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COMPUTING TOPOLOGICAL INDICES OF CRYSTALLOGRAPHIC STRUCTURES

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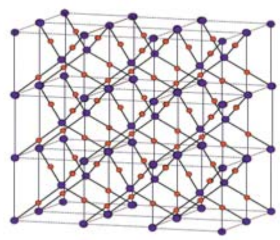
Graph theory plays a vital role in modeling and designing any chemical structure or chemical network. Chemical graph theory helps in understanding about the molecular structural properties of a molecular graph. The molecular graph is a graph consists of atoms called vertices and the chemical bond between atoms called edges. A molecular descriptors (topological index) is a numeric amount related with a graph which describes the topology of the graph and is invariant under graph automorphism. In this article, we study the chemical graphs of Titanium Difluoride TiF_2 and Crystallographic Structure of Cu_2O. Moreover, we compute and give closed formulas of degree based additive molecular descriptors (topological indices).



INTRODUCTION

Graph theory contributes a prominent role in the field of chemical sciences. This theory is proficient for modeling and designing of chemical structures and complex networks. The manipulation and examination of chemical structural information is made conceivable by using molecular descriptors. The chemical graph theory applies graph theory to mathematical modeling of molecular phenomena, which is helpful for the study of molecular structure. Chemical compounds have a variety of applications in chemical graph theory, drug design, etc. A great variety of topological indices are studied and used in theoretical chemistry, pharmaceutical researchers see.[1–3]

A chemical structure can be represented by using graph theory, where vertices denotes atoms and edges denotes molecular bond. A topological index is a numeric number which indicates some useful information about molecular structure. It is the numerical invariants of a molecular graph and are useful to correlate with their bioactivity and physio-chemical properties. Researchers have found topological index to be powerful and useful tool in the description of molecular structure. Some applications related to topological indices of molecular graphs are given in.[4,5]

There are certain chemical compounds that are useful for the survival of living things. Carbon, oxygen, hydrogen and nitrogen are the main elements that helps in the production of cells in the living things. Carbon is an essential element for human life. It is useful in the formation of proteins, carbohydrates and nucleic acids. It is vital for the growth of plants in the form of carbon dioxide. The carbon atoms can bond together in various ways, called allotropes of carbon. The well known forms are graphite and diamond. Recently, many new forms have been discovered including nanotubes, buckminster fullerene and sheets, crystal cubic structure.[6,7]

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A topological index is a numeric amount related with a graph which describes the topology of the graph and is invariant under graph automorphism. There are some real classes of topological indices, for example, distance based topological indices, degree based topological indices and numbering related polynomials and indices of graphs. The idea of topological indices introduced by Wiener.[8] The Wiener index is the first and most concentrated topological index, both from theoretical perspective and applications see.[9]

The most seasoned topological index which was presented by I. Gutman and N. Trinajstic is the first Zagreb index, in light of degree of vertices of G in.[10] Taken after by the first and second Zagreb indices, B. Furtula and I. Gutman[11] presented Forgotten topological indices which was characterized as:

$$F(G) = \sum_{pq \in E(G)} (\xi_p{}^2 + \xi_q{}^2) \qquad (1)$$

In 2015, Gutman *et. al.* argue that the prescient capacity, acentric factor and entropy of Forgotten Topological index is practically like that of first Zagreb index, and the correlation coefficients between these two is bigger than 0.95. In 2014, Sunet *et.al.* found some essential type of forgotten topological index and announced that such index can fortify the physico-chemical flexibility of Zagreb indices. Recently, Gao *et al.*[12] showed the forgotten topological index of some noteworthy medication atomic structures.

Spurred by the achievement of the ABC index, Furtula *et.al.,*[13] set forth its changed adaptation and they named it "Augmented Zagreb index" and is characterized as:

$$AZI(G) = \sum_{pq \in E(G)} \left(\frac{\xi_p \times \xi_q}{\xi_p + \xi_q - 2}\right)^3 \qquad (2)$$

Another topological index based on the vertex degree is the Balaban index.[14,15] This index for a graph G of order n, size m is defined as:

$$J(G) = \frac{m}{m-n+2} \sum_{pq \in E(G)} \frac{1}{\sqrt{\xi_p \times \xi_q}} \qquad (3)$$

where ξ_p, ξ_q are the degrees of the vertices $p, q \in V(G)$ The redefined version of the Zagreb indices were defined by Ranjini *et al.*,[16] namely, the redefined first, second and third Zagreb indices for a graph G as;

$$ReZG_1(G) = \sum_{pq \in E(G)} \frac{\xi_p + \xi_q}{\xi_p \times \xi_q} \qquad (4)$$

$$ReZG_2(G) = \sum_{pq \in E(G)} \frac{\xi_p \times \xi_q}{\xi_p + \xi_q} \qquad (5)$$

$$ReZG_3(G) = \sum_{pq \in E(G)} (\xi_p \times \xi_q)(\xi_p + \xi_q) \qquad (6)$$

For further study of topological indices of various graph families.[17–25]

Crystallographic structure of Cu_2O

Among different transition metal oxides, Cu_2O has pulled in extensive consideration as of late attributable to its recognized properties and non-toxic nature, minimal effort, plenitude, and basic creation process. These days, the promising uses of Cu_2O chiefly concentrate on chemical sensors, solar oriented cells, photocatalysis, lithium-particle batteries and catalysis. The chemical graph of Crystallographic structure of Cu_2O described in Figure 1 and Figure 2, for more information about this structure see.[11-24] 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 $m \times n$ unites in the mn −plane and then storing it up in t layers. The number of vertices and edges of $Cu_2O[m, n, t]$ are $(m + 1)(n + 1)(t + 1) + 5mnt$ and $8mnt$, respectively. In $Cu_2O[m, n, t]$ the number zero degree vertices is 4, the number of one degree vertices is $4m + 4n + 4t - 8$, the number of two degree vertices is $4mnt + 2mn + 2mt + 2nt - 4n - 4m - 4t + 6$ and the number of four degree vertices is $2nmt - nm - nt - mt + n + m + t - 1$.

Main Results for Crystallographic structure of Cu_2O

In this section, we compute the general result of topological indices for Crystallographic structure of Cu_2O. More preciously, we computed additive topological indices namely Forgotten index, Augmented index, Balaban index and Re-defined Zagreb indices for $Cu_2O[m, n. t]$. In addition, we give graphical comparison and application of these indices.

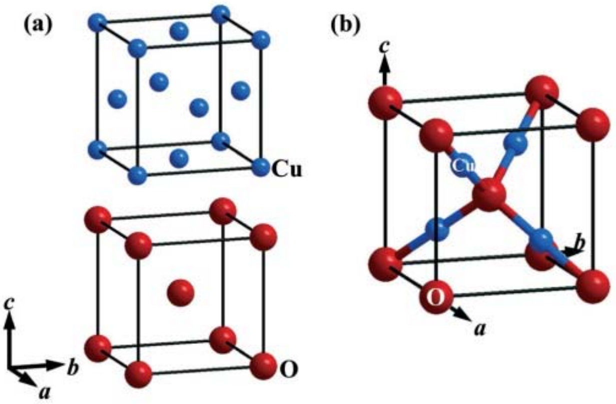

Fig. 1 – Crystallographic structure of Cu_2O. (a) In lattice of Cu_2O the structural characteristics of the atoms of Cu and O. The lattice of Cu_2O is formed by interpenetrating the lattices of Cu and O into each other. (b) Unit cell of Cu_2O, where copper and oxygen atoms are shown in small blue and in large red spheres."

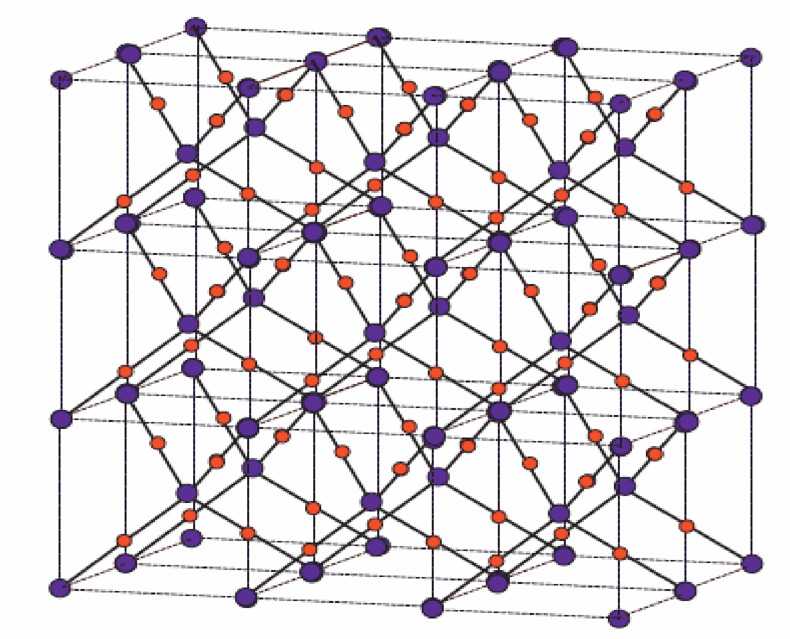

Fig. 2 – Crystallographic structure of Cu_2O [3,2,3]

Table 1

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

(ξ_p, ξ_q)	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

• **Forgotten index $F(Cu_2O[m,n,t])$**

Let G be the graph of carbon graphite $Cu_2O[m,n,t]$. Now by using equation (1) together with Table 1 we have:

$$F(G) = \sum_{pq \in E(G)} (\xi_p{}^2 + \xi_q{}^2)$$

$$F(Cu_2O[m,n,t]) = \sum_{pq\in E_1}[\xi_p{}^2+\xi_q{}^2]+\sum_{pq\in E_2}[\xi_p{}^2+\xi_q{}^2]+\sum_{pq\in E_3}[\xi_p{}^2+\xi_q{}^2]$$
$$= 5|E_1(Cu_2O[m,n,t])| + 8|E_2(Cu_2O[m,n,t])|$$
$$+20|E_3(Cu_2O[m,n,t])|$$
$$= 5(4n+4m+4t-8)+8(4nm+4nt+4mt-8n-8m-8t+12)$$
$$+20(4(2nmt-nm-nt-mt+n+m+t-1))$$
$$= 36n+36m+36t-24-48nm-48nt-48mt+160nmt.$$

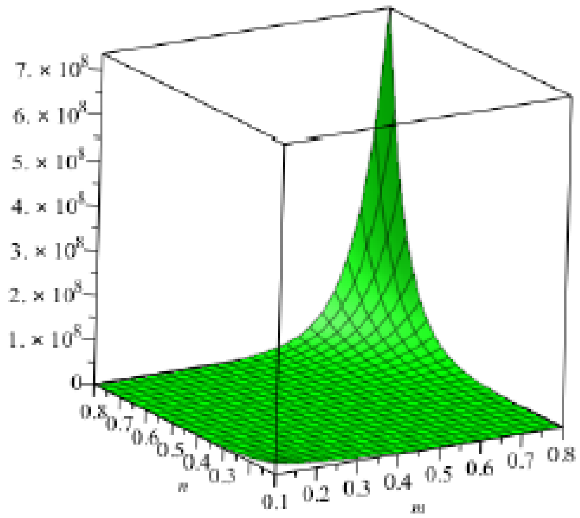

Fig. 3 – The graphical representation of Forgotten index.

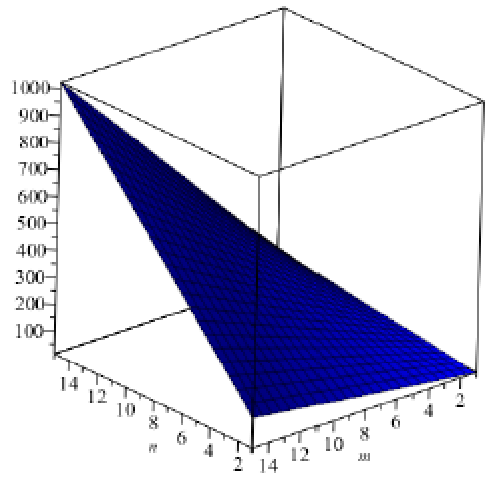

Fig. 4 – The graphical representation of Augmented Zagreb index.

• **Augmented Zagreb index $AZI(Cu_2O[m,n,t]])$**

Let G be the graph of $G \simeq Cu_2O[m,n,t]$.

Now using equation (2) together with Table 1 we have

$$AZI(G) = \sum_{pq\in E(G)}\left(\frac{\xi_p\times\xi_q}{\xi_p+\xi_q-2}\right)^3$$

$$AZI(Cu_2O[m,n,t]) = \sum_{pq\in E_1}\left(\frac{\xi_p\times\xi_q}{\xi_p+\xi_q-2}\right)^3 + \sum_{pq\in E_2}\left(\frac{\xi_p\times\xi_q}{\xi_p+\xi_q-2}\right)^3 - \sum_{pq\in E_3}\left(\frac{\xi_p\times\xi_q}{\xi_p+\xi_c-2}\right)^3$$

$$\begin{aligned}
AZI(G) &= 8|E_1(Cu_2O[m,n,t])| + 8|E_2(Cu_2O[m,n,t])| \\
&+8|E_3(Cu_2O[m,n,t])| \\
&= 8(4n+4m+4t-8) + 8(4nm+4nt+4mt-8n-8m-8t+12) \\
&+8(4(2nmt-nm-nt-mt+n+m+t-1)) \\
&= 64nmt.
\end{aligned}$$

- **Balaban index $J(Cu_2O[m,n,t])$**

Let G be the graph of $G \cong Cu_2O[m,n,t]$. Now using equation (3) together with Table 1 we have:

$$J(G) = \frac{m}{m-n+2}\sum_{pq\in E(G)}\frac{1}{\sqrt{\xi_p\times\xi_q}}$$

$$J(G) = \frac{m}{m-n+2}\left[\sum_{pq\in E_1}\frac{1}{\sqrt{\xi_p\times\xi_q}} + \sum_{pq\in E_2}\frac{1}{\sqrt{\xi_p\times\xi_q}}\right] + \frac{m}{m-n+2}\left[\sum_{pq\in E_3}\frac{1}{\sqrt{\xi_p\times\xi_q}}\right]$$

$$= \frac{8mnt}{2mnt-mn-mt-m-nt-n-t+1}$$
$$\times\left[\frac{1}{\sqrt{2}}|E_1(Cu_2O[m,n,t])| + \frac{1}{2}|E_2(Cu_2O[m,n,t])| + \frac{1}{\sqrt{8}}|E_3(Cu_2O[m,n,t])|\right]$$

$$J(G) = \frac{8mnt}{2mnt-mn-mt-m-nt-n-t+1}$$
$$\times\left[\frac{1}{\sqrt{2}}(4n+4m+4t-8) + \frac{1}{2}(4nm+4nt+4mt-8n-8m-8t+12)\right]$$
$$+\frac{8mnt}{2mnt-mn-mt-m-nt-n-t+1}$$
$$\times\left[\frac{1}{\sqrt{8}}(4(2nmt-nm-nt-mt+n+m+t-1))\right]$$

$$J(G) = \frac{8mnt}{2mnt-mn-mt-m-nt-n-t+1}\times\left[\frac{\sqrt{2}}{2}(4n+4m+4t-8)\right]$$
$$+\frac{8mnt}{2mnt-mn-mt-m-nt-n-t+1}\times[2mn+2nt+2mt-4n-4m-4t+6]$$
$$+\frac{8mnt}{2mnt-mn-mt-m-nt-n-t+1}$$
$$\times\left[\frac{\sqrt{2}}{2}(2nmt-nm-nt-mt+n+m+t-1)\right]$$

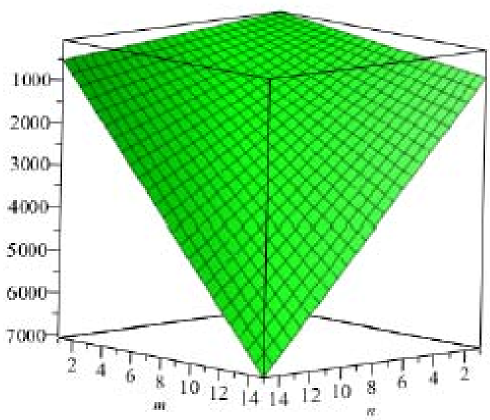

Fig. 5 – The graphical representation of Balaban index.

• **The Redefine Zagreb indices for** $Cu_2O[m,n,t]$

Let G be the graph of $G \simeq Cu_2O[m,n,t]$. Now using equations [(4)-(6)] and Table 1 we have:

$$ReG_1(G) = \sum_{p,q\in E(G)} \frac{\xi_p+\xi_q}{\xi_p\times\xi_q}$$

$$ReG_1(Cu_2O[m,n,t]) = \sum_{pq\in E_1} \frac{\xi_p+\xi_q}{\xi_p\times\xi_q} + \sum_{pq\in E_2} \frac{\xi_p+\xi_q}{\xi_p\times\xi_q} + \sum_{pq\in E_3} \frac{\xi_p+\xi_q}{\xi_p\times\xi_q}$$

$$ReG_1(Cu_2O[m,n,t]) = \frac{3}{2}|E_1(Cu_2O[m,n,t])| + 1|E_2(Cu_2O[m,n,t])|$$
$$+\frac{3}{4}|E_3(Cu_2O[m,n,t])|$$
$$=\frac{3}{2}(4n+4m+4t-8)$$
$$+(4nm+4nt+4mt-8n-8m-8t+12)$$
$$+\frac{3}{4}(4(2nmt-nm-nt-mt+n+m+t-1))$$
$$=n+m+t-3+nm+nt+mt+6nmt$$

$$ReG_2(G) = \sum_{p,q\in E(G)} \frac{\xi_p\times\xi_q}{\xi_p+\xi_q}$$

$$ReG_2(Cu_2O[m,n,t]) = \sum_{pq\in E_1} \frac{\xi_p\times\xi_q}{\xi_p+\xi_q} + \sum_{pq\in E_2} \frac{\xi_p\times\xi_q}{\xi_p+\xi_q} + \sum_{pq\in E_3} \frac{\xi_p\times\xi_q}{\xi_p+\xi_q}$$
$$=\frac{2}{3}|E_1(Cu_2O[m,n,t])| + 1|E_2(Cu_2O[m,n,t])|$$
$$+\frac{4}{3}|E_3(Cu_2O[m,n,t])|$$
$$=\frac{2}{3}(4n+4m+4t-8)$$
$$+(4nm+4nt+4mt-8n-8m-8t+12)$$
$$+\frac{4}{3}(4(2nmt-nm-nt-mt+n+m+t-1))$$
$$=\frac{4}{3}-\frac{4}{3}nm-\frac{4}{3}nt-\frac{4}{3}mt+\frac{32}{3}nmt$$

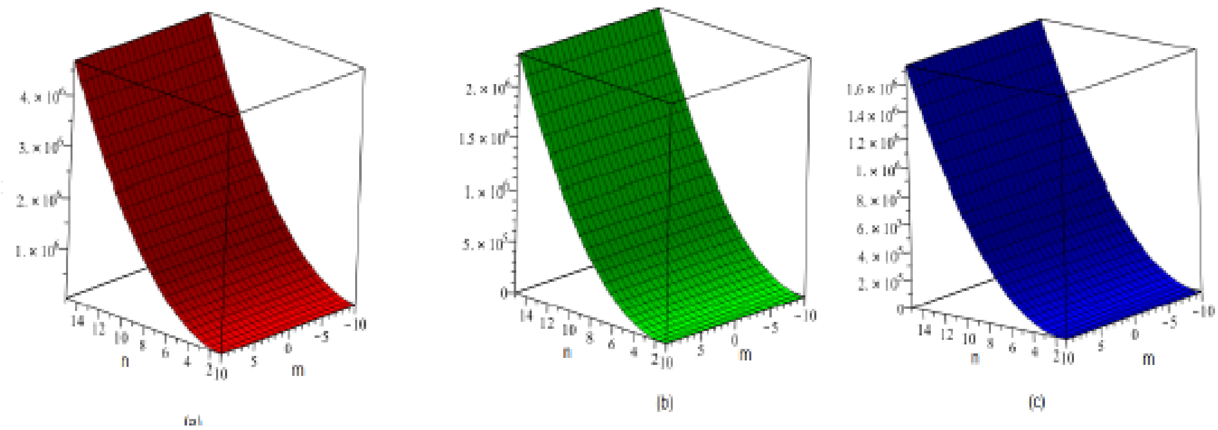

Fig. 6 – The graphical representation of (a) $ReG_1(G)$ index (b) $ReG_2(G)$ index (c) $ReG_3(G)$ index.

$$ReG_3(G) = \sum_{pq\in E(G)} (\xi_p\times\xi_q)(\xi_p+\xi_q)$$

$$ReG_3(Cu_2O[m,n,t]) = \sum_{pq\in E_1} (\xi_p\times\xi_q)(\xi_p+\xi_q) + \sum_{pq\in E_2} (\xi_p\times\xi_q)(\xi_p+\xi_q)$$
$$+\sum_{pq\in E_3} (\xi_p\times\xi_q)(\xi_p+\xi_q)$$
$$=(2)(3)|E_1(Cu_2O[m,n,t])| + (4)(4)|E_2(Cu_2O[m,n,t])|$$

$$+(8)(6)|E_3(Cu_2O[m,n,t])|$$
$$=(2)(3)(4n+4m+4t-8)$$
$$+(4)(4)(4nm+4nt+4mt-8n-8m-8t+12)$$
$$+(8)(6)(4(2nmt-nm-nt-mt+n+m+t-1))$$
$$=88n+88m+88t-48-128nm-128nt-128mt+384nmt$$

Crystal Structure of Titanium Difluoride

Titanium Difluoride is a water insoluble Titanium source for use in oxygen-sensitive applications, for example, metal production. Fluoride compounds have various applications in current advances and science, from oil refining and drawing to engineered organic chemistry and the making of pharmaceuticals.

The chemical graph of crystal structure of titanium difluoride $TiF_2[m,n,t]$ is described in Figure 7, for more details see.[25,26] 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 $m \times n$ unites in the mn —plane and then storing it up in t layers. The cardinality of vertices and edges of $TiF_2[m,n,t]$ are $12mnt+2mn+2mt+2nt+m+n+t+1$ and $32mnt$, respectively. In $TiF_2[m,n,t]$ the number of one degree vertices is 8, the number of two degree vertices is $4m+4n+4t-12$, the number of four degree vertices is $8mnt+4mn+4mt+4nt-4n-4m-4t+6$ and the number of eight degree vertices is $4mnt-2(mn+mt+nt)+m+n+t-1$.

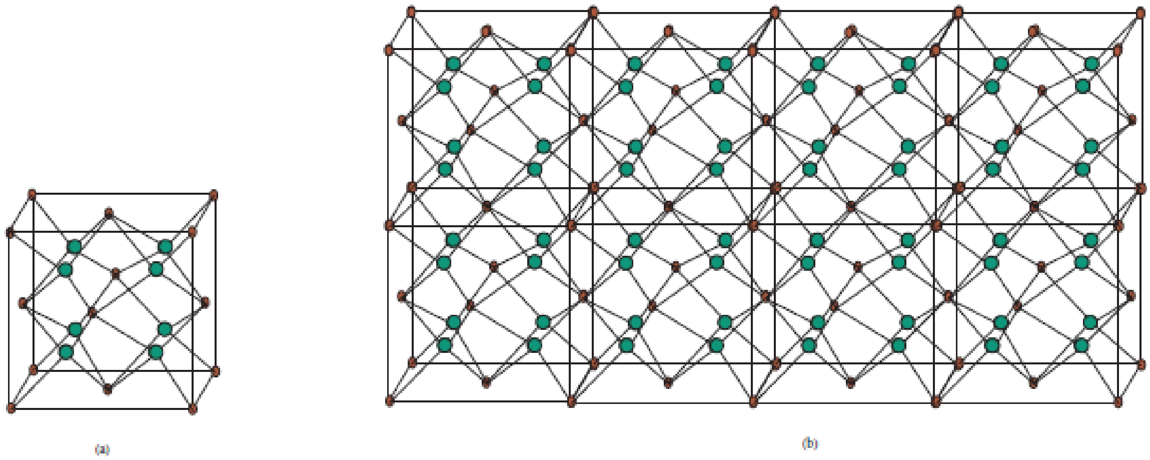

Fig. 7 – Crystal Structure Titanium Difluoride $TiF_2[m,n,t]$, (a) represents unit cell of of $TiF_2[m,n,t]$ with Ti atoms in red and F atoms in green (b) crystal structure of $TiF_2[4,1,2]$.

Table 2

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

(ξ_u, ξ_v)	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

Main Results for Crystallographic structure of $TiF_2[m,n,t]$

In this section, we compute the general result of topological indices for Crystallographic structure of $TiF_2[m,n,t]$. More preciously, we computed additive topological indices namely Forgotten index, Augmented index, Balaban index and Re-defined Zagreb indices for $TiF_2[m,n,t]$. In addition, we give graphical comparison and application of these indices.

• **Forgotten index $F(TiF_2[m,n,t])$** Let G be the graph of $G \simeq TiF_2[m,n,t]$. Now using equation (1) together with Table 2 we have

$$F(G) = \sum_{p,q\in E(G)} ({\xi_p}^2 + {\xi_q}^2)$$
$$F(TiF_2[m,n,t]) = \sum_{pq\in E_1} ({\xi_p}^2 + {\xi_q}^2) + \sum_{pq\in E_2} ({\xi_p}^2 + {\xi_q}^2)$$
$$+ \sum_{pq\in E_3} ({\xi_p}^2 + {\xi_q}^2) + \sum_{pq\in E_4} ({\xi_p}^2 + {\xi_q}^2)$$
$$= 17|E_1(TiF_2[m,n,t])| + 20|E_2(TiF_2[m,n,t])|$$
$$+32|E_3(TiF_2[m,n,t])| + 80|E_4(TiF_2[m,n,t])|$$

$$F(G) = 17(8) + 20(8(m+n+t-3)) + 32(16(mn+mt+nt)$$
$$-16(m+n+t) + 24)$$
$$+80(32mnt - 16(mt+mn+nt) + 8(m+n+t) - 8)$$
$$= -216 + 288m + 288n + 288t - 768mn - 768mt - 768nt + 2560mnt$$

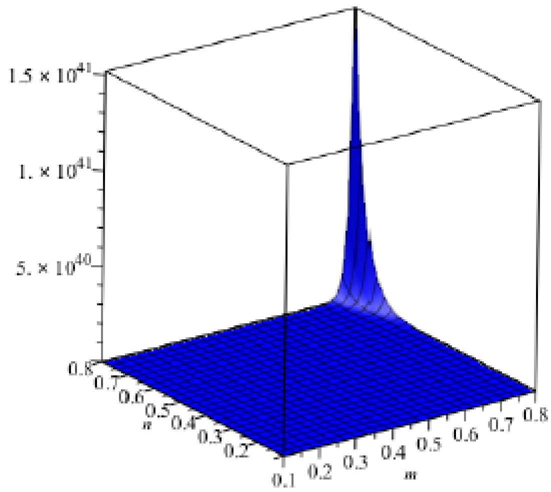

Fig. 8 – The graphical representation of Forgotten index.

• **Augmented Zagreb index $AZI(TiF_2[m,n,t])$** Let G be the graph of $G \simeq TiF_2[m,n,t]$. By using Table 2 and equation (2), we have

$$AZI(G) = \sum_{p,q\in E(G)} \left(\frac{\xi_p \times \xi_q}{\xi_p + \xi_q - 2}\right)^3$$
$$AZI(TiF_2[m,n,t]) = \sum_{pq\in E_1} \left(\frac{\xi_p \times \xi_q}{\xi_p + \xi_q - 2}\right)^3 + \sum_{pq\in E_2} \left(\frac{\xi_p \times \xi_q}{\xi_p + \xi_q - 2}\right)^3$$
$$+ \sum_{pq\in E_3} \left(\frac{\xi_p \times \xi_q}{\xi_p + \xi_q - 2}\right)^3 + \sum_{pq\in E_4} \left(\frac{\xi_p \times \xi_q}{\xi_p + \xi_q - 2}\right)^3$$
$$= \frac{64}{27}|E_1(TiF_2[m,n,t])| + 8|E_2(TiF_2[m,n,t])|$$
$$+ \frac{512}{27}|E_3(TiF_2[m,n,t])|$$
$$+ \frac{4096}{125}|E_4(TiF_2[m,n,t])|$$
$$= \frac{64}{27}(8) + 8(8(m+n+t-3))$$
$$+ \frac{512}{27}(16(mn+mt+nt) - 16(m+n+t) + 24)$$
$$+ \frac{4096}{125}(32mnt - 16(mt+mn+nt) + 8(m+n+t) - 8)$$

$$= \frac{67264}{3375} + \frac{76736}{3375}m + \frac{76736}{3375}n + \frac{76736}{3375}t - \frac{745472}{3375}mn - \frac{745472}{3375}mt - \frac{745472}{3375}nt + \frac{131072}{125}mnt$$

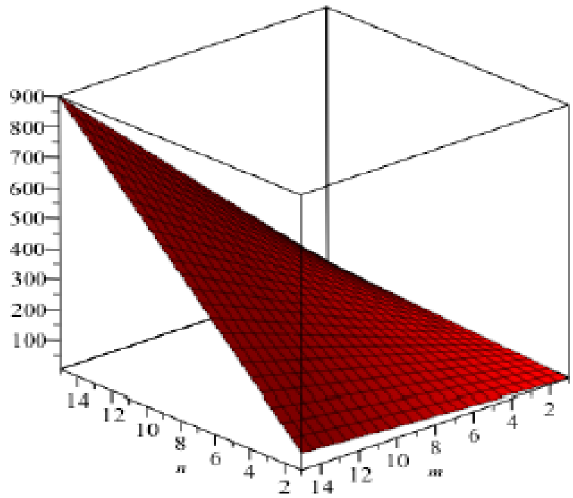

Fig. 9 – The graphical representation of Augmented Zagreb index.

• **Balaban index $J(TiF_2[m,n,t])$**

Let G be the graph of $G \cong TiF_2[m,n,t]$. Now by using Table 2 and equations (3), we have:

$$J(G) = \frac{m}{m-n+2}\sum_{p,q\in E(G)} \frac{1}{\sqrt{\xi_p \times \xi_q}}$$

$$J(TiF_2[m,n,t]) = \frac{m}{m-n+2} \times \left[\sum_{pq\in E_1} \frac{1}{\sqrt{\xi_p \times \xi_q}} + \sum_{pq\in E_2} \frac{1}{\sqrt{\xi_p \times \xi_q}}\right]$$

$$+ \frac{m}{m-n+2} \times \left[\sum_{pq\in E_3} \frac{1}{\sqrt{\xi_p \times \xi_q}} + \sum_{pq\in E_4} \frac{1}{\sqrt{\xi_p \times \xi_q}}\right]$$

$$= \frac{32mnt}{20mnt-2mn-2mt-2nt-m-n-t+1} \times$$

$$\times \left[\frac{1}{2}|E_1(TiF_2[m,n,t])| + \frac{1}{2\sqrt{2}}|E_2(TiF_2[m,n,t])|\right]$$

$$+ \left[\frac{32mnt}{20mnt-2mn-2mt-2nt-m-n-t+1}\right]$$

$$\times \left[\frac{1}{4}|E_3(TiF_2[m,n,t])| + \frac{1}{4\sqrt{2}}|E_4(TiF_2[m,n,t])|\right]$$

$$= \frac{32mnt}{20mnt-2mn-2mt-2nt-m-n-t+1}$$

$$\times \left[\frac{1}{2}(8) + \frac{1}{2\sqrt{2}}(8(m+n+t-3))\right]$$

$$+ \left[\frac{1}{4}(16(mn+mt+nt) - 16(m+n+t) + 24)\right]$$

$$+ \left[\frac{32mnt}{20mnt-2mn-2mt-2nt-m-n-t+1}\right]$$

$$\times \left[\frac{1}{4\sqrt{2}}(32mnt - 16(mt+mn+nt) + 8(m+n+t) - 8)\right]$$

$$= \left[\frac{32mnt}{20mnt-2mn-2mt-2nt-m-n-t+1}\right] \times$$

$$\times \left[10 + 2(m+n+t-3)\sqrt{2} + 4mn + 4mt + 4nt - 4m - 4n - 4t\right]$$

$$+\left[\frac{32mnt}{20mnt-2mn-2mt-2nt-m-n-t+1}\right]$$
$$\times\left[\frac{1}{8}(32nmt-16mn-16mt-16nt+8m+8n+8t-8)\sqrt{2}\right]$$

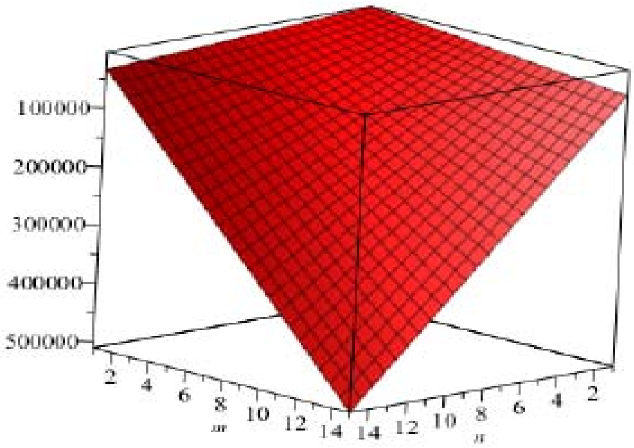

Fig. 10 – The graphical representation of Balaban index.

- **The Redefine Zagreb indices of $TiF_2[m,n,t]$**

Let G be the graph of $G \cong TiF_2[m,n,t]$. Now using equations (4-6), we have:

$$ReG_1(G)=\sum_{p,q\in E(G)}\frac{\xi_p+\xi_q}{\xi_p\times\xi_q}$$

$$F(TiF_2[m,n,t])=\sum_{pq\in E_1}\frac{\xi_p+\xi_q}{\xi_p\times\xi_q}+\sum_{pq\in E_2}\frac{\xi_p+\xi_q}{\xi_p\times\xi_q}+\sum_{pq\in E_3}\frac{\xi_p+\xi_q}{\xi_p\times\xi_q}+\sum_{pq\in E_4}\frac{\xi_p+\xi_q}{\xi_p\times\xi_q}$$
$$-\frac{5}{4}|E_1(TiF_2[m,n,t])|+\frac{3}{4}|E_2(TiF_2[m,n,t])|$$
$$+\frac{1}{2}|E_3(TiF_2[m,n,t])|+\frac{3}{8}|E_4(TiF_2[m,n,t])|$$
$$=\frac{5}{4}(8)+\frac{3}{4}(8(m+n+t-3))+\frac{1}{2}(16(mn+mt+nt)$$
$$-16(m+n+t)+24)$$
$$+\frac{3}{8}(32mnt-16(mt+mn+nt)+8(m+n+t)-8)$$
$$=1+m+n+t+2mn+2mt+2nt+12mnt$$

$$ReG_2(G)=\sum_{p,q\in E(G)}\frac{\xi_p\times\xi_q}{\xi_p+\xi_q}$$

$$ReG_2(TiF_2[m,n,t])=\sum_{pq\in E_1}\frac{\xi_p\times\xi_q}{\xi_p+\xi_q}+\sum_{pq\in E_2}\frac{\xi_p\times\xi_q}{\xi_p+\xi_q}+\sum_{pq\in E_3}\frac{\xi_p\times\xi_q}{\xi_p+\xi_q}+\sum_{pq\in E_4}\frac{\xi_p\times\xi_q}{\xi_p+\xi_q}$$
$$=\frac{4}{5}|E_1(TiF_2[m,n,t])|+\frac{4}{3}|E_2(TiF_2[m,n,t])|$$
$$+2|E_3(TiF_2[m,n,t])|+\frac{8}{3}|E_4(TiF_2[m,n,t])|$$
$$-\frac{4}{5}(8)+\frac{4}{3}(8(m+n+t-3))+2(16(mn+mt+nt)$$
$$-16(m+n+t)+24)$$
$$+\frac{8}{3}(32mnt-16(mt+mn+nt)+8(m+n+t)-8)$$
$$=\frac{16}{15}-\frac{32}{3}mn-\frac{32}{3}mt-\frac{32}{3}nt+\frac{256}{3}mnt$$

$$ReG_3(G)=\sum_{p,q\in E(G)}(\xi_p\times\xi_q)(\xi_p+\xi_q)$$

$$
\begin{aligned}
&ReG_3(TiF_2[m,n,t]\\
&= \sum_{st\in E_1} (\xi_p \times \xi_q)(\xi_p + \xi_q) + \sum_{st\in E_2} (\xi_p \times \xi_q)(\xi_p + \xi_q)\\
&+ \sum_{pq\in E_3} (\xi_p \times \xi_q)(\xi_p + \xi_q)\\
&+ \textstyle\sum_{pq\in E_4} \xi_p . \xi_q(\xi_p + \xi_q)\\
&= 4(5)|E_1(TiF_2[m,n,t])| + 6(8)|E_2(TiF_2[m,n,t])|\\
&+8(16)|E_3(TiF_2[m,n,t])| + 12(32)|E_4(TiF_2[m,n,t])|\\
&= 20(8) + 48(8(m+n+t-3)) + 128(16(nm+mt+nt)\\
&-16(m+n+t) + 24)\\
&+384(32mnt - 16(mt+mn+nt) + 8(m+n+t) - 8)\\
&= -992 + 1408m + 1408n + 1408t - 4096mn - 4096mt\\
&-4096nt + 12288mnt
\end{aligned}
$$

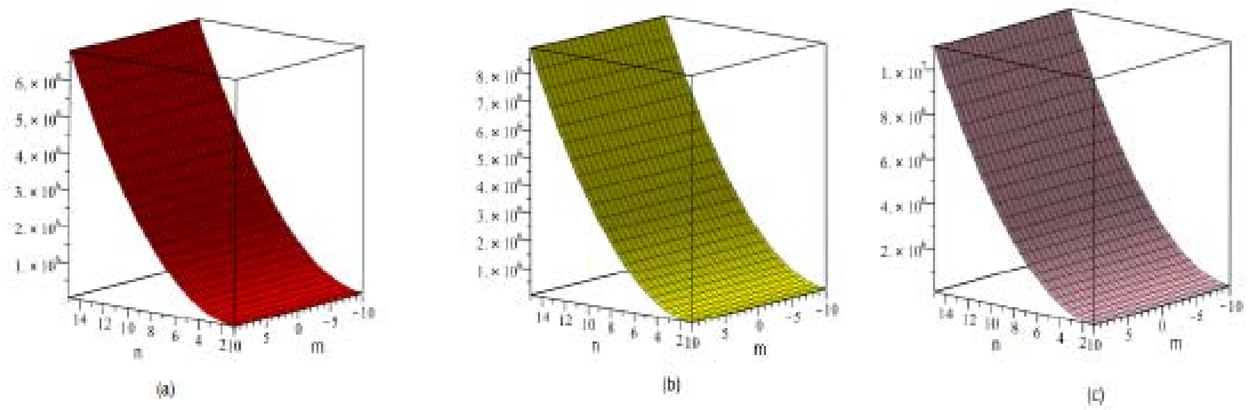

Fig. 11 – The graphical representation of (a) $ReG_1(G)$ index (b) $ReG_2(G)$ index (c) $ReG_3(G)$ index.

COMPARISONS AND DISCUSSION

• For the comparison of these indices numerically for Cu_2O, we computed all indices for different values of m, n, t. Now, from Table 3, we can easily see that all indices are in increasing order as the values of m, n, t are increasing. The graphical representations of topological indices for $Cu_2O[m,n,t]$ are depicted for Forgotten index in Figure 3. The Augmented index in Figure 4, Balaban index in Figure 5 and the redefined Zagreb indices in Figure 6 for certain values of m, n, t.

Table 3

Numerical computation of all indices for Cu_2O

$[m,n,t]$	$F(G)$	$AZI(G)$	$J(G)$	$ReZ_1(G)$	$ReZ_2(G)$	$ReZ_3(G)$
[1,1,1]	1812	2094	3.2×10^4	101	4.5×10^6	212
[2,2,2]	5176	6344	5.3×10^6	235	12.7×10^8	379
[3,3,3]	10268	12898	9.4×10^8	330	15.3×10^{10}	546
[4,4,4]	17788	21756	14.3×10^{12}	424	19.4×10^{16}	713

Table 4

Numerical computation of all indices for $TiF_2[m,n,t]$

$[m,n,t]$	$F(G)$	$AZI(G)$	$J(G)$	$ReZ_1(G)$	$ReZ_2(G)$	$ReZ_3(G)$
[1,1,1]	1812	2094	4.3×10^{6}	118	5.5×10^{7}	314
[2,2,2]	6512	7354	7.3×10^{9}	468	15.7×10^{11}	478
[3,3,3]	14258	14878	10.5×10^{12}	927	19.4×10^{15}	646
[4,4,4]	24758	32766	19.2×10^{16}	1537	24.5×10^{19}	917

• For the comparison of these indices numerically for $TiF_2[m,n,t]$, we computed all indices for different values of m,n,t. Now, from Table 4, we can easily see that all indices are in increasing order as the values of m,n,t are increasing. The graphical representations of topological indices for $TiF_2[m,n,t]$ are depicted for Forgotten index in Figure 8. The Augmented index in Figure 9, Balaban index in Figure 10 and the redefined Zagreb indices in Figure 11 for certain values of m,n.

• The forgotten topological index is helpful for testing the substance and pharmacological properties of drug nuclear structures. So in the case of Cu_2O and $TiF_2[m,n,t]$, its increasing value is useful for quick action during chemical reaction for drugs.

The augmented Zagreb index displays a good correlation with the formation heat of heptanes and octane. So our computation for AZI index is play an important rule for formation heat of heptanes and octane as its values are in increasing order.

The Balaban index shows good correlation with entropy of an octane isomers. The computation of Balaban index for Cu_2O and $TiF_2[m,n,t]$ provide a positive input for the correlation with entropy of all octane isomers.

The Zagreb types indices and polynomials were found to occur for the computation of the total π-electron energy of molecules, thus, the total π-electron energy in increasing order in the case of Cu_2O and $TiF_2[m,n,t]$, for higher values of m,n,t.

CONCLUSIONS

In this paper, we have studied and computed some degree based topological indices for the chemical graph of the crystal structure of titanium difluoride TiF_2 and crystallographic structure of cuprite Cu_2O. The exact results have been computed for additive topological indices namely Forgotten index, Augmented index, Balaban index and Re-defined Zagreb indices for $Cu_2O[m,n,t]$ and $TiF_2[m,n,t]$ for some values of $m,\ n,t$.

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

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