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On analysis of silicon dioxide based on topological indices and entropy measure via regression model

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The construction sector accounts for around 95% of the commercial usage of silicon dioxide (sand), for example, in the making of concrete. There are several uses for quartz, however in order to get a purer material, chemical processing is needed. Graph theory proved to be very beneficial for other research, especially in the applied sciences. In particular, graph theory has greatly influenced the field of chemistry. To do this, a transformation is needed to produce a graph with the vertices representing the atoms in the chemical compound and the edges indicating the bonds between the atoms. This graph then represents a chemical network or structure. In a graph, a vertex's valency (or degree) is determined by the number of edges that are incident to it. The entropy of a probability quantifies a system's level of uncertainty. In this article, we compute Zagreb-type indices and then compute the entropy measure. In order to evaluate the relevance of each kind, this article builds several edge degree-based entropies that link to the indices and establish how to adjust them. We also create the logarithmic regression model between indices and entropy.

Keywords Degree of a vertex, Chemical graph theory, Topological indices, Entropy measure, Logarithmic regression model, Silicon dioxide (SiO_2)

According to graph theory, a graph is made up of vertices $V(G)$, or groups of objects, connected by edges $E(G)$, or straight lines[1,2]. We deal with simple graphs, which means that they don't have self-loops or multiple, directed, or weighted edges. η_α represents the degree of a vertex α, which is the number of edges connected to it.

The physical, chemical, and topological characteristics of a graph are displayed by the topological index's numerical value[3,4]. Chemical graph theory allows us to model the mathematical behavior of chemical networks. It has to do with using graph theory to a complex chemical issue. In the discipline of chemical chemistry, this idea is extremely important. Information science, mathematics, and chemistry are combined to make chem-informatics[5,6]. A mathematical technique known as a topological graph index, or molecular descriptor, may be applied to any graph that represents a molecule structure. This index may be used to further study certain physicochemical aspects of a molecule and assess mathematical values. In the last 20 years, a great deal of topological indices, or numerical graph invariants, have been created and applied to correlation analysis in environmental chemistry, toxicology, theoretical chemistry, and pharmacology. To what degree these indices are associated with one another, however, has not been the subject of any comprehensive investigation[21].

Shanmukha, et al.[7,8] examined the curved regression models and chemical application of the vertex-degree-based topological index. Zhang et al.[9,10] examined the degree-based topological indexes of certain anti-cancer treatments using curve fitting models. Rasheed et al.[11] discussed the octane isomer characteristics using new degree-based topological indices. Rai et al.[13] analyzed the comparison of M-polynomial based topological indices between subdivisions and poly Hex-derived networks. Abirami et al.[15,16] computed degree-based topological indices for ruthenium bipyridine's complex structure. Kirana et al.[18] discussed the Quinolone antibiotics' different degree-based topological indices using QSPR and curvilinear regression. Tousi et al.[20,35] computed the degree-based topological indices of Titanium dioxide nanotubes' molecular graph and line graph. Yu et al.[22,23] used the logarithmic regression model's application to the topological indices and entropy metrics of the beryllunite network. Zaman et al.[24] regression models and degree-based topological indicators were utilised in the QSPR study of a few new medications used to treat blood cancer.

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In this paper, we discuss degree-based topological indices. In 1972, the $M_1(G)$, $M_2(G)$ indices were presented by Gutman[25] and defined in Eq.1 and Eq.2 as follows:

$$M_1(G) = \sum_{\alpha\beta \in E(G)} (\eta_\alpha + \eta_\beta). \tag{1}$$

$$M_2(G) = \sum_{\alpha\beta \in E(G)} (\eta_\alpha \times \eta_\beta). \tag{2}$$

Tang et al.[26] defined the third, fourth, and fifth Zagreb indices shown in Eq. 3 and Eq. 4.

$$M_4(G) = \sum_{\alpha\beta \in E(G)} \eta_\alpha(\eta_\alpha + \eta_\beta). \tag{3}$$

$$M_5(G) = \sum_{\alpha\beta \in E(G)} \eta_\beta(\eta_\alpha + \eta_\beta). \tag{4}$$

In 2016, Gao[27] discussed their work and defined redefined Zagreb indices as shown in Eq. 5, Eq. 6, and Eq. 7:

$$ReZG_1(G) = \sum_{\alpha\beta \in E(G)} \frac{\eta_\alpha + \eta_\beta}{\eta_\alpha \times \eta_\beta}. \tag{5}$$

$$ReZG_2(G) = \sum_{\alpha\beta \in E(G)} \frac{\eta_\alpha \times \eta_\beta}{\eta_\alpha + \eta_\beta}. \tag{6}$$

$$ReZG_3(G) = \sum_{\alpha\beta \in E(G)} (\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta). \tag{7}$$

The entropy of a probability quantifies the degree of uncertainty in a system. The statistical methods serve as a solid foundation for this idea. It is mostly used for chemical structures and the graphs that go with them. It also offers details on chemical topologies and graph structure. It was initially employed as a concept in 1955. Entropy has uses in a wide range of technological and scientific domains. This determines both intrinsic and extrinsic entries. Mondal, S., and Das, K. C.[12,29] discussed the degree-based graph entropy in Structure-Property Modeling. Emadi Kouchak et al.[14,30] danalyzed the structural irregularity in networks using graph entropies-graph energies indices. Jacob et al.[31] computed Entropy measurements and topological characterisation of tetragonal zeolite merlinoites. Ishfaq[32] discussed the diamond structure entropies and topological indices. Networks as information functionalities are investigated using the concept of degree power. The concept of entropy for various topological indices is proposed by the writers. The basis discussed in[28] is the entropy of probability distributions. The information entropy is defined as:

$$ENT_\psi(G) = -\sum_{i=1}^{q} N_i \frac{G(\alpha_i\beta_i)}{TI} \log \frac{G(\alpha_i\beta_i)}{TI} = \log(TI) - \frac{1}{TI}\sum_{i=1}^{q} N_i G(\alpha_i\beta_i) \log G(\alpha_i\beta_i). \tag{8}$$

- **First Zagreb Entropy**

If $G(\alpha\beta) = (\eta_\alpha + \eta_\beta)$, then

$$\sum_{\alpha\beta \in E} G(\alpha\beta) = \sum_{\alpha\beta \in E} (\eta_\alpha + \eta_\beta) = M_1$$

Now Eq. (8) represents the first Zagreb entropy.

$$ENT_{M_1}(G) = \log\left(M_1\right) - \frac{1}{\left(M_1\right)} \sum_{i=1}^{q} \sum_{\alpha\beta \in E_i} [(\eta_\alpha + \eta_\beta)] \log\left[(\eta_\alpha + \eta_\beta)\right]. \tag{9}$$

- **Second Zagreb Entropy**

If $G(\alpha\beta) = (\eta_\alpha \times \eta_\beta)$, then

$$\sum_{\alpha\beta \in E} G(\alpha\beta) = \sum_{\alpha\beta \in E} (\eta_\alpha \times \eta_\beta) = M_2$$

Now Equation (8) represents the second Zagreb entropy.

$$ENT_{M_2}(G) = \log\big(M_2\big) - \frac{1}{\big(M_2\big)} \sum_{i=1}^{q} \sum_{\alpha\beta \in E_i} [(\eta_\alpha \times \eta_\beta)] \log\big[(\eta_\alpha \times \eta_\beta)\big]. \tag{10}$$

- **Fourth Zagreb Entropy**

If $G(\alpha\beta) = \eta_\alpha(\eta_\alpha + \eta_\beta)$, then

$$\sum_{\alpha\beta \in E} G(\alpha\beta) = \sum_{\alpha\beta \in E} \eta_\alpha(\eta_\alpha + \eta_\beta) = M_4$$

Now Equation (8) represents the fourth Zagreb entropy.

$$ENT_{M_4}(G) = \log\big(M_4\big) - \frac{1}{\big(M_4\big)} \sum_{i=1}^{q} \sum_{\alpha\beta \in E_i} [\eta_\alpha(\eta_\alpha + \eta_\beta)] \log\big[\eta_\alpha(\eta_\alpha + \eta_\beta)\big]. \tag{11}$$

- **Fifth Zagreb Entropy**

If $G(\alpha\beta) = \eta_\beta(\eta_\alpha + \eta_\beta)$, then

$$\sum_{\alpha\beta \in E} G(\alpha\beta) = \sum_{\alpha\beta \in E} \eta_\beta(\eta_\alpha + \eta_\beta) = M_5$$

Now Equation (8) represents the fifth Zagreb entropy.

$$ENT_{M_5}(G) = \log\big(M_5\big) - \frac{1}{\big(M_5\big)} \sum_{i=1}^{q} \sum_{\alpha\beta \in E_i} [\eta_\beta(\eta_\alpha + \eta_\beta)] \log\big[\eta_\beta(\eta_\alpha + \eta_\beta)\big]. \tag{12}$$

- **Redefined First Zagreb Entropy**

If $G(\alpha\beta) = \frac{\eta_\alpha + \eta_\beta}{\eta_\alpha \times \eta_\beta}$, then

$$\sum_{\alpha\beta \in E} G(\alpha\beta) = \sum_{\alpha\beta \in E} \frac{\eta_\alpha + \eta_\beta}{\eta_\alpha \times \eta_\beta} = ReZG_1$$

Now Equation (8) represents the redefined first Zagreb Entropy.

$$ENT_{ReZ_1}(G) = \log\big(ReZG_1\big) - \frac{1}{\big(ReZG_1\big)} \sum_{i=1}^{q} \sum_{\alpha\beta \in E_i} [\frac{\eta_\alpha + \eta_\beta}{\eta_\alpha \times \eta_\beta}] \log\big[\frac{\eta_\alpha + \eta_\beta}{\eta_\alpha \times \eta_\beta}\big]. \tag{13}$$

- **Redefined Second Zagreb Entropy**

If $G(\alpha\beta) = \frac{\eta_\alpha \times \eta_\beta}{\eta_\alpha + \eta_\beta}$, then

$$\sum_{\alpha\beta \in E} G(\alpha\beta) = \sum_{\alpha\beta \in E} \frac{\eta_\alpha \times \eta_\beta}{\eta_\alpha + \eta_\beta} = ReZG_2$$

Now Equation (8) represents the redefined second Zagreb entropy.

$$ENT_{ReZG_2}(G) = \log\big(ReZG_2\big) - \frac{1}{\big(ReZG_2\big)} \sum_{i=1}^{q} \sum_{\alpha\beta \in E_i} [\frac{\eta_\alpha \times \eta_\beta}{\eta_\alpha + \eta_\beta}] \log\big[\frac{\eta_\alpha \times \eta_\beta}{\eta_\alpha + \eta_\beta}\big]. \tag{14}$$

- **Redefined third Zagreb Entropy**

If $G(\alpha\beta) = (\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta)$, then

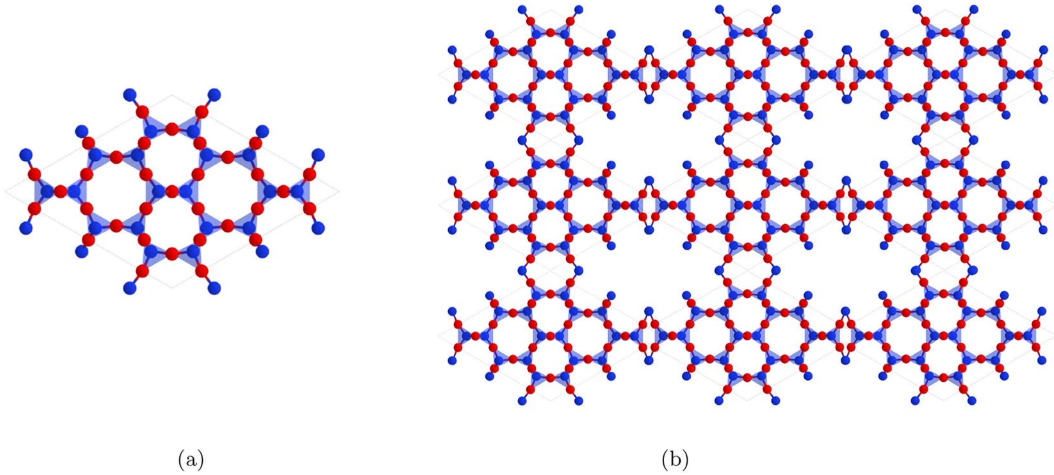


Fig. 1. (**a**) Silicon dioxide SiO_2 unit cell; (**b**) Silicon dioxide for $m = 3 = n$.

$Indices\backslash[m,n]$	**[1, 1]**	**[2, 2]**	**[3, 3]**	**[4, 4]**	**[5, 5]**	**[6, 6]**	**[7, 7]**	**[8, 8]**
$M_1(SiO_2)$	306	1240	2802	4992	7810	11256	15330	20032
$M_2(SiO_2)$	348	1424	3228	5760	9020	13008	17724	23168
$M_4(SiO_2)$	576	2384	5424	9696	15200	21936	29904	39104
$M_5(SiO_2)$	882	3560	8034	14304	22370	32232	43890	57344
$ReZG_1(SiO_2)$	63	244	543	960	1495	2148	2919	3808
$ReZG_2(SiO_2)$	72.8	296.53	671.2	1196.8	1873.33	2700.8	3679.2	4808.53
$ReZG_3(SiO_2)$	1692	6928	15708	28032	43900	63312	86268	112768

Table 1. Comparison of topological indices numerically.

$$\sum_{\alpha\beta\in E} G(\alpha\beta) = \sum_{\alpha\beta\in E} (\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta) = ReZG_3$$

Now Equation (8) represents the redefined third Zagreb Entropy.

$$ENT_{ReZG_3}(G) = \log\big(ReZG_3\big) - \frac{1}{(ReZG_3)} \sum_{i=1}^{q} \sum_{\alpha\beta\in E_i} [(\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta)] \log\big[(\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta)\big]. \quad (15)$$

The majority of silicon dioxide is produced by mining, which also includes quartz purification and sand mining. Quartz may be used for a variety of tasks, but in order to create a purer or more useful material, chemical processing is needed. The main component used in the creation of most glass is silica[17]. The moment at which freezing occurs Melting silica with other minerals reduces the melting point of the mixture and increases fluidity thanks to the depression idea.[19,33]. Similar to the odd physical properties of liquid water, molten silica possesses the following properties: A minimal heat capacity, a maximum density at temperatures below $5000°$C, and negative temperature expansion[34].

The unit structure and copies of the structure of Silicon dioxide are shown in Figure 1. Using Figure 1 we partitioned edges into 8 sets based on the degree of vertices.

$$E_{(2,2)} = \{\alpha\beta \in E(SiO_2) : \eta_\alpha = 2, \eta_\beta = 2\}$$
$$E_{(1,2)} = \{\alpha\beta \in E(SiO_2) : \eta_\alpha = 1, \eta_\beta = 2\}$$
$$E_{(2,3)} = \{\alpha\beta \in E(SiO_2) : \eta_\alpha = 2, \eta_\beta = 3\}$$

The cardinality of $E_{(1,2)}$ is $4m + 4n + 4mn$, $E_{(2,2)}$ is $-4m - 4n + 8mn$, and $E_{(2,3)}$ is $54mn$.

Main result

We have calculated Zagreb-type indices.

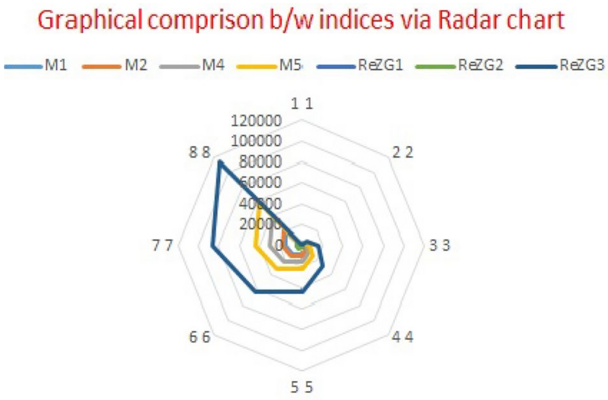


Fig. 2. Comparing indices via Radar chart.

$Indices \backslash [m, n]$	[1, 1]	[2, 2]	[3, 3]	[4, 4]	[5, 5]	[6, 6]	[7, 7]	[8, 8]
$ENT_{M_1}(SiO_2)$	1.812	2.416	2.769	3.019	3.213	3.372	3.506	3.622
$ENT_{M_2}(SiO_2)$	1.796	2.404	2.758	3.009	3.204	3.363	3.497	3.613
$ENT_{M_4}(SiO_2)$	1.793	2.403	2.758	3.009	3.204	3.363	3.497	3.613
$ENT_{M_5}(SiO_2)$	1.801	2.406	2.759	3.010	3.204	3.362	3.496	3.612
$ENT_{ReZG_1}(SiO_2)$	1.805	2.411	2.764	3.015	3.209	3.368	3.502	3.618
$ENT_{ReZG_2}(SiO_2)$	1.811	2.415	2.768	3.018	3.212	3.371	3.505	3.621
$ENT_{ReZG_3}(SiO_2)$	1.781	2.392	2.748	2.999	3.194	3.353	3.487	3.604

Table 2. Comparing entropy measures numerically.

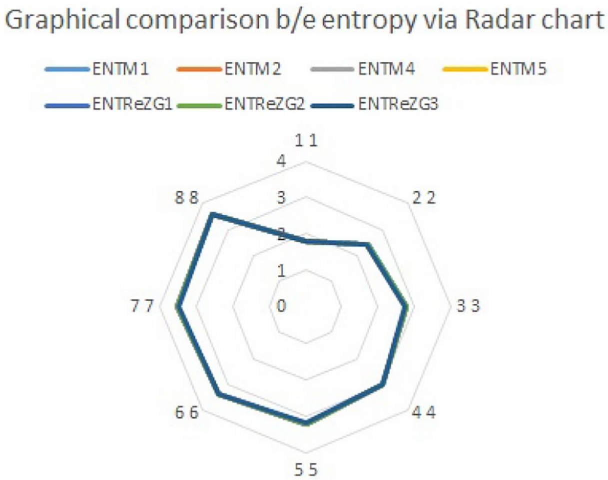
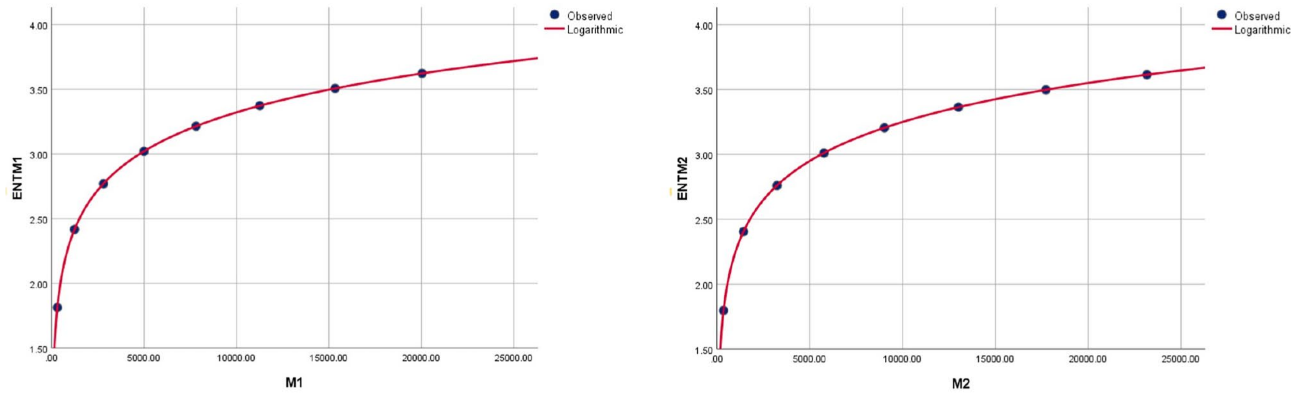


Fig. 3. Comparing entropy via Radar chart.

Model	***R***	R^2	S_E	***F***	***Sign***
$ENT_{M_1} = 0.433\ln[M_1] - 0.665$	1	1	0.001	5041268.294	0.000
$ENT_{M_2} = 0.433\ln[M_2] - 0.738$	1	1	0.001	6180203.675	0.000

Table 3. Model of logarithmic regression between different indices of entropies.

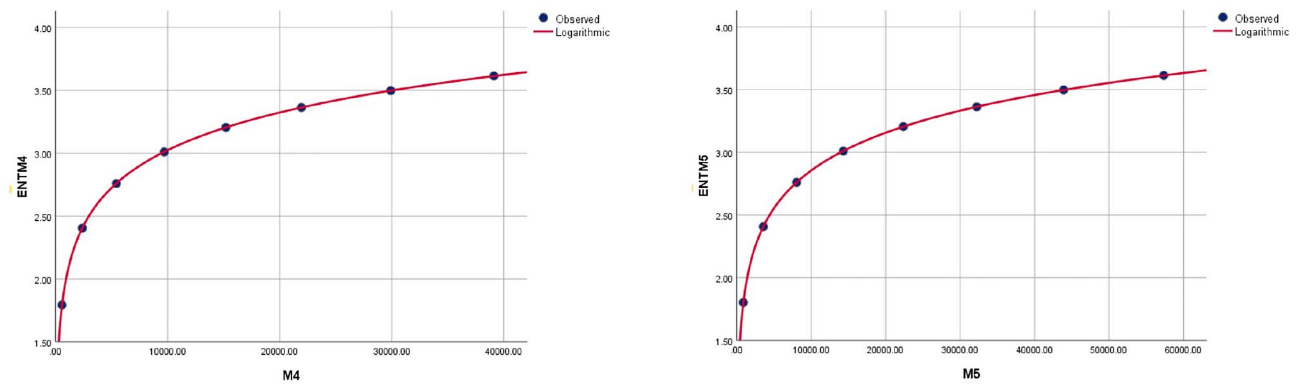


(a) $M_1(G)$ VS $ENT_{M_1}(G)$ (b) $M_1(G)$ VS $ENT_{M_1}(G)$

Fig. 4. Logarithmic regression's visual behaviour.

Model	*R*	R^2	S_E	*F*	*Sign*
$ENT_{M_4} = 0.432\ln[M_4] - 0.953$	1	1	0.001	1880448.754	0.000
$ENT_{M_5} = 0.434\ln[M_5] - 1.141$	1	1	0.001	53458895.12	0.000

Table 4. Model of logarithmic regression between different indices of entropies.



(a) $M_4(G)$ VS $ENT_{M_4}(G)$ (b) $M_5(G)$ VS $ENT_{M_5}(G)$

Fig. 5. Logarithmic regression's visual behaviour.

Model	*R*	R^2	S_E	*F*	*Sign*
$ENT_{ReZG_1} = 0.442\ln[ReZG_1] - 0.020$	1	1	0.003	261751.313	0.000
$ENT_{ReZG_2} = 0.432\ln[ReZG_2] - 0.441$	1	1	0.001	2641046.855	0.000
$ENT_{ReZG_3} = 0.434\ln[ReZG_3] - 1.447$	1	1	0.0001	965703871.7	0.000

Table 5. Model of logarithmic regression between different indices of entropies.

- **First Zagreb Index**

Put degree-based partition into Eq. 1, in this way, we derive the first Zagreb index: :

$$\begin{aligned}M_1(G) =&\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}(\eta_\alpha+\eta_\beta)\\ =&(1+2)(4m+4n+4mn)+(2+2)(-4m-4n+8mn)+(2+3)(54mn)\\ =&(3)(4m+4n+4mn)+(4)(-4m-4n+8mn)+(5)(54mn)\\ =&314mn-4m-4n.\end{aligned}$$

- **Second Zagreb Index**

Put degree-based partition into Eq. 2, in this way, we derive the second Zagreb index:

$$\begin{aligned}M_2(G) =&\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}\eta_\alpha\times\eta_\beta\\ =&(1\times 2)(4m+4n+4mn)+(2\times 2)(-4m-4n+8mn)+(2\times 3)(54mn)\\ =&(2)(4m+4n+4mn)+(4)(-4m-4n+8mn)+(6)(54mn)\\ =&364mn-8m-8n.\end{aligned}$$

- **Fourth Zagreb Index**

Put degree-based partition into Eq. 3, we obtain the fourth Zagreb index as follows:

$$\begin{aligned}M_4(G) =&\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}\eta_\alpha(\eta_\alpha+\eta_\beta)\\ =&1(1+2)(4m+4n+4mn)+2(2+2)(-4m-4n+8mn)+2(2+3)(54mn)\\ =&(3)(4m+4n+4mn)+(8)(-4m-4n+8mn)+(10)(54mn)\\ =&616mn-20m-20n.\end{aligned}$$

Put degree-based partition into Eq. 4, we obtain the fifth Zagreb index as follows:

- **Fifth Zagreb Index**

$$\begin{aligned}M_5(G) =&\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}\eta_\beta(\eta_\alpha+\eta_\beta)\\ =&2(1+2)(4m+4n+4mn)+2(2+2)(-4m-4n+8mn)+3(2+3)(54mn)\\ =&(6)(4m+4n+4mn)+(8)(-4m-4n+8mn)+(15)(54mn)\\ =&898mn-8m-8n.\end{aligned}$$

- **First Redefined Zagreb Index**

Put degree-based partition into Eq. 5, in this way, we derive the redefined first Zagreb index:

$$\begin{aligned}ReZG_1(G) =&\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}\frac{\eta_\alpha+\eta_\beta}{\eta_\alpha\times\eta_\beta}\\ =&\left(\frac{1+2}{1\times 2}\right)(4m+4n+4mn)+\left(\frac{2+2}{2\times 2}\right)(-4m-4n+8mn)+\left(\frac{2+3}{2\times 3}\right)(54mn)\\ =&\left(\frac{3}{2}\right)(4m+4n+4mn)+\left(\frac{4}{4}\right)(-4m-4n+8mn)+\left(\frac{5}{6}\right)(54mn)\\ =&59mn+2m+2n.\end{aligned}$$

- **Second Redefined Zagreb Index**

Put degree-based partition into Eq. 6, in this way, we derive the redefined second Zagreb index:

$$\begin{aligned}ReZG_2(G) &= \sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}\frac{\eta_\alpha\times\eta_\beta}{\eta_\alpha+\eta_\beta}\\ &= \left(\frac{1\times 2}{1+2}\right)(4m+4n+4mn)+\left(\frac{2\times 2}{2+2}\right)(-4m-4n+8mn)+\left(\frac{2\times 3}{2+3}\right)(54mn)\\ &= \left(\frac{2}{3}\right)(4m+4n+4mn)+\left(\frac{4}{4}\right)(-4m-4n+8mn)+\left(\frac{6}{5}\right)(54mn)\\ &= 75.46666667mn-1.333333333m-1.333333333n.\end{aligned}$$

- **Third Redefined Zagreb Index**

Put degree-based partition into Eq. 7, in this way, we derive the redefined third Zagreb index:

$$ReZG_3(G) = \sum_{i=1}^{3}\sum_{\alpha\beta\in E_i(G)}\Big((\eta_\alpha\times\eta_\beta)(\eta_\alpha+\eta_\beta)\Big)$$

$$\begin{aligned}&= ((1\times 2)(1+2))(4m+4n+4mn)+((2\times 2)(2+2))(-4m-4n+8mn)+((2\times 3)(2+3))(54mn)\\ &= (6)(4m+4n+4mn)+(16)(-4m-4n+8mn)+(30)(54mn)\\ &= 1772mn-40m-40n.\end{aligned}$$

A thorough numerical and graphical comparison of different indices when the parameters (*m*) and (*n*) are increased is shown in Table 1 and Figure 2. The results unambiguously demonstrate a positive association by showing that all indices rise with greater values of (*m*) and (*n*). The indicators' respective rates of rise, however, differ. The radar chart, in particular, indicates that the $ReZG_3$ index is rising faster than the other indexes. This implies that $ReZG_3$, maybe as a result of its underlying computation technique, is more susceptible to variations in (*m*) and (*n*). $ReZG_3$sharp increase highlights its potential as a highly responsive measure, which may be especially helpful in applications that need quick or high-sensitivity change detection.

- **First Zagreb Entropy**

Put down the computed first Zagreb index and edge partition into Eq.9, then the first Zagreb entropy is:

$$ENT_{M_1}(G) = \log\big(M_1\big)-\frac{1}{\big(M_1\big)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[(\eta_\alpha+\eta_\beta)]\log\big[(\eta_\alpha+\eta_\beta)\big]$$

$$\begin{aligned}ENT_{M_1}(G) &= \log\big(314mn-4m-4n\big)-\frac{(3)(4m+4n+4mn)\log(3)}{\big(314mn-4m-4n\big)}-\frac{(4)(-4m-4n+8mn)\log(4)}{\big(314mn-4m-4n\big)}\\ &\quad-\frac{(5)(54mn)\log(5)}{\big(314mn-4m-4n\big)}.\end{aligned}$$

- **Second Zagreb Entropy**

Put down the computed second Zagreb index and edge partition into Eq.10, then the second Zagreb entropy is:

$$ENT_{M_2}(G) = \log\big(M_2\big)-\frac{1}{\big(M_2\big)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[(\eta_\alpha\times\eta_\beta)]\log\big[(\eta_\alpha\times\eta_\beta)\big]$$

$$\begin{aligned}ENT_{M_2}(G) &= \log\big(364mn-8m-8n\big)-\frac{(2)(4m+4n+4mn)\log(2)}{\big(364mn-8m-8n\big)}-\frac{(4)(-4m-4n+8mn)\log(4)}{\big(364mn-8m-8n\big)}\\ &\quad-\frac{(6)(54mn)\log(6)}{\big(364mn-8m-8n\big)}.\end{aligned}$$

- **Fourth Zagreb Entropy**

Put down the computed fourth Zagreb index and edge partition into Eq.11, then the fourth Zagreb entropy is:

$$ENT_{M_4}(G) = \log\left(M_4\right) - \frac{1}{\left(M_4\right)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[\eta_\alpha(\eta_\alpha+\eta_\beta)]\log\left[\eta_\alpha(\eta_\alpha+\eta_\beta)\right]$$

$$ENT_{M_4}(G) = \log\left(616mn-20m-20n\right) - \frac{(3)(4m+4n+4mn)\log(3)}{\left(616mn-20m-20n\right)} - \frac{(8)(-4m-4n+8mn)\log(8)}{\left(616mn-20m-20n\right)} - \frac{(10)(54mn)\log(10)}{\left(616mn-20m-20n\right)}.$$

- **Fifth Zagreb Entropy**

Put down the computed fifth Zagreb index and edge partition into Eq.12, then the fifth Zagreb entropy is:

$$ENT_{M_5}(G) = \log\left(M_5\right) - \frac{1}{\left(M_5\right)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[\eta_\beta(\eta_\alpha+\eta_\beta)]\log\left[\eta_\beta(\eta_\alpha+\eta_\beta)\right]$$

$$ENT_{M_5}(G) = \log\left(898mn-8m-8n\right) - \frac{(6)(4m+4n+4mn)\log(6)}{\left(898mn-8m-8n\right)} - \frac{(8)(-4m-4n+8mn)\log(8)}{\left(898mn-8m-8n\right)} - \frac{(15)(54mn)\log(15)}{\left(898mn-8m-8n\right)}$$

- **Redefined First Zagreb Entropy**

Put down the computed redefined first Zagreb index and edge partition into Eq.13, then the redefined first Zagreb entropy is:

$$ENT_{ReZ_1}(G) = \log\left(ReZG_1\right) - \frac{1}{\left(ReZG_1\right)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[\frac{\eta_\alpha+\eta_\beta}{\eta_\alpha\times\eta_\beta}]\log\left[\frac{\eta_\alpha+\eta_\beta}{\eta_\alpha\times\eta_\beta}\right]$$

$$ENT_{ReZ_1}(G) = \log\left(59mn+2m+2n\right) - \frac{(\frac{3}{2})(4m+4n+4mn)\log(\frac{3}{2})}{\left(59mn+2m+2n\right)} - \frac{(\frac{4}{4})(-4m-4n+8mn)\log(\frac{4}{4})}{\left(59mn+2m+2n\right)} - \frac{(\frac{5}{6})(54mn)\log(\frac{5}{6})}{\left(59mn+2m+2n\right)}.$$

- **Redefined Second Zagreb Entropy**

Put down the computed redefined second Zagreb index and edge partition into Eq.14, then the redefined second Zagreb entropy is:

$$ENT_{ReZG_2}(G) = \log\left(ReZG_2\right) - \frac{1}{\left(ReZG_2\right)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[\frac{\eta_\alpha\times\eta_\beta}{\eta_\alpha+\eta_\beta}]\log\left[\frac{\eta_\alpha\times\eta_\beta}{\eta_\alpha+\eta_\beta}\right]$$

$$ENT_{ReZ_2}(G) = \log\left(75.46666667mn-1.333333333m-1.333333333n\right) - \frac{(\frac{2}{3})(4m+4n+4mn)\log(\frac{3}{2})}{\left(75.46666667mn-1.333333333m-1.333333333n\right)} - \frac{(\frac{4}{4})(-4m-4n+8mn)\log(\frac{4}{4})}{\left(75.46666667mn-1.333333333m-1.333333333n\right)} - \frac{(\frac{6}{5})(54mn)\log(\frac{6}{5})}{\left(75.46666667mn-1.333333333m-1.333333333n\right)}.$$

- **Redefined Third Zagreb Entropy**

Put down the computed redefined third Zagreb index and edge partition into Eq.15, then the redefined third Zagreb entropy is:

$$ENT_{ReZG_3}(G) = \log\left(ReZG_3\right) - \frac{1}{\left(ReZG_3\right)}\sum_{i=1}^{3}\sum_{\alpha\beta\in E_i}[(\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta)]\log\left[(\eta_\alpha \times \eta_\beta)(\eta_\alpha + \eta_\beta)\right]$$

$$ENT_{ReZ_3}(G) = \log\left(1772mn - 40m - 40n\right) - \frac{(6)(4m+4n+4mn)\log(6)}{\left(1772mn - 40m - 40n\right)} - \frac{(16)(-4m-4n+8mn)\log(16)}{\left(1772mn - 40m - 40n\right)} - \frac{(30)(54mn)\log(30)}{\left(1772mn - 40m - 40n\right)}.$$

A thorough numerical and graphical comparison of different entropy when the parameters (*m*) and (*n*) are increased is shown in Table 2 and Figure 3. The results unambiguously demonstrate a positive association by showing that all indices rise with greater values of (*m*) and (*n*). The indicators' respective rates of rise, however, differ. The radar chart, in particular, indicates that the ENT_{ReZG3} entropy is rising faster than the other entropy. This implies that ENT_{ReZG3}, maybe as a result of its underlying computation technique, is more susceptible to variations in (*m*) and (*n*). ENT_{ReZG3}sharp increase highlights its potential as a highly responsive measure, which may be especially helpful in applications that need quick or high-sensitivity change detection.

Regression model

The logarithmic regression model is a sort of nonlinear regression that is employed in scenarios where the dependent variable has a logarithmic pattern but has little to no association with one or more variables. The dependent variable in this model is the response's natural logarithm, whereas the independent variable, entropy, is plotted against the independent variable indices. Simply said, the exponential growth or decay phenomena is employed or used in every sector these days, including biology, economics, finance, and many more. The logarithmic regression model has the following form.

$$ENT(TI) = a\ln{(TI)} + b.$$

where *ENT*(*TI*) is the dependent variable, (*TI*) is the independent variable, $\ln(TI)$ represents the natural logarithm of *TI* and *a* and *b* are coefficients to be estimated from the data. This is particularly helpful when there is a change in the independent variable and a corresponding increase or fall in the dependent variable at different rates during the course of the computed periods. When there are saturation effects or when the rate of returns progressively declines, this is very helpful. When determining associations between variables and creating better prediction models, logarithmic regression may be a better option than line regressions in some situations.

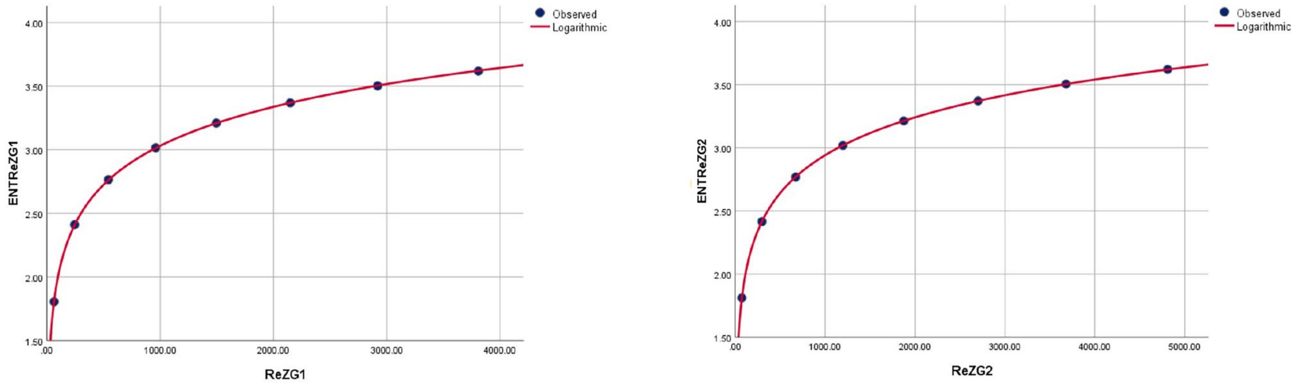
Two different logarithmic regression models are summarised in Table 3, and Figure 4. The entropy measure is predicted by these models using the natural logarithm of multiple indices (M_1, and M_2). With a R^2 value of 1, the model perfectly fits the data. This indicates that the whole fluctuation in the entropy measure can be explained by the natural logarithm of $M_1(G)$. It has a strong linear connection. This indicates that the whole fluctuation in the entropy measure can be explained by the natural logarithm of $M_2(G)$. It has a strong linear connection. Relatively modest, the number (0.433) shows precise coefficient calculations. The strong *F* statistic $(5041268.294 - 6180203.675)$ at a significance level of 0.000 indicates.

Two different logarithmic regression models are summarised in Table 4, and Figure 5. The entropy measure is predicted by these models using the natural logarithm of several indices (M_4, and M_5). The R^2 squared value of 1 indicates that the model matches the data exactly. This indicates that the whole fluctuation in the entropy measure can be explained by the natural logarithm of $M_5(G)$. It has a strong linear connection. This indicates that the whole fluctuation in the entropy measure can be explained by the natural logarithm of $M_2(G)$. It has a strong linear connection. Relatively modest, the number $(0.432 - 0.433)$ shows precise coefficient calculations. The strong *F* statistic $(1880448.754 - 53458895.12)$ at a significance level of 0.000.

Three different logarithmic regression models are summarised in Table 5, and Figure 6 and Figure 7. The entropy measure is predicted by these models using the natural logarithm of several indices, $ReZG_1$, $ReZG_2$, and $ReZG_3$. The R^2 squared value of 1 indicates that the model matches the data exactly. This indicates that the whole fluctuation in the entropy measure can be explained by the natural logarithm of $ReZG_1(G)$ and $ReZG_2(G)$. It has a strong linear connection. This indicates that the whole fluctuation in the entropy measure can be explained by the natural logarithm of $ReZG_3(G)$. It has a strong linear connection. Relatively modest, the number $(0.432 - 0.433)$ shows precise coefficient calculations. The strong *F* statistic $(261751.313 - 965703871.7)$ at a significance level of 0.000.

Conclusion

Our analysis in this work has focused on the computation of numerous Zagreb-type indices and their link with entropy measurements, as well as the mathematical and computational characterization of silicon dioxide (SiO_2). The application of topological indices from the chemical graph theory subfield, known as Zagreb indices, can help explain the molecular structure of silicon dioxide. Subsequently, the silicon dioxide entropy value was ascertained, serving as a quantifiable indicator of the unpredictability present in the chemical system. We constructed logarithmic regression models relating entropy measurements to indices. We see that the greatest value of R and R squared is 1, as we can see. It indicates that entropy and indices have a significant relationship.



(a) $ReZG_1(G)$ VS $ENT_{ReZG_1}(G)$ (b) $ReZG_2(G)$ VS $ENT_{ReZG_2}(G)$

Fig. 6. Logarithmic regression's visual behaviour.

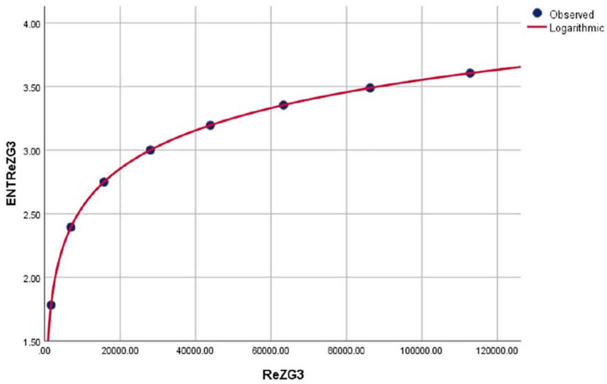


Fig. 7. $ReZG_3(G)$ VS $ENT_{ReZG_3}(G)$.

Data availability

The datasets used and/or analysed during the current study are available from the corresponding author on reasonable request.

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Author contributions
Rongbing Huang contributed to the data analysis, computation, funding resources, calculation verifications, and wrote the initial draft of the paper. Muhammad Farhan Hanif contributed to the computation and investigated and approved the final draft of the paper. Muhammad Kamran Siddiqui contributed to supervision, conceptualization, Methodology, Matlab calculations, Maple graphs improvement project administration. Muhammad Faisal Hanif contributed to the Investigation, analyzing the data curation, designing the experiments. Brima Gegbe contributes to formal analyzing experiments, software, validation, and funding. All authors read and approved the final version.

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Declarations

Competing interests
The authors declares no competing interests.

Additional information
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