

Investigation of some new results of entropy for titanium difluoride

Muhammad Kamran Naseer [†]

Department of Mathematics

Lahore Leads University

Lahore 54000

Pakistan

Bushra Kadhum Awaad [‡]

Department of Mathematics

College of Education for Pure Sciences

University of Kerbala

Karbala 56001

Iraq

Hayder Abdulameer Yousif Al-Iessa [§]

Department of Computer Engineering

Institute of Graduate Programs

Al-Turath University

Al Mansour

Baghdad 10013

Iraq

Muhammad Saqlain Zaki [‡]

Department of Mathematics

COMSATS University Islamabad

Sahiwal Campus

Sahiwal 57000

Pakistan

[†] ORCID-ID: 0000-0002-1846-3877

[‡] ORCID-ID: 0009-0003-8224-5393

[§] ORCID-ID: 0009-0005-8362-0524

[‡] ORCID-ID: 0000-0002-3671-1643

[†] E-mail: kamrannaseer92@gmail.com

[‡] E-mail: Bushra.k@uokerbala.edu.iq

[§] E-mail: hayder.abdulameer@uoturath.edu.iq

[‡] E-mail: saqlainsaqisial786@gmail.com

Abdul Waheed [@]

*Department of Mathematics
University of Peshawar
District Peshawar
Khyber-Pakhtunkhwa 24840
Pakistan*

Sumit Kaushal [#]

*Institute of Engineering and Technology
Centre for Research Impact & Outcome
Chitkara University
Rajpura 140401
Punjab
India*

Zuhra Muter Saleh ^{\$}

*Department of Pharmacy
Al-Manara College For Medical Sciences
Maysan 62006
Iraq*

Wissam Aziz Yousif [^]

*Department of Medical Laboratories Technology
Al-Nisour University College
Nisour Seq. Karkh
Baghdad 10013
Iraq*

Misbah Arshad [%]

*Department of Mathematics
COMSATS University Islamabad
Sahiwal Campus
Sahiwal 57000
Pakistan*

[@] ORCID-ID: 0009-0003-0137-5146

[#] ORCID-ID: 0009-0003-3286-7194

^{\$} ORCID-ID: 0000-0002-6690-848X

[^] ORCID-ID: 0000-0002-6162-8198

[%] ORCID-ID: 0000-0002-7225-8786

[@] E-mail: Waheeduop22@outlook.com

[#] E-mail: Sumit_Kaushal1@outlook.com

^{\$} E-mail: zuhramutersaleh@uomanara.edu.iq

[^] E-mail: wissam.rad@nuc.edu.iq

[%] E-mail: misbah@cuisahiwal.edu.pk

Mohammad Reza Farahani [&]

Mehdi Alaeiyan ^{*}

Department of Mathematics and Computer Science

Iran University of Science and Technology (IUST)

Narmak 16844

Tehran

Iran

Murat Cancan [~]

Department of Mathematics

Faculty of Education

Yuzuncu Yil University

Van

Turkey

Abstract

In this study, we delve into the evaluation of graph entropy through the lens of topological properties inherent in crystallographic structures. Specifically, we focus on the crystallographic structure of $TiF_2[i,j,t]$ (Figure 1). By employing various topological indices to compute the entropies of $TiF_2[i,j,t]$. This comprehensive approach allows for a deeper understanding of the entropy characteristics of this particular crystallographic structure, offering insights into its inherent properties.

Subject Classification (2020): 05C85, 05C90, 05C62, 05C12.

Keywords: Entropy, First zagreb index, Second zagreb index, Modified second zagreb index, Augmented zagreb Index, Hyper zagreb 2nd index, Entropies of $TiF_2[i,j,t]$ crystallographic structure, Entropy of $TiF_2[i,j,t]$.

Introduction

The solution of the seven-bridge problem by Leonhard Euler marked the beginning of graph theory. Seven bridge-related puzzles were resolved by Leonhard Euler in 1735. Concerning graphs and structure, graph theory is a significant area of practical mathematics. A graph is any item that consists of

[&] ORCID-ID: 0000-0003-2969-4280

^{*} ORCID-ID: 0000-0003-2185-5967

[~] ORCID-ID: 0000-0002-8606-2274

[&] E-mail: mohammad_farahani@mathdep.iust.ac.ir;
mrfarhani88@gmail.com

^{*} E-mail: alaeiyan@iust.ac.ir (Corresponding Author)

[~] E-mail: mcancan@yyu.edu.tr

points and connections. A directed graph, sometimes called a digraph, is a graph in which all of the connections are one-way.

Graph theory has use in several domains of life. In computer science, for instance, a network of communication, computing devices, data organisation, computation flow, etc. are all constructed and displayed using graphs. In physics, biology, and chemistry, it is also employed to investigate the characteristics of molecules. Real numbers represent topological indices for any graph of compounds and graph networks. The characteristics of intriguing substances are predicted using the topological index, which is invariant. In the subject of hem informatics, topological indices in conjunction with the quantitative structure-property and quantitative structure-activity relationships are required to research the characteristics and chemical bioactivity of substances. Numerous applications in network theory are also supported by polynomials, such as topological indices. The Wiener polynomial, also known as the Hosoya polynomial [1], for instance, aids in the creation of topological indices that are dependent on distance. The M-polynomial was first presented to determine degree-dependent topological indices. In chemistry, the valence and degree have a tight relationship [2]. It is possible to clarify the entire narrative by saying that the topological index functions as a function that gives a real number to each molecule structure. First and second Zagreb indices are degree-based graph invariants that have been extensively explored since the 1970s. We go over several kinds of graph indices below.

Definition 2.1: [3] The First Zagreb index is defined as $M_1(G) = \sum_{st \in E(G)} (d_s + d_t)$

Definition 2.2: [3] The Second Zagreb index is represented by $M_2(G)$ and it's defined as $M_2(G) = \sum_{st \in E(G)} (d_s \cdot d_t)$

Definition 2.3: [4] The modified second Zagreb index is denoted by ${}^mM_2(G)$ and it's defined as ${}^mM_2(G) = \sum_{st \in E(G)} \frac{1}{d_s \cdot d_t}$

Definition 2.4: [5] Augmented Zagreb Index is represented by $AZI(G)$ and it's defined as $AZI(G) = \sum_{st \in E(G)} \left(\frac{d_s d_t}{d_s + d_t - 2} \right)^3$

Definition 2.5: [6] Hyper Zagreb 2nd Index is denoted by $H_2(G)$ and it's defined as $H_2(G) = \sum_{st \in E(G)} (d_s \cdot d_t)^2$

Definition 2.6: Suppose that we have a probability density function $P_{ij} = \frac{w(st)}{\sum w(st)}$

In [7, 8], The entropy for any graph G is defined as $I(G, w) = -\sum P_{ij} \log(P_{ij})$

Chemical Graph Theory is a significant area of graph theory. It works with chemistry-related graphs. Graph theory is the study of graphs in mathematics.

Graphs are the main subjects of study in discrete mathematics. Mathematical constructs called graphs are used to study pairwise relationships between items.

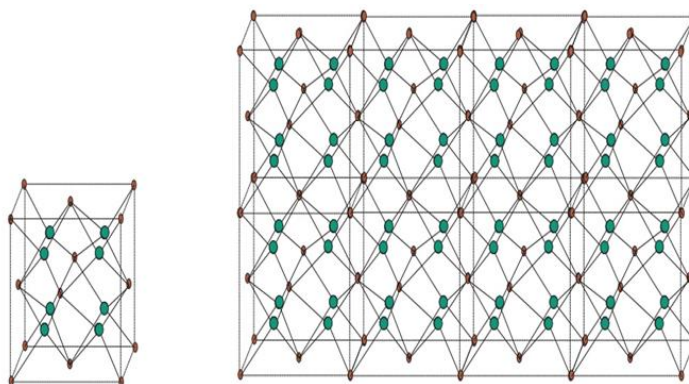


Figure 1

Crystal structure titanium difluoride $TiF_2[i,j,t]$. (a) The unit cell of $TiF_2[i,j,t]$ with Ti atoms in red and F atoms in green. (b) Crystal structure of $TiF_2[4,1,2]$.

In recent years Chemical graph theory has fascinated increasing research interest. In 1988, a number of scholars published about 500 publications a year, all of which were with chemical graph theory. Chemical indices in graph theory, which have their roots in chemistry and provide findings that chemists utilize, emerged as the most significant theme across a wide range of works. The Wiener index, general hyper-Wiener index, Randic index, harmonic index, sum-connectivity index, general Randic index, general sum connectivity index, and the first and second Zagreb indices are a few well-known chemical indicators [9-13]. In the middle of the 20th century, theoretical chemists discovered important knowledge on several aspects of organic material's molecular structure. By examining correctly constructed invariants of the underlying molecular graph, these molecular structures may be identified. Graph invariants that are useful for chemical determinations are known as topological indices. For the quantitative structure-property relation (QSPR) and the quantitative structure-activity relation (QSAR), several topological indices are crucial to employ [14-29]. Structure refers to the molecular structure in this context, while property refers to any physical or chemical feature.

Results and Discussion

In this section, we will find the entropy of chemical structure by using some topological indices.

Table 1

Edge partition of $TiF_2[i,j,t] \geq 1$ based on the degrees of end vertices of each edge.

(d_s, d_t)	Frequency	Set of dges
(1,4)	8	E_1

(2,4)	$8(i+j+t-3)$	E_2
(4,4)	$16(ij+it+jt)-16(i+j+t)-24$	E_3
(4,8)	$32ijt-16(ij+it+jt)+8(i+j+t)-8$	E_4

We can now immediately obtain the following results from this edge partition from Table 1.

Theorem 4.1: *The entropy of $TiF_2[i,j,t] \geq 1$ with first Zagreb Index is*

$$I(TiF_2[i,j,t], M_1) = \log \left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right] - \frac{1}{\left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right]} \left[\begin{array}{l} 414.40559848(ijt) - \\ 91.60728(ij + it + jt) + \\ 22.35714(i + j + t) - \\ 14.3031 \end{array} \right]$$

Proof: By definition 1. We have $M_1(TiF_2[i,j,t]) = 8[(48ijt - 8(ij + it + jt) + 2(i + j + t) - 1)]$

$$I(TiF_2, M_1) = \log \left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right] - \frac{1}{\left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right]} \left[\begin{array}{l} (1 + 4)|E_1| \log(1 + 4) + \\ (2 + 2)|E_2| \log(2 + 4) + \\ (4 + 4)|E_3| \log(4 + 4) + \\ (4 + 8)|E_4| \log(4 + 8) \end{array} \right]$$

$$I(TiF_2, M_1) = \log \left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right] - \frac{1}{\left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right]} \left[\begin{array}{l} (5)|E_1| \log(5) + \\ (6)|E_2| \log(6) + \\ (24)|E_3| \log(2) + \\ (12)|E_4| \log(12) \end{array} \right]$$

$$I(TiF_2, M_1) = \log \left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right] - \frac{1}{\left[\frac{8(48ijt - 8(ij + it + jt))}{+2(i + j + t) - 1} \right]}$$

$$\begin{aligned}
& \left[\begin{array}{c} \log 2(768ijt + 48(i+j+t) - \\ 192(i+j+t) + 56) + 384 \\ \log 3(384ijt - 192(ij+it+jt) + \\ 144(i+j+t) - 240) + \\ \log 5(40) \end{array} \right] \\
(TiF_2[i, j, t], M_1) = & \log \left[\begin{array}{c} 8(48ijt - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1) \end{array} \right] - \frac{1}{\left[\begin{array}{c} 8(48ijt - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1) \end{array} \right]} \\
& \left[\begin{array}{c} 414.40559848(ijt) - \\ 91.60728(ij + it + jt) + \\ 22.35714(i + j + t) - \\ 14.3031 \end{array} \right]
\end{aligned}$$

Theorem 4.2: The entropy of $TiF_2[i, j, t] \geq 1$ with second Zagreb Index is

$$\begin{aligned}
I(TiF_2, M_2) = & \log \left[\begin{array}{c} -32[(32ijt) - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1] \end{array} \right] - \frac{1}{\left[\begin{array}{c} -32[(32ijt - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1)] \end{array} \right]} \\
& \left[\begin{array}{c} 1541.273578(ijt) - \\ 462.382073(ij + it + jt) + \\ 134.861438(i + j + t) - \\ 850.108708 \end{array} \right]
\end{aligned}$$

Proof: By definition 1, we have $M_2(TiF_2) = -32[8ijt - 8(ij + it + jt) + 2(i + j + t) - 1]$

$$\begin{aligned}
I(TiF_2, M_2) = & \log \left[\begin{array}{c} -32[(32ijt) - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1] \end{array} \right] - \frac{1}{\left[\begin{array}{c} -32[(32ijt - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1)] \end{array} \right]} \\
& \left[\begin{array}{c} (1.4)|E_1| \log(1.4) + \\ (2.2)|E_2| \log(2.4) + \\ (4.4)|E_3| \log(4.4) + \\ (4.8)|E_4| \log(4.8) \end{array} \right] \\
I(TiF_2, M_2) = & \log \left[\begin{array}{c} -32[(32ijt) - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1] \end{array} \right] - \frac{1}{\left[\begin{array}{c} -32[(32ijt - \\ 8(ij + it + jt) \\ + 2(i + j + t) - 1)] \end{array} \right]} \\
& \left[\begin{array}{c} 8|E_1| \log(2) + \\ 24|E_2| \log 2 + \\ 64|E_3| \log 2 + \\ 160|E_4| \log 2 \end{array} \right]
\end{aligned}$$

$$I(TiF_2, M_2) = \log \left[\frac{-32[(32ijt) - 8(ij + it + jt) + 2(i + j + t) - 1]}{1} \right] - \frac{1}{\left[\frac{-32[(32ijt) - 8(ij + it + jt) + 2(i + j + t) - 1]}{1} \right]}$$

$$I(TiF_2[i, j, t], M_2) = \log \left[\frac{-32[(32ijt) - 8(ij + it + jt) + 2(i + j + t) - 1]}{1} \right] - \frac{1}{\left[\frac{-32[(32ijt) - 8(ij + it + jt) + 2(i + j + t) - 1]}{1} \right]}$$

$$\left[\log 2(64 + 64(16(ij + it + jt) + 24(8(i + j + t) - 3) - 16(i + j + t) - 24 + 160[32ijt - 16(ij + it + jt) + 8(i + j + t) - 8]) \right]$$

$$\left[\frac{1541.273578(ijt) - 462.382073(ij + it + jt) + 134.861438(i + j + t) - 850.108708}{1} \right]$$

Theorem 4.3: The entropy of $TiF_2[i, j, t] \geq l$ with modified 2nd Zagreb weight is

$$I(TiF_2, {}^m M_2) = \log \left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right] - \frac{1}{\left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right]}$$

$$\left[\frac{1.505149(ijt) + 1.956694(ij + it + jt) - 1.279376(i + j + t) + 5.719566}{1} \right]$$

Proof: By definition 1, we have ${}^m M_2(TiF_2) = \frac{1}{2}(2ijt + ij + it + jt + i + j + t)$

$$I(TiF_2, {}^m M_2) = \log \left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right] - \frac{\left[\frac{1}{14}|E_1| \log \frac{1}{14} + \frac{1}{22}|E_2| \log \frac{1}{22} + \frac{1}{44}|E_3| \log \frac{1}{44} + \frac{1}{48}|E_4| \log \frac{1}{48} \right]}{\left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right]}$$

$$= \log \left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right] - \frac{\left[\frac{1}{4}|E_1| \log \frac{1}{4} + \frac{1}{16}|E_2| \log \frac{1}{16} + \frac{1}{32}|E_3| \log \frac{1}{32} + \frac{1}{32}|E_4| \log \frac{1}{32} \right]}{\left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right]}$$

$$= \log \left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right] - \frac{\left[\log 2(-5ijt - \frac{3}{2}(ij + it + jt) - \frac{1}{4}(i + j + t) + \frac{39}{4}) \right]}{\left[\frac{ijt + \frac{1}{2}(ij + it + jt) + \frac{1}{4}(i + j + t) - \frac{19}{4}}{1} \right]}$$

Theorem 4.4: The entropy of $TiF_2[i,j,t] \geq l$ with Augmented Zagreb weight is

$$I(TiF_2, AZI) = \log(64ijt) - \frac{1}{64ijt} [57.797759ijt]$$

Proof: By definition 1, we have

$$AZI(TiF_2) = \left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right]$$

$$I(TiF_2, AZI)$$

$$\begin{aligned} &= \log \left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right] \\ &\quad - \left[\frac{\left(\frac{1.4}{1+4-2} \right)^3 |E_1| \log \left(\frac{1.4}{1+4-2} \right)^3 + \left(\frac{2.2}{2+2-2} \right)^3 |E_2| \log \left(\frac{2.2}{2+2-2} \right)^3}{\left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right]} \right. \\ &\quad \left. + \left(\frac{4.4}{4+4-2} \right)^3 |E_3| \log \left(\frac{4.4}{4+4-2} \right)^3 + \left(\frac{4.8}{4+8-2} \right)^3 |E_3| \log \left(\frac{4.8}{4+8-2} \right)^3 \right] \\ &= \log \left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right] \\ &\quad - \left[\frac{24 |E_1| \log 2 + 24 |E_2| \log 2 + 24 |E_3| \log 2}{\left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right]} \right] \\ &= \log \left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right] \\ &\quad - \left[\frac{24 \log 2 (8ijt)}{\left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right]} \right] \\ &= \log \left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right] \\ &\quad - \left[\frac{57.797759ijt}{\left[\frac{131072}{125}ijt - \frac{745472}{3375}(ij + it + jt) + \frac{40768}{125}(i + j + t) - \frac{1013912}{1125} \right]} \right] \end{aligned}$$

Theorem 4.5: The entropy of $TiF_2[i,j,t] \geq l$ with hyper Zagreb second weight is

$$I(TiF_2, H_2) = \log \left[\frac{512(ijt) - 192(ij + jt + it)}{+144(i + j + t) - 106} \right] - \frac{924.7641466798(ijt) - 376.28749458(ij + jt + it) + 317.8876754212(i + j + t) - 250.4569563924}{[512(ijt) - 192(ij + jt + it) + 144(i + j + t) - 106]}$$

Proof: By definition 1, we have

$$H_2(TiF_2) = [512(ijt) - 192(ij + jt + it) + 144(i + j + t) - 106]:$$

$$I(TiF_2, H_2)$$

$$\begin{aligned} &= \log \left[\frac{512(ijt) - 192(ij + jt + it)}{+144(i + j + t) - 106} \right] - \frac{[(1.2)^2 |E_1| \log (1.2)^2 + (2.2)^2 |E_2| \log (2.2)^2 + (2.4)^2 |E_3| \log (2.4)^2]}{[512(ijt) - 192(ij + jt + it) + 144(i + j + t) - 106]} \\ &= \log \left[\frac{512(ijt) - 192(ij + jt + it)}{+144(i + j + t) - 106} \right] - \frac{[8 |E_1| \log 2 + 64 |E_2| \log 2 + 384 |E_3| \log 2]}{[512(ijt) - 192(ij + jt + it) + 144(i + j + t) - 106]} \end{aligned}$$

$$\begin{aligned}
&= \log \left[\frac{512(ijt) - 192(ij + jt + it)}{+144(i+j+t) - 106} \right] - \frac{\left[\log 2(8|E_1| + 64|E_2| + 384|E_3|) \right]}{[512(ijt) - 192(ij + jt + it) + 144(i+j+t) - 106]} \\
&= \log \left[\frac{512(ijt) - 192(ij + jt + it)}{+144(i+j+t) - 106} \right] - \frac{\log 2(3072(ijt) - 1250(ij + jt + it) + 1056(i+j+t) - 832)}{[512(ijt) - 192(ij + jt + it) + 144(i+j+t) - 106]}
\end{aligned}$$

Table 2

Edge partition of $TiF_2[i, j, t] \geq 2$ based on the degrees of end vertices of each edge.

(d_s, d_t)	Frequency	Set of Edges
(2,4)	$4(i+j+t)-8$	E_1
(4,6)	$4(ij+it+jt)-8(i+j+t)+12$	E_2
(5,8)	$4(i+j+t)-8$	E_3
(6,8)	$4(ij+it+jt)-8(i+j+t)+12$	E_4
(8,8)	$8ijt-8(ij+it+jt)+8(i+j+t)-8$	E_5

We can now immediately obtain the following results from this edge partition from Table 2.

Theorem 4.6: The entropy of $TiF_2[i, j, t] \geq 2$ with first Zagreb Index is

$$I(TiF_2[i, j, t], M_1) = \log \left[\frac{128ijt - 32(ij + it + jt)}{+12(i+j+t) + 8} \right] - \frac{\left[154.1273578(ijt) - 49.9441878(ij + it + jt) + 22.3617021(i+j+t) + 5.2207836 \right]}{[128ijt - 32(ij + it + jt) + 12(i+j+t) + 8]}$$

Proof: By definition 1. We have $M_1(TiF_2) = (128ijt - 32(ij + it + jt) + 12(i + j + t) + 8)$:

$$I(TiF_2[i, j, t], M_1)$$

$$\begin{aligned}
&= \log \left[\frac{128ijt - 32(ij + it + jt)}{+12(i+j+t) + 8} \right] - \frac{\left[(2+4)|E_1| \log(2+4) + (4+6)|E_2| \log(4+6) + (5+8)|E_3| \log(5+8) + (6+8)|E_4| \log(6+8) + (8+8)|E_5| \log(8+8) \right]}{[128ijt - 32(ij + it + jt) + 12(i+j+t) + 8]} \\
&= \log \left[\frac{128ijt - 32(ij + it + jt)}{+12(i+j+t) + 8} \right] - \frac{\left[6|E_1| \log 6 + 10|E_2| \log 10 + 13|E_3| \log 13 + 14|E_4| \log 14 + 16|E_5| \log 16 \right]}{[128ijt - 32(ij + it + jt) + 12(i+j+t) + 8]} \\
&= \log \left[\frac{128ijt - 32(ij + it + jt)}{+12(i+j+t) + 8} \right] - \frac{\left[\log 6(24(i+j+t) - 48) + \log 10(40(ij + it + jt) - 80(i+j+t) + 120) + \log 13(52(i+j+t) - 104) + \log 14(56(ij + it + jt) - 112(i+j+t) + 158) + 112 \log 16(ijt - (ij + it + jt) + (i+j+t) - 1) \right]}{[128ijt - 32(ij + it + jt) + 12(i+j+t) + 8]}
\end{aligned}$$

Theorem 4.7: The entropy of $TiF_2[i, j, t] \geq 2$ with second Zagreb Index is

$$I(TiF_2[i, j, t], M_2) = \log \left[\frac{512ijt - 244(ij + it + jt)}{+128(i+j+t) - 32} \right] - \frac{\left[924.7641467(ijt) - 642.8588274(ij + it + jt) + 299.3954313(i+j+t) - 241.1605134 \right]}{[512ijt - 244(ij + it + jt) + 128(i+j+t) - 32]}$$

Proof: By definition 1, we have $M_2(TiF_2) = (512ijt - 244(ij + it + jt) + 128(i + j + t) - 32$:

$$\begin{aligned}
 I(TiF_2[i, j, t], M_2) &= \log \left[\frac{512ijt - 244(ij + it + jt)}{+128(i + j + t) - 32} \right] - \frac{\left[\begin{array}{l} (2.4)|E_1|\log(2.4) + (4.6)|E_2|\log(4.6) + \\ (5.8)|E_3|\log(5.8) + (6.8)|E_4|\log(6.8) + (8.8)|E_5|\log(8.8) \end{array} \right]}{[512ijt - 244(ij + it + jt) + 128(i + j + t) - 32]} \\
 &= \log \left[\frac{512ijt - 244(ij + it + jt)}{+128(i + j + t) - 32} \right] - \frac{\left[\begin{array}{l} 8|E_1|\log 8 + 24|E_2|\log 24 + \\ 40|E_3|\log 40 + 48|E_4|\log 48 + 64|E_5|\log 64 \end{array} \right]}{[512ijt - 244(ij + it + jt) + 128(i + j + t) - 32]} \\
 &= \log \left[\frac{512ijt - 244(ij + it + jt)}{+128(i + j + t) - 32} \right] - \frac{\left[\begin{array}{l} 8\log 8(4(i + j + t) - 8) + 24\log 24[4(ij + it + jt) - 8(i + j + t) + 12] \\ + 40\log 40(4(i + j + t) - 8) + 48\log 48[4(ij + it + jt) - 8(i + j + t) + 12] \\ + 64\log 64[8ijt - 8(ij + it + jt) + 8(i + j + t) - 8] \end{array} \right]}{[512ijt - 244(ij + it + jt) + 128(i + j + t) - 32]}
 \end{aligned}$$

Theorem 4.8: The entropy of $TiF_2[i, j, t] \geq 2$ with modified 2nd Zagreb weight is

$$\begin{aligned}
 I(TiF_2, {}^mM_2) &= \log \left[\frac{\frac{1}{8}(ijt)}{+ \frac{1}{8}(ij + it + jt)} \right] - \frac{1}{\left[\begin{array}{l} \frac{1}{8}(ijt) \\ + \frac{1}{8}(ij + it + jt) \\ + \frac{9}{40}(i + j + t) - \frac{23}{40} \end{array} \right]} \\
 &\quad \left[\begin{array}{l} -0.225742(ijt) - \\ 0.144366(ij + it + jt) - \\ 0.097246(i + j + t) + \\ 0.338859 \end{array} \right]
 \end{aligned}$$

Proof: By definition 1, we have ${}^mM_2(TiF_2) = \frac{1}{2}(2ijt + ij + it + jt + i + j + t)$

$$\begin{aligned}
 I(TiF_2, {}^mM_2) &= \log \left[\frac{\frac{1}{8}(ijt)}{+ \frac{1}{8}(ij + it + jt)} \right] - \frac{1}{\left[\begin{array}{l} \frac{1}{8}(ijt) \\ + \frac{1}{8}(ij + it + jt) \\ + \frac{9}{40}(i + j + t) - \frac{23}{40} \end{array} \right]} \\
 &\quad \left[\begin{array}{l} \frac{1}{2.4}|E_1|\log \frac{1}{2.4} + \frac{1}{4.6}|E_2|\log \frac{1}{4.6} + \\ \frac{1}{5.8}|E_3|\log \frac{1}{5.8} + \frac{1}{6.8}|E_4|\log \frac{1}{6.8} + \\ \frac{1}{8.8}|E_5|\log \frac{1}{8.8} \end{array} \right]
 \end{aligned}$$

$$\begin{aligned}
I(TiF_2, {}^mM_2) &= -\log \left[\begin{array}{c} \frac{1}{8}(ijt) \\ +\frac{1}{8}(ij+it+jt) \\ +\frac{9}{40}(i+j+t)-\frac{23}{40} \end{array} \right] + \frac{1}{\left[\begin{array}{c} \frac{1}{8}(ijt) \\ +\frac{1}{8}(ij+it+jt) \\ +\frac{9}{40}(i+j+t)-\frac{23}{40} \end{array} \right]} \\
&\quad \left[\begin{array}{c} \frac{1}{8}|E_1|\log \frac{1}{8} + \frac{1}{24}|E_2|\log \frac{1}{24} + \\ \frac{1}{40}|E_3|\log \frac{1}{40} + \frac{1}{48}|E_4|\log \frac{1}{48} + \\ \frac{1}{64}|E_5|\log \frac{1}{64} \end{array} \right] \\
I(TiF_2, {}^mM_2) &= -\log \left[\begin{array}{c} \frac{1}{8}(ijt) \\ +\frac{1}{8}(ij+it+jt) \\ +\frac{9}{40}(i+j+t)-\frac{23}{40} \end{array} \right] + \frac{1}{\left[\begin{array}{c} \frac{1}{8}(ijt) \\ +\frac{1}{8}(ij+it+jt) \\ +\frac{9}{40}(i+j+t)-\frac{23}{40} \end{array} \right]} \\
&\quad \left[\begin{array}{c} \frac{1}{8}\{4(i+j+t)-8\}\log \frac{1}{8} + \frac{1}{24}\{4(ij+it+jt)-8(i+j+t)+12\}\log \frac{1}{24} + \\ \frac{1}{40}\{4(i+j+t)-8\}\log \frac{1}{40} + \frac{1}{48}\{4(ij+it+jt)-8(i+j+t)+12\}\log \frac{1}{48} + \\ \frac{1}{64}\{8ijt-8(ij+it+jt)+8(i+j+t)-8\}\log \frac{1}{64} \end{array} \right] \\
I(TiF_2, {}^mM_2) &= \log \left[\begin{array}{c} \frac{1}{8}(ijt) \\ +\frac{1}{8}(ij+it+jt) \\ +\frac{9}{40}(i+j+t)-\frac{23}{40} \end{array} \right] - \frac{1}{\left[\begin{array}{c} \frac{1}{8}(ijt) \\ +\frac{1}{8}(ij+it+jt) \\ +\frac{9}{40}(i+j+t)-\frac{23}{40} \end{array} \right]} \\
&\quad \left[\begin{array}{c} -0.225742(ijt) - \\ 0.144366(ij+it+jt) - \\ 0.097246(i+j+t) + \\ 0.338859 \end{array} \right]
\end{aligned}$$

Theorem 4.9: The entropy of $TiF_2[i,j,t] \geq 2$ with Augmented Zagreb weight is (TiF_2, AZI)

$$= \log \left[\begin{array}{c} \frac{262144}{343}(ijt) - \frac{137292}{343}(ij+it+jt) \\ + \frac{95558696}{113533}(i+j+t) - \frac{55213740}{456533} \end{array} \right] - \left[\begin{array}{c} \frac{1513.37016310667(ijt) - 896.40080323762(ij+it+jt)}{+631.84083470165(i+j+t) - 367.28086616568} \\ \frac{262144}{343}(ijt) - \frac{137292}{343}(ij+it+jt) + \frac{95558696}{113533}(i+j+t) - \frac{55213740}{456533} \end{array} \right]$$

Proof: By definition 1, we have

$$\begin{aligned}
 AZI(TiF_2) &= \left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + jt + it) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right] \\
 (TiF_2, AZI) &= \log \left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + it + jt) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right] \\
 &\quad - \frac{\left[\left(\frac{2.4}{2+4-2} \right)^3 |E_1| \log \left(\frac{2.4}{2+4-2} \right)^3 + \left(\frac{4.6}{4+6-2} \right)^3 |E_2| \log \left(\frac{4.6}{4+6-2} \right)^3 + \left(\frac{5.8}{5+8-2} \right)^3 |E_3| \log \left(\frac{5.8}{5+8-2} \right)^3 + \right. \\
 &\quad \left. \left(\frac{6.8}{6+8-2} \right)^3 |E_3| \log \left(\frac{6.8}{6+8-2} \right)^3 + \left(\frac{8.8}{8+8-2} \right)^3 |E_3| \log \left(\frac{8.8}{8+8-2} \right)^3 \right]}{\left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + it + jt) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right]} \\
 (TiF_2, AZI) &= \log \left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + it + jt) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right] \\
 &\quad - \frac{\left[24|E_1| \log 2 + 81|E_2| \log 3 + \frac{576000}{1331}|E_3| \log 2 + \frac{192000}{1331}|E_3| \log 5 - \frac{192000}{1331}|E_3| \log 11 \right]}{\left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + it + jt) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right]} \\
 (TiF_2, AZI) &= \log \left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + it + jt) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right] \\
 &\quad - \frac{\left[\log 2 \left(\frac{3932160}{343}(ijt) - \frac{3405312}{343}(ij + it + jt) + \frac{4665334752}{456533}(i + j + t) - \frac{4798199232}{466533} \right) \right. \\
 &\quad \left. + \log 3(324(ij + it + jt) - 648(i + j + t) + 972) + \log 5 \left(\frac{768000}{1331}(i + j + t) - \frac{1536000}{1331} \right) \right. \\
 &\quad \left. - \log 7 \left(\frac{786432}{343} \right) ((ijt) - (ij + it + jt) + (i + j + t)) - \log 11 \left(\frac{768000}{1331}(i + j + t) - \frac{1536000}{1331} \right) \right]}{\left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + it + jt) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533} \right]}
 \end{aligned}$$

Theorem 4.10: The entropy of $TiF_2[i, j, t] \geq 2$ with hyper Zagreb second weight is

$$\begin{aligned}
 I(TiF_2, H_2) &= \log \left[32768(ijt) - 21248(ij + jt + it) + 16384(i + j + t) - 11520 \right] \\
 &\quad - \frac{\left[118369.81077500801(ijt) - 84201.16558679765(ij + jt + it) + \right. \\
 &\quad \left. 62143.92246597906(i + j + t) - 40086.67934516046 \right]}{\left[32768(ijt) - 21248(ij + jt + it) + 16384(i + j + t) - 11520 \right]}
 \end{aligned}$$

Proof: By definition 1, we have

$$\begin{aligned}
 H_2(TiF_2) &= [32768(ijt) - 21248(ij + jt + it) + 16384(i + j + t) - 11520] \\
 (TiF_2, H_2) &= \log \left[\frac{32768(ijt) - 21248(ij + jt + it) + 16384(i + j + t) - 11520}{1} \right] - \frac{1}{\left[\frac{32768(ijt) - 21248(ij + jt + it) + 16384(i + j + t) - 11520}{1} \right]}
 \end{aligned}$$

$$\begin{aligned}
I(TiF_2, H_2) &= \log \left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right] - \frac{1}{\left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right]} \\
&\quad \left[\begin{array}{c} (2.4)^2 |E_1| \log(2.4)^2 + \\ (4.6)^2 |E_2| \log(4.6)^2 + \\ (5.8)^2 |E_3| \log(5.8)^2 + \\ (6.8)^2 |E_4| \log(6.8)^2 + \\ (8.8)^2 |E_5| \log(8.8)^2 \end{array} \right] \\
I(TiF_2, H_2) &= \log \left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right] - \frac{1}{\left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right]} \\
&\quad \left[\begin{array}{c} 128 |E_1| \log(8) + \\ 1152 |E_2| \log(24) + \\ 3200 |E_3| \log(40) + \\ 4608 |E_4| \log(48) + \\ 8192 |E_5| \log(64) \end{array} \right] \\
I(TiF_2, H_2) &= \log \left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right] - \frac{1}{\left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right]} \\
&\quad \left[\begin{array}{c} 128 \log 8 (4(i + j + t) - 8) + \\ 1152 \log 24 \left[\begin{array}{c} 4(ij + it + jt) - \\ 8(i + j + t) + 12 \end{array} \right] + \\ 3200 \log 40 (4(i + j + t) - 8) + \\ 4608 \log 48 \left[\begin{array}{c} 4(ij + it + jt) - \\ 8(i + j + t) + 12 \end{array} \right] + \\ 8192 \log 64 \left[\begin{array}{c} 8ijt - 8(ij + it + jt) + \\ 8(i + j + t) - 8 \end{array} \right] \end{array} \right] \\
I(TiF_2, H_2) &= \log \left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right] - \frac{1}{\left[\begin{array}{c} 32768(ijt) - \\ 21248(ij + jt + it) + \\ 16384(i + j + t) \\ -11520 \end{array} \right]} \\
&\quad \left[\begin{array}{c} 118369.8107750(ijt) - \\ 84201.1655868(ij + jt + it) + \\ 62143.922466(i + j + t) - \\ 40086.6793452 \end{array} \right]
\end{aligned}$$

Conclusion

In this paper, we studied crystallographic structure cu_2o . We work on the structure of Crystallographic Structure $TiF_2[i,j,t]$ and apply the definition of entropy to it. In particular, we compute the entropy for Crystallographic

Structure $TiF_2[i,j,t]$ by using some topological indices as weight such as First Zagreb index, Second Zagreb index, modified second Zagreb index, Augmented Zagreb Index, Hyper Zagreb 2nd Index, and using this result we compute general results of entropies for $TiF_2[i,j,t]$.

References

- [1] I. Gutman, Some properties of the Wiener polynomials, *Graph Theory Notes New York*, vol. 125, pp. 13-18 (1993).
- [2] M. Munir, W. Nazeer, Z. Shahzadi, and S. Kang, "Some Invariants of Circulant Graphs," *Symmetry*, vol. 8, no. 11, pp. 134-134 (2016). [Online] Available: <https://doi.org/10.3390/sym8110134>.
- [3] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535-538, Dec. (1972). [Online] Available: [https://doi.org/10.1016/0009-2614\(72\)85099-1](https://doi.org/10.1016/0009-2614(72)85099-1).
- [4] A. Miličević, S. Nikolić, and N. Trinajstić, "On reformulated Zagreb indices," *Molecular Diversity*, vol. 8, no. 4, pp. 393-399 (2004). [Online] Available: <https://doi.org/10.1023/b:modi.0000047504.14261.2a>.
- [5] B. Furtula, A. Graovac, and D. Vukičević, "Augmented Zagreb index," *J. Math. Chem.* vol. 48, no. 2, pp. 370-380, Apr. (2010). [Online] Available: <https://doi.org/10.1007/s10910-010-9677-3>.
- [6] G.H Shirdel, H. Rezapour, and A.M. Sayadi, "The Hyper-Zagreb Index of Graph Operations," *Iranian J. Math. Chem.*, vol. 4, no. 2, pp. 213-220 (2013). [Online] Available: <https://doi.org/10.22052/ijmc.2013.5294>.
- [7] D. Vukicevic, and M. Gaperov, "Bond Additive Modeling 1. Adriatic Indices," *Croatica Chemica Acta*, vol. 83, no. 3, pp. 243-260, Oct. (2010).
- [8] D. Crescenzo and M. Longobardi, "On Weighted Residual and Past Entropies," arXiv (Cornell University) (2007). [Online] Available: <https://doi.org/10.48550/arxiv.math/0703489>.
- [9] M. Randic, "Characterization of molecular branching," *J. Am. Chem. Soc.* vol. 97, no. 23, pp. 6609-6615 (1975). [Online] Available: <https://doi.org/10.1021/ja00856a001>.
- [10] M.S. Zakir, M. Arshad, M.K. Naseer, and M. Cancan, One Study of Weighted Entropy Based on Topological Indices for Triazine-Based Dendrimer: A Mathematical Chemistry Approach. *Eur. Chem. Bull.*

- vol. 12, no. 1, pp. 2770-2788 (2023). [Online] Available: <https://doi.org/10.31838/ECB/2023.12.s1-B.277>.
- [11] M.S. Zakir, M. Arshad, M.K. Naseer, Z. Kanwal, I. Ahmad, and M. Cancan, Evaluation of Weighted Entropies Based on Topological Indices for Poly Propyl Ether Imine Dendrimers. *Eur. Chem. Bull.*, vol. 12, no. 8, pp. 7120-7130 (2023).
- [12] W. Gao and M.R. Farahani, "The hyper-zagreb index for an infinite family of nanostar dendrimer," *J. Discrete Math. Sci. Cryptography*, vol. 20, no. 2, pp. 515-523 (2017). [Online] Available: <https://doi.org/10.1080/09720529.2016.1220088>.
- [13] W. Gao, L. Shi, and M.R. Farahani. Distance-Based Indices for Some Families of Dendrimer Nanostars. " *IAENG Int. J. Appl. Math.*, 46(2), 168-186 (2016).
- [14] J.-B. Liu, A.Q. Baig, M. Imran, W. Khalid, M. Saeed, and M.R. Farahani, "Computation of bond incident degree (BID) indices of complex structures in drugs," *Eurasian Chemical Communications*, vol. 2, no. 6, pp. 672-679 (2020). [Online] Available: <https://doi.org/10.33945/sami/ecc.2020.6.4>.
- [15] M.R. Farahani, A.Q. Baig and W.Sajjad. The second eccentric Zagreb index of the Nth growth of nanostar dendrimer D3[N]. *J. Math. Nanosci.* vol. 7, no. 1, pp. 23-28 (2017). [Online] Available: <https://doi.org/10.22061/jmns.2017.670>.
- [16] M. Cancan, S. Ediz, H. Mutee-Ur-Rehman, and D. Afzal, "M-polynomial and topological indices Poly (EThyleneAmidoAmine) dendrimers," *J Inform Optim Sci.*, vol. 41, no. 4, pp. 1117-1131 (2020). [Online] Available: <https://doi.org/10.1080/02522667.2020.1745383>.
- [17] A.J.M. Khalaf, A. Javed, M.K. Jamil, M. Alaeiyan, and M.R. Farahani, "Topological properties of four types of porphyrin dendrimers," *Proyecciones (Antofagasta)*, vol. 39, no. 4, pp. 979-993 (2020). [Online] Available: <https://doi.org/10.22199/issn.0717-6279-2020-04-0061>.
- [18] M. Imran, M.K. Siddiqui, S. Ahmad, M.F. Hanif, M.H. Muhammad, and M.R. Farahani, "Topological properties of benzenoid, phenylenes and nanostar dendrimers," *J. Discrete Math. Sci. Cryptography*, vol. 22, no. 7, pp. 1229-1248 (2019). [Online] Available: <https://doi.org/10.1080/09720529.2019.1701267>.
- [19] M. Alaeiyan, F. Afzal, M.R. Farahani, and M.A. Rostami, "An exact formulas for the Wiener polarity index of nanostar dendrimers," *J*

- Inform Optim Sci.*, vol. 41, no. 4, pp. 933-939 (2020). [Online] Available: <https://doi.org/10.1080/02522667.2020.1748274>.
- [20] M.K. Hashmi, F. Chaudhry, A. Jalil, and M.R. Farahani, "Investigation of dendrimer structures by means of reverse atomic bond connectivity index," *J. Discrete Math. Sci. Cryptography*, vol. 24, no. 2, pp. 473-485 (2021). [Online] Available: <https://doi.org/10.1080/09720529.2021.1882161>.
- [21] I.G. Farkoush, M. Alaeiyan, M.R. Farahani, and M. Maghasedi, "Computing the Narumi-Katayama Index and Modified Narumi-Katayama Index of Some Families of Dendrimers and Tetrathiafulvalene," *J. Math.*, vol. 2021, pp. 1-3 (2021). [Online] Available: <https://doi.org/10.1155/2021/8492991>.
- [22] W. Zhao, M.C. Shanmukha, A. Usha, M.R. Farahani, and K.C. Shilpa, "Computing SS Index of Certain Dendrimers." *J. Math.* vol. 2021, pp. 1-14 (2021). [Online] Available: <https://doi.org/10.1155/2021/7483508>.
- [23] H. Yang, M. Naeem, A.Q. Baig, H. Shaker, and M.K. Siddiqui, "Vertex Szeged index of crystal cubic carbon structure," *J. Discrete Math. Sci. Cryptography*, vol. 22, no. 7, pp. 1177-1187 (2019). [Online] Available: <https://doi.org/10.1080/09720529.2019.1688966>.
- [24] M. Imran, M. Naeem, A. Q. Baig, M.K. Siddiqui, M.A. Zahid, and W. Gao, "Modified eccentric descriptors of crystal cubic carbon," *J. Discrete Math. Sci. Cryptography*, vol. 22, no. 7, pp. 1215-1228 (2019). [Online] Available: <https://doi.org/10.1080/09720529.2019.1700922>.
- [25] M. Imran, M.R. Farahani, M. Cancan, M. Alaeiyan, and A. Akgöl, "On topological indices of certain families of graphs," *Physica Scripta*, vol 100, pp. 1-14 (2024). [Online] Available: <https://doi.org/10.1088/1402-4896/ad9065>.
- [26] L. Ragoub, A. Baby, D.A. Xavier, M.U. Ghani, E.S. Varghese, T.Nair, M.R. Farahani and M. Cancan. "Molecular Descriptors Of Certain Class Of Carbon Nanocone Networks Through Quotient Graph Approach," *J. Comb. Math. Comb. Comput.* vol. 120, pp. 301-313. [Online] Available: <https://doi.org/10.61091/jcmcc120-027>.
- [27] M.S. Zakir, M.K. Naseer, M.R. Farahani, I. Ahmad, Z. Kanwal, M. Alaeiyan and M. Cancan. "On Exploring the Topological Aspects of the Chemical Structure of the Nanotube HAC5C7[w;t]. *Utilitas Mathematica*, vol. 119, no. 1, pp. 17-24 (2024). [Online] Available: <https://doi.org/10.61091/um119-03>.

- [28] N. Nigar, S.M. Alam, M.W. Rasheed, M.R. Farahani, M. Alaeiyan and M. Cancan, "On Ve-Degree and Ev-Degree Based Topological Invariants of Chemical Structures," *Utilitas Mathematica*, vol. 119, no. 1, pp. 25-35, Mar. (2024). [Online] Available: <https://doi.org/10.61091/um119-04>.
- [29] M.C. Shanmukha, A. Usha, M.R. Farahani, M. Alaeiyan, and M. Cancan, "Numerical Descriptors of Top Ranked Zinc Databased Inhibitors of Sars Cov-2," *Archives des Sciences.*, vol. 74, no. 3, pp. 51-55 (2024). [Online] Available: <https://doi.org/10.62227/as/74309>.

Received February, 2025