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GRAPH-THEORETICAL APPROACHES TO ENTROPY IN CU_2O CRYSTALLINE STRUCTURES: IMPLICATIONS FOR BIOMEDICAL AND ENERGY APPLICATIONS

SORAN NOORI SALEH[1], MUHAMMAD KAMRAN NASEER[2], NASIR ALI[3,*], ÜMIT KARABIYIK[4,*], MUHAMMAD SAQLAIN ZAKIR[4], MISBAH ARSHAD[5]

[1]Ministry of Education, General Directorate of Education of Sulaimani, Directorate of Education Chamchamal, Chamchamal, Iraq

[2]Department of Mathematics, Lahore Leads University, Lahore, Pakistan

[3]Department of Mathematics, COMSATS University Islamabad, Vehari Campus, Vehari, 61100, Pakistan

[4]Department of Mathematics and Computer Science, Necmettin Erbakan University, Konya, Turkey

[5]Department of Mathematics, COMSATS University Islamabad, Sahiwal Campus, Sahiwal, 57000, Pakistan

Abstract: In molecular science, understanding the intricate connections between molecular structures and their biomedical and pharmacological properties has been a focal point of research, aided by experimental and computational approaches. A key tool in this exploration is the use of Topological Indices, which are numerical descriptors that reveal fundamental characteristics of molecular frameworks. These indices are particularly crucial in predicting the biological activity of new chemical compounds and pharmaceuticals by quantifying weighted entropies. In this study, we examine the concept of graph entropy in relation to the topological properties of the copper oxide crystalline structure $(Cu_2O[i,j,t])$. Our goal is to unravel the mathematical complexity of $Cu_2O[i,j,t]$ by integrating entropy with various topological indices, including weighted measures. We also present a graphical comparison that illustrates the interplay between these computed indices and their corresponding entropies, offering new insights into the structural and mathematical elegance of $Cu_2O[i,j,t]$. This analysis broadens our understanding

*Corresponding author
E-mail address: nasirzawar@gmail.com
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of the material's potential applications across fields such as chemical sensors, solar cells, photocatalysis, and energy storage, where the unique crystallography of Cu_2O plays a pivotal role.

Keywords*:* entropy; crystallography review; topological indices; entropy measure; weighted entropies of $cu_2o[i, j, t]$; crystallographic structure; entropy of $cu_2o[i, j, t]$; graph theory.

2020 AMS Subject Classification: 05C30, 92E10.

1. INTRODUCTION

Graph theory, the foundation of which can be traced back to Leonhard Euler's ingenious solution to the Seven Bridges Problem in 1735, stands as a crucial branch of applied mathematics that revolves around the study of graphs and their structural intricacies.

In mathematical terms, graph theory delves into the realm of graphs, which are fundamental objects of investigation in discrete mathematics. A graph is essentially a collection of vertices (also known as nodes) interconnected by edges (the connecting lines). These graphs serve as versatile mathematical structures, enabling us to explore the relationships between pairs of objects. When all connections within a graph are one-way, it is referred to as a directed graph or a digraph.

The significance of graph theory extends to a multitude of fields. In the realm of computer science, graphs play a pivotal role in constructing and illustrating communication networks, computational devices, data organization, and the flow of computations, among other applications. Moreover, this mathematical framework finds its utility in studying the properties of molecules in fields such as chemistry, physics, and biology. Readers may see the applications of graph theory in [24,25,26,27]. The quantification of weighted entropies through these indices offers a robust framework for anticipating relevant characteristics, thereby contributing to the advancement of medical and pharmaceutical applications see [24].

One intriguing aspect of graph theory is the concept of topological indices, which are real numbers associated with compounds and graph networks. These indices are instrumental in predicting the properties of various compounds and remain constant, making them valuable tools in chemoinformatics. To delve into the properties and chemical bioactivity of compounds, scientists rely on quantitative structure-property relationships and structure-activity relationships, often in conjunction with topological indices.

In the realm of network theory, various polynomials, such as the Wiener polynomial and the Hosoya polynomial [1], come into play, enabling the creation of distance-dependent topological indices. For degree-dependent topological indices, the M-polynomial has been introduced, closely intertwined with the concept of valence in chemistry [2]. This amalgamation of graph theory and chemistry has been instrumental in assigning each molecular structure a real number, paving the way for the study of compounds' properties.

Since the 1970s, degree-based, invariant graphs, known as the First and Second Zagreb indices, have garnered extensive attention and study. Moreover, We demonstrate the relevance of topological indices-based entropy calculations in facilitating accurate QSAR estimations, particularly in the domain of antiparasitic drug development. Our findings underscore the utility of these methods for enhancing predictive modeling and contributing to advancements in drug discovery.

The investigation conducted by the researchers involves the computation of entropy-based graphical indices for the crystallographic structure of molecular copper oxide. The methods employed and the results obtained exhibit a sound analytical foundation. Some Graphical indices and thermodynamic properties can be seen in [19,20,21]

Moreover, the crystallographic structure of copper oxide holds significant chemical importance. The arrangement of atoms in a crystal lattice provides crucial insights into the material's properties and behavior. In the case of copper oxide, understanding its crystallographic structure is fundamental for unraveling its electronic, magnetic, and catalytic properties. Readers may see [30,31,32] for Graphical indices and physicochemical properties. Furthermore, some quantum-theoretic applications of graphical indices can be seen in [36,37,38].

These indices, along with various other graph indices, are discussed in more detail below, unveiling the rich tapestry of applications and discoveries within the realm of graph theory.

Definition 1.1. [3] For a graph G, First Zagreb index is denoted and defined as:

$$M_1(G) = \sum_{xy \in E(G)} (d_x + d_y)$$

Definition 1.2. [3] For a graph, The Second Zagreb index is denoted and defined as:

$$M_2(G) = \sum_{xy \in E(G)} (d_x d_y)$$

Definition 1.3. [4] For a graph, The modified second Zagreb index is denoted and defined as:

$$Modified\ M_2(G) = \sum_{xy \in E(G)} \frac{1}{d_x d_y}$$

Definition 1.4. [5] For a graph G, The augmented Zagreb Index is denoted and defined as:

$$AZI(G) = \sum_{xy \in E(G)} \left(\frac{d_x d_y}{d_x + d_y - 2}\right)^3$$

Definition 1.5. [6] For a graph G, Hyper Zagreb 2nd Index is denoted and defined as:

$$H_2(G) = \sum_{xy \in E(G)} \left(d_x d_y\right)^2$$

Definition 1.6. [7] For a graph G, Redefined 1st Zagreb Index is denoted and defined as:

$$ReZ\ G_1(G) = \sum_{xy \in E(G)} \frac{d_x + d_y}{d_x d_y}$$

Definition 1.7. [8] For a graph G, Redefined 2nd Zagreb Index is denoted and defined as:

$$ReZ\ G_2(G) = \sum_{xy \in E(G)} \frac{d_x d_y}{d_x + d_y}$$

Definition 1.8. [8] For a graph G, Redefined 3rd Zagreb Index is denoted and defined as:as

$$ReZ\ G_3(G) = \sum_{xy \in E(G)} \left((d_x d_y)(d_x + d_y)\right)$$

Definition 1.9. [9] Suppose that we have a probability density function

$$P_{ij} = \frac{w(xy)}{\sum W(xy)}$$

The Entropy for any graph *G* it's defined as

$$I(G, w) = -\sum P_{ij} \log\left(P_{ij}\right)$$

One fascinating branch of graph theory that has been gaining significant attention is Chemical Graph Theory, which delves into the intriguing relationship between graphs and chemistry. In recent years, the field of Chemical Graph Theory has sparked my growing interest in research. Back in 1988, numerous researchers were generating around 500 articles annually, each centered on the intersections of chemistry and graph theory.

Among the myriad topics covered in these articles, chemical indices in graph theory have emerged as a particularly vital subject. These indices find their roots in the field of chemistry and yield valuable insights that chemists actively utilize in their work. Notable examples of these chemical indices include the First and Second Zagreb indices, multiplicative Zagreb indices, the Wiener index, the general hyper-Wiener index, the Randic index, the harmonic index, the sum-connectivity index, the general Randic index, and the general sum-connectivity index, among others [10,11,12,13].

Theoretical chemists, as far back as the mid-20th century, recognized the potential of these graph-based invariants to reveal essential insights about the molecular structures of organic materials. By observing appropriately designed invariants of the fundamental molecular graph, they could unveil critical information. These invariants, often referred to as topological indices, serve as graph invariants that offer valuable insights for making chemical determinations.

These topological indices play a pivotal role in various aspects of chemistry, including Numerical Structure-Property Relations (QSPR) and Quantitative Structure-Activity Relations (QSAR). The detailed applicability can be seen in [12,13,14,15,16,17]. They enable chemists to make data-driven decisions and predictions based on the structural characteristics of chemical compounds, underscoring the profound impact of Chemical Graph Theory on the field of chemistry [14, 15, 16, 17, and 18]. The Pauli rejection postulate proposes that two or more electrons do not have the same quantum numbers in a molecule. Thus, if two particular atoms associate to arrange diatomic molecules and every orbit of the atom divert into two molecular orbitals which have distinct energy, it allows electrons in an earlier atomic orbital that possess a new framework of orbits, and each has not have the same energy. Commonly, if any huge number M of atoms are identical to overlap to make a solid substance, like a crystal lattice (See Figure 1), the atomic orbital of atoms overlies each other [19].

Here we will discuss topological indices and how to use them $cu_2o[i,j,t]$

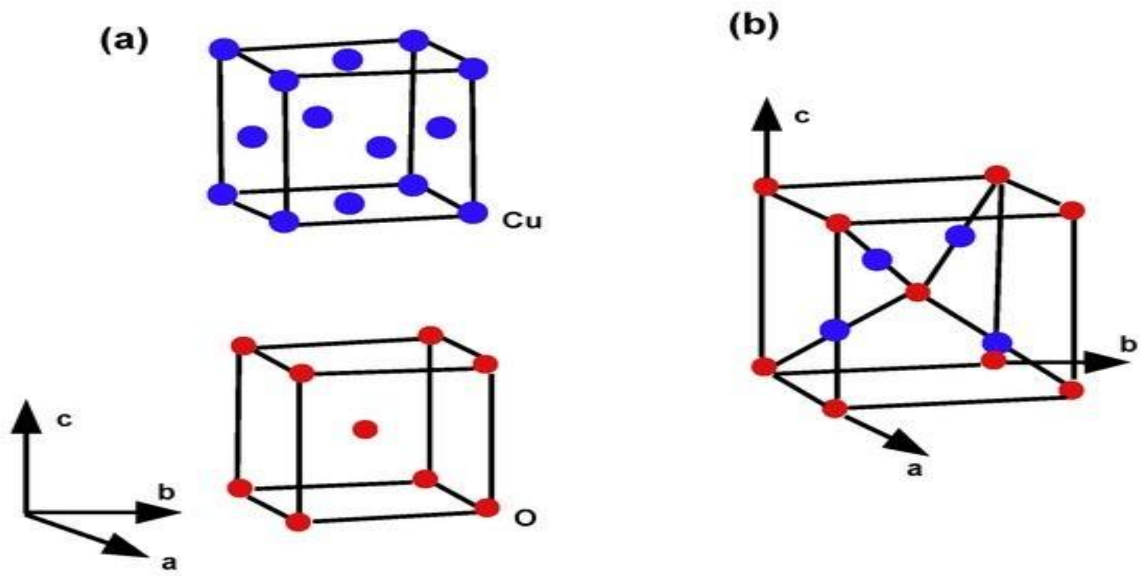


Figure 1:Crystallographic molecule

Structure of the crystallographic molecule Cu_2O

(a) Cu and O structural features atoms in the lattice of Cu_2O. The lattice of Cu_2O (See Figure 2) is formed by interpenetrating the lattices of Cu and O with the other one.

(b) Cu_2O Unit Cell. As small blue spheres, copper atoms are seen, and oxygen atoms they're seen as big red spheres. Each Cu atom is coordinated in the Cu_2O lattice with two O atoms and each atom of O is coordinated by four atoms of Cu.

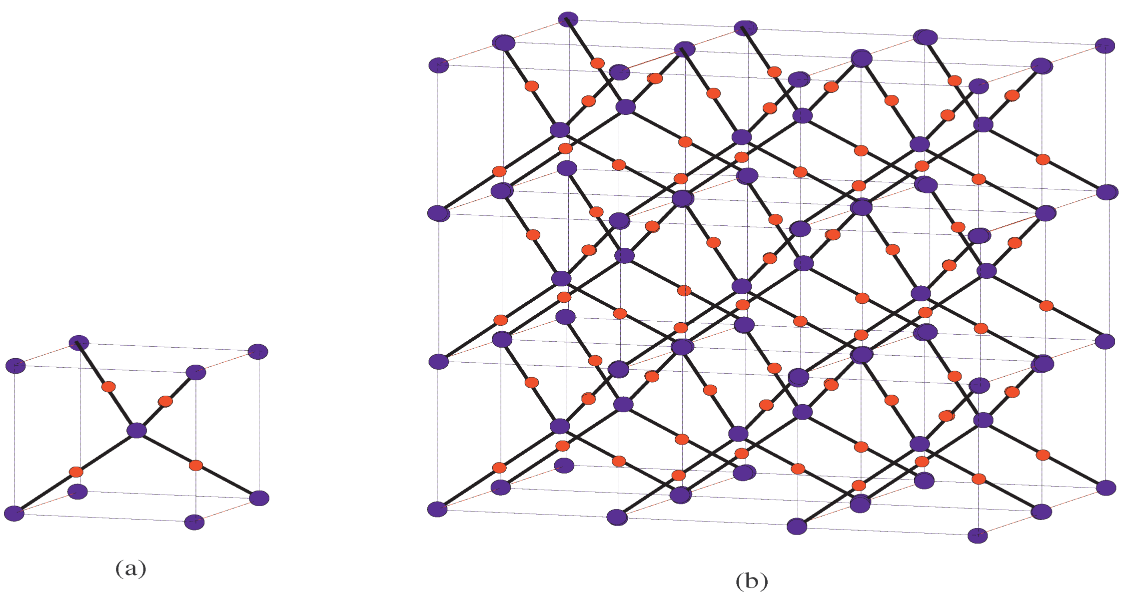


Figure 2: (a)Cu_2O[1,1,1] unit cell, (b) Cu_2O[3,2,3] crystallographic structure.

Set of Edges	(d_s, d_t)	Frequency
E_1	(1,2)	$4i + 4j + 4t - 8$
E_2	(2,2)	$4ij + 4jt + 4it - 8i - 8j - 8t + 12$
E_3	(2,4)	$4(2ijt - ij - it - jt + i + j + t - 1)$

Table 1: Edge partition of $cu_2o[i,j,t] \geq 1$ based on the degrees of end vertices of each edge.

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

Table 2: Edge partition of $cu_2o[i,j,t] \geq 2$ based on the degrees of end vertices of each edge

Based on edge partitions given in Table 1 and Table 2, we will discuss topological indices as we wait and Compute the Weighted Entropy for $cu_2o[i,j,t]$

2. MAIN RESULTS

Corollary 1: The Modified second Zagreb index ${}^{m}M_2(G)$ of cu_2o

$$Modified\ M_2(G) = \sum_{xy \in E(G)} \frac{1}{d_x d_y}$$

$${}^{m}M_2(cu_2o) = \frac{1}{2.4}|E_1| + \frac{1}{4.6}|E_2| + \frac{1}{5.8}|E_3| + \frac{1}{6.8}|E_4| + \frac{1}{8.8}|E_5|$$

$${}^{m}M_2(cu_2o) = \begin{bmatrix} \frac{1}{2}(i+j+t) - 1 + \frac{1}{6}(ij+it+jt) - \frac{1}{3}(i+j+t) + \frac{1}{2} + \frac{1}{10}(i+j+t) - \frac{1}{5} \\ + \frac{1}{12}(ij+it+jt) - \frac{1}{6}(i+j+t) + \frac{1}{4} + \frac{1}{8}(ijt) - \frac{1}{8}(ij+it+jt) \\ + \frac{1}{8}(i+j+t) - \frac{1}{8} \end{bmatrix}$$

$${}^{m}M_2(cu_2o) = \frac{1}{8}(ijt) + \frac{1}{8}(ij+it+jt) + \frac{9}{40}(i+j+t) - \frac{23}{40}$$

Corollary 2: The Redefined 1st Zagreb Index is $ReZ\ G_1(cu_2o)$

$$ReZ\ G_1(G) = \sum_{xy\in E(G)} \frac{d_x + d_y}{d_x d_y}$$

$$ReZG_1(cu_2o) = \frac{3}{4}|E_1| + \frac{5}{12}|E_2| + \frac{13}{40}|E_3| + \frac{7}{24}|E_4| + \frac{1}{4}|E_5|$$

$ReZG_1(cu_2o)$

$$= \begin{bmatrix} 3(i+j+t) - 6 + \frac{5}{3}(ij+it+jt) - \frac{10}{3}(i+j+t) + 5 + \frac{13}{10}(i+j+t) - \frac{13}{5} \\ +\frac{7}{6}(ij+it+jt) - \frac{7}{3}(i+j+t) + \frac{7}{2} + 2(ijt) - 2(ij+it+jt) \\ +2(i+j+t) - 2 \end{bmatrix}$$

$$ReZG_1(cu_2o) = 2(ijt) + \frac{5}{6}(ij+it+jt) + \frac{19}{30}(i+j+t) - \frac{21}{10}$$

Corollary 3: The Redefined Second Zagreb Index is $ReZG_2(cu_2o)$)

$$ReZ\ G_1(G) = \sum_{xy\in E(G)} \frac{d_x . d_y}{d_x + d_y}$$

$$ReZG_1(cu_2o) = \frac{4}{3}|E_1| + \frac{12}{5}|E_2| + \frac{40}{13}|E_3| + \frac{24}{7}|E_4| + 4|E_5|$$

$$ReZG_1(cu_2o) = \begin{bmatrix} \frac{16}{3}(i+j+t) - \frac{32}{3} + \frac{48}{5}(ij+it+jt) - \frac{96}{5}(i+j+t) + \frac{144}{5} + \\ \frac{160}{13}(i+j+t) - \frac{320}{13} + \frac{96}{7}(ij+it+jt) - \frac{192}{7}(i+j+t) + \frac{288}{7} + \\ 32(ijt) - 32(ij+it+jt) + 32(i+j+t) - 32 \end{bmatrix}$$

$$ReZG_1(cu_2o) = 32(ijt) - \frac{304}{35}(ij+it+jt) + \frac{4112}{1365}(i+j+t) + \frac{3632}{1365}$$

Corollary 3: The Redefined Third Zagreb Index is $ReZG_3(cu_2o)$

$$ReZ\ G_3(cu_2o) = \sum_{xy\in E(G)} (d_x + d_y)(d_x . d_y)$$

$$ReZG_3(cu_2o) = 48|E_1| + 240|E_2| + 520|E_3| + 672|E_4| + 1024|E_5|$$

$$ReZG_3(cu_2o) = \begin{bmatrix} 192(i+j+t) - 384 + 960(ij+it+jt) - 1920(i+j+t) + 2880 + \\ 2080(i+j+t) - 4160 + 2688(ij+it+jt) - 5376(i+j+t) + 8064 + \\ 8192(ijt) - 8192(ij+it+jt) + 8192(i+j+t) - 8192 \end{bmatrix}$$

$$ReZG_3(cu_2o) = 8192(ijt) - 4544(ij+it+jt) + 3176(i+j+t) + 1792$$

Theorem 1: Weighted Entropy of $cu_2o[i,j,t] \geq 1$ with the first Zagreb Index is

$$I(cu_2o[i,j,t],M_1) = \log\begin{bmatrix} 4(12ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{4\begin{bmatrix} (12ijt - \\ 2(ij + it + jt) + \\ i + j + t) \end{bmatrix}}\begin{bmatrix} 37.3512600(ijt) - \\ 9.04267014796(ij + it + jt) + \\ 5.13516534335(i + j + t) - \\ 1.22766053874 \end{bmatrix}$$

Proof. By definition (1.1). We have,

$$M_1(cu_2o) = 4(12ijt - 2(ij + it + jt) + i + j + t)$$

By definition (1.9). We have,

$$I(cu_2o,M_1) = \log\begin{bmatrix} 4(12ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{4\begin{bmatrix} (12ijt - \\ 2(ij + it + jt) + \\ i + j + t) \end{bmatrix}}\begin{bmatrix} (1+2)|E_1|\log(1+2) + \\ (2+2)|E_2|\log(2+2) + \\ (2+4)|E_3|\log(2+4) \end{bmatrix}$$

$$I(cu_2o,M_1) = \log\begin{bmatrix} 4(12ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{4\begin{bmatrix} (12ijt - \\ 2(ij + it + jt) + \\ i + j + t) \end{bmatrix}}\begin{bmatrix} 3|E_1|\log(3) + 4|E_2|\log 4 \\ +6|E_3|\log 6 \end{bmatrix}$$

$$I(cu_2o,M_1) = \log\begin{bmatrix} 4(12ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{4\begin{bmatrix} (12ijt - \\ 2(ij + it + jt) + \\ i + j + t) \end{bmatrix}}\begin{bmatrix} \log 2(48ijt + 8ij + 8it + 8jt \\ -40i - 40j - 40t + 72) + \\ \log 3(48ijt - 24ij - 24it - 24jt + \\ 36i + 36j + 36t - 48) \end{bmatrix}$$

$$I(cu_2o[i,j,t],M_1) = \log\begin{bmatrix} 4(12ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{4\begin{bmatrix} (12ijt - \\ 2(ij + it + jt) + \\ i + j + t) \end{bmatrix}}\begin{bmatrix} 37.3512600(ijt) - \\ 9.04267014796(ij + it + jt) + \\ 5.13516534335(i + j + t) - \\ 1.22766053874 \end{bmatrix} \quad \square$$

Theorem 2: Weighted Entropy of $cu_2o[i,j,t] \geq 1$ with the second Zagreb Index is

$$I(cu_2o,M_2) = \log\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix}}\begin{bmatrix} 57.79775916748(ijt) - \\ 19.26591972249(ij + it + jt) + \\ 9.63295986125(i + j + t) - \\ 4.81647993062 \end{bmatrix}$$

Proof. By definition (1.2). We have,

$$M_2(cu_2o) = 8(8ijt - 2(ij + it + jt) + i + j + t)$$

By definition (1.9). We have,

$$I(cu_2o, M_2) = \log\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} (1.2)|E_1|\log(1.2) + \\ (2.2)|E_2|\log(2.2) + \\ (2\,.4)|E_3|\log(2.4) \end{bmatrix}$$

$$I(cu_2o, M_2) = \log\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} 2|E_1|\log(2) + \\ 4|E_2|\log 4 + \\ 8|E_3|\log 8 \end{bmatrix}$$

$$I(cu_2o, M_2) = \log\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} \log 2(192ijt - 64ij - 64it - 64jt \\ +32i + 32j + 32t - 16) \end{bmatrix}$$

$$I(cu_2o[i,j,t], M_2) = \log\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} 8(8ijt - \\ 2(ij + it + jt) \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} 57.79775916748(ijt) - \\ 19.26591972249(ij + it + jt) + \\ 9.63295986125(i + j + t) - \\ 4.81647993062 \end{bmatrix}$$

□

Theorem 3: The Entropy of $cu_2o[i,j,t] \geq 1$ with modified 2nd Zagreb weight is

$$\mathrm{I}\,(cu_2o\ , {}^{m}M_2) = \log\begin{bmatrix} \frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} \frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} -0.90308998699(ijt) - \\ 0.15051499783(ij + it + jt) + \\ 0.15051499783(i + j + t) - \\ 0.15051499783 \end{bmatrix}$$

Proof. By definition (1.3). We have,

$${}^{m}\mathrm{M}_2(cu_2o) = \frac{1}{2}(2ijt + ij + it + jt + i + j + t)$$

By definition (1.9). We have,

$$\mathrm{I}\,(cu_2o, {}^{m}\mathrm{M}_2) = \log\begin{bmatrix} \frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} \frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} \frac{1}{1.2}|E_1|log\frac{1}{1.2} + \\ \frac{1}{2.2}|E_2|log\frac{1}{2.2} + \\ \frac{1}{2.4}|E_3|log\frac{1}{2.4} \end{bmatrix}$$

$$\mathrm{I}\,(cu_2o, {}^{m}\mathrm{M}_2) = \log\begin{bmatrix} \frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t) \end{bmatrix} - \frac{1}{\begin{bmatrix} \frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t) \end{bmatrix}} \begin{bmatrix} \frac{1}{2}|E_1|log\frac{1}{2} + \\ \frac{1}{4}|E_2|log\frac{1}{4} + \\ \frac{1}{8}|E_3|log\frac{1}{8} \end{bmatrix}$$

$$I\,(cu_2o, {}^{m}M_2) = \log\begin{bmatrix}\frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t)\end{bmatrix} - \frac{1}{\begin{bmatrix}\frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t)\end{bmatrix}}\left[\frac{1}{2}\log 2\begin{pmatrix}-6ijt - (ij + it + jt) + \\ (i + j + t) - 1\end{pmatrix}\right]$$

$$I\,(cu_2o\ , {}^{m}M_2) = \log\begin{bmatrix}\frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t)\end{bmatrix} - \frac{1}{\begin{bmatrix}\frac{1}{2}(2ijt \\ +ij + it + jt \\ + i + j + t)\end{bmatrix}}\begin{bmatrix}-0.90308998699(ijt) - \\ 0.15051499783(ij + it + jt) + \\ 0.15051499783(i + j + t) - \\ 0.15051499783\end{bmatrix}$$

□

Theorem 4: *The Entropy of* $cu_2o[i, j, t] \geq 1$ *with Augmented Zagreb weight is*

$$I(cu_2o, AZI) = \log(64ijt) - \frac{1}{64ijt}[57.797759ijt]$$

Proof. By definition (1.4). We have,

$$AZI(cu_2o) = 64ijt$$

By definition (1.9). We have,

$$I(cu_2o, AZI) = log(64ijt) - \frac{1}{64ijt}\begin{bmatrix}\left(\frac{1.2}{1+2-2}\right)^3 |E_1| log\left(\frac{1.2}{1+2-2}\right)^3 + \\ \left(\frac{2.2}{2+2-2}\right)^3 |E_2| log\left(\frac{2.2}{2+2-2}\right)^3 \\ + \left(\frac{2.4}{2+4-2}\right)^3 |E_3| log\left(\frac{2.4}{2+4-2}\right)^3 +\end{bmatrix}$$

$$I(cu_2o, AZI) = log(64ijt) - \frac{1}{64ijt}\begin{bmatrix}24|E_1|log2 + \\ 24|E_2|log2 + \\ 24|E_3|log2\end{bmatrix}$$

$$I(cu_2o, AZI) = log(64ijt) - \frac{1}{64ijt}[24log2(8ijt)]$$

$$(cu_2o, AZI) = \log(64ijt) - \frac{1}{64ijt}[57.797759ijt]$$ □

Theorem 5: *The Entropy of* $cu_2o[i, j, t] \geq 1$ *with hyper Zagreb second weight is*

$$I(cu_2o, H_2) = \log\begin{bmatrix}512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106\end{bmatrix} - \frac{1}{\begin{bmatrix}512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106\end{bmatrix}}\begin{bmatrix}924.7641466798(ijt) - \\ 376.28749458(ij + jt + it) + \\ 317.8876754212(i + j + t) - \\ 250.4569563924\end{bmatrix}$$

Proof. By definition (1.5). We have,

$H_2(cu_2o) = [512(ijt) - 192(ij + jt + it) + 144(i + j + t) - 106]$

By definition (1.9). We have,

$$I(cu_2o, H_2) = \log\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix} - \frac{1}{\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix}}\begin{bmatrix} (1.2)^2|E_1|log(1.2)^2 + \\ (2.2)^2|E_2|log(2.2)^2 + \\ (2.4)^2|E_3|log(2.4)^2 \end{bmatrix}$$

$$I(cu_2o, H_2) = \log\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix} - \frac{1}{\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix}}\begin{bmatrix} 8|E_1|log2 + \\ 64|E_2|log2 + \\ 384|E_3|log2 \end{bmatrix}$$

$$I(cu_2o, H_2) = \log\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix} - \frac{1}{\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix}}[log2(8|E_1| + 64|E_2| + 384|E_3|)]$$

$$I(cu_2o, H_2) = \log\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix} - \frac{1}{\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix}}\left[log2\begin{pmatrix} 3072(ijt) - 1250(ij + jt + it) + \\ 1056(i + j + t) - 832 \end{pmatrix}\right]$$

$$I(cu_2o, H_2) = \log\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix} - \frac{1}{\begin{bmatrix} 512(ijt) - \\ 192(ij + jt + it) + \\ 144(i + j + t) - 106 \end{bmatrix}}\begin{bmatrix} 924.7641466798(ijt) - \\ 376.28749458(ij + jt + it) + \\ 317.8876754212(i + j + t) - \\ 250.4569563924 \end{bmatrix} \square$$

Theorem 6: *The Entropy of* $cu_2o[i, j, t] \geq 1$ *with redefined first Zagreb weight is*

$$I(cu_2o, ReZ(G_1)) = \log\begin{bmatrix} 6(ijt) + \\ (ij + jt + it) + \\ i + j + t - 3 \end{bmatrix} - \frac{1}{\begin{bmatrix} 6(ijt) + \\ (ij + jt + it) + \\ i + j + t - 3 \end{bmatrix}}\begin{bmatrix} -0.749632(ijt) + \\ 0.374816(ij + jt + it) + \\ 0.681731(i + j + t) - \\ 1.738279 \end{bmatrix}$$

Proof. By definition (1.6). We have,

$ReZG_1(cu_2o) = [6(ijt) + ij + jt + it + i + j + t - 3]$

By definition (1.9). We have,

$$I(cu_2o, ReZ(G_1)) = \log\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix} - \frac{1}{\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix}}\begin{bmatrix} \frac{1+2}{1.2}|E_1|log\frac{1+2}{1.2} + \frac{2+2}{2.2}|E_2|log\frac{2+2}{2.2} + \\ \frac{2+4}{2.4}|E_3|log\frac{2+4}{2.4} \end{bmatrix}$$

$$I(cu_2o, ReZ(G_1)) = \log\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix} - \frac{1}{\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix}}\begin{bmatrix} \frac{3}{2}|E_1|log3 - \frac{3}{2}|E_1|log2 + \\ \frac{3}{4}|E_3|log3 - \frac{3}{2}|E_3|log2 \end{bmatrix}$$

$$I(cu_2o, ReZ(G_1)) = \log\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix} - \frac{1}{\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix}}\begin{bmatrix} -\frac{3}{2}log2(|E_1| + |E_3|) + \\ log3\left(\frac{3}{2}|E_1| + \frac{3}{4}|E_3|\right) \end{bmatrix}$$

$$I(cu_2o, ReZ(G_1)) = \log\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix} - \frac{1}{\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix}}\begin{bmatrix} -\frac{3}{2}log2\begin{pmatrix} 8(ijt) - 4(ij+it+jt) + \\ 8(i+j+t) - 12 \end{pmatrix} + \\ log3\begin{pmatrix} 6(ijt) - 3(ij+it+jt) + \\ 9(i+j+t) - 15 \end{pmatrix} \end{bmatrix}$$

$$I(cu_2o, ReZ(G_1)) = \log\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix} - \frac{1}{\begin{bmatrix} 6(ijt) + \\ (ij+jt+it) + \\ i+j+t-3 \end{bmatrix}}\begin{bmatrix} -0.749632(ijt) + \\ 0.374816(ij+jt+it) + \\ 0.681731(i+j+t) - \\ 1.738279 \end{bmatrix} \square$$

Theorem 7: *The Entropy of* $cu_2o[i,j,t] \geq 1$ *with redefined second Zagreb weight is*

$$I(cu_2o, ReZ(G_2)) = \log\left[\frac{1}{3}\begin{bmatrix} 32(ijt) - \\ 4(ij+jt+it-1) \end{bmatrix}\right] - \frac{1}{\left[\frac{1}{3}\begin{bmatrix} 32(ijt) - \\ 4(ij+jt+it-1) \end{bmatrix}\right]}\begin{bmatrix} 1.33267985716(ijt) - \\ 0.66633992858(ij+it+jt) + \\ 0.19676323776(i+j+t) + \\ 0.27281345305 \end{bmatrix}$$

Proof. By definition (1.7). We have,

$$ReZG_2(cu_2o,) = \frac{1}{3}[32(ijt) - 4(ij+jt+it-1)]$$

By definition (1.9). We have,

$$I(cu_2o, ReZ(G_2)) = \log\left[\frac{1}{3}\begin{bmatrix} 32(ijt) - \\ 4(ij+jt+it-1) \end{bmatrix}\right] - \frac{1}{\left[\frac{1}{3}\begin{bmatrix} 32(ijt) - \\ 4(ij+jt+it-1) \end{bmatrix}\right]}\begin{bmatrix} \frac{1.2}{1+2}|E_1|log\frac{1.2}{1+2} + \frac{2.2}{2+2}|E_2|log\frac{2.2}{2+2} + \\ \frac{2.4}{2+4}|E_3|log\frac{2.4}{2+4} \end{bmatrix}$$

$$I(cu_2o, ReZ(G_2)) = \log\left[\frac{1}{3}\begin{bmatrix} 32(ijt) - \\ 4(ij+jt+it-1) \end{bmatrix}\right] - \frac{1}{\left[\frac{1}{3}\begin{bmatrix} 32(ijt) - \\ 4(ij+jt+it-1) \end{bmatrix}\right]}\begin{bmatrix} \frac{2}{3}|E_1|log2 - \frac{2}{3}|E_1|log3 + \\ \frac{8}{3}|E_3|log2 - \frac{4}{3}|E_3|log3 \end{bmatrix}$$

$$I(cu_2o,ReZ(G_2)) = \log\left[\frac{1}{3}\left[\begin{matrix}32(ijt)-\\4(ij+jt+it-1)\end{matrix}\right]\right] - \frac{1}{\left[\frac{1}{3}\left[\begin{matrix}32(ijt)-\\4(ij+jt+it-1)\end{matrix}\right]\right]}\left[\begin{matrix}\frac{2}{3}log2(|E_1|+4|E_3|)-\\\frac{2}{3}log3(|E_1|+2|E_3|)\end{matrix}\right]$$

$$I(cu_2o,ReZ(G_2)) = \log\left[\frac{1}{3}\left[\begin{matrix}32(ijt)-\\4(ij+jt+it-1)\end{matrix}\right]\right] - \frac{1}{\left[\frac{1}{3}\left[\begin{matrix}32(ijt)-\\4(ij+jt+it-1)\end{matrix}\right]\right]}\left[\begin{matrix}\frac{2}{3}log2\begin{pmatrix}32(ijt)-16(ij+it+jt)+\\20(i+j+t)-24\end{pmatrix}-\\\frac{2}{3}log3\begin{pmatrix}16(ijt)-8(ij+it+jt)+\\12(i+j+t)-16\end{pmatrix}\end{matrix}\right]$$

$$I(cu_2o,ReZ(G_2)) = \log\left[\frac{1}{3}\left[\begin{matrix}32(ijt)-\\4(ij+jt+it-1)\end{matrix}\right]\right] - \frac{1}{\left[\frac{1}{3}\left[\begin{matrix}32(ijt)-\\4(ij+jt+it-1)\end{matrix}\right]\right]}\left[\begin{matrix}1.33267985716(ijt)-\\0.66633992858(ij+it+jt)+\\0.19676323776(i+j+t)+\\0.27281345305\end{matrix}\right]\square$$

Theorem 8: *The Entropy of* $cu_2o[i,j,t] \geq 1$ *with redefined third Zagreb weight is*

$$I(cu_2o,ReZ(G_3)) = \log\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right] - \frac{1}{\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right]}\left[\begin{matrix}645.59663515(ijt)-\\245.734639(ij+jt+it)-\\458.25004534686(i+j+t)-\\128.95854092\end{matrix}\right]$$

Proof. By definition (1.8). We have, Entropy with

$$ReZG_3(cu_2o) = [384(ijt) - 128(ij+jt+it) + 88(i+j+t) - 48]$$

By definition (1.9). We have,

$$I(cu_2o,ReZ(G_3)) = \log\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right] - \frac{1}{\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right]}\left[\begin{matrix}(1.2)(1+2)|E_1|\log(1.2)(1+2)+\\(2.2)(2+2)|E_2|\log(2.2)(2+2)+\\(2\,.4)(2+4)|E_3|\log(2.3)\,(2+3)+\end{matrix}\right]$$

$$I(cu_2o,ReZ(G_3)) = \log\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right] - \frac{1}{\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right]}\left[\begin{matrix}6|E_1|\log 6+16|E_2|\log 16+\\48|E_3|\log 48\end{matrix}\right]$$

$$I(cu_2o,ReZ(G_3)) = \log\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right] - \frac{1}{\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right]}\left[\begin{matrix}[24(i+j+t)-48]log6+\\(64(ij+jt+it)-128(i+j+t)+192)log16+\\\begin{pmatrix}384(ijt)-192(ij+it+jt)-\\192(i+j+t)-192\end{pmatrix}log48\end{matrix}\right]$$

$$I(cu_2o,ReZ(G_3)) = \log\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right] - \frac{1}{\left[\begin{matrix}384(ijt)-\\128(ij+jt+it)+\\88(i+j+t)-48\end{matrix}\right]}\left[\begin{matrix}645.59663515(ijt)-\\245.734639(ij+jt+it)-\\458.25004534686(i+j+t)-\\128.95854092\end{matrix}\right]\square$$

Theorem 9: Weighted Entropy of $cu_2o[i,j,t] \geq 2$ with the first Zagreb Index is

$$I(cu_2o[i,j,t],M_1)=\log\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}-\frac{1}{\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}}\begin{bmatrix}154.1273578(ijt)-\\49.9441878(\mathrm{ij}+\mathrm{it}+\mathrm{jt})+\\22.3617021(i+j+t)+\\5.2207836\end{bmatrix}$$

Proof. By definition (1.1). We have,

$$M_1(cu_2o)=(128ijt-32(ij+it+jt)+12(i+j+t)+8$$

By definition (1.9). We have,

$$I(cu_2o,M_1)=\log\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}-\frac{1}{\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}}\begin{bmatrix}(2+4)|E_1|\log(2+4)+\\(4+6)|E_2|\log(4+6)+\\(5+8)|E_3|\log(5+8)+\\(6+8)|E_4|\log(6+8)+\\(8+8)|E_5|\log(8+8)\end{bmatrix}$$

$$I(cu_2o,M_1)=\log\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}-\frac{1}{\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}}\begin{bmatrix}6|E_1|\log(6)+\\10|E_2|\log 10+\\13|E_3|\log 13+\\14|E_4|\log 14+\\16|E_5|\log 16\end{bmatrix}$$

$$I(cu_2o,M_1)=\log\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}-\frac{1}{\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}}\begin{bmatrix}\log 6(24(i+j+t)-48)+\\\log 10\begin{bmatrix}40(ij+it+jt)-\\80(i+j+t)+120\end{bmatrix}+\\\log 13(52(i+j+t)-104)+\\\log 14\begin{bmatrix}56(ij+it+jt)-\\112(i+j+t)+168\end{bmatrix}+\\128\log 16\begin{bmatrix}ijt-(ij+it+jt)+\\(i+j+t)-1\end{bmatrix}\end{bmatrix}$$

$$I(cu_2o[i,j,t],M_1)=\log\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}-\frac{1}{\begin{bmatrix}(128ijt-\\32(ij+it+jt)\\+12(i+j+t)+8\end{bmatrix}}\begin{bmatrix}154.1273578(ijt)-\\49.9441878(ij+it+jt)+\\22.3617021(i+j+t)+\\5.2207836\end{bmatrix}\ \square$$

Theorem 10: Weighted Entropy of $cu_2o[i,j,t] \geq 2$ with the second Zagreb Index is

$$I(cu_2o[i,j,t],M_2)=\log\begin{bmatrix}(512ijt-\\244(ij+it+jt)\\+128(i+j+t)\\-32\end{bmatrix}-\frac{1}{\begin{bmatrix}(512ijt-\\244(ij+it+jt)\\+128(i+j+t)\\-32\end{bmatrix}}\begin{bmatrix}924.7641467(ijt)-\\469.465549899(ij+it+jt)+\\299.3954313(i+j+t)-\\129.3253127309\end{bmatrix}$$

Proof. By definition (1.2). We have,

$M_2(cu_2o) = 512ijt - 244(ij + it + jt) + 128(i + j + t) - 32$

By definition (1.9). We have,

$$I(cu_2o, M_2) = \log\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) - 32\end{bmatrix} - \frac{1}{\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) - 32\end{bmatrix}}\begin{bmatrix}(2.4)|E_1|\log(2.4) + \\ (4.6)|E_2|\log(4.6) + \\ (5.8)|E_3|\log(5.8) + \\ (6.8)|E_4|\log(6.8) + \\ (8.8)|E_5|\log(8.8)\end{bmatrix}$$

$$I(cu_2o, M_2) = \log\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) - 32\end{bmatrix} - \frac{1}{\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) - 32\end{bmatrix}}\begin{bmatrix}8|E_1|\log(8) + \\ 24|E_2|\log(24) + \\ 40|E_3|\log(40) + \\ 48|E_4|\log(48) + \\ 64|E_5|\log(64)\end{bmatrix}$$

$$I(cu_2o, M_2) = \log\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) \\ -32\end{bmatrix} - \frac{1}{\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) \\ -32\end{bmatrix}}\begin{bmatrix}8\log 8(4(i+j+t) - 8) + \\ 24\log 24\begin{bmatrix}4(ij+it+jt) - \\ 8(i+j+t) + 12\end{bmatrix} + \\ 40\log 40(4(i+j+t) - 8) + \\ 48\log 48\begin{bmatrix}4(ij+it+jt) - \\ 8(i+j+t) + 12\end{bmatrix} + \\ 64\log 64\begin{bmatrix}8ijt - 8(ij+it+jt) + \\ 8(i+j+t) - 8\end{bmatrix}\end{bmatrix}$$

$$I(cu_2o[i,j,t], M_2) = \log\begin{bmatrix}512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) \\ -32\end{bmatrix} - \frac{1}{\begin{bmatrix}(512ijt - \\ 244(ij + it + jt) \\ +128(i + j + t) \\ -32\end{bmatrix}}\begin{bmatrix}924.7641467(ijt) - \\ 469.465549899(ij + it + jt) + \\ 299.3954313(i + j + t) - \\ 129.3253127309\end{bmatrix} \square$$

Theorem 11: *The Entropy of* $cu_2o[i,j,t] \geq 2$ *with Augmented Zagreb weight is*

$$(cu_2o, AZI) = log\begin{bmatrix}\frac{262144}{343}(ijt) - \\ \frac{137292}{343}(ij + it + jt) \\ +\frac{95558696}{113533}(i + j + t) \\ -\frac{55213740}{456533}\end{bmatrix} - \frac{1}{\begin{bmatrix}\frac{262144}{343}(ijt) - \\ \frac{137292}{343}(ij + it + jt) \\ +\frac{95558696}{113533}(i + j + t) \\ -\frac{55213740}{456533}\end{bmatrix}}\begin{bmatrix}1513.37016310667(ijt) - \\ 896.40080323762(\mathrm{ij} + \mathrm{it} + \mathrm{jt}) + \\ 631.84083470165(i + j + t) - \\ 367.28086616568\end{bmatrix}$$

Proof. By definition (1.4). We have,

$$AZI(cu_2o) = \left[\frac{262144}{343}(ijt) - \frac{137292}{343}(ij + jt + it) + \frac{95558696}{113533}(i + j + t) - \frac{55213740}{456533}\right]$$

By definition (1.9). We have,

$$I(cu_2o, AZI) = log\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right] - \frac{1}{\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right]}\left[\begin{array}{c}\left(\frac{2.4}{2+4-2}\right)^3|E_1|log\left(\frac{2.4}{2+4-2}\right)^3+ \\ \left(\frac{4.6}{4+6-2}\right)^3|E_2|log\left(\frac{4.6}{4+6-2}\right)^3+ \\ \left(\frac{5.8}{5+8-2}\right)^3|E_3|log\left(\frac{5.8}{5+8-2}\right)^3+ \\ \left(\frac{6.8}{6+8-2}\right)^3|E_3|log\left(\frac{6.8}{6+8-2}\right)^3+ \\ \left(\frac{8.8}{8+8-2}\right)^3|E_3|log\left(\frac{8.8}{8+8-2}\right)^3\end{array}\right]$$

$$I(cu_2o, AZI) = log\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right] - \frac{1}{\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right]}\left[\begin{array}{c}24|E_1|log2+81|E_2|log3+ \\ \frac{576000}{1331}|E_3|log2+\frac{192000}{1331}|E_3|log5 \\ -\frac{192000}{1331}|E_3|log11+384|E_4|log2+ \\ \frac{491520}{343}|E_5|log2-\frac{98304}{343}|E_5|log7\end{array}\right]$$

$$I(cu_2o, AZI) = log\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right] - \frac{1}{\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right]}\left[\begin{array}{c}log2\left(\begin{array}{c}\frac{3932160}{343}(ijt)- \\ \frac{3405312}{343}(ij+it+jt)+ \\ \frac{4665334752}{456533}(i+j+t)- \\ \frac{4798199232}{466533}\end{array}\right)+ \\ log3\left(\begin{array}{c}324(ij+it+jt)- \\ 648(i+j+t)+972\end{array}\right)+ \\ log5\left(\frac{768000}{1331}(i+j+t)-\frac{1536000}{1331}\right) \\ -log7\left(\begin{array}{c}\frac{786432}{343}(ijt)- \\ \frac{786432}{343}(ij+it+jt)+ \\ \frac{786432}{343}(i+j+t)- \\ \frac{786432}{343}\end{array}\right)- \\ log11\left(\frac{768000}{1331}(i+j+t)-\frac{1536000}{1331}\right)\end{array}\right]$$

$$(cu_2o, AZI) = log\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right] - \frac{1}{\left[\begin{array}{c}\frac{262144}{343}(ijt)- \\ \frac{137292}{343}(ij+it+jt) \\ +\frac{95558696}{113533}(i+j+t) \\ -\frac{55213740}{456533}\end{array}\right]}\left[\begin{array}{c}1513.37016310667(ijt)- \\ 896.40080323762(ij+it+jt)+ \\ 631.84083470165(i+j+t)- \\ 367.28086616568\end{array}\right]\square$$

Theorem 12: *The Entropy of* $cu_2o[i,j,t] \geq 2$ *with hyper Zagreb second weight is*

$$I(cu_2o, H_2) = \log\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix} - \frac{1}{\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix}}\begin{bmatrix} 118369.81077500801(ijt) - \\ 81021.1588858941(ij+jt+it) + \\ 64641.25695911797(i+j+t) - \\ 48261.35503234189 \end{bmatrix}$$

Proof. By definition (1.5). We have,

$$H_2(cu_2o) = [32768(ijt) - 21248(ij+jt+it) + 16384(i+j+t) - 11520]$$

By definition (1.9). We have,

$$I(cu_2o, H_2) = \log\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix} - \frac{1}{\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix}}\begin{bmatrix} (2.4)^2|E_1|log(2.4)^2 + \\ (4.6)^2|E_2|log(4.6)^2 + \\ (5.8)^2|E_3|log(5.8)^2 + \\ (6.8)^2|E_4|log(6.8)^2 + \\ (8.8)^2|E_5|log(8.8)^2 \end{bmatrix}$$

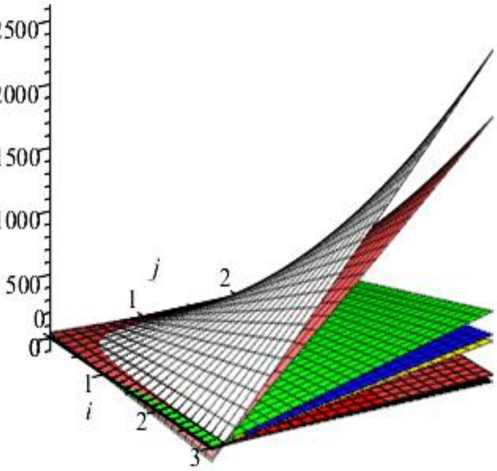
$$I(cu_2o, H_2) = \log\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix} - \frac{1}{\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix}}\begin{bmatrix} 128|E_1|\log(8) + \\ 1152|E_2|\log(24) + \\ 3200|E_3|\log(40) + \\ 4608|E_4|\log(48) + \\ 8192|E_5|\log(64) \end{bmatrix}$$

$$I(cu_2o, H_2) = \log\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix} - \frac{1}{\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix}}\begin{bmatrix} 128\log 8(4(i+j+t)-8) + \\ 1152\log 24\begin{bmatrix} 4(ij+it+jt) - \\ 8(i+j+t)+12 \end{bmatrix} + \\ 3200\log 40(4(i+j+t)-8) + \\ 4608\log 48\begin{bmatrix} 4(ij+it+jt) - \\ 8(i+j+t)+12 \end{bmatrix} + \\ 8192\log 64\begin{bmatrix} 8ijt - 8(ij+it+jt) + \\ 8(i+j+t)-8 \end{bmatrix} \end{bmatrix}$$

$$I(cu_2o, H_2) = log\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix} - \frac{1}{\begin{bmatrix} 32768(ijt) - \\ 21248(ij+jt+it) + \\ 16384(i+j+t) \\ -11520 \end{bmatrix}}\begin{bmatrix} 118369.81077500801(ijt) - \\ 81021.1588858941(ij+jt+it) + \\ 64641.25695911797(i+j+t) - \\ 48261.35503234189 \end{bmatrix}\square$$

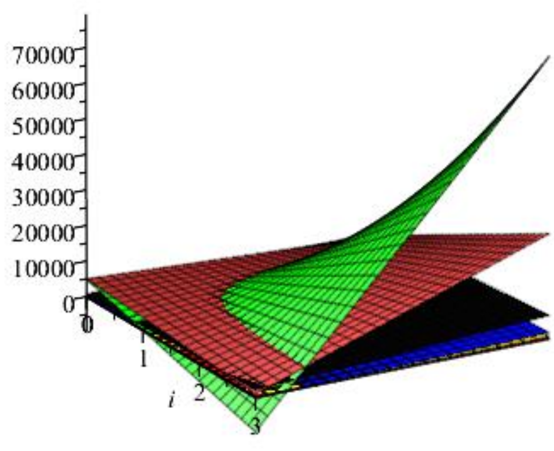
Graphical Comparison of the Results:

One can see the graphical comparison of our results in Figure 3, Figure 4, Figure 5 and Figure 6.



Yellow=first Zagreb Index , Blue=Second Zagreb Index, Black=Modified 2nd Zagreb Index, Green=Augmented Zagreb Index, Pink=Hyper Second Zagreb Index, Red=Redefined first Zagreb Index, Orange= Redefined second Zagreb Index, Brown=Redefined third Zagreb Index

Figure 3: *Comparison of Topological Indices for* $cu_2o[i,j,t] \geq 1$



Yellow=first Zagreb Index , Blue=Second Zagreb Index, Black=Modified 2nd Zagreb Index, Green=Augmented Zagreb Index, Pink=Hyper Second Zagreb Index, Red=Redefined first Zagreb Index, Orange= Redefined second Zagreb Index, Brown=Redefined third Zagreb Index

Figure 4*: Comparison of Topological Indices for* $cu_2o[i,j,t] \geq 2$

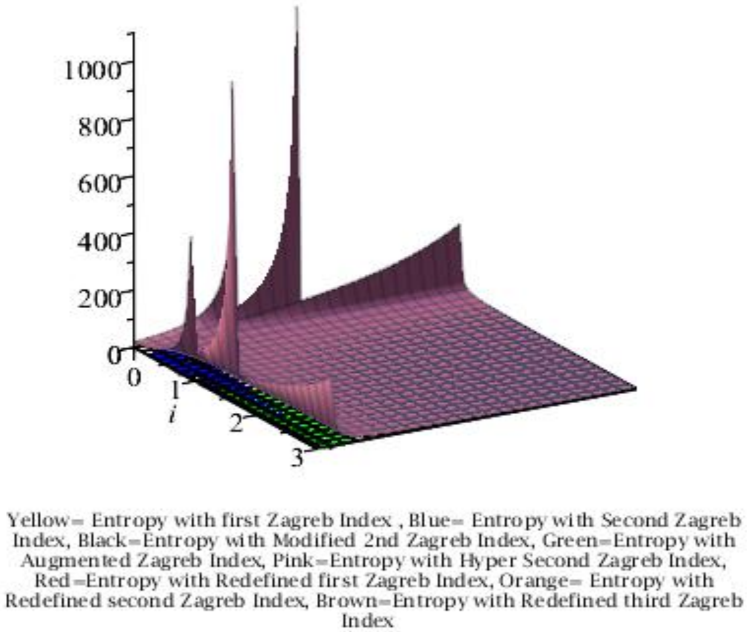


Figure 5: *Comparison of Entropies for* $cu_2o[i,j,t] \geq 1$

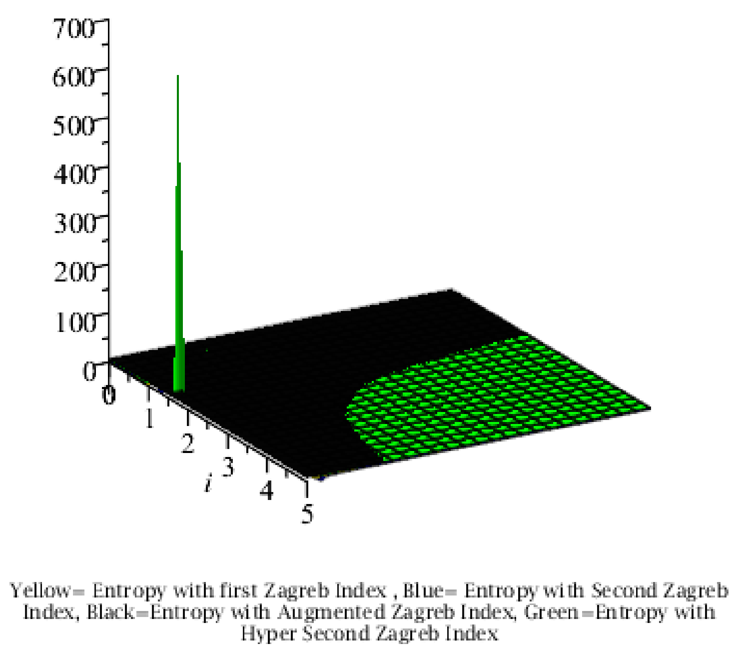


Figure 6: *Comparison of Entropies for* $cu_2o[i,j,t] \geq 2$

CONCLUSION

In this paper, we studied the crystallographic structure cu_2o. We work on the structure of Crystallographic Structure of the molecule $cu_2o[i,j,t]$ and apply the definition of entropies based on topological indices to it. Methods to calculate entropies based on topological indices have opened the door to many diverse applications, such as antiparasitic drug QSAR estimations. Topological descriptors help us understand the graphs and networks that underlie topologies. Various chemical graph entropies calculated on topological-based assessments can tackle many complicated schemes in biomedicine, bioinformatics, and chem-informatics, among other fields. This topological study may help in the electronic and atomic structure of oxygen-dosed and clean of for cu_2o single-crystal surfaces and all new experimental information may concern the defect structure in non-stoichiometric for cu_2o. The results are comprehensively calculated and can bring future outcomes. In the future, we are interested in calculating the entropies based on different distance-based topological indices for the chemical structure of for cu_2o.

DATA AVAILABILITY STATEMENT

All data generated or analyzed during this study are included in this published article.

AUTHORS' CONTRIBUTION

All authors contributed to the study as follows: Soran Noori Saleh was responsible for conceptualization, methodology, and formal analysis; Muhammad Kamran Naseer handled software, data curation, and visualization; Nasir Ali contributed to writing the original draft, supervision, and project administration; Ümit Karabiyik focused on validation, resources, and writing – review and editing; Muhammad Saqlain Zakir managed investigation, data curation, and software; and Misbah Arshad contributed to validation, resources, and writing – review and editing.

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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