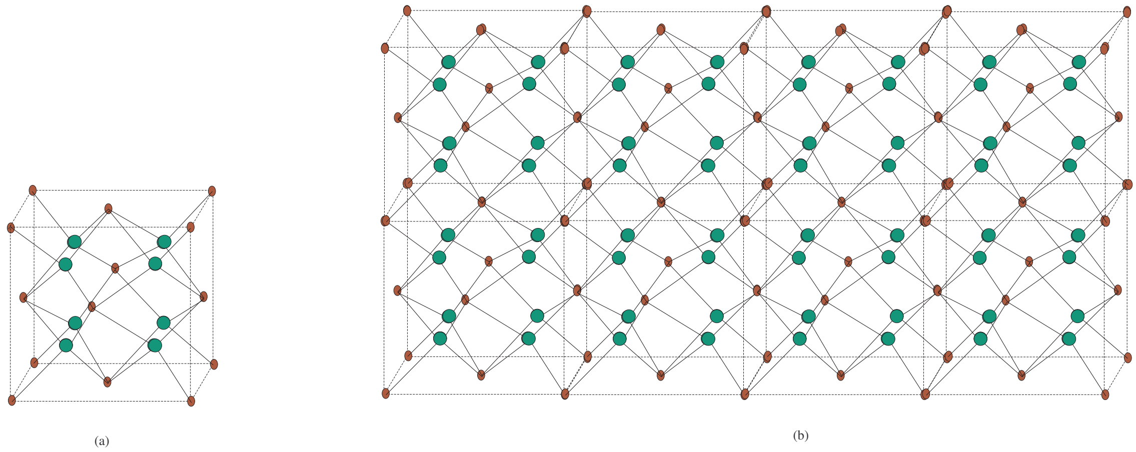

Figure 3. (**a**)The unit cell of of $TiF_2[m, n, t]$ with Ti atoms in red and F atoms in green; (**b**) the crystal structure of $TiF_2[4, 1, 2]$.

Table 3. Edge partition of $TiF_2[m, n, t]$ based on the degrees of end vertices of each edge.

$(d_s,\ d_t)$	Frequency	Set of Edges
(1, 4)	8	E_1
(2, 4)	$8(m+n+t-3)$	E_2
(4, 4)	$16(mn+mt+nt)-16(m+n+t)+24$	E_3
(4, 8)	$32mnt-16(mt+mn+nt)+8(m+n+t)-8$	E_4

Theorem 7. *Consider the graph $G \cong TiF_2[m, n, t]$ with $m, n, t \geq 1$, then its general Randić index is equal to,*

$$R_\alpha G = \begin{cases} 32\big[32mnt - 8(mn+mt+nt) + 2(m+n+t) - 1\big], & \text{if } \alpha = 1, \\ \frac{1}{4}(4mnt + 2(mn+mt+nt) + m+n+t+1), & \text{if } \alpha = -1, \\ 16\big(8\sqrt{2}mnt + 4(1-\sqrt{2})(mn+mt+nt) & \\ +(3\sqrt{2}-4)(m+n+t) - 5\sqrt{2} + 7\big), & \text{if } \alpha = \frac{1}{2}, \\ 4\sqrt{2}mnt + 2(2-\sqrt{2})(mn+mt+nt) & \\ +(3\sqrt{2}-4)(m+n+t) - 7\sqrt{2} + 10, & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Let $G \cong TiF_2[m, n, t]$ be the crystal structure of titanium difluoride. The general Randić index,

For $\alpha = 1$.

$$\begin{aligned} R_1(G) &= \sum_{st \in E(G)} (d_s \times d_t) \\ &= \sum_{st \in E_1(G)} (d_s \times d_t) + \sum_{st \in E_2(G)} (d_s \times d_t) + \sum_{st \in E_3(G)} (d_s \times d_t) + \sum_{st \in E_4(G)} (d_s \times d_t) \\ &= (8)(1 \times 4) + (8m + 8n + 8t - 24)(2 \times 4) \\ &+ \big(16(mn+mt+nt) - 16(m+n+t) + 24\big)(4 \times 4) \\ &+ \big(32mnt - 16(mn+mt+nt) + 8(m+n+t) - 8\big)(4 \times 8) \\ &= 32\big[32mnt - 8(mn+mt+nt) + 2(m+n+t) - 1\big] \end{aligned}$$

For $\alpha = -1$,

$$R_{-1}(G) = \sum_{st\in E(G)} \frac{1}{(d_s \times d_t)}$$
$$= \sum_{st\in E_1(G)} \frac{1}{(d_s \times d_t)} + \sum_{st\in E_2(G)} \frac{1}{(d_s \times d_t)} + \sum_{st\in E_3(G)} \frac{1}{(d_s \times d_t)} + \sum_{st\in E_4(G)} \frac{1}{(d_s \times d_t)}$$

$$\begin{aligned} R_{-1}(G) &= (8)\frac{1}{(1\times 4)} + (8m+8n+8t-24)\frac{1}{(2\times 4)} \\ &+ \big(16(mn+mt+nt) - 16(m+n+t) + 24\big)\frac{1}{(4\times 4)} \\ &+ \big(32mnt - 16(mn+mt+nt) + 8(m+n+t) - 8\big)\frac{1}{(4\times 8)} \\ &= \frac{1}{4}(4mnt + 2(mn+mt+nt) + m+n+t+1) \end{aligned}$$

For $\alpha = \frac{1}{2}$,

$$\begin{aligned} R_{\frac{1}{2}}(G) &= \sum_{st\in E(G)} \sqrt{(d_s \times d_t)} \\ &= \sum_{st\in E_1(G)} \sqrt{(d_s \times d_t)} + \sum_{st\in E_2(G)} \sqrt{(d_s \times d_t)} + \sum_{st\in E_3(G)} \sqrt{(d_s \times d_t)} + \sum_{st\in E_4(G)} \sqrt{(d_s \times d_t)} \\ &= (8)\sqrt{(1\times 4)} + (8m+8n+8t-24)\sqrt{(2\times 4)} \\ &+ \big(16(mn+mt+nt) - 16(m+n+t) + 24\big)\sqrt{(4\times 4)} \\ &+ \big(32mnt - 16(mn+mt+nt) + 8(m+n+t) - 8\big)\sqrt{(4\times 8)} \\ &= 16\big(8\sqrt{2}mnt + 4(1-\sqrt{2})(mn+mt+nt) + (3\sqrt{2}-4)(m+n+t) - 5\sqrt{2} + 7\big) \end{aligned}$$

For $\alpha = -\frac{1}{2}$,

$$\begin{aligned} R_{-\frac{1}{2}}(G) &= \sum_{st\in E(G)} \frac{1}{\sqrt{(d_s \times d_t)}} \\ &= \sum_{st\in E_1(G)} \frac{1}{\sqrt{(d_s \times d_t)}} + \sum_{st\in E_2(G)} \frac{1}{\sqrt{(d_s \times d_t)}} + \sum_{st\in E_3(G)} \frac{1}{\sqrt{(d_s \times d_t)}} + \sum_{st\in E_4(G)} \frac{1}{\sqrt{(d_s \times d_t)}} \\ &= (8)\frac{1}{\sqrt{(1\times 4)}} + (8m+8n+8t-24)\frac{1}{\sqrt{(2\times 4)}} \\ &+ \big(16(mn+mt+nt) - 16(m+n+t) + 24\big)\frac{1}{\sqrt{(4\times 4)}} \\ &+ \big(32mnt - 16(mn+mt+nt) + 8(m+n+t) - 8\big)\frac{1}{\sqrt{(4\times 8)}} \\ &= 4\sqrt{2}mnt + 2(2-\sqrt{2})(mn+mt+nt) + (3\sqrt{2}-4)(m+n+t) - 7\sqrt{2} + 10 \end{aligned}$$

□

Theorem 8. *Consider the graph $G \cong TiF_2[m,n,t]$ with $m,n,t \geq 1$, then its atom bond connectivity index is equal to,*

$$\begin{aligned} ABC(G) &= 2\big[4\sqrt{5}mnt - 2(\sqrt{5}-\sqrt{6})(mn+mt+nt) + (2\sqrt{2}+\sqrt{5}-2\sqrt{6})(m+n+t)\big] \\ &+ 2\big[-6\sqrt{2}+2\sqrt{3}-\sqrt{5}+3\sqrt{6}\big] \end{aligned}$$

Proof. Let $G \cong TiF_2[m,n,t]$ be the crystal structure of titanium difluoride. The atom bond connectivity index can be calculated by using Table 3 in the following equation.

$$\begin{aligned} ABC(G) &= \textstyle\sum_{st\in E(G)} \sqrt{\frac{d_s+d_t-2}{d_sd_t}} \\ &= \textstyle\sum_{st\in E_1(G)} \sqrt{\frac{d_s+d_t-2}{d_sd_t}} + \sum_{st\in E_2(G)} \sqrt{\frac{d_s+d_t-2}{d_sd_t}} + \sum_{st\in E_3(G)} \sqrt{\frac{d_s+d_t-2}{d_sd_t}} + \sum_{st\in E_4(G)} \sqrt{\frac{d_s+d_t-2}{d_sd_t}} \\ &= (8)\sqrt{\tfrac{1+4-2}{1\times 4}} + (8m+8n+8t-24)\sqrt{\tfrac{2+4-2}{2\times 4}} \\ &+ \big(16(mn+mt+nt)-16(m+n+t)+24\big)\sqrt{\tfrac{4+4-2}{4\times 4}} \\ &+ \big(32mnt-16(mn+mt+nt)+8(m+n+t)-8\big)\sqrt{\tfrac{4+8-2}{4\times 8}} \\ &= 2\big[4\sqrt{5}mnt - 2(\sqrt{5}-\sqrt{6})(mn+mt+nt) + (2\sqrt{2}+\sqrt{5}-2\sqrt{6})(m+n+t)\big] \\ &+ 2\big[-6\sqrt{2}+2\sqrt{3}-\sqrt{5}+3\sqrt{6}\big] \end{aligned}$$

□

Theorem 9. *Consider the graph $G \cong TiF_2[m,n,t]$ with $m,n,t \geq 1$, then its geometric arithmetic index is equal to,*

$$GA(G) = 8\Big[\frac{8\sqrt{2}(mnt-1)}{3} - \big(\frac{4\sqrt{2}}{3}-2\big)(mn+mt+nt-m-n-t) + \frac{19}{5}\Big]$$

Proof. Let $G \cong TiF_2[m,n,t]$ be the crystal structure of titanium difluoride. The geometric arithmetic index is computed as below:

$$\begin{aligned} GA(G) &= \sum_{st\in E(G)} \frac{2\sqrt{d_sd_t}}{d_s+d_t} \\ &= \sum_{st\in E_1(G)} \frac{2\sqrt{d_sd_t}}{d_s+d_t} + \sum_{st\in E_2(G)} \frac{2\sqrt{d_sd_t}}{d_s+d_t} + \sum_{st\in E_3(G)} \frac{2\sqrt{d_sd_t}}{d_s+d_t} + \sum_{st\in E_4(G)} \frac{2\sqrt{d_sd_t}}{d_s+d_t} \\ &= (8)\frac{2\sqrt{1\times 4}}{1+4} + (8m+8n+8t-24)\frac{2\sqrt{2\times 4}}{2+4} \\ &+ \big(16(mn+mt+nt)-16(m+n+t)+24\big)\frac{2\sqrt{4\times 4}}{4+4} \\ &+ \big(32mnt-16(mn+mt+nt)+8(m+n+t)-8\big)\frac{2\sqrt{4\times 8}}{4+8} \\ &= 8\Big[\frac{8\sqrt{2}(mnt-1)}{3} - \big(\frac{4\sqrt{2}}{3}-2\big)(mn+mt+nt-m-n-t) + \frac{19}{5}\Big] \end{aligned}$$

□

Theorem 10. *Consider the graph $G \cong TiF_2[m,n,t]$ with $m,n,t \geq 1$, then its first and second Zagreb indices are equal to,*

$$M_1(G) = 8\big[48mnt - 8(mn+mt+nt) + 2(m+n+t) - 1\big],$$
$$M_2(G) = 32\big[32mnt - 8(mn+mt+nt) + 2(m+n+t) - 1\big].$$

Proof. Let $G \cong TiF_2[m,n,t]$ be the crystal structure of titanium difluoride. The first and second Zagreb indices are computed as below:

$$\begin{aligned}
M_1(G) &= \textstyle\sum_{st\in E(G)}(d_s+d_t) \\
&= \textstyle\sum_{st\in E_1(G)}(d_s+d_t) + \sum_{st\in E_2(G)}(d_s+d_t) + \sum_{st\in E_3(G)}(d_s+d_t) + \sum_{st\in E_4(G)}(d_s+d_t) \\
&= (8)(1+4) + (8m+8n+8t-24)(2+4) + \big(16(mn+mt+nt) - 16(m+n+t) + 24\big)(4+4) \\
&+ \big(32mnt - 16(mn+mt+nt) + 8(m+n+t) - 8\big)(4+8) \\
&= 8\big(48mnt - 8(mn+mt+nt) + 2(m+n+t) - 1\big)
\end{aligned}$$

$$\begin{aligned}
M_2(G) &= \textstyle\sum_{st\in E(G)}(d_sd_t) \\
&= \textstyle\sum_{st\in E_1(G)}(d_sd_t) + \sum_{st\in E_2(G)}(d_sd_t) + \sum_{st\in E_3(G)}(d_sd_t) + \sum_{st\in E_4(G)}(d_sd_t) \\
&= (8)(1\times 4) + (8m+8n+8t-24)(2\times 4) + \big(16(mn+mt+nt) - 16(m+n+t) + 24\big)(4\times 4) \\
&+ \big(32mnt - 16(mn+mt+nt) + 8(m+n+t) - 8\big)(4\times 8) \\
&= 32\big[32mnt - 8(mn+mt+nt) + 2(m+n+t) - 1\big]
\end{aligned}$$

□

Table 4 shows the edge partition of the chemical graph $TiF_2[m,n,t]$ based on the degree sum of the end vertices of each edge.

Table 4. Edge partition of $TiF_2[m,n,t]$, $m,n,s \geq 2$ based on the degree sum of the end vertices of each edge.

$(S_s,\ S_t)$	Frequency	Set of Edges
(4, 13)	8	E_1
(8, 18)	$8(m+n+t-3)$	E_2
(13, 16)	16	E_3
(16, 18)	$16(mn+mt+nt) - 16(m+n+t) + 8$	E_4
(16, 24)	$32mnt - 16(mn+mt+nt) + 8$	E_5
(18, 32)	$8(m+n+t-2)$	E_6

Theorem 11. *Consider the graph $G \cong TiF_2[m,n,t]$ with $m,n,t > 1$, then its fourth atom bond connectivity index is equal to,*

$$\begin{aligned}
ABC_4(G) &= \frac{4\sqrt{57}mnt}{3} - \Big(\frac{2\sqrt{57}}{3} - \frac{16}{3}\Big)(mn+mt+nt) + \Big(\frac{4}{\sqrt{3}} + \frac{4\sqrt{6}}{3} - \frac{16}{3}\Big)(m+n+t) \\
&- 4\sqrt{6} - \frac{8}{\sqrt{3}} + \frac{12\sqrt{39}}{13} + \frac{\sqrt{57}}{3} + \frac{4\sqrt{195}}{13} + \frac{8}{3}
\end{aligned}$$

Proof. Let $G \cong TiF_2[m,n,t]$ be the crystal structure of titanium difluoride. The fourth atom bond connectivity index is computed as below:

$$\begin{aligned}
ABC_4(G) &= \sum_{st\in E(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} \\
&= \sum_{st\in E_1(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st\in E_2(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st\in E_3(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} \\
&+ \sum_{st\in E_4(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st\in E_5(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}} + \sum_{st\in E_6(G)} \sqrt{\frac{S_s+S_t-2}{S_sS_t}}
\end{aligned}$$

$$\begin{aligned}
ABC_4(G) &= (8)\sqrt{\frac{4+13-2}{4\times 13}} + (8m+8n+8t-24)\sqrt{\frac{8+18-2}{8\times 18}} + (16)\sqrt{\frac{13+16-2}{13\times 16}} \\
&+ \big(16(mn+mt+nt)-16(m+n+t)+8\big)\sqrt{\frac{16+18-2}{16\times 18}} \\
&+ \big(32mnt-16(mn+mt+nt)+8\big)\sqrt{\frac{16+24-2}{16\times 24}} + (8m+8n+8t-16)\sqrt{\frac{18+32-2}{18\times 32}} \\
&= \frac{4\sqrt{57}mnt}{3} - \Big(\frac{2\sqrt{57}}{3} - \frac{16}{3}\Big)(mn+mt+nt) + \Big(\frac{4}{\sqrt{3}} + \frac{4\sqrt{6}}{3} - \frac{16}{3}\Big)(m+n+t) \\
&- 4\sqrt{6} - \frac{8}{\sqrt{3}} + \frac{12\sqrt{39}}{13} + \frac{\sqrt{57}}{3} + \frac{4\sqrt{195}}{13} + \frac{8}{3}
\end{aligned}$$

□

Theorem 12. *Consider the graph $G \cong TiF_2[m,n,t]$ with $m,n,t \geq 2$, then its fifth geometric arithmetic index is equal to,*

$$\begin{aligned}
GA_5(G) &= \frac{64\sqrt{6}mnt}{5} + \Big(\frac{192\sqrt{2}}{17} - \frac{32\sqrt{6}}{5}\Big)(mn+mt+nt) - \Big(\frac{192\sqrt{2}}{17} - \frac{4896}{325}\Big)(m+n+t) \\
&+ \frac{96\sqrt{2}}{17} + \frac{16\sqrt{6}}{5} + \frac{3104\sqrt{13}}{493} - \frac{12192}{325}
\end{aligned}$$

Proof. Let $G \cong TiF_2[m,n,t]$ be the crystal structure of titanium difluoride. The fifth geometric arithmetic index is computed as below:

$$
\begin{aligned}
GA_5(G) &= \sum_{st\in E(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} \\
&= \sum_{st\in E_1(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} + \sum_{st\in E_2(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} + \sum_{st\in E_3(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} \\
&+ \sum_{st\in E_4(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} + \sum_{st\in E_5(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} + \sum_{st\in E_6(G)} \frac{2\sqrt{S_sS_t}}{S_s+S_t} \\
&= (8)\frac{2\sqrt{4\times 13}}{4+13} + (8m+8n+8t-24)\frac{2\sqrt{8\times 18}}{8+18} + (16)\frac{2\sqrt{13\times 16}}{13+16} \\
&+ \big(16(mn+mt+nt)-16(m+n+t)+8\big)\frac{2\sqrt{16\times 18}}{16+18} \\
&+ \big(32mnt-16(mn+mt+nt)+8\big)\frac{2\sqrt{16\times 24}}{16+24} + (8m+8n+8t-16)\frac{2\sqrt{18\times 32}}{18+32} \\
&= \frac{64\sqrt{6}mnt}{5} + \Big(\frac{192\sqrt{2}}{17} - \frac{32\sqrt{6}}{5}\Big)(mn+mt+nt) - \Big(\frac{192\sqrt{2}}{17} - \frac{4896}{325}\Big)(m+n+t) \\
&+ \frac{96\sqrt{2}}{17} + \frac{16\sqrt{6}}{5} + \frac{3104\sqrt{13}}{493} - \frac{12192}{325}
\end{aligned}
$$

□

6. Discussion

Since the topological indices have many applications in different branches of science, namely pharmaceutical, chemistry and biological drugs, the graphical representation of these calculated results is helpful to scientists. The graphical representations of topological indices for $Cu_2O[m,n,t]$ are depicted for Randić indices in Figures 4 and 5. The atomic bond connectivity index and geometric arithmetic index for $Cu_2O[m,n,t]$ are depicted in Figure 6. The first and second Zagreb indices for $Cu_2O[m,n,t]$ are depicted in Figure 7. The fourth atomic bond connectivity index and the fifth geometric arithmetic index for $Cu_2O[m,n,t]$ are depicted in Figure 8.

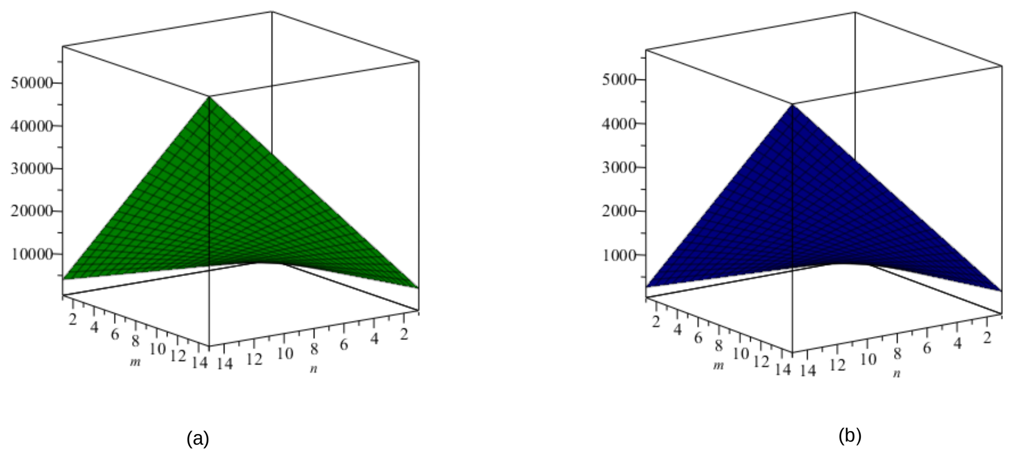

Figure 4. The graphical representation of the Randić index for (**a**) $\alpha = 1$ and (**b**) for $\alpha = -1$.

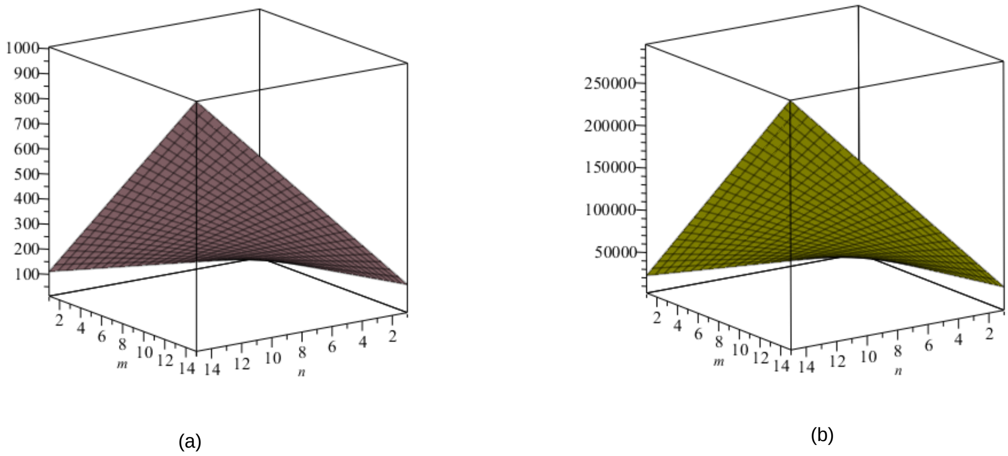

Figure 5. The graphical representation of the Randić index for (**a**) $\alpha = \frac{1}{2}$ and (**b**) for $\alpha = \frac{-1}{2}$.

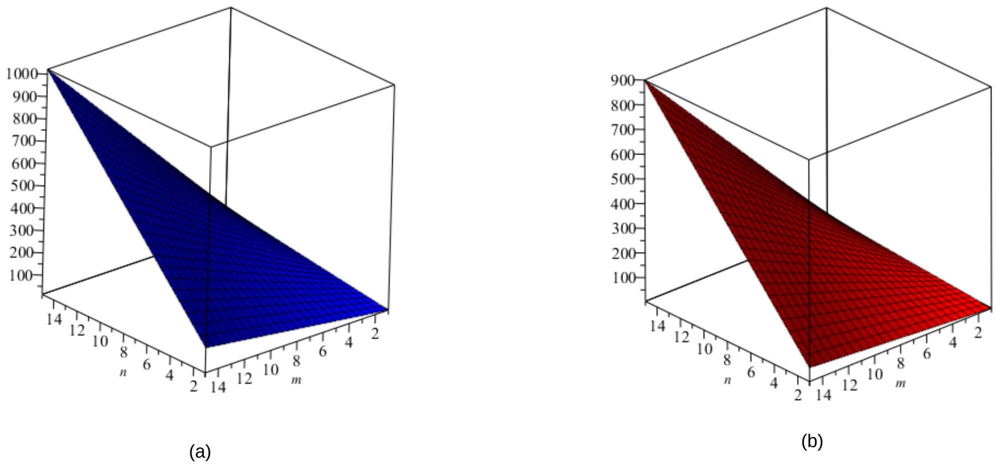

Figure 6. The graphical representation of the (**a**) ABC index and (**b**) GA index.

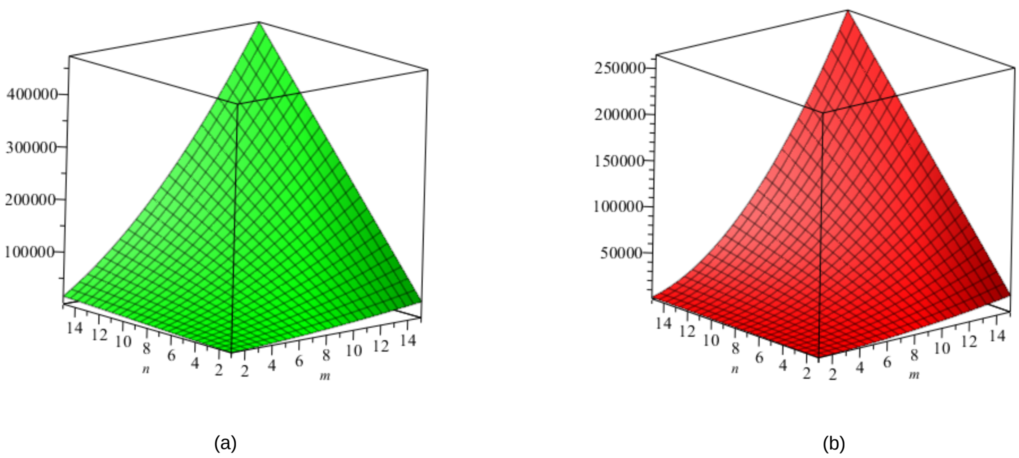

Figure 7. The graphical representation of the (**a**) first Zagreb index and (**b**) second Zagreb index.

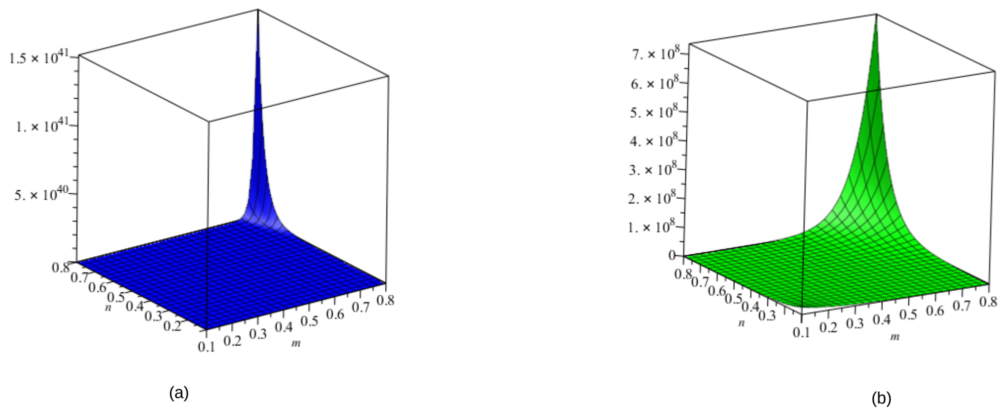

Figure 8. The graphical representation of the (**a**) ABC_4 index and (**b**) GA_5 index.

The graphical representations of topological indices for titanium difluoride TiF_2 are depicted for Randić indices in Figures 9 and 10. The atomic bond connectivity index and geometric arithmetic index for titanium difluoride TiF_2 are depicted in Figure 11. The first and second Zagreb indices for titanium difluoride TiF_2 are depicted in Figure 12. The fourth atomic bond connectivity index and the fifth geometric arithmetic index for titanium difluoride TiF_2 are depicted in Figure 13.

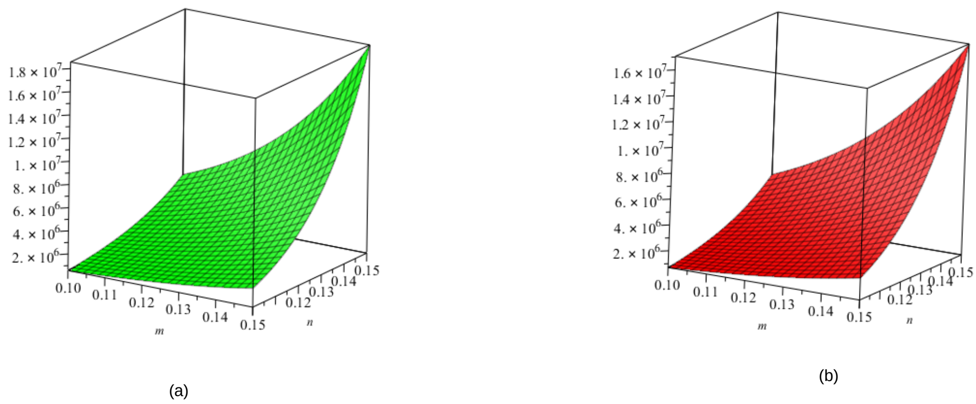

Figure 9. The graphical representation of the Randić index for (**a**) $\alpha = 1$ and (**b**) for $\alpha = -1$.

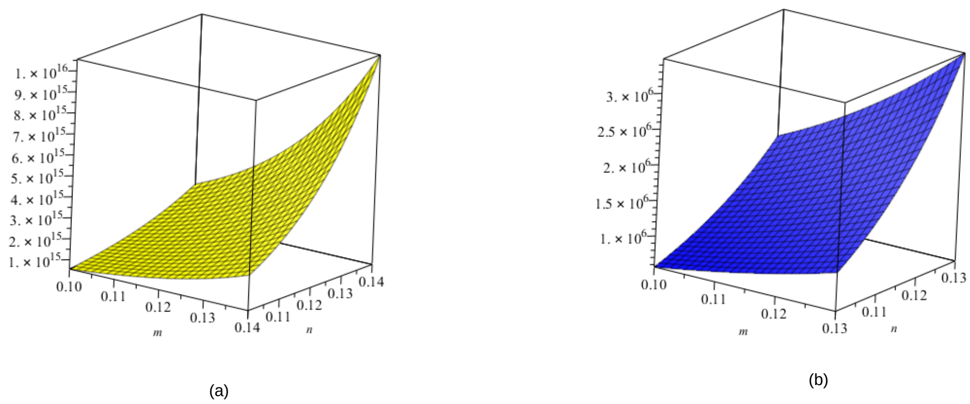

Figure 10. The graphical representation of the Randić index for (**a**) $\alpha = \frac{1}{2}$ and (**b**) for $\alpha = \frac{-1}{2}$.

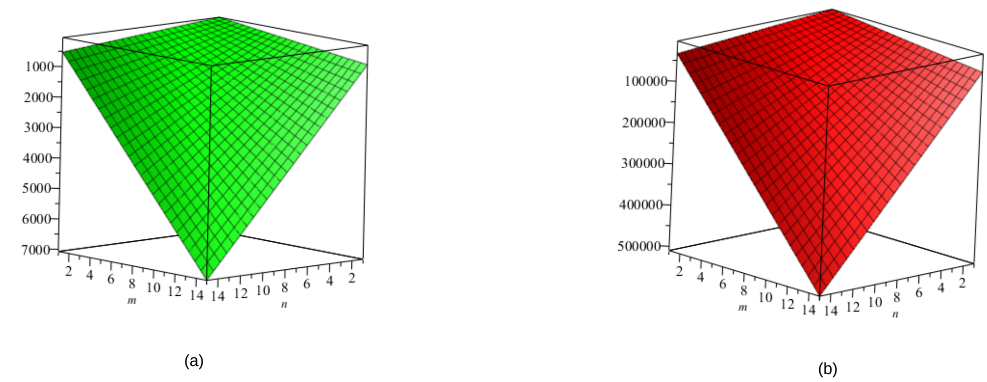

Figure 11. The graphical representation of the (**a**) ABC index and (**b**) GA index.

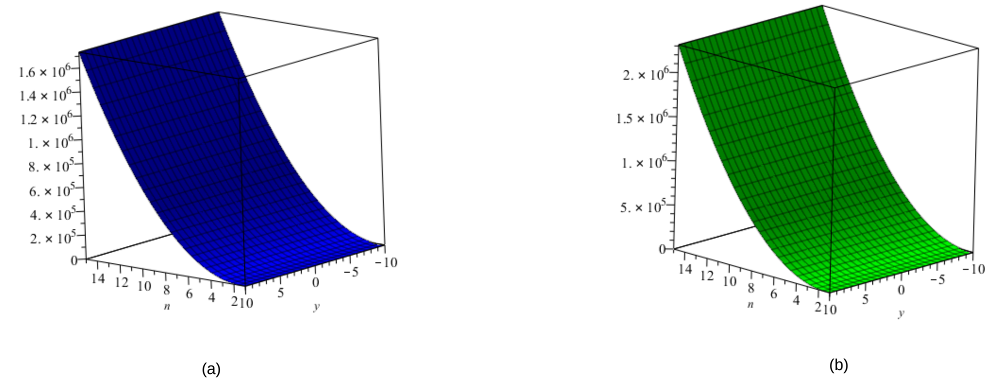

Figure 12. The graphical representation of the (**a**) first Zagreb index and (**b**) second Zagreb index.

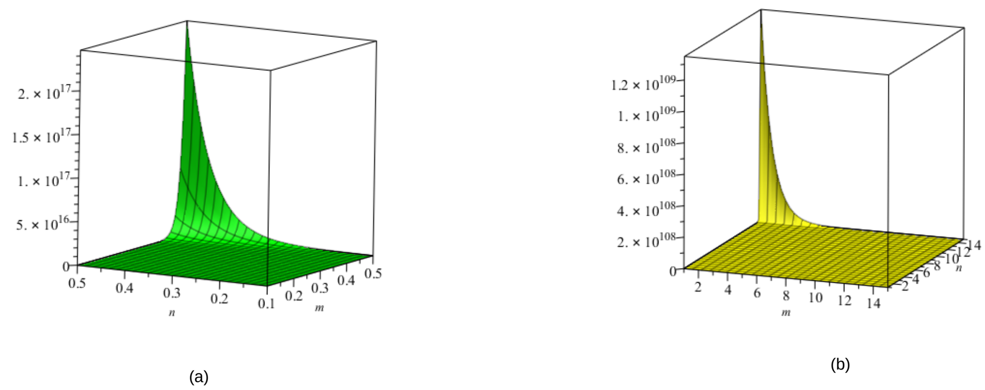

Figure 13. The graphical representation of the (**a**) ABC_4 index and (**b**) GA_5 index.

7. Conclusions

In this paper, we have computed some degree-based topological indices, namely the atom bond connectivity index ABC, the geometric arithmetic index GA, the general Randić index, the GA_5 index, the ABC_4 index and the first and second Zagreb indices for the chemical graph of the crystal structure of titanium difluoride TiF_2 and crystallographic structure of cuprite Cu_2O.

In the future, we are interested in computing the distance-based and counting-related topological indices for these structures.

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Conflicts of Interest: The authors declare no conflict of interest.

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