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Entropy-Based Topological Characterization of Magnesium Silicide

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Abstract. Chemical graph theory focuses on the physical features of molecular structures using topological descriptors, where topological descriptors are mathematical formulas that represents a molecular structure and can be applied to any graph. Chemical graph theory depends extensively on topological descriptors, particularly in relation with chemical features of molecules. According to the structural characteristics of the graphs implemented in their computation, they can be categorised. This research paper focuses on several types of Zagreb descriptors for magnesium silicide's molecular structure. The structure denoted by (Mg_2Si), comprises of eight magnesium Mg and four silicon Si atoms. The structure and shape of the molecular graph are commonly described by the Zagreb indices. The significance of these indices in simulating the chemical characteristics of the magnesium silicide network is emphasised in the paper.

AMS (MOS) Subject Classification Codes: 05C09; 05C92
Key Words: Topological descriptors; Molecular complexity; Magnesium silicide; Graph entropy

1. INTRODUCTION

Entropy, a basis in thermodynamics, is a measurement of randomness or disorder, important in system evolution based on the second law [36]. It is a basis in statistical mechanics in physics [5], linking micro and macro properties [6]. Entropy is applied in reaction spontaneity calculations by chemists with the Gibbs free energy, where δS (change in entropy) is a deciding equilibrium. In information theory, Shannon reformulated entropy as a measure of uncertainty in information transmission. Entropy is utilized in ecosystems and cellular functions by biologists, where order and disorder are balanced in metabolism. In chemical graph theory, molecules are graphically mapped (nodes into atoms, and edges into bonds). Entropy in such a system is a structure complexity measurement useful in prediction of chemical properties. Entropy in a graph is a Shannon-derived quantity based on node degree distribution or topological indices and connectivity patterns. Architectural variability is implied with high entropy and is a source of increased reactivity or instability. They are useful in drug design in QSAR analyses where molecular structure is related with bioactivity. Topological indices are numerical features based on a chemical substance's molecular graph and are a structure reflection independent of geometric and space-related properties. Topological indices are increasingly utilized in chemical graph theory with a future in representing physicochemical properties, bioactivity prediction, and designing new molecules in cheminformatics and drug design.

Topological indices such as Randic Index [34], Zagreb Indices [17], and the Wiener Index [41] are important in QSAR/QSPR research. They are applied in prediction of molecular properties such as pharmacokinetics and drug design and in material science and in prediction of molecular properties such as boiling points and stability. In pharmaceutical chemistry, topological indices are used with a view to assessing molecular similarity and leading the design of better drug candidates [11, 43, 19]. The Randic Connectivity Index, for example, has been used with a view to screening compounds possessing potential bioactivity versus a specific target molecule [14].

In nanoscience, geometric-arithmetic index and atom-bond connectivity index play a significant role in simulating the electronic properties and the stability of nanomaterials such as nanotubes and fullerenes [20, 29, 37]. Topological indices are also applied in estimating chemical risks in the environment based on bioaccumulation and degradation properties. The Balaban Index is applied in estimating the ecological risks posed by pollutants, among other applications. Outside the chemical discipline, these indices are applied in bionetworks where they are applied in protein-protein research, in the study of metabolism pathways, and in simulating biological systems.

Entropy-based molecular descriptors have been explored in recent times with increased frequency because they are useful in characterizing molecular structure. Entropy-based descriptors have been investigated in simulated and actual chemical compounds by Dehmer et al. [9] and found useful in models based on statistics. Entropy measures have been applied in a vast array of polycyclic aromatic compounds (PAHs). Entropy calculations have also been applied in research on metal-organic frameworks (MOFs) and finding important structure and thermodynamic properties [22].

In graph theory and chemical graph entropies, Kavitha et al. [26] investigated kekulene structure tessellations and their implications in the field of thermochemistry and spectroscopy. Likewise, Rahul et al. [35] utilized Shannon entropy in degree-based entropy investigation in the field of graphyne and graphdiyne and provided insights about their structure. Machine learning methods have been applied in the prediction of entropy, and a prime example is provided by Aldosari et al. [3] who utilized machine intelligence in order to forecast entropy and heat capacity in hydrocarbons

Topological indices and entropy metrics have been widely investigated in the structure of zeolites. Jacob et al. [24] identified tetragonal zeolite merlinoites based on entropy metrics and gave insights on their crystal properties. In a second investigation, Paul et al. [33] made a comparison between multiplicative and scalar multiplicative descriptors in QSAR/QSPR research and examined their entropy-driven efficiency.

Now a days, the most of researcher are focusing on entropy based descriptors for specific molecular networks. Zuo et al. [44] calculated the entropy of benzenoid structures and Shanmukha et al. [38] determine the expectation values of Sombor indices and their entropy for a graph associated with a graphene related graphs. These researchers' effort strengthen the position of entropy descriptors in computational chemistry and materials science. Entropy descriptors have proved valuable in molecular modelling, pharmaceutical chemistry, nanomaterials research, and QSAR/QSPR analyses. The further development of entropy-based descriptors combined with machine learning and regression approaches will increase the predictive power of molecular characterization techniques. Recently, many authors worked on different types topological indices that helps to calculate the entropy measures of different graphs. Answar *al. et* [4] determine the intuitionistic Sombor indices via mathematical approach. By using the machine learning approach entropy based QSPR analysis of drugs and Sombor indices of molecular graphs are studied in [1]. The latest approaches to exploring the topological indices for different drugs [32] and flavonoid molecular structures are considered [18]. In these papers, the authors used the new techniques and methods that will helps the new researchers in future.

Magnesium silicide (Mg_2Si) is a magnesium and silicon inorganic chemical and a metal silicide [31]. It is a semiconductor with special properties and is a key substance in technology. Structurally, Mg_2Si is in the arrangement type referred to as antifluorite and is a face-centered cubic (FCC) system with space group $Fm\bar{3}m$. The magnesium atoms are in positions where fluorine is in CaF_2, and silicon atoms are in positions where there is calcium, and there is a resulting ionic substance with metallic and semiconductor properties. The crystal structure is what makes it stable and efficient in heat and is significant in high-temperature uses.

The physical and chemical properties are also the cause of utility in the case of Mg_2Si [30, 27]. It has a molecular weight of 76.71 g/mol, a density of about 1.94 g/cm^3, and a melting point about 1,100 C. It is a semiconductor with a band gap with a value about 0.78 eV and is, therefore, used in electronics and thermos-electronics. It is insoluble in water but acid-reactive and emits silane gas (SiH_4), a useful feature in special chemical reactions. The thermal stability is high in the case of Mg_2Si, and owing to this, it is used in conditions where there is a requirement for a substance with thermal decomposition resistance. The existing study in [16] discovers the application of the Magnesium Iodide structure by using modified M-polynomials to evaluate its topological and chemical properties.

Magnesium silicide finds numerous uses in numerous sectors. One significant usage is in thermoelectric power generation where magnesium silicide is a thermoelectric generator with a potential ability to convert power wasted in heat into electrical power [7]. It is particularly useful in space exploration and in recovering process heat in the industry [28]. In the field of optoelectronics, Mg_2Si is utilized in the fabrication of sensors in the infrared and in photonic devices because there is a favorable band gap in the infrared [25, 15]. Another significant usage is in alloys with light metal where magnesium silicide is a hard phase in magnesium-aluminum-silicon (Mg-Al-Si) alloys. These alloys are utilized in numerous ways in the space, automotive, and electronics sectors in order to harden a substance while keeping low density [42].

2. PRELIMINARIES

The first topological index depending on the initial vertex degree was proposed by Randi in 1975 under the name connectivity index or Randi index [34]. In all the formulas γ_1, γ_2 are the vertices of the graph. The mathematical definition of this index is:

$$R_{-\frac{1}{2}}(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \frac{1}{\sqrt{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}} \tag{2. 1}$$

The first and second Zagreb indices were introduced in 1972 by Gutman [17]

$$M_1(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} (\Upsilon(\gamma_1) + \Upsilon(\gamma_2)) \tag{2. 2}$$

$$M_2(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} (\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)) \tag{2. 3}$$

In 2013, Shirdel et al. [39] introduced the hyper Zagreb index

$$HM(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} (\Upsilon(\gamma_1) + \Upsilon(\gamma_2))^2 \tag{2. 4}$$

Estrada et al. [10] introduced the atom-bond connectivity index:

$$ABC(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \sqrt{\frac{\Upsilon(\gamma_1) + \Upsilon(\gamma_2)}{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}} \tag{2. 5}$$

The geometric arithmetic index was introduced by Vukicević et al. [40] in 2009:

$$GA(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \frac{2\sqrt{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}}{\Upsilon(\gamma_1) + \Upsilon(\gamma_2)} \tag{2. 6}$$

Furtula and Gutman [13] presented the forgotten topological index in 2015

$$F(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} (\Upsilon(\gamma_1)^2 + \Upsilon(\gamma_2)^2) \tag{2. 7}$$

Furtula et al. [12] defined the augmented Zagreb index in 2010

$$AZI(M_g) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \left(\frac{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}{\Upsilon(\gamma_1) + \Upsilon(\gamma_2) - 2} \right)^3 \tag{2. 8}$$

Dehmer [8] presented the following notion:

Definition 2.1. [8]. *Let $M_G = (V, \Xi)$ be a connected graph and ψ be an arbitrary information functional. Then entropy of M_G is defined by*

$$E_\Lambda(M_g) = -\sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \frac{\Lambda(\gamma_1\gamma_2)}{\sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \Lambda(\gamma_1\gamma_2)} \ln \left[\frac{\Lambda(\gamma_1\gamma_2)}{\sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \Lambda(\gamma_1\gamma_2)} \right] \tag{2. 9}$$

Randić entropy If $\Lambda(\gamma_1\gamma_2) = \frac{1}{\sqrt{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}}$, then

$$\sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \Lambda(\gamma_1\gamma_2) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \left(\frac{1}{\sqrt{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}} \right) = R_{-\frac{1}{2}}(M_g)$$

The first Zagreb entropy is obtained by simplifying Equation (2. 9) as follows:

$$E_{R_{-\frac{1}{2}}}(M_g) = \ln\left(R_{-\frac{1}{2}}(M_g)\right) - \frac{1}{R_{-\frac{1}{2}}(M_g)} \ln \left[\prod_{\gamma_1\gamma_2 \in \Xi(M_g)} \left(\frac{1}{\sqrt{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}} \right)^{\frac{1}{\sqrt{\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)}}} \right] \tag{2. 10}$$

First Zagreb entropy
If $\Lambda(\gamma_1\gamma_2) = \Upsilon(\gamma_1) + \Upsilon(\gamma_2)$, then

$$\sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \Lambda(\gamma_1\gamma_2) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \big(\Upsilon(\gamma_1) + \Upsilon(\gamma_2)\big) = M_1(M_g)$$

The first Zagreb entropy is obtained by simplifying Equation (2. 9) as follows:

$$E_{M_1(M_g)} = \ln\big(M_1(M_g)\big) - \frac{1}{M_1(M_g)} \ln \left[\prod_{\gamma_1\gamma_2 \in \Xi(M_g)} \big(\Upsilon(\gamma_1) + \Upsilon(\gamma_2)\big)^{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)} \right] \tag{2. 11}$$

Second Zagreb entropy
If $\Lambda(\gamma_1\gamma_2) = \Upsilon(\gamma_1) \times \Upsilon(\gamma_2)$, then

$$\sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \Lambda(\gamma_1\gamma_2) = \sum_{\gamma_1\gamma_2 \in \Xi(M_g)} \big(\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)\big) = M_2(M_g)$$

The second Zagreb entropy is obtained by simplifying Equation (2. 9) as follows:

$$E_{M_2(M_g)} = \ln\left(M_2(M_g)\right) - \frac{1}{\big(M_2(M_g)\big)} \ln \left[\prod_{\gamma_1\gamma_2 \in \Xi(M_g)} \big[\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)\big]^{\left[\Upsilon(\gamma_1) \times \Upsilon(\gamma_2)\right]} \right] \tag{2. 12}$$

Hyper Zagreb entropy

$$E_{HM(M_g)} = \ln\left(HM(M_g)\right) - \frac{1}{\big(HM(M_g)\big)} \ln \left[\prod_{\gamma_1\gamma_2 \in \Xi(M_g)} \big[(\Upsilon(\gamma_1) + \Upsilon(\gamma_2))^2\big]^{\left[(\Upsilon(\gamma_1)+\Upsilon(\gamma_2))^2\right]} \right] \tag{2. 13}$$

Atom bond connectivity entropy

$$E_{ABC(M_g)} = \ln\big(ABC(M_g)\big) - \frac{1}{\big(ABC(M_g)\big)} \ln\left[\prod_{\gamma_1\gamma_2\in\Xi(M_g)}\left[\sqrt{\frac{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)}{\Upsilon(\gamma_1)\times\Upsilon(\gamma_2)}}\right]^{\left[\sqrt{\frac{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)}{\Upsilon(\gamma_1)\times\Upsilon(\gamma_2)}}\right]}\right] \tag{2. 14}$$

Geometrical arithmetic entropy

$$E_{GA(M_g)} = \ln\big(GA(M_g)\big) - \frac{1}{\big(GA(M_g)\big)} \ln\left[\prod_{\gamma_1\gamma_2\in\Xi(M_g)}\left[\frac{2\sqrt{\Upsilon(\gamma_1)\times\Upsilon(\gamma_2)}}{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)}\right]^{\left[\frac{2\sqrt{\Upsilon(\gamma_1)\times\Upsilon(\gamma_2)}}{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)}\right]}\right] \tag{2. 15}$$

Forgotten entropy The forgotten entropy is defined as follows:

$$E_{F(M_g)} = \ln\big(F(M_g)\big) - \frac{1}{\big(F(M_g)\big)} \ln\left[\prod_{\gamma_1\gamma_2\in\Xi(M_g)}\left[(\Upsilon(\gamma_1)^2+\Upsilon(\gamma_2)^2)\right]^{\left[\Upsilon(\gamma_1)^2+\Upsilon(\gamma_2)^2\right]}\right] \tag{2. 16}$$

Augmented Zagreb entropy

$$E_{AZI(M_g)} = \ln\big(AZI(M_g)\big) - \frac{1}{\big(AZI(M_g)\big)} \ln\left[\prod_{\gamma_1\gamma_2\in\Xi(M_g)}\left[\left(\frac{\Upsilon(\gamma_1)\times\Upsilon(\gamma_2)}{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)-2}\right)^3\right]^{\left[\left(\frac{\Upsilon(\gamma_1)\times\Upsilon(\gamma_2)}{\Upsilon(\gamma_1)+\Upsilon(\gamma_2)-2}\right)^3\right]}\right] \tag{2. 17}$$

Recently, some researchers determine the entropy of different families of graph with new approaches. Ismail *al. et* [23] determine the entropy and topological indices of phenylacetone monooxygenase by using Python coding, this will motivate the new researcher to work in this direction with different coding techniques. Huang *al. et* [21] investigate the entropy measure of cage network with subdivision via regression analysis. The entropy-based modeling of chain hex-derived networks are determined by Ahmed [2] in 2024. These new approaches will open up new horizons for future research and provide valuable directions for further exploration in the field.

3. Main Results

In this section, we present the entropy-based characterization of the Magnesium Silicide molecular structure using various topological entropy measures.

3.1. **Construction of Magnesium-Silicide Graph.** Let $M_g = Mg_2Si$ be a molecular graph with $\alpha_1 \times \alpha_2 \times \alpha_3$ cells see Figure 1. The cardinalities of the vertex set of this graph is given by $12\alpha_1\alpha_2\alpha_3 + 2\alpha_1\alpha_2 + 2\alpha_2\alpha_3 + 2\alpha_1\alpha_3 + \alpha_1 + \alpha_2 + \alpha_3 + 1$, and the edge set is given by $32\alpha_1\alpha_2\alpha_3$. There are four distinct types of vertex degrees 1, 2, 4, and 8. Specifically, there are 8 vertices of degree 1, $4\alpha_1 + 4\alpha_2 + 4\alpha_3 - 12$ vertices of degree 2, $8\alpha_1\alpha_2\alpha_3 + 4\alpha_1\alpha_2 + 4\alpha_2\alpha_3 + 4\alpha_1\alpha_3 - 4\alpha_1 - 4\alpha_2 - 4\alpha_3 + 6$ vertices of degree 4, and $4\alpha_1\alpha_2\alpha_3 - 2\alpha_1\alpha_2 - 2\alpha_2\alpha_3 - 2\alpha_1\alpha_3 + \alpha_1 + \alpha_2 + \alpha_3 - 1$ vertices of degree 8.

The edges of the molecular graph of Mg_2Si are classified based on the degree pairs of the two vertices they connect. In particular, edges connecting degree-1 and degree-4 vertices are collected in the set E_1, and there are a total of 8 such edges. Edges connecting degree-2 and degree-4 vertices are in the set E_2, and there are a total of $8\alpha_1+8\alpha_2+8\alpha_3-24$ such edges. Edges connecting degree-4 and degree-4 vertices are in the set E_3, and there

are a total of $16\alpha_1\alpha_2 + 16\alpha_2\alpha_3 + 16\alpha_1\alpha_3 - 16\alpha_1 - 16\alpha_2 - 16\alpha_3 + 24$ such edges. Finally, edges with degree-4 and degree-8 vertices are in the set E_4, and there are a total of $32\alpha_1\alpha_2\alpha_3 - 16\alpha_1\alpha_2 - 16\alpha_2\alpha_3 - 16\alpha_1\alpha_3 + 8\alpha_1 + 8\alpha_2 + 8\alpha_3 - 8$ such edges. These four edge partitions are the only possible pairs of degree pairs in the molecular structure of Mg_2Si See, Figure 1.

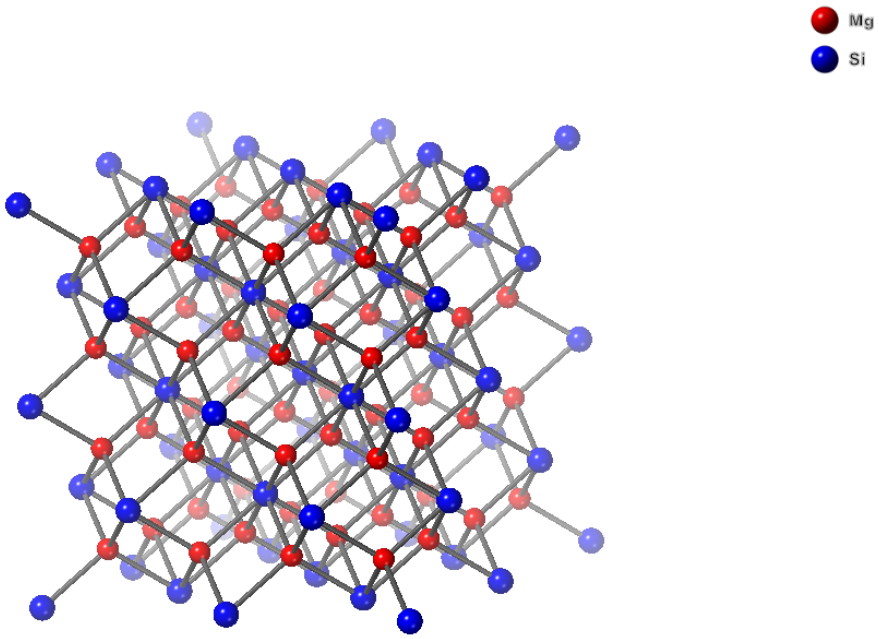

FIGURE 1. Structure of Mg_2Si for $\alpha_1 = \alpha_2 = \alpha_3 = 2$

3.2. **Entropy of Magnesium Silicide.** Now, we determine Randić entropy, first, second and hyper Zagreb entropy, Atom bond connectivity entropy, Forgotten entropy and Augmented Zagreb entropy as follows:

3.2.1. *Randić entropy.* To compute the Randić entropy, we first calculate the Randić index. Using the edge partitions and Eq. (2. 1), we get:

$$R_{-\frac{1}{2}}(M_g) = 10 + \frac{(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}}{4} + 4\alpha_1\alpha_2 + 4\alpha_1\alpha_3 + 4\alpha_2\alpha_3 - 4\alpha_1 - 4\alpha_2 - 4\alpha_3 + \frac{(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}}{8}$$

The Randić entropy is computed using the Eq. (2. 10):

$$E_{R_{-\frac{1}{2}}}(M_g) = \ln\Big(10 + \frac{\sqrt{2}\,(8\alpha_1+8\alpha_2+8\alpha_3-24)}{4} + 4\alpha_1\alpha_2 + 4\alpha_1\alpha_3 + 4\alpha_2\alpha_3 - 4\alpha_1 - 4\alpha_2 - 4\alpha_3 +$$

$$\frac{\sqrt{2}\,(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)}{8}\Big) - \Bigg[4\ln(2) + \frac{(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}\,\ln\left(\frac{\sqrt{2}}{4}\right)}{4} - \frac{(16\alpha_1\alpha_2+16\alpha_1\alpha_3+16\alpha_2\alpha_3-16\alpha_1-16\alpha_2-16\alpha_3+24)\ln(2)}{2} + \frac{(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}\,\ln\left(\frac{\sqrt{2}}{8}\right)}{8}\Bigg] \Bigg/ \Bigg[10 + \frac{(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}}{4} + 4\alpha_1\alpha_2 + 4\alpha_1\alpha_3 + 4\alpha_2\alpha_3 - 4\alpha_1 - 4\alpha_2 - 4\alpha_3 + \frac{(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}}{8}\Bigg]$$

After, simplification we get:

$$E_{R_{-\frac{1}{2}}}(M_g) = \ln(0.1006 + 0.2427\alpha_1 + 0.2427\alpha_2 + 0.2427\alpha_3 + 1.1716\alpha_1\alpha_2 + 1.1716\alpha_1\alpha_3 + 1.1716\alpha_2\alpha_3 + 5.6568\alpha_1\alpha_2\alpha_3) - \frac{1.0(0.1817+0.1540\alpha_1+0.1540\alpha_2+0.1540\alpha_3-0.6440\alpha_1\alpha_2-0.6440\alpha_1\alpha_3-0.6440\alpha_2\alpha_3-9.8020\alpha_1\alpha_2\alpha_3)}{0.1006+0.2427\alpha_1+0.2427\alpha_2+0.2427\alpha_3+1.1716\alpha_1\alpha_2+1.1716\alpha_1\alpha_3+1.1716\alpha_2\alpha_3+5.6568\alpha_1\alpha_2\alpha_3}$$

3.2.2. *First Zagreb entropy.* First Zagreb entropy is computed using the Equations (2. 2) and (2. 11).

$$M_1(M_g) = 384\alpha_1\alpha_2\alpha_3 - 64\alpha_1\alpha_2 - 64\alpha_1\alpha_3 - 64\alpha_2\alpha_3 + 16\alpha_1 + 16\alpha_2 + 16\alpha_3 - 8$$

$$E_{M_1}(M_g) = \ln(384\alpha_1\alpha_2\alpha_3 - 64\alpha_1\alpha_2 - 64\alpha_1\alpha_3 - 64\alpha_2\alpha_3 + 16\alpha_1 + 16\alpha_2 + 16\alpha_3 - 8) - \frac{40\ln(5)+6(8\alpha_1+8\alpha_2+8\alpha_3-24)\ln(6)+24(16\alpha_1\alpha_2+16\alpha_1\alpha_3+16\alpha_2\alpha_3-16\alpha_1-16\alpha_2-16\alpha_3+24)\ln(2)}{384\alpha_1\alpha_2\alpha_3-64\alpha_1\alpha_2-64\alpha_1\alpha_3-64\alpha_2\alpha_3+16\alpha_1+16\alpha_2+16\alpha_3-8} + \frac{12(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\ln(12)}{384\alpha_1\alpha_2\alpha_3-64\alpha_1\alpha_2-64\alpha_1\alpha_3-64\alpha_2\alpha_3+16\alpha_1+16\alpha_2+16\alpha_3-8}$$

$$E_{M_1}(M_g) = \ln(384\alpha_1\alpha_2\alpha_3 - 64\alpha_1\alpha_2 - 64\alpha_1\alpha_3 - 64\alpha_2\alpha_3 + 16\alpha_1 + 16\alpha_2 + 16\alpha_3 - 8) - \frac{(-32.93+58.39\alpha_1+58.39\alpha_2+58.39\alpha_3-210.94\alpha_1\alpha_2-210.94\alpha_1\alpha_3-210.94\alpha_2\alpha_3+954.20\alpha_1\alpha_2\alpha_3)}{384\alpha_1\alpha_2\alpha_3-64\alpha_1\alpha_2-64\alpha_1\alpha_3-64\alpha_2\alpha_3+16\alpha_1+16\alpha_2+16\alpha_3-8}$$

3.2.3. *Second Zagreb entropy.* Second Zagreb entropy is computed using the Equations (2. 3) and (2. 12).

$$M_2(M_g) = 1024\alpha_1\alpha_2\alpha_3 - 256\alpha_1\alpha_2 - 256\alpha_1\alpha_3 - 256\alpha_2\alpha_3 + 64\alpha_1 + 64\alpha_2 + 64\alpha_3 - 32$$

$$E_{M_2}(M_g) = \ln(1024\alpha_1\alpha_2\alpha_3 - 256\alpha_1\alpha_2 - 256\alpha_1\alpha_3 - 256\alpha_2\alpha_3 + 64\alpha_1 + 64\alpha_2 + 64\alpha_3 - 32) - \frac{64\ln(2)+24(8\alpha_1+8\alpha_2+8\alpha_3-24)\ln(2)+64(16\alpha_1\alpha_2+16\alpha_1\alpha_3+16\alpha_2\alpha_3-16\alpha_1-16\alpha_2-16\alpha_3+24)\ln(2)}{1024\alpha_1\alpha_2\alpha_3-256\alpha_1\alpha_2-256\alpha_1\alpha_3-256\alpha_2\alpha_3+64\alpha_1+64\alpha_2+64\alpha_3-32} + \frac{160(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\ln(2)}{1024\alpha_1\alpha_2\alpha_3-256\alpha_1\alpha_2-256\alpha_1\alpha_3-256\alpha_2\alpha_3+64\alpha_1+64\alpha_2+64\alpha_3-32}$$

$$E_{M_2}(M_g) = \ln(1024\alpha_1\alpha_2\alpha_3 - 256\alpha_1\alpha_2 - 256\alpha_1\alpha_3 - 256\alpha_2\alpha_3 + 64\alpha_1 + 64\alpha_2 + 64\alpha_3 - 32) - \frac{(-177.43+310.54\alpha_1+310.54\alpha_2+310.54\alpha_3-1064.6\alpha_1\alpha_2-1064.6\alpha_1\alpha_3-1064.6\alpha_2\alpha_3+3549\alpha_1\alpha_2\alpha_3)}{1024\alpha_1\alpha_2\alpha_3-256\alpha_1\alpha_2-256\alpha_1\alpha_3-256\alpha_2\alpha_3+64\alpha_1+64\alpha_2+64\alpha_3-32}$$

3.2.4. *Hyper Zagreb entropy.* Hyper Zagreb entropy is obtained using the Equations (2. 4) and (2. 13).

$$HM(M_g) = 4608\alpha_1\alpha_2\alpha_3 - 1280\alpha_1\alpha_2 - 1280\alpha_1\alpha_3 - 1280\alpha_2\alpha_3 + 416\alpha_1 + 416\alpha_2 + 416\alpha_3 - 280$$

$E_{HM(M_g)} = \ln(4608\alpha_1\alpha_2\alpha_3 - 1280\alpha_1\alpha_2 - 1280\alpha_1\alpha_3 - 1280\alpha_2\alpha_3 + 416\alpha_1 + 416\alpha_2 + 416\alpha_3 - 280) -$
$\frac{400\ln(5)+72(8\alpha_1+8\alpha_2+8\alpha_3-24)\ln(6)+384(16\alpha_1\alpha_2+16\alpha_1\alpha_3+16\alpha_2\alpha_3-16\alpha_1-16\alpha_2-16\alpha_3+24)\ln(2)}{4608\alpha_1\alpha_2\alpha_3-1280\alpha_1\alpha_2-1280\alpha_1\alpha_3-1280\alpha_2\alpha_3+416\alpha_1+416\alpha_2+416\alpha_3-280} +$
$\frac{288(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\ln(12)}{4608\alpha_1\alpha_2\alpha_3-1280\alpha_1\alpha_2-1280\alpha_1\alpha_3-1280\alpha_2\alpha_3+416\alpha_1+416\alpha_2+416\alpha_3-280}$
$E_{HM(M_g)} = \ln(4608\alpha_1\alpha_2\alpha_3 - 1280\alpha_1\alpha_2 - 1280\alpha_1\alpha_3 - 1280\alpha_2\alpha_3 + 416\alpha_1 + 416\alpha_2 + 416\alpha_3 - 280) -$

$\frac{(-1789.4+2498.6\alpha_1+2498.6\alpha_2+2498.6\alpha_3-7191.4\alpha_1\alpha_2-7191.4\alpha_1\alpha_3-7191.4\alpha_2\alpha_3+22901\alpha_1\alpha_2\alpha_3)}{4608\alpha_1\alpha_2\alpha_3-1280\alpha_1\alpha_2-1280\alpha_1\alpha_3-1280\alpha_2\alpha_3+416\alpha_1+416\alpha_2+416\alpha_3-280}$

3.2.5. *Atom bond connectivity entropy.* Atom bond connectivity entropy is computed using the Equations (2. 5) and (2. 14).

$ABC(M_g) = 4\sqrt{3}+\frac{(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}}{2}+\frac{(16\alpha_1\alpha_2+16\alpha_1\alpha_3+16\alpha_2\alpha_3-16\alpha_1-16\alpha_2-16\alpha_3+24)\sqrt{6}}{4}+$
$\frac{(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{5}}{4}$

$E_{ABC(M_g)} = \ln\big(2\left(-6+\left(3+2\left(\alpha_2+\alpha_3-1\right)\alpha_1+2\left(\alpha_3-1\right)\alpha_2-2\alpha_3\right)\sqrt{3}+2\alpha_1+2\alpha_2+2\alpha_3\right)\sqrt{2}+4\sqrt{3}+$
$2\left(-1+\left(1+2\left(2\alpha_3-1\right)\alpha_2-2\alpha_3\right)\alpha_1+\left(-2\alpha_3+1\right)\alpha_2+\alpha_3\right)\sqrt{5}\big)+$
$\frac{-2\sqrt{6}\left((\alpha_2+\alpha_3-1)\alpha_1+(\alpha_3-1)\alpha_2-\alpha_3+\frac{3}{2}\right)\ln\left(\frac{\sqrt{6}}{4}\right)-2(\alpha_1+\alpha_2+\alpha_3-3)\sqrt{2}\ln\left(\frac{\sqrt{2}}{2}\right)-2\sqrt{3}\ln\left(\frac{\sqrt{3}}{2}\right)-4\sqrt{5}\left(\left(\alpha_2-\frac{1}{2}\right)\left(\alpha_3-\frac{1}{2}\right)\alpha_1+\left(-\frac{\alpha_3}{2}+\frac{1}{4}\right)\alpha_2+\frac{\alpha_3}{4}-\frac{1}{4}\right)\ln\left(\frac{\sqrt{5}}{4}\right)}{\left(\left((2\alpha_2+2\alpha_3-2)\alpha_1+(2\alpha_3-2)\alpha_2-2\alpha_3+3\right)\sqrt{3}+2\alpha_1+2\alpha_2+2\alpha_3-6\right)\sqrt{2}+2\sqrt{3}+\left(\left((4\alpha_3-2)\alpha_2+1-2\alpha_3\right)\alpha_1+(-2\alpha_3+1)\alpha_2-1+\alpha_3\right)\sqrt{5}}$

3.2.6. *Geometrical arithmetic entropy.* Geometrical arithmetic entropy is computed using Equations (2. 6) and (2. 15)

$GA(M_g) = \frac{152}{5} + \frac{2(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}}{3} + 16\alpha_1\alpha_2 + 16\alpha_1\alpha_3 + 16\alpha_2\alpha_3 - 16\alpha_1 - 16\alpha_2 - 16\alpha_3+$
$\frac{2(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}}{3}$

$E_{GA(M_g)} = \ln\Big(\frac{152}{5} + \frac{2(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}}{3} + 16\alpha_1\alpha_2 + 16\alpha_1\alpha_3 + 16\alpha_2\alpha_3 - 16\alpha_1 - 16\alpha_2 - 16\alpha_3$
$+\frac{2(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}}{3}\Big) -$
$\left(\frac{32\ln\left(\frac{4}{5}\right)}{5} + \frac{2(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}\ln\left(\frac{2\sqrt{2}}{3}\right)}{3} + \frac{2(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}\ln\left(\frac{2\sqrt{2}}{3}\right)}{3}\right)\times$
$1\Big/\Big[\ln\Big(\frac{152}{5} + \frac{2(8\alpha_1+8\alpha_2+8\alpha_3-24)\sqrt{2}}{3} + 16\alpha_1\alpha_2 + 16\alpha_1\alpha_3 + 16\alpha_2\alpha_3 - 16\alpha_1 - 16\alpha_2 - 16\alpha_3$
$+\frac{2(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\sqrt{2}}{3}\Big)\Big]$

3.2.7. *Forgotten entropy.* The forgotten entropy is obtained as follows:

$E_{F(M_g)} = \ln(2560\alpha_1\alpha_2\alpha_3 - 768\alpha_1\alpha_2 - 768\alpha_1\alpha_3 - 768\alpha_2\alpha_3 + 288\alpha_1 + 288\alpha_2 + 288\alpha_3 - 216) -$
$[136\ln(17) + 20\left(8\alpha_1 + 8\alpha_2 + 8\alpha_3 - 24\right)\ln(20) + 160\left(16\alpha_1\alpha_2 + 16\alpha_1\alpha_3 + 16\alpha_2\alpha_3 - 16\alpha_1 - 16\alpha_2 - 16\alpha_3 + 24\right)$
$\ln(2) + 80\left(32\alpha_1\alpha_2\alpha_3 - 16\alpha_1\alpha_2 - 16\alpha_1\alpha_3 - 16\alpha_2\alpha_3 + 8\alpha_1 + 8\alpha_2 + 8\alpha_3 - 8\right)\ln(80)]\Big/[2560\alpha_1\alpha_2\alpha_3 - 768\alpha_1\alpha_2$
$-768\alpha_1\alpha_3 - 768\alpha_2\alpha_3 + 288\alpha_1 + 288\alpha_2 + 288\alpha_3 - 216]$

3.2.8. *Augmented Zagreb entropy.* Similarly, augmented Zagreb entropy is:

$E_{AZI(M_g)} = \ln\big(\frac{67264}{3375} + \frac{76736}{3375}\alpha_1 + \frac{76736}{3375}\alpha_2 + \frac{76736}{3375}\alpha_3 - \frac{745472}{3375}\alpha_1\alpha_2 - \frac{745472}{3375}\alpha_1\alpha_3 - \frac{745472}{3375}\alpha_2\alpha_3$
$+\frac{131072}{125}\alpha_1\alpha_2\alpha_3\big) - \Big[\frac{512\ln\left(\frac{64}{27}\right)}{27} + 24\left(8\alpha_1 + 8\alpha_2 + 8\alpha_3 - 24\right)\ln(2) +$
$\frac{512(16\alpha_1\alpha_2+16\alpha_1\alpha_3+16\alpha_2\alpha_3-16\alpha_1-16\alpha_2-16\alpha_3+24)\ln\left(\frac{512}{27}\right)}{27}+$

$$\frac{4096(32\alpha_1\alpha_2\alpha_3-16\alpha_1\alpha_2-16\alpha_1\alpha_3-16\alpha_2\alpha_3+8\alpha_1+8\alpha_2+8\alpha_3-8)\ln\left(\frac{4096}{125}\right)}{125}\Bigg] \Bigg/$$
$$\left[\frac{67264}{3375}+\frac{76736}{3375}\alpha_1+\frac{76736}{3375}\alpha_2+\frac{76736}{3375}\alpha_3-\frac{745472}{3375}\alpha_1\alpha_2-\frac{745472}{3375}\alpha_1\alpha_3-\frac{745472}{3375}\alpha_2\alpha_3+\frac{131072}{125}\alpha_1\alpha_2\alpha_3\right]$$

4. COMPARATIVE ANALYSIS

Calculation of different entropy values for the Magnesium Silicide network provides valuable information about its structural complexity and chemical potential. The entropy values calculated for Randi entropy, Zagreb entropy (First and Second), Hyper Zagreb entropy, ABC entropy, GA entropy, Forgotten entropy, and Augmented Zagreb entropy indicate how a number of topological indices behave under changing molecular arrangements.

$[\alpha_1, \alpha_2, \alpha_3]$	Randić entropy	First Zagreb entropy	Second Zagreb entropy
$[1, 1, 1]$	3.4116	3.4482	3.3647
$[2, 2, 2]$	5.5058	5.5141	5.4457
$[3, 3, 3]$	6.7319	6.7370	6.6905
$[4, 4, 4]$	7.6010	7.6047	7.5695
$[5, 5, 5]$	8.2744	8.2777	8.2500
$[6, 6, 6]$	8.8242	8.8272	8.8038
$[7, 7, 7]$	9.2888	9.2901	9.2714
$[8, 8, 8]$	9.6910	9.6931	9.6764
$[9, 9, 9]$	10.046	10.048	10.033
$[10, 10, 10]$	10.363	10.365	10.351

TABLE 1. Comparison of Randić entropy, First Zagreb entropy, and Second Zagreb entropy for different α values.

The Randić entropy, First Zagreb entropy, and Second Zagreb entropy are compared Table 1, and Figure 2 and found to exhibit a consistent increasing trend with $[\alpha_1, \alpha_2, \alpha_3]$ values. Though similar growth trends are observed in all three entropy measures, First Zagreb entropy is consistently greater than Randi entropy and Second Zagreb entropy for all values under examination. This suggests that structural complexity in Mg_2Si as described by the Zagreb indices is more sensitive to vertex degree sums than degree-product-based descriptors like Randi entropy. The small difference between First and Second Zagreb entropies indicates that both descriptors are efficient in representing molecular connectivity with minimal variation in weight distribution.

The Geometric-Arithmetic (GA) and Atom-Bond Connectivity (ABC) entropy values Figure 3, Table 2) follow a similar trend with other entropy values. GA entropy is always higher than ABC entropy at every point since previously reported in molecular graph theory where GA indexes overestimate connectivity effects due to their emphasis on geometric mean relations. The closeness of both entropy values suggests that both indexes are reliable in representing the electronic properties and stability of Mg_2Si.

The Hyper Zagreb entropy, Forgotten entropy, and Augmented Zagreb entropy Table 3 and Figure 4 are seen to exhibit interesting deviations from other entropies. The Hyper Zagreb entropy values are generally a bit lower than those of Forgotten and Augmented Zagreb entropies at higher α values. This would suggest that squared-degree-based Hyper

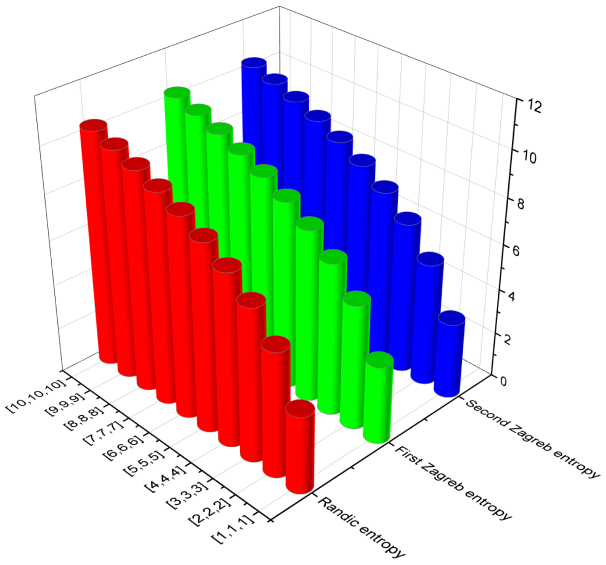

FIGURE 2. Graphical Randić entropy, first Zagreb entropy, and second Zagreb entropy for different α values

$[\alpha_1, \alpha_2, \alpha_3]$	ABC entropy	GA entropy
$[1, 1, 1]$	3.4533	3.4614
$[2, 2, 2]$	5.5401	5.5442
$[3, 3, 3]$	6.7586	6.7611
$[4, 4, 4]$	7.6225	7.6241
$[5, 5, 5]$	8.2925	8.2937
$[6, 6, 6]$	8.8397	8.8407
$[7, 7, 7]$	9.3024	9.3032
$[8, 8, 8]$	9.7031	9.7037
$[9, 9, 9]$	10.057	10.057
$[10, 10, 10]$	10.373	10.374

TABLE 2. Comparison of ABC entropy and GA entropy for different α values.

Zagreb entropy is underestimating certain features of connectivity in relation to Forgotten entropy that places more importance on contributions from higher-degree vertices. The Augmented Zagreb entropy with an additional exponential weighting factor provides higher values for more complex molecular structures and is more sensitive to increasing molecular complexity.

The consistently higher values of Augmented Zagreb entropy in comparison to other descriptors reflect its enhanced sensitivity to both high-degree vertices and non-linear bonding configurations. In the context of Mg_2Si, which features a cubic antifluorite structure with varying local environments for magnesium and silicon atoms, this sensitivity becomes

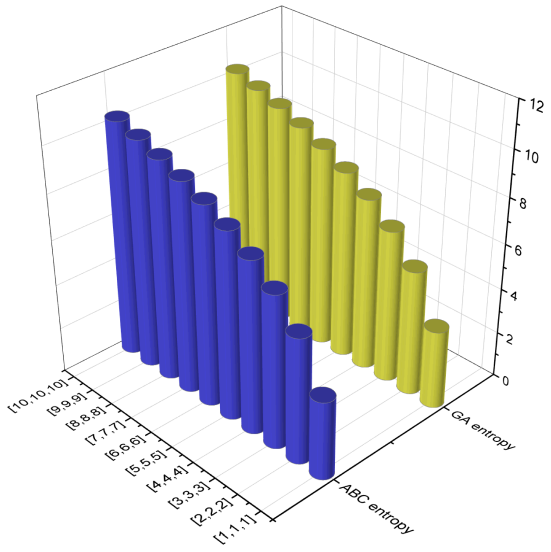

FIGURE 3. Graphical comparison of ABC entropy and GA entropy for different α values

$[\alpha_1, \alpha_2, \alpha_3]$	Hyper Zagreb entropy	Forgotten entropy	Augmented Zagreb entropy
$[1, 1, 1]$	3.4087	3.4362	3.3021
$[2, 2, 2]$	5.4322	5.4173	5.4578
$[3, 3, 3]$	6.6774	6.6625	6.7037
$[4, 4, 4]$	7.5577	7.5471	7.5831
$[5, 5, 5]$	8.2406	8.2306	8.2613
$[6, 6, 6]$	8.7950	8.7866	8.8134
$[7, 7, 7]$	9.2645	9.2572	9.2809
$[8, 8, 8]$	9.6691	9.6632	9.6826
$[9, 9, 9]$	10.027	10.021	10.040
$[10, 10, 10]$	10.345	10.340	10.356

TABLE 3. Comparison of Hyper Zagreb entropy, Forgotten entropy, and Augmented Zagreb entropy for different α values.

particularly significant. A higher Augmented Zagreb entropy suggests increased local connectivity complexity, which may correlate with enhanced charge delocalization pathways and richer electronic density distributions. This, in turn, can influence carrier mobility, thermoelectric efficiency, and overall electronic conductivity. Furthermore, higher entropy values can signal the potential for stronger lattice vibrations and phonon scattering, which are critical in determining thermal conductivity. Thus, the Augmented Zagreb entropy

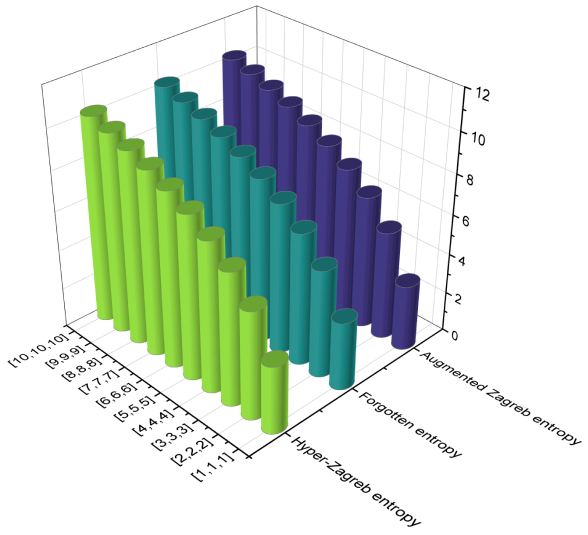

FIGURE 4. Graphical comparison of hyper Zagreb entropy, forgotten entropy, and augmented Zagreb entropy for different α values

not only serves as a topological marker but also provides deeper insights into the physicochemical and electronic behavior of the magnesium silicide network, particularly under high-temperature and thermoelectric conditions.

5. CONCLUSION

The comparative analysis verifies that different entropy measures provide varying yet complementary information on molecular structure in Mg_2Si. Randi, ABC, and GA entropies consider patterns of connectivity, whereas node-degree-based contributions are stressed by Zagreb and Hyper Zagreb entropies. Forgotten and Augmented Zagreb entropies are more sensitive to molecular size and connectivity and are hence useful in explaining stability and electron behavior in magnesium silicide. These findings verify the significance of entropy-based descriptors in predicting thermodynamics and electronics in metal silicides and open new avenues for future material and chemical sciences computation. All measures of entropy are found to be increasing with scaled-up molecular structure and point towards higher topological complexity in large-scale magnesium silicide networks. First, Second, and Hyper Zagreb-based entropies consistently produce higher values than Randi entropy and substantiate their role in modeling chemical properties based on connectivity. ABC and GA entropies are comparable and differ by a small margin with GA entropy consistently producing higher values. Forgotten and Augmented Zagreb entropies are more sensitive to topological features and are highest among all calculated values in the case of Augmented Zagreb entropy.

CONFLICT OF INTEREST

The author declares that he has no conflict of interest.

AUTHOR CONTRIBUTION STATEMENT

- Ali Ahmad: Conceptualization, Methodology, Investigation, Writing - Review & Editing, Supervision
- Mir Asma: Methodology, Verification, Investigation, Data Curation, Writing - Review & Editing, Visualization, Project administration,
- Anwar L. Bilgrami: Validation, Verification, Formal analysis, Resources, Data Curation, Writing - Original Draft, Funding acquisition
- Muhammad Faisal Nadeem: Conceptualization, Software, Validation, Resources, Writing - Original Draft, Supervision

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