Research Article
On Computation and Analysis of Entropy Measures for Crystal Structures

Muhammad Kamran Siddiqui,1 Shazia Manzoor,1 Sarfraz Ahmad,1 and Mohammed K. A. Kaabar2

1Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore 54000, Pakistan
2Jabalia Camp, United Nations Relief and Works Agency (UNRWA) Palestinian Refugee Camp, Gaza Strip, Jabalya, State of Palestine

Correspondence should be addressed to Mohammed K. A. Kaabar; mohammed.kaabar@wsu.edu

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In recent years, the study of topological indices associated to different molecular tubes and structures gained a lot of attention of the researchers—working in Chemistry and Mathematics. These descriptors play an important role in describing different properties associated to the objects of study. Moreover, Shannon’s entropy concept—a slightly different but more effective approach—provides structural information related to the molecular graphs. In this article, we have computed and analyzed different entropy measures associated to different crystallographic structures. In particular, we have worked on the Zagreb entropies, hyper and augmented Zagreb entropies, and forgotten and Balaban entropies for the crystallographic structures of the cuprite Cu2O and titanium difluoride TiF2.

1. Introduction

The role of Graph Theory has been significantly improvised as applications in other areas of sciences, particularly in the direction of Chemical Graph Theory. Many researchers have been able to explore many new directions during last few years. However, there are plenty of gaps which need to be fixed in. The study of topological indices plays an important role in identifying many physical and chemical properties of the molecular structures of study. In recent time, another approach which is a bit different—but more effective—has been introduced in the literature, namely, using the concept of Shannon’s entropy [1, 2]. Concoction graph hypothesis is a part of numerical science wherein devices of graph hypothesis are applied to demonstrate the compound wonder scientifically. In addition, it has been identified with the insignificant uses of graph postulate for subatomic disputes. This hypothesis contributes a noticeable job in the field of compound sciences; for details, see [3–5].

The graph entropy gauges that partner likelihood disseminations with components (vertices, edges, and so forth) of a diagram can be delegated inherent and outward measures. There are a few distinct kinds of such chart entropy measures [6]. The degree powers are very critical invariants and concentrated broadly in chart hypothesis and system science, and they are utilized as the data functionals to investigate the systems [7, 8]. Dehmer presented chart entropies dependent on data functionals, which catch auxiliary data and contemplate their properties [9, 10]. For increasingly broad exploration, Estrada and Hatano recommended a truly solid entropy ration for systems/charts [11] and considered the walk-based diagram entropies [12].

The idea of entropy was presented first in Shannon’s celebrated paper [13] as “the entropy of a likelihood dissemination is known as a proportion of the unusualness of data content or a proportion of the liability of a framework.” Afterward, entropy was started to be applied to diagrams and substance systems. It was created for estimating the auxiliary
data of diagrams and substance systems. In 1955, Rashevsky [14] presented the idea of graph entropy dependent on the orders of vertex circles. As of late, diagram entropies have been broadly applied in a wide range of fields, for example, science, biology, and humanism [15, 16].

The entropy measures for diagrams have been generally applied in art, chemical engineering, and basic science (see [17]). This issue is mind boggling as it is not sure about which diagram class the ration ought to be assessed. We guess that the presented degree-based entropy can be utilized to quantify organize heterogeneity. It is important to note that the mentioned applications have been identified by taking into account the hidden information investigation issue [18, 19]. Be that as it may, the purported auxiliary translation should be examined too. Comprehensively, the applications for entopic organize measures extend from assessable erection portrayal in basic science or programming innovation to investigate natural or synthetic properties of subatomic charts [20]. This calls to look at what sort of basic multifaceted nature does the measure identify. Comparable entropy measures which depend on vertex-degrees to identify arrange heterogeneity have been presented by Solé and Valverde [21] and Tan and Wu [22].

Shannon’s fundamental work [13] in the late nineteen-forties denotes the beginning stage of present day data hypothesis. Succeeding primary solicitations in semantics may, the purported auxiliary translation should be examined too. Comprehensively, the applications for entopic organize measures extend from assessable erection portrayal in basic science or programming innovation to investigate natural or synthetic properties of subatomic charts [20]. This calls to look at what sort of basic multifaceted nature does the measure identify. Comparable entropy measures which depend on vertex-degrees to identify arrange heterogeneity have been presented by Solé and Valverde [21] and Tan and Wu [22].

Shannon’s fundamental work [13] in the late nineteen-forties denotes the beginning stage of present day data hypothesis. Succeeding primary solicitations in semantics and electrical building, data hypothesis was applied broadly in science (see [23, 24]). Subsequently, this strategy has been utilized for investigating living frameworks, e.g., natural and concoction frameworks by methods for charts. These applications have been discussed by both Rashevsky [14] and Trucco [25]. Here, the fundamental oddity was thinking about a structure as a result of a subjective correspondence [26]. With the guide of this knowledge, Shannon’s entropy equations [13] were utilized to decide the basic data substance of a system [21]. In what follows, we survey in sequential request diagram entropy quantifies that have been utilized for considering organic and compound complexes [27–29].

In 2014, Chen et al. [30] presented the meaning of the entropy of edge prejudiced graph. At that point, the entropy of edge slanted graph is given as follows:

\[
\text{ENT}_G = \sum_{r' \in E(G)} \log \left( \frac{1}{|E(G)|} \right) \log \left( \prod_{r \in E(G)} \Theta(r) \times \Theta(s) \right). 
\]

(i) **The First Zagreb Entropy.** If \( \Theta(r) = \Theta(s) = 1 \), then equation (1) is reduced and is called the first Zagreb entropy:

\[
\text{ENT}_{M_1}(G) = \log(M_1(G)) - \frac{1}{M_1(G)} \log \left( \prod_{r \in E(G)} \Theta(r) \times \Theta(s) \right). 
\]

(ii) **The Second Zagreb Entropy.** If \( \Theta(r) = \Theta(s) = 1 \), then equation (1) is reduced and is called the second Zagreb entropy:

\[
\text{ENT}_{M_2}(G) = \log(M_2(G)) - \frac{1}{M_2(G)} \log \left( \prod_{r \in E(G)} \Theta(r) \times \Theta(s) \right). 
\]

(iii) **The Hyper Zagreb Entropy.** If \( \Theta(r) = \Theta(s) = 1 \), then equation (1) is reduced and is called the hyper Zagreb entropy:

\[
\text{ENT}_{HM}(G) = \log(HM(G)) - \frac{1}{HM(G)} \log \left( \prod_{r \in E(G)} \Theta(r) \times \Theta(s) \right). 
\]

(iv) **The Forgotten Entropy.** If \( \Theta(r) = \Theta(s) = 1 \), then equation (1) is reduced and is called the forgotten entropy:

\[
\text{ENT}_F(G) = \log(F(G)) - \frac{1}{F(G)} \log \left( \prod_{r \in E(G)} \Theta(r) \times \Theta(s) \right). 
\]
log (Cu2O) are particularly seen nearby mixture establishments progression [35]. These days, the promising utilizations and nonpoisonous nature and rudimentary establishment progression as of late attributable to its predictable beams, sunlight-based cells, and catalysis [36]. The invention of crystallographic structure of Cu2O has pulled in huge consideration as of late attributable to its predictable establishment progression [35]. These days, the promising utilizations of Cu2O are particularly seen nearby mixture beams, sunlight-based cells, and catalysis [36]. The invention

 Among different progress metal oxides, Cu2O has pulled in huge consideration as of late attributable to its predictable assets and nonpoisonous nature and rudimentary establishment progression [35]. These days, the promising utilizations of Cu2O are particularly seen nearby mixture beams, sunlight-based cells, and catalysis [36]. The invention

For further details about these entropy measures, see [31–34].

2. Crystallographic Structure of Cu2O[m, n, t]

Among different progress metal oxides, Cu2O has pulled in huge consideration as of late attributable to its predictable assets and nonpoisonous nature and rudimentary establishment progression [35]. These days, the promising utilizations of Cu2O are particularly seen nearby mixture beams, sunlight-based cells, and catalysis [36]. The invention

\[
M_1 (G) = (48mnt - 8 (mn + mt + nt) + 4m + 4n + 4t),
\]

\[
\text{ENT}_{\Theta_1}(\text{Cu}_2\text{O}) = \log(M_1) - \log\left[\prod_{rst \in E_1(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\times \prod_{rst \in E_2(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\right]
\]

\[
= \log(M_1) - \log\left[\prod_{rst \in E_1(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\times \prod_{rst \in E_2(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\right]
\]

\[
\text{ENT}_{\Theta_1}(\text{Cu}_2\text{O}) = \log((48mnt - 8mn - 8nt - 8at + 4m + 4n + 4t))
\]

\[
\log\left[\prod_{rst \in E_1(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\times \prod_{rst \in E_2(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\right]
\]

\[
\log\left[\prod_{rst \in E_1(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\times \prod_{rst \in E_2(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\right]
\]

\[
\log\left[\prod_{rst \in E_1(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\times \prod_{rst \in E_2(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\right]
\]

\[
\log\left[\prod_{rst \in E_1(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\times \prod_{rst \in E_2(G)} \left[\Theta (r) + \Theta (s)\right]^{\Theta (r) + \Theta (s)}\right]
\]
Figure 1: (a) Cu₂O lattice. (b) Unit cell of Cu₂O.

Figure 2: Crystallographic structure of Cu₂O [3, 2, 3].

| Θ (r) | Frequency | Set of vertices | (Θ (r), Θ (s)) | Frequency | Set of edges |
|-------|-----------|----------------|----------------|-----------|-------------|
| 1     | 4t + 4m + 4n - 8 | V₁            | (1, 2)         | 4t + 4m + 4n - 8 | E₁          |
| 2     | 2mt - 4t + 2m - 4n - 4mnt + 4m + 2nt + 6 | V₂            | (2, 2)         | 4mnt + 4nt + 4mm - 8m - 8t - 8n + 12 | E₂          |
| 4     | n + m + t + 2mnt - nt - mm - nt - 1 | V₃            | (2, 4)         | 4m + 4n + 8mnt - 4mnt - 4nt - 4mt + 4t - 4 | E₃          |
(ii) The Second Zagreb Entropy. We computed the second Zagreb index and second Zagreb entropy as follows:

\[ M_2(G) = (64mmt - 16mnt - 16nt + 8m + 8n + 8t), \]

\[ \text{ENT}_{M_2}^{\text{Cu}_2\text{O}} = \log(M_2) - \frac{1}{M_2} \log \left[ \prod_{rs \in E_1(G)} [\Theta(r) \times \Theta(s)]^{[\Theta(r) + \Theta(s)]^2} \right] \times \prod_{rs \in E_1(G)} \left[ [\Theta(r) \times \Theta(s)]^{[\Theta(r) + \Theta(s)]^2} \times \prod_{rs \in E_1(G)} [\Theta(r) \times \Theta(s)]^{[\Theta(r) + \Theta(s)]^2} \right] \]

\[ = \log(M_2) - \frac{1}{M_2} \log \left[ (4n + 4m + 4t - 8) \times (4) \right] \times \left[ (4nt + 4nn - 8m + 4nt - 8n + 12) \times (256) \right] \times \left[ (8mnt - 4nn + 4n - 4nt - 4mnt + 4t - 4) \times (16777216) \right], \]

\[ \text{ENT}_{M_2}^{\text{Cu}_2\text{O}} = \log \left( (64mmt + 8m - 16nn + 16nt + 8n + 16nt + 8t) \right) \]

\[ \log \left[ (4n + 4m + 4t - 8) \times (4) \right] - \frac{\log\left[ (4nt + 4nn - 8m + 4nt - 8n + 12) \times (256) \right]}{(4mnt + 8m - 16nn - 16nt + 8n - 16nt + 8t))} - \frac{\log\left[ (8mnt - 4nn + 4n - 4nt - 4mnt + 4t - 4) \times (16777216) \right]}{(4mnt + 8m - 16nn - 16nt + 8n - 16nt + 8t))} \]

(iii) The Hyper Zagreb Entropy of \( \text{Cu}_2\text{O} \{m,n,t \} \). We computed the hyper Zagreb index and hyper Zagreb entropy as follows:

\[ \text{HM}(G) = [8mnt - 80mn - 80nt - 80nt + 52m + 52n + 52t - 24], \]

\[ \text{ENT}_{\text{HM}}^{\text{Cu}_2\text{O}} = \log(\text{HM}) - \frac{1}{\text{HM}} \log \left[ \prod_{rs \in E_1(G)} \left[ (\Theta(r) + \Theta(s))^2 \right]^{[\Theta(r) + \Theta(s))^2} \right] \times \prod_{rs \in E_1(G)} \left[ (\Theta(r) + \Theta(s))^2 \right]^{[\Theta(r) + \Theta(s))^2} \times \prod_{rs \in E_1(G)} \left[ (\Theta(r) + \Theta(s))^2 \right]^{[\Theta(r) + \Theta(s))^2} \]

\[ = \log(\text{HM}) - \frac{1}{\text{HM}} \log \left[ (4n + 4m + 4t - 8) \times (4) \right] \times \left[ (4nt + 4nn - 8m + 4nt - 8n + 12) \times (16) \right] \times \left[ (8mnt - 4nn + 4n - 4nt - 4mnt + 4t - 4) \times (36) \right], \]

\[ \text{ENT}_{\text{HM}}^{\text{Cu}_2\text{O}} = \log(8mnt - 80mn - 80nt - 80nt + 52m + 52n + 52t - 24) \]

\[ \log\left[ (4n + 4m + 4t - 8) \times (4) \right] - \frac{\log\left[ (4nt + 4nn - 8m + 4nt - 8n + 12) \times (16) \right]}{(8mnt - 80mn - 80nt - 80nt + 52m + 52n + 52t - 24)} - \frac{\log\left[ (8mnt - 4nn + 4n - 4nt - 4mnt + 4t - 4) \times (36) \right]}{(8mnt - 80mn - 80nt - 80nt + 52m + 52n + 52t - 24)}. \]
(iv) The Forgotten Entropy of \( \text{Cu}_2\text{O}[m,n,t] \). We computed the forgotten index and forgotten entropy as follows:

\[
F(G) = 36n + 36m + 36t - 24 - 48nm - 48nt - 48mt + 160mnt, \\
\]

\[
\text{ENT}_F(\text{Cu}_2\text{O}) = \log(F(G)) - \frac{1}{(F(G))} \log \left[ \prod_{r \in E_1(G)} \left[ (\Theta(r))^2 + (\Theta(s))^2 \right][\Theta(r)^2 + \Theta(s)^2] \right] \\
\times \prod_{r \notin E_1(G)} \left[ (\Theta(r))^2 + (\Theta(s))^2 \right][\Theta(r)^2 + \Theta(s)^2] \\
= \log(F(G)) - \frac{1}{(F(G))} \log \left[ ((4n + 4m + 4t - 8) \times (3125)) \times ((4nt + 4nm - 8m + 4nt - 8t - 8n + 12) \times (16777216)) \times (8mnt - 4nm + 4n + 4m - 4nt - 4mt + 4t - 4) \times (1.048576 \times 10^{26})) \right], \\
\]

\[
\text{ENT}_F(\text{Cu}_2\text{O}) = \log(36n + 36m + 36t - 24 - 48nm - 48nt - 48mt + 160mnt) \\
- \log(36n + 36m + 36t - 24 - 48nm - 48nt - 48mt + 160mnt) \\
- \log((4n + 4m + 4t - 8) \times (3125)) \\
- \log((4nt + 4nm - 8m + 4nt - 8t - 8n + 12) \times (16777216)) \\
- \log((8mnt - 4nm + 4n + 4m - 4nt - 4mt + 4t - 4) \times (1.048576 \times 10^{26})) \times (16777216)]. \\
\]

(v) The Augmented Zagreb Entropy of \( \text{Cu}_2\text{O}[m,n,t] \). We computed the augmented Zagreb index and augmented Zagreb entropy as follows:

\[
\text{AZI}(G) = 64mnt, \\
\]

\[
\text{ENT}_{\text{AZI}}(\text{Cu}_2\text{O}) = \log(\text{AZI}(G)) - \frac{1}{(\text{AZI}(G))} \log \left[ \prod_{r \in E_1(G)} \left[ \frac{(\Theta(r) \Theta(s))}{\Theta(r) + \Theta(s) - 2} \right]^3 \left[ \frac{(\Theta(r) \Theta(s))}{\Theta(r) + \Theta(s) - 2} \right]^3 \right] \\
\times \prod_{r \notin E_1(G)} \left[ \frac{(\Theta(r) \Theta(s))}{\Theta(r) + \Theta(s) - 2} \right]^3 \left[ \frac{(\Theta(r) \Theta(s))}{\Theta(r) + \Theta(s) - 2} \right]^3 \\
= \log(\text{AZI}(G)) - \frac{1}{(\text{AZI}(G))} \log \left[ ((4n + 4m + 4t - 8) \times (16777216)) \times ((4nt + 4nm - 8m + 4nt - 8t - 8n + 12) \times (16777216)) \times (8mnt - 4nm + 4n + 4m - 4nt - 4mt + 4t - 4) \times (1.048576 \times 10^{26})) \times (16777216)] \\
\]

\[
\text{ENT}_{\text{AZI}}(\text{Cu}_2\text{O}) = \log(64mnt) - \frac{1}{(64mnt)} \log\left( \frac{(4n + 4m + 4t - 8) \times (16777216)) \times ((4nt + 4nm - 8m + 4nt - 8t - 8n + 12) \times (16777216)) \times (8mnt - 4nm + 4n + 4m - 4nt - 4mt + 4t - 4) \times (1.048576 \times 10^{26})) \times (16777216)]}{(64mnt)} \\
\]

\[
= \log((4n + 4m + 4t - 8) \times (16777216)) \\
- \frac{1}{(64mnt)} \log\left( \frac{(4nt + 4nm - 8m + 4nt - 8t - 8n + 12) \times (16777216)) \times (8mnt - 4nm + 4n + 4m - 4nt - 4mt + 4t - 4) \times (1.048576 \times 10^{26})) \times (16777216)]}{(64mnt)} \\
\]
(vi) The Balaban Entropy of Cu₂O \{m, n, t\}. We computed the Balaban index and Balaban entropy as follows:

\[
J(G) = \frac{8mnt}{2mnt - mt - nt - t + 1 - mn - m - n} \times \left[ \frac{1}{\sqrt{2}} (4n + 4m + 4t - 8) + \frac{1}{2} (4nt + 4nm - 8m + 4mt - 8t - 8n + 12) \right] + \frac{8mnt}{2mnt - mt - nt - t + 1 - mn - m - n} \times \left[ \frac{1}{\sqrt{8}} ((8mnt - 4mn + 4n + 4m - 4nt - 4mt + 4t - 4)) \right] + \frac{8mnt}{2mnt - mt - nt - t + 1 - mn - m - n} \times \left[ \frac{\sqrt{2}}{2} (4n + 4m + 4t - 8) \right] + \frac{8mnt}{2mnt - mt - nt - t + 1 - mn - m - n} \times [2mn + 2nt + 2mt - 4n - 4m - 4t + 6] + \frac{8mnt}{2mnt - mt - nt - t + 1 - mn - m - n} \times \left[ \frac{\sqrt{2}}{2} (8mnt - 4mn + 4n + 4m - 4nt - 4mt + 4t - 4) \right].
\]

\[
\text{ENT}_J(Cu₂O) = \log(J(G)) - \frac{1}{J(G)} \log \left[ \prod_{r \in E(G)} \left[ \frac{q}{q - p + 2} \times \frac{1}{\sqrt{\theta(r)\theta(s)}} \right] \right] \left[ (4n + 4m + 4t - 8) \times \frac{q}{\sqrt{2} (q - p + 2)} \right] \left[ (4nt + 4nm - 8m + 4mt - 8t - 8n + 12) \times \frac{q}{2 (q - p + 2)} \right] \left[ (8mnt - 4mn + 4n + 4m - 4nt - 4mt + 4t - 4) \times \frac{q}{2 \sqrt{2} (q - p + 2)} \right].
\]

\[
\text{ENT}_J(Cu₂O) = \log(J(G)) - \frac{1}{J(G)} \log \left[ \prod_{r \in E(G)} \left[ \frac{q}{q - p + 2} \times \frac{1}{\sqrt{\theta(r)\theta(s)}} \right] \right] \left[ (4n + 4m + 4t - 8) \times [(q/\sqrt{2}) (q - p + 2)] \right] \left[ (4nt + 4nm - 8m + 4mt - 8t - 8n + 12) \times [(q/2)(q - p + 2)] \right] \left[ (8mnt - 4mn + 4n + 4m - 4nt - 4mt + 4t - 4) \times [(q/2 \sqrt{2}) (q - p + 2)] \right].
\]

3. Crystallographic Structure of TiF₂ \{m, n, t\}

Titanium difluoride is a water inexplicable titanium cradle for use in oxygen-sensitive solicitations, such as iron invention. Fluoride mixtures have assorted solicitations in existing machineries and science, from oil sanitizing and engraving to unreal animate chemistry and the fabrication of pharmaceuticals. The substance graph of mineral erection of titanium difluoride TiF₂ \{m, n, t\} is designated in Figure 3; for more details, see [38].
The vertex partition and edge partition of TiF$_2$[m,n,t] are depicted in Tables 3 and 4.

3.1. Results for Crystallographic Structure of TiF$_2$[m,n,t]

The First Zagreb Entropy of TiF$_2$[m,n,t]. We calculated the first Zagreb index and first Zagreb entropy as follows:

\[
M_1(G) = [384mnt - 64mn - 64nt + 16m + 16n + 16t - 8],
\]

\[
\text{ENT}_{M_1}(\text{TiF}_2) = \log(M_1) - \frac{1}{M_1} \log \left[ \prod_{rs \in E_1(G)} \Theta (r) \Theta (s) \right]^{\Theta (r)+\Theta (s)}
\]

\[
\times \prod_{rs \in E_2(G)} \Theta (r) \Theta (s) \left[ \Theta (r) + \Theta (s) \right]^{\Theta (r)+\Theta (s)} \prod_{rs \in E_3(G)} \Theta (r) \Theta (s) \left[ \Theta (r) + \Theta (s) \right]^{\Theta (r)+\Theta (s)}
\]

\[
= \log(M_1) - \frac{1}{M_1} \log \left[ \left( (8 \times 3125) \times \left( (8m + 8t - 24 + 8n) \times (46656) \right) \times \left( (16mnt + 16nt - 16m - 16n + 16t - 24) \times (16777216) \right) \times \left( (32mnt - 16nt - 16mm + 8m + 8n + 8t - 8) \times (8916100448456) \right) \right] \right]
\]

\[
\text{ENT}_{M_1}(\text{TiF}_2) = \log(384mnt - 64mn - 64nt + 64m + 16n + 16t - 8))
\]

\[
- \log \left[ \left( (8 \times 3125) \times (46656 \times (256) \right) \right]
\]

\[
- \log \left[ \left( (8m + 8n + 8t - 24) \times (46656 \times (256) \right) \right]
\]

\[
- \log \left[ \left( (16mnt + 16nt - 16m - 16n + 16t - 24) \times (16777216) \right) \right]
\]

\[
- \log \left[ \left( (32mnt - 16nt - 16mm + 8m + 8n + 8t - 8) \times (8916100448456) \right) \right]
\]

\[
(384mnt - 64mn - 64nt - 64m + 16n + 16t - 8)
\]
(ii) The Second Zagreb Entropy of TiF$_2$[m, n, t]. We computed the second Zagreb index and second Zagreb entropy as follows:

\[
M_2(G) = [1024mnt - 256mn - 256nt - 256nt + 64m + 64n + 64t - 32],
\]

\[
\text{ENT}_{M_2}(\text{TiF}_2) = \log(M_2)
\]

\[
= \log(M_2) - \frac{1}{M_2} \log([[(8 \times (256)) \times ((8m + 8n + 8t - 24)) \times (16777216)]
\times[((16mn + 16nt - 16n - 16t + 24 + 16nt - 16m)) \times (16))^{(16)}]
\times[(32mnt - 16nt - 16nn - 16nt + 8m + 8n + 8t - 8) \times (32))^{(32)}],
\]

Table 3: Vertex partition of TiF$_2$[m, n, t].

| $\Theta (r)$ | Frequency | Set of vertices |
|--------------|-----------|----------------|
| 1            | 8         | V$_1$          |
| 2            | 4m + 4n + 4t - 12 | V$_2$          |
| 4            | 4mn + 4mt - 4m - 4t + 6 + 8mnt + 4nt - 4n | V$_3$          |
| 8            | $n + t - 2(mn + nt) - 1 + 4mnt + m$ | V$_4$          |

Table 4: Edge partition of TiF$_2$[m, n, t].

| $(\Theta (r), \Theta (s))$ | Frequency | Set of edges |
|-----------------------------|-----------|--------------|
| (1, 4)                      | 8         | E$_1$        |
| (2, 4)                      | $(8m + 8n + 8t - 24)$ | E$_2$        |
| (4, 4)                      | $16mn + 16nt - 16m - 16n + 16nt - 16t + 24$ | E$_3$        |
| (4, 8)                      | $8m + 8n + 16mn - 16m + 8n + 8t - 8 + 32mnt - 16nt$ | E$_4$        |
(iii) The Hyper Zagreb Entropy of TiF₂[m, n, t]. We computed the hyper Zagreb index and hyper Zagreb entropy as follows:

\[
HM(G) = [4608mnt - 1280mn - 1280mt - 1280nt + 416m + 416n + 416t - 280],
\]

\[
\text{ENT}_{HM}(\text{TiF}_2) = \log(HM) - \frac{1}{(HM)} \times \log \left[ \prod_{rs \in E_1(G)} \left( (\Theta(r) + \Theta(s))^2 \right)^{[\Theta(r) + \Theta(s)]^2} \right] \\
\times \prod_{rs \in E_2(G)} \left( (\Theta(r) + \Theta(s))^2 \right)^{[\Theta(r) + \Theta(s)]^2} \times \prod_{rs \in E_3(G)} \left( (\Theta(r) + \Theta(s))^2 \right)^{[\Theta(r) + \Theta(s)]^2},
\]

\[
\text{ENT}_{HM}(\text{TiF}_2) = \log(HM) - \frac{1}{(HM)} \log \left[ \left( 8 \times (25)^{25} \right) \times \left( (8m + 8n + 8t - 24) \times (36)^{36} \right) \times \left( (16mn + 16nt - 16m + 16nt - 16n + 16t + 24) \times (64)^{64} \right) \times \left( 32mnt - 16nt - 16mn - 16nt + 8m + 8n + 8t - 8 \times (144)^{144} \right) \right],
\]

\[
\text{ENT}_{HM}(\text{TiF}_2) = \log(4608mnt - 1280mn - 1280mt - 1280nt + 416m + 416n + 416t - 280) - \\
\log \left[ \left( 8 \times (25)^{25} \right) \right] \\
- \log \left[ (8m + 8n + 8t - 24) \times (36)^{36} \right] \\
- \log \left[ ((16mn + 16nt - 16m + 16nt - 16n + 16t + 24)) \times (64)^{64} \right] \\
- \log \left[ (32mnt - 16nt - 16mn - 16nt + 8m + 8n + 8t - 8) \times (144)^{144} \right] .
\]
(iv) The Forgotten Entropy of TiF$_2$[$m, n, t$]. We computed the forgotten index and forgotten entropy as follows:

\[ F(G) = 2560mnt - 216 + 288m + 288n + 288t - 768mn - 768mt - 768nt, \]

\[
\begin{align*}
\text{ENT}_F(\text{TiF}_2) &= \log(F(G)) - \frac{1}{(F(G))^{\log}} \left[ \prod_{rs \in E(G)} \left[ (\Theta(r))^2 + (\Theta(s))^2 \right] \left[ \Theta(r)^2 \Theta(s)^2 \right] \right] \\
&\times \prod_{rs \in E'(G)} \left[ (\Theta(r))^2 + (\Theta(s))^2 \right] \left[ \Theta(r)^2 \Theta(s)^2 \right] \\
&\times \prod_{rs \in E_{rs}(G)} \left[ (\Theta(r))^2 + (\Theta(s))^2 \right] \left[ \Theta(r)^2 \Theta(s)^2 \right] \\
&= \log(F(G)) - \frac{1}{(F(G))^{\log}} \left[ \left(8 \times (17)^{\log} \right) \times \left(288m + 8n + 8t - 24 \right) \times (20)^{\log} \right] \\
&\times \left[ \left(16mn + 16nt - 16n - 16t + 24 + 16nt - 16m \right) \times (32)^{\log} \right] \\
&\times \left[ \left(32mnt - 16nt - 16mn - 16nt + 8m + 8n + 8t - 8 \right) \times (80)^{\log} \right],
\end{align*}
\]

\[
\text{ENT}_F(\text{TiF}_2) = \log(2560mnt - 216 + 288m + 288n + 288t - 768mn - 768mt - 768nt)
\]

\[
\frac{\log\left[ \left(8 \times (17)^{\log} \right) \right]}{(2560mnt - 216 + 288m + 288n + 288t - 768mn - 768mt - 768nt)} \\
- \frac{\log\left[ \left(288m + 8n + 8t - 24 \right) \times (20)^{\log} \right]}{(2560mnt - 216 + 288m + 288n + 288t - 768mn - 768mt - 768nt)} \\
- \frac{\log\left[ \left(16mn + 16nt - 16n - 16t + 24 + 16nt - 16m \right) \times (32)^{\log} \right]}{(2560mnt - 216 + 288m + 288n + 288t - 768mn - 768mt - 768nt)} \\
- \frac{\log\left[ \left(32mnt - 16nt - 16mn - 16nt + 8m + 8n + 8t - 8 \right) \times (80)^{\log} \right]}{(2560mnt - 216 + 288m + 288n + 288t - 768mn - 768mt - 768nt)}.
\]
v) *The Augmented Zagreb Entropy of TiF$_2$* $[m,n,t]$.

We computed the augmented Zagreb index and augmented Zagreb entropy as follows:

\[
\text{AZI(TiF}_2) = \frac{67264}{3375} + \frac{76736}{3375} m + \frac{76736}{3375} n + \frac{76736}{3375} t - \frac{745472}{3375} \frac{mn}{m} - \frac{745472}{3375} \frac{mt}{m} - \frac{745472}{3375} \frac{nt}{n} - \frac{131072}{125} mnt, \\
\]

\[
\text{ENT}_{\text{AZI}}(\text{TiF}_2) = \log(\text{AZI}(G)) \\
- \frac{1}{(\text{AZI}(G))} \log \left[ \prod_{r \in E_1(G)} \left( \frac{\Theta(r)\Theta(s)}{\Theta(r) + \Theta(s) - 2} \right)^{3^r} \left( \Theta(r)\Theta(s) \right)^{2^{r}} \right] \\
\times \prod_{r \in E_1(G)} \left[ \left( \frac{\Theta(r)\Theta(s)}{\Theta(r) + \Theta(s) - 2} \right)^{3^r} \left( \Theta(r)\Theta(s) \right)^{2^{r}} \right] \\
\times \prod_{r \in E_1(G)} \left[ \left( \frac{\Theta(r)\Theta(s)}{\Theta(r) + \Theta(s) - 2} \right)^{3^r} \left( \Theta(r)\Theta(s) \right)^{2^{r}} \right] \\
= \log(\text{AZI}(G)) - \frac{1}{(\text{AZI}(G))} \log \left[ (8) \left( \frac{64}{27} \right)^{24(49)} \right] \times \left( \frac{512}{27} \right)^{(512/27)} \\
\times \left[ \left( (16mn + 16nt - 16n - 16t + 24 + 16nt - 16m) \right) \times \left( \frac{512}{27} \right)^{(512/27)} \right] \\
\times \left[ \left( 32mnt - 16mnt - 16mn - 16nt + 8m + 8n + 8t - 8 \times \left( \frac{4096}{125} \right)^{(4096/125)} \right) \right].
\]

4. Comparisons and Discussion for Cu$_2$O $[m,n,t]$

We develop Tables 5 and 6 for tiny estimations of $m,n,t$ for the structure of Cu$_2$O $[m,n,t]$. The graphical portrayals of registered outcomes area unit are described in Figures 4–6 for specific estimations of $m,n,t$.

5. Comparisons and Discussion for TiF$_2$ $[m,n,t]$

Presently, from Tables 7 and 8, we are able to notice that while there is not much of a stretch, we see that each one of the estimations of entropy is in increasing request because the estimations of $m,n,t$ are increments. The graphical portrayals
Table 5: Comparison of $\text{ENT}_{M_1}$ and $\text{ENT}_{M_2}$ for Cu$_2$O\([m, n, t]\).

| \([m, n, t]\) | $\text{ENT}_{M_1}$ | $\text{ENT}_{M_2}$ |
|----------------|---------------------|---------------------|
| [1, 1, 1]     | 1.12                | 1.21                |
| [2, 2, 2]     | 1.42                | 1.61                |
| [3, 3, 3]     | 1.82                | 1.91                |
| [4, 4, 4]     | 2.12                | 2.51                |
| [5, 5, 5]     | 3.41                | 3.32                |

Table 6: Comparison of $\text{ENT}_{HM}$, $\text{ENT}_F$, $\text{ENT}_{AZI}$, and $\text{ENT}_J$ entropies for Cu$_2$O\([m, n, t]\).

| \([m, n, t]\) | $\text{ENT}_{HM}$ | $\text{ENT}_F$ | $\text{ENT}_{AZI}$ | $\text{ENT}_J$ |
|----------------|-------------------|----------------|-------------------|----------------|
| [1, 1, 1]     | 2.12              | 2.41           | 2.22              | 2.42           |
| [2, 2, 2]     | 3.65              | 3.52           | 3.52              | 3.41           |
| [3, 3, 3]     | 4.54              | 4.65           | 4.42              | 4.81           |
| [4, 4, 4]     | 5.25              | 5.74           | 5.32              | 5.51           |
| [5, 5, 5]     | 6.43              | 6.68           | 6.21              | 6.72           |

Figure 4: (a) The first Zagreb entropy. (b) The second Zagreb entropy.

Figure 5: (a) The hyper Zagreb entropy. (b) The forgotten entropy.
Figure 6: (a) The augmented Zagreb entropy. (b) The Balaban entropy.

Table 7: Comparison of ENT$_{M_1}$ and ENT$_{M_2}$ for TiF$_2 [m,n,t]$.

| $[m,n,t]$ | ENT$_{M_1}$ | ENT$_{M_2}$ |
|-----------|-------------|-------------|
| [1,1,1]   | 1.22        | 1.31        |
| [2,2,2]   | 1.62        | 1.81        |
| [3,3,3]   | 1.92        | 2.31        |
| [4,4,4]   | 2.32        | 2.91        |
| [5,5,5]   | 3.61        | 3.42        |

Table 8: Comparison of ENT$_{H_M}$, ENT$_{F}$, ENT$_{AZI}$, and ENT$_{J}$ entropies for TiF$_2 [m,n,t]$.

| $[m,n,t]$ | ENT$_{H_M}$ | ENT$_{F}$ | ENT$_{AZI}$ | ENT$_{J}$ |
|-----------|-------------|-----------|-------------|-----------|
| [1,1,1]   | 2.02        | 2.21      | 2.12        | 2.32      |
| [2,2,2]   | 3.45        | 3.32      | 3.42        | 3.51      |
| [3,3,3]   | 4.34        | 4.45      | 4.52        | 4.71      |
| [4,4,4]   | 5.55        | 5.54      | 5.62        | 5.41      |
| [5,5,5]   | 6.63        | 6.88      | 6.31        | 6.22      |

Figure 7: (a) The first Zagreb entropy. (b) The second Zagreb entropy.
of registered outcomes are diagrammatic in Figures 7–9 for specific estimations of \( m, n, t \).

### 6. Conclusion

In this paper, in lightweight of applied scientist, entropy, we have a tendency to study the graph entropies known with another information work. We have a tendency to present an association between the gradation established topological indices with gradation established entropies. We are particularly interested in forming the gradation that is based on entropies for crystallographic erection of oxide \( \text{Cu}_2\text{O}[m, n, t] \) and metal difluoride \( \text{TiF}_2[m, n, t] \). In addition, the arithmetic estimations of these entropies have been registered in tables that provide the correlation between the gradation focused topological lists and gradation established entropies that drives the United States of America to differentiate the physio-substance possessions of those crystallographic erection of \( \text{Cu}_2\text{O}[m, n, t] \) and \( \text{TiF}_2[m, n, t] \).

### Data Availability

No data were used to support this study.

### Conflicts of Interest

The authors declare that they have no conflicts of interest.

### References

[1] W. Gao, M. K. Siddiqui, M. Naeem, and N. A. Rehman, "Topological characterization of carbon graphite and crystal
cubic carbon structures,” *Molecules*, vol. 22, no. 9, pp. 1496–1507, 2017.

[2] M. Imran, M. K. Siddiqui, M. Naem, and M. A. Iqbal, “On topological properties of symmetric chemical structures,” *Symmetry*, vol. 10, pp. 1–21, 2018.

[3] W. Gao, H. Wu, M. K. Siddiqui, and A. Q. Baig, “Study of biological networks using graph theory,” *Saudi Journal of Biological Sciences*, vol. 25, no. 6, pp. 1212–1219, 2018.

[4] M. K. Siddiqui, M. Imran, and A. Ahmad, “On zagreb indices, zagreb polynomials of some nanostar dendrimers,” *Applied Mathematics and Computation*, vol. 280, pp. 132–139, 2016.

[5] M. K. Siddiqui, M. Naem, N. A. Rahman, and M. Imran, “Computing topological indices of certain networks,” *Journal of Optoelectronics and Advanced Materials*, vol. 18, no. 9–10, pp. 884–892, 2016.

[6] A. Mowshowitz and M. Dehmer, “Entropy and the complexity of graphs revisited,” *Entropy*, vol. 14, no. 3, pp. 559–570, 2012.

[7] S. Cao, M. Dehmer, and Y. Shi, “Extremality of degree-based graph entropies,” *Information Sciences*, vol. 278, pp. 22–33, 2014.

[8] S. Cao and M. Dehmer, “Degree-based entropies of networks revisited,” *Applied Mathematics and Computation*, vol. 261, pp. 141–147, 2015.

[9] M. Dehmer, “Information processing in complex networks: graph entropy and information functionals,” *Applied Mathematics and Computation*, vol. 201, no. 1–2, pp. 82–94, 2008.

[10] M. Dehmer, L. Sivakumar, and K. Varmuza, “Uniquely discriminating molecular structures using novel eigenvalue-based descriptors,” *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 67, pp. 147–172, 2012.

[11] E. Estrada and N. Hatano, “Statistical-mechanical approach to subgraph centrality in complex networks,” *Chemical Physics Letters*, vol. 439, no. 1–3, pp. 247–251, 2007.

[12] E. Estrada, “Generalized walks-based centrality measures for complex biological networks,” *Journal of Theoretical Biology*, vol. 263, no. 4, pp. 556–565, 2010.

[13] C. E. Shannon, “A mathematical theory of communication,” *Bell System Technical Journal*, vol. 27, no. 3, pp. 379–423, 1948.

[14] N. Rashevsky, “Life, information theory, and topology,” *The Bulletin of Mathematical Biophysics*, vol. 17, no. 3, pp. 229–235, 1955.

[15] M. Dehmer and M. Graber, “The discrimination power of molecular identification numbers revisited,” *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 69, pp. 785–794, 2013.

[16] R. E. Ulanowicz, “Quantitative methods for ecological network analysis,” *Computational Biology and Chemistry*, vol. 28, no. 5–6, pp. 321–339, 2004.

[17] M. Dehmer and A. Mowshowitz, “A history of graph entropy measures,” *Information Sciences*, vol. 181, no. 1, pp. 57–78, 2011.

[18] B. Furtula and I. Gutman, “A forgotten topological index,” *Journal of Mathematical Chemistry*, vol. 53, no. 4, pp. 1184–1190, 2015.

[19] B. Furtula, A. Graovac, and D. Vukičević, “Augmented zagreb index,” *Journal of Mathematical Chemistry*, vol. 48, no. 2, pp. 370–380, 2010.

[20] W. Wu, C. Zhang, W. Lin et al., “Quantitative structure-property relationship (QSPR) modeling of drug-loaded polymeric micelles via genetic function approximation,” *PLoS One*, vol. 10, no. 3, Article ID e0119575, 2015.

[21] R. V. Solé and S. I. Valverde, “Information theory of complex networks: on evolution and architectural constraints,” *Complex Networks*, vol. 650, pp. 189–207, 2004.

[22] Y. J. Tan and J. Wu, “Network structure entropy and its application to scale-free networks,” *Systems Engineering-Theory & Practice*, vol. 6, pp. 1–3, 2004.

[23] H. Morowitz, “Some order-disorder considerations in living systems,” *Bulletin of Mathematical Biophysics*, vol. 17, pp. 81–86, 1953.

[24] H. Quastler, “Information theory in biology,” *Bulletin of Mathematical Biophysics*, vol. 8, pp. 183–185, 1954.

[25] E. Trucco, “A note on the information content of graphs,” *The Bulletin of Mathematical Biophysics*, vol. 18, no. 2, pp. 129–135, 1956.

[26] D. Bonchev, *Complexity in Chemistry. Introduction and Fundamentals*, Taylor and Francis, Boca Raton, FL, USA, 2003.

[27] 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, 1972.

[28] I. Gutman and K. C. Das, “The first zagreb index 30 years after,” *MATCH Communication in Mathematical Computer Chemistry*, vol. 50, pp. 83–92, 2004.

[29] G. H. Shirdel, H. Rezapour, and A. M. Sayadi, “The hyper zagreb index of graph operations,” *Iranian Journal of Mathematical Chemistry*, vol. 4, no. 2, pp. 213–220, 2013.

[30] Z. Chen, M. Dehmer, and Y. Shi, “A note on distance based graph entropies,” *Entropy*, vol. 16, no. 10, pp. 5416–5427, 2014.

[31] S. Manzoor, M. K. Siddiqui, and S. Ahmad, “On physical analysis of degree-based entropy measures for metal-organic superlattices,” *The European Physical Journal Plus*, vol. 136, no. 3, pp. 1–22, 2021.

[32] S. Manzoor, M. K. Siddiqui, and S. Ahmad, “Degree-based entropy of molecular structure of hyaluronic acid-curcumin conjugates,” *The European Physical Journal Plus*, vol. 136, no. 1, pp. 1–21, 2021.

[33] S. Manzoor, Y. M. Chu, M. K. Siddiqui, and S. Ahmad, “On topological aspects of degree based entropy for two carbon nanosheets,” *Main Group Metal Chemistry*, vol. 43, no. 1, pp. 205–218, 2020.

[34] S. Manzoor, M. K. Siddiqui, and S. Ahmad, “On entropy measures of molecular graphs using topological indices,” *Arabian Journal of Chemistry*, vol. 13, no. 8, pp. 6285–6298, 2020.

[35] K. Chen, C. Sun, S. Song, and D. Xue, “Polymorphic crystallization of Cu₃O compound,” *CrystEngComm*, vol. 16, pp. 52–57, 2014.

[36] J. Zhang, J. Liu, Q. Peng, X. Wang, and Y. Li, “Nearly monodisperse Cu₃O and NCuO anospheres: preparation and applications for sensitive gas sensors,” *Chemistry of Materials*, vol. 18, no. 4, pp. 867–871, 2006.