TOPOLOGICAL PROPERTIES OF CHEMICAL STRUCTURES

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Graph theory plays an important role in modeling and designing any chemical structure or network. The molecular topological descriptors are the numerical invariants of a molecular graph and are very useful for predicting their bioactivity. In this paper, we have studied the chemical graph of crystal structure of titanium difluoride TiF_2, crystallographic structure of cuprite Cu_2O and Boron-Carbon crystal structure of $P\bar{4}m2BC_3[s,t,n]$. We have discussed and computed exact results for degree based topological indices namely Zagreb indices, Zagreb coindices and Sanskruti index.
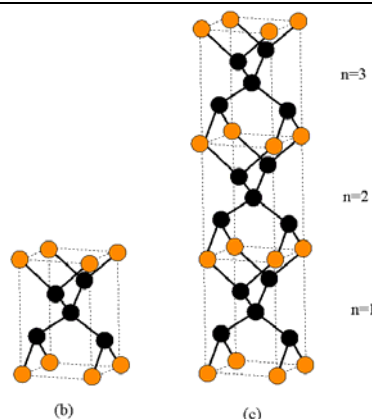
INTRODUCTION

Graph theory is a standout amongst the most extraordinary and one of a kind branch of mathematics by which the showing of any structure is made possible. As of late, it achieves much consideration among scientists on account of its extensive variety of utilizations in Computer science, electrical systems (network), interconnected systems (network), biological networks, and in chemistry, and so forth. The chemical graph theory (*CGT*) is the quickly developing zone among scientists. It helps in comprehension about the basic properties of a molecular graph. There are a considerable measure of molecular compounds, which have assortment of utilizations in the fields of business, commercial, industrial, pharmaceutical chemistry, in every day life and in research facility.

A relationship exists between molecular compounds and their atomic structures. The control and examination of molecular compounds data is made possible utilizing molecular descriptors. Chemical graph theory is a branch of mathematical chemistry in which apparatuses of graph theory are applied to model the chemical phenomenon mathematically. Likewise, it identifies with the nontrivial uses of graph theory for solving molecular problems. This theory contributes a noticeable part in the field of chemical sciences.

A new subject namely Chem-informatics which is a combination of chemistry, mathematics and information science helps to analyzes (*QSAR*) and (*QSPR*) connections that are used to predict the bioactivity and physiochemical properties of chemical compounds. A topological index is a

numerical esteem that is processed mathematically from the molecular graph. It is related with chemical constitution demonstrating for correlation of chemical structure with numerous physical, chemical properties and biological activities, see details.[1,10]

For a given $G = (V, E)$ graph where V to be the vertex set and E be the edge set of G. The degree d_p of p is the quantity of edges of G incident with p. The length of a most limited path in a graph G is a distance $d(p, q)$ amongst p and q represented by a polynomial, a numerical value or by matrix form. There are sure sorts of topological indices primarily eccentric based, degree based and distance based indices etc. In this paper, we have dealt with degree based topological indices.

The Zagreb indices were conceived in 1972 by Gutman and Trinajestic,[11,12] they are characterized as:

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q) \qquad (1)$$

$$M_2(G) = \sum_{pq \in E(G)} (d_p \times d_q) \qquad (2)$$

In 2008, Došlić put forward the first Zagreb coindex and second Zagreb coindex, defined as[4]

$$\overline{M_1} = \overline{M_1}(G) = \sum_{pq \notin E(G)} [d_p + d_q] \qquad (3)$$

$$\overline{M_2} = \overline{M_2}(G) = \sum_{pq \notin E(G)} d_p \times d_q \qquad (4)$$

In 2016, I. Gutman *et al.*[7] proves the following Theorems:

Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges. Then

$$\overline{M_1}(G) = 2|E(G)|(|V(G)| - 1) - M_1(G). \qquad (5)$$

Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges. Then

$$\overline{M_2}(G) = 2|E(G)|^2 - \frac{1}{2} M_1(G) - M_2(G) \qquad (6)$$

In 2016, S. M. Hosamani[14] introduced the Sanskruti index $S(G)$ for a molecular graph G, defined as:

$$S(G) = \sum_{pq \in E(G)} \left(\frac{S_p \times S_q}{S_p + S_q - 2} \right)^3 \qquad (7)$$

For further study and research about the topological indices see.[1,6,13,16,21–28]

Main results

In this section, additive topological indices mainly first and second zegreb indices, first and second zegreb coindices and Sanskruti index of $Cu_2O[m, n, t]$, $TiF_2[m, n, t]$ and $P\overline{4}m2BC_3[s, t, n]$ are computed. Moreover, the exact values are derived for these indices of the chemical graphs $Cu_2O[m, n, t]$, $TiF_2[m, n, t]$ and $P\overline{4}m2BC_3[s, t, n]$.

Crystallographic structure of *Cu₂O*

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 portrayed in Figure 1 and Figure 2, for more data about this structure see.[2,30,31] 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 develop this graph first by taking $m \times n$ units in the mn —plane and after that leveling up in t layers. The quantity 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 $2mnt - nm - nt - mt + n + m + 1$.

In the next Theorem, we have computed the exact result of first and second Zagreb index for the chemical graph Cu_2O [*m,n,t*].

Theorem 3.1. Consider the graph of $G \cong Cu_2O[m, n, t]$ with $m, n, t \geq 1$, then its first and second Zagreb index is equal to,

$$M_1(G) - 48mnt - 8mn - 8mt - 8nt + 4m + 4n + 4t \qquad (8)$$

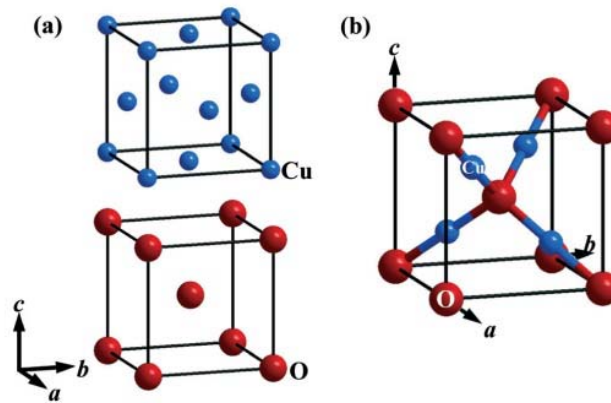$$M_2(G) = 64mnt - 16mn - 16mt - 16nt + 8m + 8n + 8t. \qquad (9)$$

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. In the lattice of Cu_2O, every Cu atom is connected with two O atoms, and every O atom is connected with four Cu atoms.

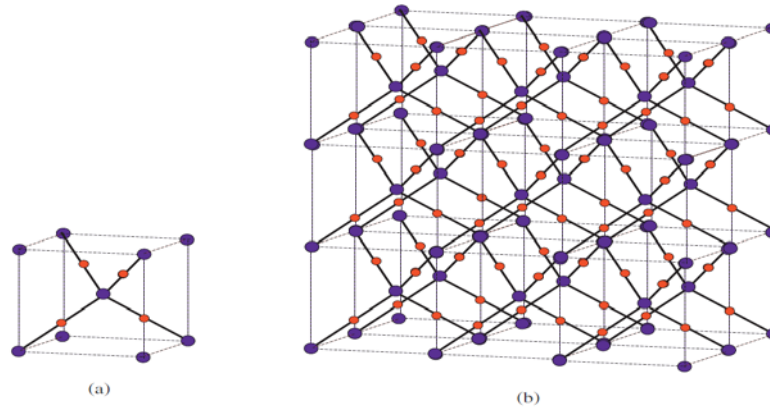

Fig. 2 – Crystallographic structure of $Cu_2O[3,2,3]$.

Table 1

Degree based partition of edges of Cu_2O [m,n,t], of end vertices of each edge

(d_p, d_q)	Frequency
(1,2)	$4n + 4m + 4t - 8$
(2,2)	$4nm + 4nt + 4mt - 8n - 8m - 8t + 12$
(2,4)	$4(2nmt - nm - nt - mt + n + m + t - 1)$

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

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q)$$

$$M_1(G) = (4m + 4n + 4t - 8)(1 + 2) + (4mn + 4mt + 4nt - 8m - 8n - 8t + 12)(2 + 2)$$
$$+ (8mnt - 4mn - 4mt - 4nt + 4m + 4n + 4t - 4)(2 + 4)$$
$$M_1(G) = 48mnt - 8mn - 8mt - 8nt + 4m + 4n + 4t.$$

By using Table 1 and Equation (1) the second Zagreb index are computed as below:

$$M_2(G) = \sum_{pq \in E(G)} (d_p d_q)$$

$$M_2(G) = (4m + 4n + 4t - 8) \cdot (1 \times 2) + (4mn + 4mt + 4nt - 8m - 8n - 8t + 12)(2 \times 2)$$
$$+ (8mnt - 4mn - 4mt - 4nt + 4m + 4n + 4t - 4)(2 \times 4)$$
$$= 64mnt - 16mn - 16mt - 16nt + 8m + 8n + 8t.$$

The first and second Zagreb coindices for the chemical graph $Cu_2O[m, n, t]$ computed are in the next Theorem.

Theorem 3.2. Consider the graph of $G \cong Cu_2O[m, n, t]$ with $m, n, t \geq 1$, then its first and second Zagreb coindices are equal to,

$$\overline{M_1}(G) = 80m^2n^2t^2 + 16mnt(m + 1)(n + 1)(t + 1) - 64mnt + 8mn + 8mt$$
$$+ 8nt - 4m - 4n - 4t$$

$$\overline{M_2}(G) = 128m^2n^2t^2 - 88mnt + 20mn + 20mt + 20nt - 10m - 10n - 10t$$

Proof. Let G be the crystallographic structure of $Cu_2O[m, n, t]$. Then by using Equations (3),(5)

and Theorem 1 first Zagreb coindex is computed as below:

$$M_1(G) = \sum_{pq \notin E(G)} (d_p + d_q)$$

$$\overline{M_1}(G) = 2|E(G)|(|V(G)| - 1) - M_1(G)$$
$$= 2(8mnt)((m + 1)(n + 1)(t + 1) + 5mnt - 1)$$
$$- (48mnt - 8mn - 8mt - 8nt + 4m + 4n + 4t)$$
$$= 80m^2n^2t^2 + 16mnt(m + 1)(n + 1)(t + 1) - 64mnt + 8mn + 8mt$$
$$+ 8nt - 4m - 4n - 4t.$$

Now, by using Equations (4),(6) and Theorem 1 second Zagreb coindex is computed as below:

$$\overline{M_2}(G) = \sum_{pq \notin E(G)} (d_p d_q)$$
$$= 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G)$$
$$\overline{M_2}(G) = 2(8mnt)^2 - \frac{1}{2}(48mnt - 8mn - 8mt - 8nt + 4m + 4n + 4t)$$
$$- (64mnt - 16mn - 16mt - 16nt + 8m + 8n + 8t)$$
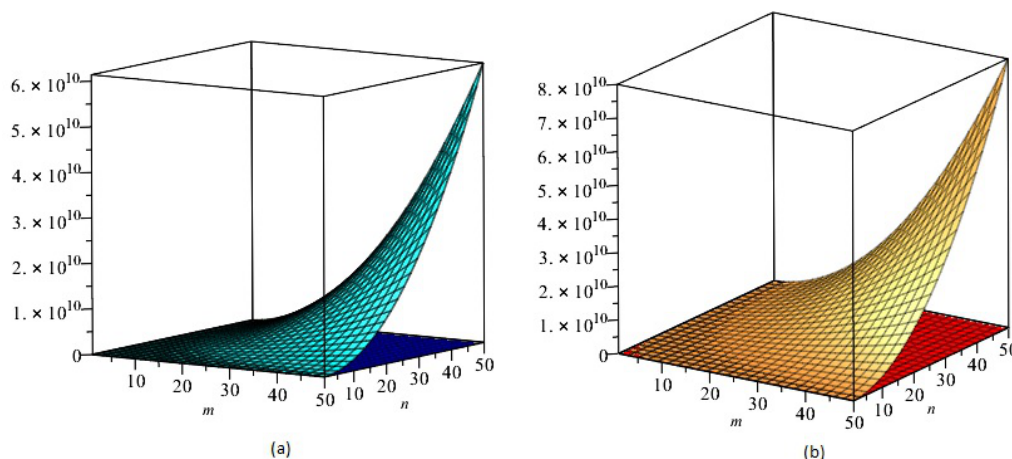$$= 128m^2n^2t^2 - 88mnt + 20mn + 20mt + 20nt - 10m - 10n - 10t$$

Fig. 3 – Comparison of indices of $G \cong Cu_2O[m, n, t]$, for fix $t = 10$: in (a) first Zagreb index $M_1(G)$ and first Zagreb coindex $\overline{M_1}(G)$ are compared. The blue and cyan colors represents $M_1(G)$ and $\overline{M_1}(G)$, respectively. Its easy to see that in the given domain $\overline{M_1}(G)$ is more dominating. In (b) second Zagreb index $M_2(G)$ and second Zagreb coindex $\overline{M_2}(G)$ are compared. The red and gold colors represents $M_2(G)$ and $\overline{M_2}(G)$, respectively. Its easy to see that in the given domain $\overline{M_2}(G)$ is more dominating. over the values of $\overline{M_2}(G)$ are largest and the values of $M_1(G)$ are smallest.

Table 2

Based on sum of degrees of neighborhood of end vertices of each edge the partition of edges of Cu_2O [m,n,t], with $m,n,t \geq 2$

(S_p, S_q)	Frequency
(2,4)	$4m + 4n + 4t - 8$
(4,6)	$4mn + 4mt + 4nt - 8m - 8n - 8t + 12$
(5,8)	$4n + 4m + 4t - 8$
(6,8)	$4mn + 4mt + 4nt - 8m - 8n - 8t + 12$
(8,8)	$8mnt - 8mn - 8nt + 8m + 8n + 8t - 8$

The Table 2 shows partition of edges of the chemical graph $Cu_2O[m, n, t]$ depending on the sum of degrees of the neighbouring vertices of end vertices of each edge. The next Theorem shows the exact value of Sanskruti index of $Cu_2O[m, n, t]$.

Theorem 3.3. Consider the graph $G \cong Cu_2O[m, n, t]$ with $m, n, t \geq 2$, then its Sanskruti index $S(G)$ is equal to

$$S(G) = \frac{262144mnt}{343} - \frac{137292mn}{343} - \frac{137292mt}{343} - \frac{137292nt}{343} + \frac{118974696n}{456533} + \frac{118974696t}{456533} + \frac{118974696m}{456533} - \frac{55213740}{456533}$$

Proof. Let G be the crystallographic structure of $Cu_2O[m, n, t]$. Then by using Table 2 and equation (7) the Sanskruti index $S(G)$ is computed as follows.

$$S(G) = \sum_{pq \in E(G)} \left(\frac{S_p \times S_q}{S_p + S_q - 2}\right)^3$$

$$S(G) = (4m + 4n + 4t - 8)\left(\frac{2 \times 4}{2 + 4 - 2}\right)^3 + (4mn + 4nt + 4mt - 8m - 8n - 8t + 12)\left(\frac{4 \times 6}{4 + 6 - 2}\right)^3 + (4m + 4n + 4t - 8)\left(\frac{5 \times 8}{5 + 8 - 2}\right)^3$$

$$+ (4mn + 4nt + 4mt - 8m - 8n - 8t + 12)\left(\frac{6 \times 8}{6 + 8 - 2}\right)^3 + (8mnt - 8mn - 8mt - 8nt + 8m + 8n + 8t - 8)\left(\frac{8 \times 8}{8 + 8 - 2}\right)^3$$

$$S(G) = \frac{262144mnt}{343} - \frac{137292mn}{343} - \frac{137292mt}{343} - \frac{137292nt}{343} + \frac{118974696n}{456533} + \frac{118974696t}{456533} + \frac{118974696m}{456533} - \frac{55213740}{456533}$$

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 4, for more details see.[3,10] 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 number 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 $4mnt - 2(mn + mt + nt) + m$.
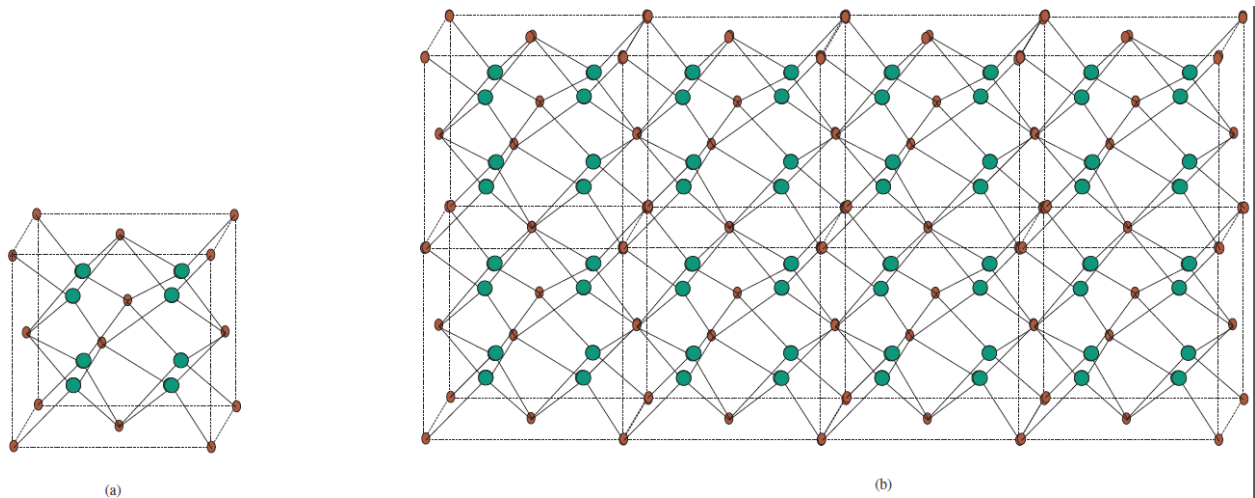

Fig. 4 – Crystal Structure Titanium Difluoride *TiF₂[m,n,t]*, (a) represents unit cell of of *TiF₂[m,n,t]*, with *Ti* atoms in red and *F* atoms in green (b) crystal structure of *TiF₂*[4,1,2].

Table 3

Degree based partition of edges of *TiF₂[m,n,t]*, of end vertices of each edge

(d_p, d_q)	Frequency
(1,4)	8
(2,4)	$8(m + n + t - 3)$
(4,4)	$16(mn + mt + nt) - 16(m + n + t) + 24$
(4,8)	$32mnt - 16(mt + mn + nt) - 8$

The exact result of the first and second Zagreb index for the chemical graph $TiF_2[m, n, t]$ is computed in the following theorem.

Theorem 4.1. Consider the graph $G \cong TiF_2[m, n, t]$ with $m, n, t \geq 1$, then its first and second Zagreb index is equal to,

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

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

Proof. Let $G \cong TiF_2[m, n, t]$ be the crystal structure of titanium difluoride. Then by using Table 3 and the equation (1) the first Zagreb index is computed as below:

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q)$$

$$M_1(G) = (8)(1 + 4) + (8m + 8n + 8t - 24)(2 + 4) + (16(mn + mt + nt) - 16(m + n + t) + 24)(8) + (32mnt - 16(mn + mt + nt) + 8(m + n + t) - 8)(4 + 8)$$
$$M_1(G) = 384mnt - 64mn - 64mt - 64nt + 16m + 16n + 16t - 8$$

Now, by using Table 3 and the equation (2) the second Zagreb index is computed as below:

$$M_2(G) = \sum_{pq \in E(G)} (d_p d_q)$$

$$M_2(G) = (8)(1 \times 4) + (8m + 8n + 8t - 24)(2 \times 4) + (16(mn + mt + nt) - 16(m + n + t) + 24)(4 \times 4) + (32mnt - 16(mn + mt + nt) + 8(m + n + t) - 8)(4 \times 8)$$

$$M_2(G) = 1024mnt - 256mn - 256mt - 256nt + 64m + 64n + 64t - 32.$$

The first and second Zagreb coindices for the chemical graph $TiF_2[m, n, t]$ computed are in the next Theorem.

Theorem 4.2. Consider the graph of $G \cong TiF_2[m, n, t]$ with $m, n, t > 1$, then its first and second Zagreb coindices are equal to,

$$\overline{M_1}(G) = 64mnt(12mnt + 2mn + 2mt + 2nt + m + n + t)$$
$$-384mnt + 64mn + 64mt + 64nt - 16m - 16n - 16t + 8.$$

$$\overline{M_2}(G) = 2048m^2n^2t^2 - 1216mnt + 288mn + 288mt + 288nt - 72m - 72n - 72t + 36$$

Proof. Let G be the crystallographic structure of $TiF_2[m, n, t]$. Then by using Equations (3),(5)

and Theorem 3 first Zagreb coindex is computed as below:

$$\overline{M_1}(G) = \sum_{pq \notin E(G)} (d_p + d_q)$$
$$\overline{M_1}(G) = 2|E(G)|(|V(G)| - 1) - M_1(G)$$
$$= 2(32mnt)(12mnt + 2mn + 2mt + 2nt + m + n + t + 1 - 1)$$
$$-(384mnt - 64mn - 64mt - 64nt + 16m + 16n + 16t - 8)$$
$$= 64mnt(12mnt + 2mn + 2mt + 2nt + m + n + t)$$
$$-384mnt + 64mn + 64mt + 64nt - 16m - 16n - 16t + 8.$$

Now, by using Equations (4),(6) and Theorem 3 second Zagreb coindex is computed as below:

$$\overline{M_2}(G) = \sum_{pq \notin E(G)} (d_p d_q)$$
$$\overline{M_2}(G) = 2|E(G)| - \frac{1}{2}M_1(G) - M_2(G)$$
$$= 2(32mnt)^2 - \frac{1}{2}(384mnt - 64mn - 64mt - 64nt + 16m + 16n + 16t - 8)$$
$$-(1024mnt - 256mn - 256mt - 256nt + 64m + 64n + 64t - 32)$$
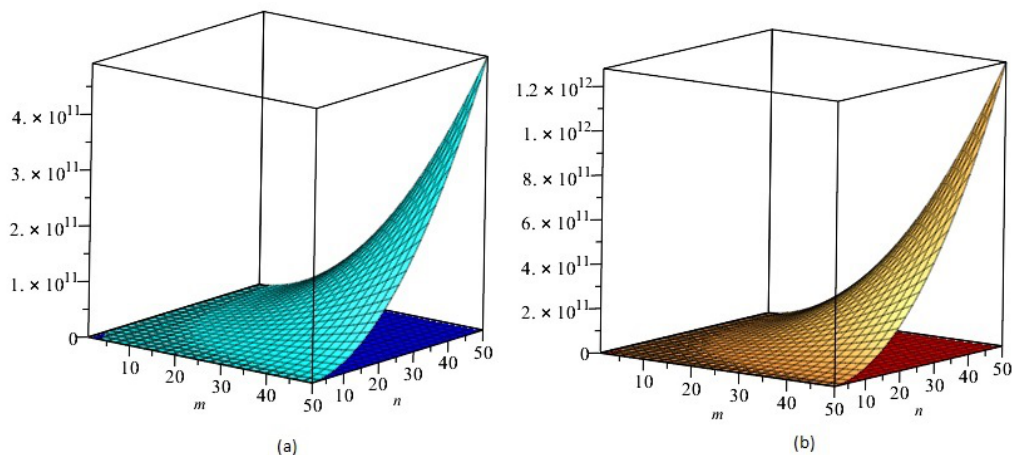$$= 2048m^2n^2t^2 - 1216mnt + 288mn + 288mt + 288nt - 72m - 72n - 72t + 36$$

Fig. 5 – Comparison of indices of $G \cong TiF_2[m,n,t]$ for fix $t = 10$: in (a) first Zagreb index $M_1(G)$ and first Zagreb coindex $\overline{M}_1(G)$ are compared. The blue and cyan colors represents $M_1(G)$ and $\overline{M}_1(G)$, respectively. Its easy to see that in the given domain $\overline{M}_1(G)$ is more dominating. In (b) second Zagreb index $M_2(G)$ and second Zagreb coindex $\overline{M}_2(G)$ are compared. The red and gold colors represents $M_2(G)$ and $\overline{M}_2(G)$, respectively. Its easy to see that in the given domain $\overline{M}_2(G)$ is more dominating. over the values of $\overline{M}_2(G)$ are largest and the values of $M_1(G)$ are smallest.

Table 4

Edge partition of *TiF$_2$[m,n,t]*, $m,n,s \geq 2$ based on degree sum of end vertices of each edge

(S_p, S_q)	Frequency
(4,13)	8
(8, 18)	$8(m + n + t - 3)$
(13,16)	16
(16, 18)	$16(mn + mt + nt) - 16(m + n + t) + 8$
(16, 24)	$32mnt - 16(mn + mt + nt) + 8$
(18, 32)	$8(m + n + t - 2)$

The Table 4 shows the edge partition of the chemical graph $TiF_2[m, n, t]$, $m, n, s \geq 2$ based on the degree sum of end vertices of each edge. The next Theorem shows the exact value of Sanskruti index of $TiF_2[m, n, t]$, $m, n, s > 2$.

Theorem 4.3. Consider the graph $G \cong TiF_2[m, n, t]$ with $m, n, t \geq 2$, then its Sanskruti index $S(G)$ is equal to

$$S(G) = \frac{226492416}{6859}mnt - \frac{33242832}{6859}mn + \frac{46760544}{6859}nt - \frac{113246208}{6859}mt + 3888m + 3888n + 3888t - \frac{18725852570869\,6}{16875712125}$$

Proof. Let G be the crystallographic structure of $TiF_2[m, n, t]$. Then by using Table 4 and equation (7) the Sanskruti index $S(G)$ is computed as follows.

$$S(G) = \sum_{pq \in E(G)} \left(\frac{S_p \times S_q}{S_p + S_q - 2}\right)^3$$

$$S(G) = (8)\left(\frac{4 \times 13}{4 + 13 - 2}\right)^3 + 8(m + n + t - 3)\left(\frac{8 \times 18}{8 + 18 - 2}\right)^3$$
$$+ (16)\left(\frac{13 \times 16}{13 + 16 - 2}\right)^3 + (16(mn + mt + nt) - 16(m + n + t) + 8)\left(\frac{16 \times 18}{16 + 18 - 2}\right)^3$$
$$+ (32mnt - 16(mn + mt + nt) + 8)\left(\frac{16 \times 24}{16 + 24 - 2}\right)^3 + 8(m + n + t - 2)\left(\frac{18 \times 32}{18 + 32 - 2}\right)^3$$

$$= \frac{226492416}{6859}mnt - \frac{33242832}{6859}mn + \frac{46760544}{6859}nt - \frac{113246208}{6859}mt + 3888m + 3888n + 3888t - \frac{18725852570869\,6}{16375712125}$$

Boron-Carbon crystal structure of $P\overline{4}m2BC_3[s,t,n]$

The vast majority of Boron and Carbon systems denoted as B-C binary systems show high imperviousness to oxidation furthermore, response with ferrous metals, contrasted and the carbon-based materials.[9,15,18] Boron carbide B_4C is a hard crystal that can be created at surrounding pressure, 8,17 while *B*-doped diamond demonstrates a superconducting progress temperature of $4K$.[5] It is of extraordinary enthusiasm for diamond-like BC_x systems to seek after predominant superhard crystals that are not just thermally and chemically more stable(steady) than diamond, yet in addition have intriguing electrical properties.[9,20,29]

Liu *et al.*[19] investigated the crystal structures with particle swarm optimization (PSO) algorithm consolidated with first-principles structural optimizations. Three metallic setups, to be specific $Pmma - a$, $Pmma - b$ and $P\overline{4}m2$ stages were revealed. With the bond resistance demonstrate, the Vickers hardness for all three stages is bigger than 60 GPa, demonstrating the superhard nature of these polymorphs, which ought to be tested experimentally. Furthermore, all stages have a superconductive transition at low temperature.

Let $G = P\overline{4}m2BC_3[s, t, n]$ be the chemical graph of $P\overline{4}m2BC_3$ with $s \times t$ unit cells in the plane and n layers. We construct this graph first by taking $s \times t$ unites in the st −plane and then storing it up in n layers. Some description of the construction are given in Figure 6 and Figure 7. The number of vertices and edges of $P\overline{4}m2BC_3[s, t, n]$ are $(s + 1)(t + 1) +$

$+ n(2s + 1)(2t + 1)$ and $n(8st + 2s + 2t)$. In $P\bar{4}m2BC_3[s,t,n]$ the number of one degree vertices is $2(s + t + 2)$, the number of two degree vertices is $2(st + 2n - 3)$, the number of three degree vertices is $2n(s + t) + 2(n - 1)(s + t - 2)$ and the number of four degree vertices is $4snt - 2sn - st - 2tn + n + s + t$. The edges of $P\bar{4}m2BC_3|s,t,n|$ are partitioned into seven sets, say E_1, E_2, E_3, E_4, E_5, E_6 and E_7. The set E_1 contains 8 edges pq, where $d_p = 3$ and $d_q = 1$. The set E_2 contains $2(s + t) - 4$ edges pq, where $d_p = 4$ and $d_q = 1$. The set E_3 contains $4(t + s + 2n - 4)$ edges pq, where $d_p = 3$ and $d_q = 2$. The set E_4 contains $4(s - 1)(t - 1)$ edges pq, where $d_p = 4$ and $d_q = 2$. The set E_5 contains $4(n - 1)(t + s - 2)$ edges pq, where $d_p - d_q - 3$. The set E_6 contains $2n(s + t) + 2(n - 1)(s + t - 2)$ edges pq, where $d_p = 4$ and $d_q = 3$. The set E_7 contains $8snt - 6sn - 4st - 6nt + 4s + 4n + 4t - 4$ edges pq, where $d_p = d_q = 4$. The edge partition is shown in Table 5 of $P\bar{4}m2BC_3[s,t,n]$ with $s, t, n \geq 1$.
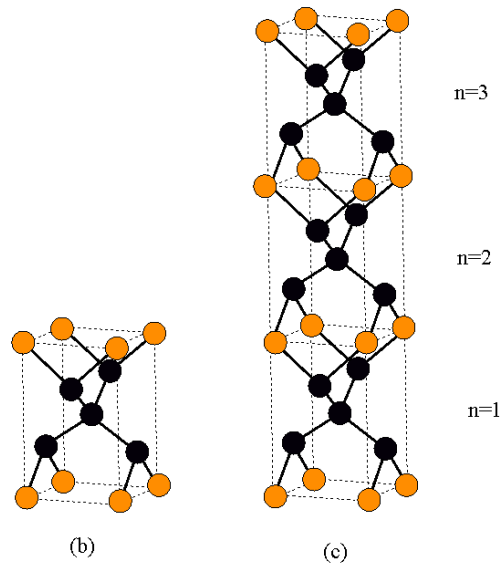

Fig. 6 – Crystal structures of $P\bar{4}m2BC_3[s,t,n]$, (a) chemical graph of unit cell,
(b) $P\bar{4}m2BC_3[1,1,3]$ with $s = t = 1$ and $n = 3$ layers. Carbon atom are black Boron atoms are brown.
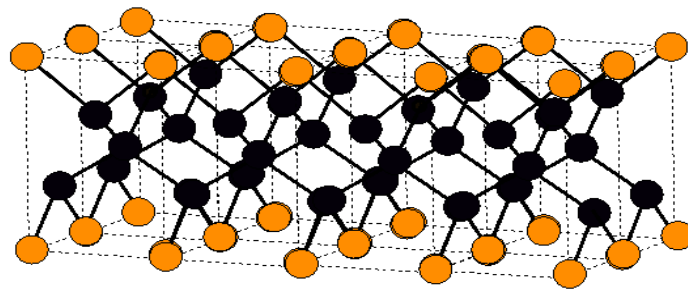

Fig. 7 – Crystal structures of $P\bar{4}m2BC_3[4,2,1]$.

Table 5

Degree based partition of edges of $P\bar{4}m2BC_3[s,t,n]$, of end vertices of each edge

(d_p, d_q)	Frequency
(3,1)	8
(4,1)	$2(s + t) - 4$
(3,2)	$4(t + s + 2n - 4)$

Table 5 (continued)

(4,2)	$4(s-1)(t-1)$
(3,3)	$4(n-1)(t+s-2)$
(4,3)	$2n(s+t)+2(n-1)(s+t-2)$
(4,4)	$8snt-6sn-4st-6nt+4s+4n+4t-4$

In the following Theorems we have computed the first and second Zagreb indices, the first and second Zagreb coindices of the chemical graph $P\overline{4}m2BC_3[s,t,n]$.

Theorem 5.1. Consider the graph $G \cong P\overline{4}m2BC_3[s,t,n]$, for $s,t,n \geq 1$, then its first and second Zagreb indices are equal to

$$M_1(G) = 64snt - 10sn - 8st - 10nt - 4n$$
$$M_2(G) = 128snt - 36sn - 32st - 36nt + 4s - 8n + 4t.$$

Proof. Let G be the graph of $P4m2BC_3[s,t,n]$. Then by using Table 5 and the equations (1),(2) the first and second Zagreb indices are computed as below:

$$M_1(G) = \sum_{pq\in \bar{s}(G)} (d_p + \acute{d}_q).$$

$$M_1(G) = (8)(3+1)+(2s+2t-4)(4+1)+4(t+s+2n-4)(3+2)+4(s-1)(t-1)(4+2)$$

$$+4(n-1)(t+s-2)(3+3)+2(n-1)(t+s-2)(4+3)$$
$$+(8snt-6sn-4st-6nt+4s+4n+4t-4)(4+4)$$
$$M_1(G) = 64snt - 10sn - 8st - 10nt - 4n$$

$$M_2(G) = \sum_{pq\in\bar{s}(G)} (d_p d_q) = B_1(G)$$
$$M_2(G) = (8)(3\times 1)+(2s+2t-4)(4\times 1)+4(t+s+2n-4)(3\times 2)$$
$$+4(s-1)(t-1)(4\times 2)+4(n-1)(t+s-2)(3\times 3)+2(n-1)(t+s$$
$$-2)(4\times 3)+(8snt-6sn-4st-6nt+4s+4n+4t-4)(4\times 4).$$
$$M_2(G) = 128snt - 36sn - 32st - 36nt + 4s - 8n + 4t$$

Theorem 5.2. Consider the graph of $G \cong P\overline{4}m2BC_3[s,t,n]$ with $m,n,t \geq 1$, then its first and second Zagreb coindices are equal to,

$$\overline{M_1}(G) = 2n(8st+2s+2t)((s+1)(t+1)+n(2s+1)(2t+1)-1)-64snt-10sn+10nt+10st+4n.$$

$$\overline{M_2}(G) = 2048m^2n^2t^2 - 1216mnt + 288mn + 288mt + 288nt - 72m - 72n - 72t + 36$$

Proof. Let G be the crystallographic structure of $P\overline{4}m2BC_3[s,t,n]$. Then by using Equations (3),(5) and Theorem 5 first Zagreb coindex is computed as below:

$$\overline{M_1}(G) = \sum_{pq\notin E(G)} (d_p + d_q)$$
$$\overline{M_1}(G) = 2|E(G)|(|V(G)|-1) - M_1(G)$$
$$= 2(n(8st+2s+2t))((s+1)(t+1)+n(2s+1)(2t+1)-1)$$
$$-(64snt-10sn-8st-10nt-4n)$$
$$= 2n(8st+2s+2t)((s+1)(t+1)+n(2s+1)(2t+1)-1)-64snt-10sn+10nt+10st+4n.$$

Now, by using Equations (4),(6) and Theorem 5 second Zagreb coindex is computed as below:

$$\overline{M_2}(G) = \sum_{pq \notin E(G)} (d_p d_q)$$

$$\overline{M_2}(G) = 2|E(G)| - \frac{1}{2}M_1(G) - M_2(G)$$

$$= 2(n(8st + 2s + 2t))^2 - \frac{1}{2}(64snt - 10sn - 8st - 10nt - 4n)$$

$$- (128snt - 36sn - 32st - 36nt + 4s - 8n + 4t)$$

$$= 2n^2(8st + 2s + 2t)^2 - 160snt + 31sn + 41nt + 37st + 10n - 4s - 4t$$

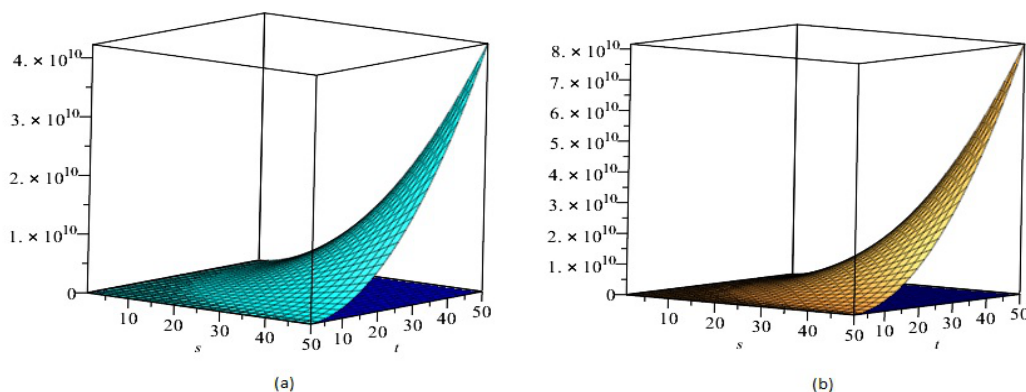(a)   (b)

Fig. 8 – Comparison of indices of $G \cong P\overline{4}m2BC_3[s,t,n]$ for fix $t = 10$: in (a) first Zagreb index $M_1(G)$ and first Zagreb coindex

$\overline{M}_1(G)$ are compared. The blue and cyan colors represents $M_1(G)$ and $\overline{M}_1(G)$, respectively. Its easy to see that in the given

domain $\overline{M}_1(G)$ is more dominating. In (b) second Zagreb index $M_2(G)$ and second Zagreb coindex $\overline{M}_2(G)$ are compared. The red

and gold colors represents $M_2(G)$ and $\overline{M}_2(G)$, respectively. Its easy to see that in the given domain $\overline{M}_2(G)$ is more dominating.

over the values of $\overline{M}_2(G)$ are largest and the values of $M_1(G)$ are smallest.

The Table 6 shows the edge partition of the chemical graph $P\overline{4}m2BC_3[s,t,n]$, $s, t, n \geq 2$ based on the degree sum of end vertices of each edge. The next Theorem shows the exact value of Sanskruti index of $P\overline{4}m2BC_3[s,t,n]$, $s, t, n \geq 2$.

Table 6

Edge partition of $P\overline{4}m2BC_3[s,t,n]$ based on degree sum of end vertices of each edge

(S_p, S_q)	Frequency
(7,3)	8
(11,4)	$2(s + t - 4)$
(7,6)	8
(8,6)	$4(s + t) - 16$
(9,6)	$8(n - 1)$
(12,8)	$4(s - 1)(t - 1)$
(10,9)	$8(n - 1)$
(10,10)	$4(n - 1)(t + s - 1)$
(12,7)	$8n$
(14,8)	$2n(s + t - 4)$
(15,10)	$2(n - 1)(s + t - 2)$
(14,11)	8
(15,11)	$4(s + t - 4)$
(15,12)	$2(s + t - 4)$
(16,12)	$4(t - 2)(s - 2)$
(14,15)	$8(n - 1)$
(15,15)	$4(n - 1)(s + t - 4)$
(15,16)	$4(n - 1)(s + t - 4)$
(16,16)	$8snt - 14sn - 8st - 14nt + 14s + 28n + 14t - 28$

Theorem 5.3. Consider the graph $G \cong TiF_2[m,n,t]$ with $m,n,t \geq 2$, then its Sanskruti index $S(G)$ is equal to

$$S(G) = \frac{2349621566328732}{983590583625}n + \frac{10515259523357}{949104000}t + \frac{10515259523357}{949104000}s + \frac{43904}{125}n(s+t-4)$$
$$- \frac{29360128}{3375}sn - \frac{29360128}{3375}nt + \frac{16777216}{3375}snt - \frac{16777216}{3375}st + \frac{4096(4s-4)(t-1)}{27}$$
$$+ \frac{49066953842012 5(4n-4)(s+t-4)}{390297362112} + \frac{3375000(2n-2)(s+t-2)}{12167} + \frac{884736(4t-8)(s-2)}{(2197}$$
$$- \frac{6799657069268862335998539}{2033852310824309008300}$$

Proof. Let G be the crystallographic structure of $TiF_2[m,n,t]$. Then by using Table 4 and equation (7) the Sanskruti index $S(G)$ is computed as follows.

$$S(G) = \sum_{pq \in E(G)} \left(\frac{S_p \times S_q}{S_p + S_q - 2}\right)^3$$

$$S(G) = (8)\left(\frac{7 \times 3}{7+3-2}\right)^3 + 2(s+t-4)\left(\frac{11 \times 4}{11+4-2}\right)^3 + (8)\left(\frac{7 \times 6}{7+6-2}\right)^3$$
$$+ (4(s+t)-16)\left(\frac{8 \times 6}{8+6-2}\right)^3 + 8(n-1)\left(\frac{9 \times 6}{9+6-2}\right)^3 + 4(s-1)(t-1)\left(\frac{12 \times 8}{12+8-2}\right)^3$$
$$+ 8(n-1)\left(\frac{10 \times 9}{10+9-2}\right)^3 + 4(n-1)(t+s-4)\left(\frac{10 \times 10}{10+10-2}\right)^3 + 8n\left(\frac{12 \times 7}{12+7-2}\right)^3$$

$$+ 2n(s+t-4)\left(\frac{14 \times 8}{14+8-2}\right)^3 + 2(n-1)(s+t-2)\left(\frac{15 \times 10}{15+10-2}\right)^3 + 8\left(\frac{14 \times 11}{14+11-2}\right)^3$$
$$+ 4(s+t-4)\left(\frac{15 \times 11}{15+11-2}\right)^3 + 2(s+t-4)\left(\frac{15 \times 12}{15+12-2}\right)^3 + 4(t-2)(s-2)\left(\frac{16 \times 12}{16+12-2}\right)^3$$
$$+ 8(n-1)\left(\frac{14 \times 15}{14+15-2}\right)^3 + 4(n-1)(s+t-4)\left(\frac{15 \times 15}{15+15-2}\right)^3$$
$$+ 4(n-1)(s+t-4)\left(\frac{15 \times 16}{15+16-2}\right)^3$$
$$+ (8snt - 14sn - 8st - 14nt + 14s + 28n + 14t - 28)\left(\frac{16 \times 16}{16+16-2}\right)^3$$

$$= \frac{2349621566328732}{983590583625}n + \frac{10515259523357}{949104000}t + \frac{10515259523357}{949104000}s + \frac{43904}{125}n(s+t-4)$$
$$- \frac{29360128}{3375}sn - \frac{29360128}{3375}nt + \frac{16777216}{3375}snt - \frac{16777216}{3375}st + \frac{4096(4s-4)(t-1)}{27}$$
$$+ \frac{49066953842012 5(4n-4)(s+t-4)}{390297362112} + \frac{3375000(2n-2)(s+t-2)}{12167} + \frac{884736(4t-8)(s-2)}{2197}$$
$$- \frac{6799657069268862335998539}{2033852310824309008300}$$

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, crystallographic structure of cuprite Cu_2O and Boron-Carbon crystal structure of $P\bar{4}m2BC_3[s,t,n]$. The exact results have been computed of the first and second Zagreb indices, first and second Zagreb coindices and Sanskruti index for TiF_2, Cu_2O and $P\bar{4}m2BC_3[s,t,n]$.

The graphical representations of Zagreb indices of $Cu_2O[m,n,t]$ and $TiF_2[m,n,t]$ are depicted in Figure 3 and Figure 5 for certain values of (m,n) and fix t. By varying the value of m,n the Zagreb indices behaves differently. The graphical representations of Zagreb indices of $P\bar{4}m2BC_3[s,t,n]$ are depicted in Figure 5 for certain values of s,t and fix n. By varying the value of s,t the Zagreb indices behaves differently.

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