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INVESTIGATING DEGREE-BASED TOPOLOGICAL INDICES AND ENTROPY IN SILICATE NETWORKS

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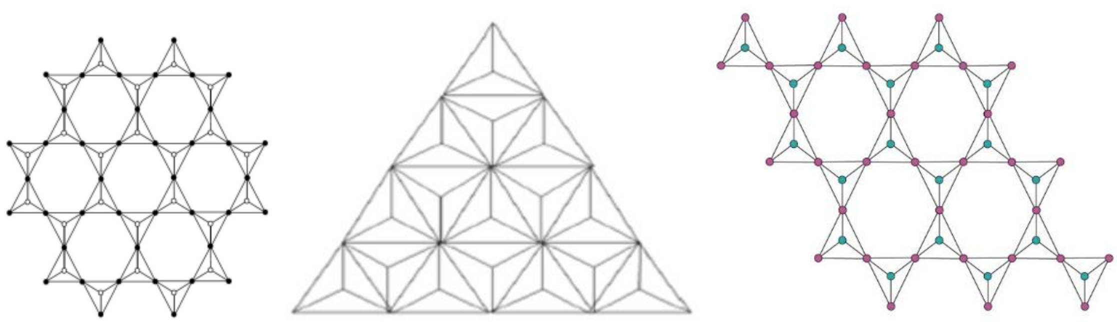
Abstract

Topological indices are numerical parameters that reflect the structural features of molecular systems. This research compute some degree based topological indices of 2-Dimensional, Triangular, and Rhombus Silicate networks using graph theory, which is a representation of complicated chemical and physical networks. In particular, we evaluate the Harmonic K-Banhatti Index (HKB), K-Banhatti Somber Index (KBS), K-Banhatti Somber Reduced Index (KBSR), and other related classes of entropy to measure the structural complexity and growth phenomena of these networks. The results of this study also confirm the conjecture that KBS R index is the most sensitive to the topological changes and growth dominates networks with the highest entropy. Performance and entropy analysis of structures reflections reveals that with certain values of the size parameter k there exists some level of network complexity . This study investigates the mathematical expression of silicate networks, intermediate between network science, chemical modeling, materials science, and provides the precise computational tools with modern algorithm via MATLAB.

Keywords:
Silicate Networks, Topological Indices, Harmonic K-Banhatti Index, K-Banhatti Somber Index, K-Banhatti Somber Reduced Index, Network Entropy,

Introduction

A graph is a mathematical structure that consists of nodes (or vertices) and edges. The nodes represent entities or points, and the edges represent the relationships or connections between them. Graphs can be both directed or undirected Graph is widely used inside the analysis and design of communication networks, which includes computer networks, social networks, and transportation networks. It allows optimize the drift of facts, have a look at connectivity styles, and layout green conversation structures. Graphs are used to model and resolve troubles in operations research, logistics, and optimization. They assist discover the maximum efficient paths, allocate sources, and optimize procedures in numerous industries. Graphs are employed to version biological and chemical systems, along with molecular structures and protein interactions (Mathew et al., 2021). A chemical graph is a graphical representation of a chemical compound, illustrating its molecular structure in a simplified and visual manner. In a chemical graph, atoms are represented as nodes or vertices, and chemical bonds between atoms are depicted as edges or lines connecting these nodes (Trinajstic, 1992). A silicate community refers to a three-dimensional structure composed of silicon (Si), oxygen (O), and other factors, generally forming a network of interconnected tetrahedral. Silicates are a big and numerous organization of minerals that make up a big part of the Earth's crust. The basic building block of silicate minerals is the silicon-oxygen tetrahedron, in which a silicon atom is surrounded via 4 oxygen atoms. Silicate minerals, forming silicate networks, are the maximum considerable minerals inside the Earth's crust (Morrison et al., 2024). They constitute a first-rate part of rocks, soils, and minerals, influencing the geology and composition of the Earth's surface. Silicate networks exhibit various systems, ranging from simple structures in minerals like olivine to complicated frameworks in minerals like quartz or feldspar. This structural variety contributes to the huge range of physical and chemical properties found in silicate minerals. Silicate minerals play an essential function in geological procedures together with weathering, erosion, and the formation of soils. The breakdown of silicate minerals contributes to the cycling of elements and the development of landscapes (Muñoz et al., 2024). Silicates are created through the fusion of metal oxides or metal carbonates with sand. The representation of a silicate network is denoted by SL_k, where the value of n corresponds to the count of hexagons located between the central point and the outer boundary of SL_k. These are class of Silicate Networks: Ortho Silicate, Pyro Silicate, Chain Silicate, Cyclic Silicate, Sheet Silicate, 2-Dimensional Silicate, Triangular Silicate & Rhombus Silicate Networks is shown in Figure 1.



(a) (b) (c)

Figure 1: A Class of Silicate Network (a) 2-Dimensional silicate Network (b) Triangular silicate Network (c) Rhombus silicate Network

Topological indices are like numbers that inform us about the shape of molecules. In the context of chemistry and molecular structures, these indices quantify various aspects of the arrangement of atoms and bonds within a molecule. Topological indices may be used to predict and correlate molecular houses without requiring specific 3-dimensional structural information. This makes them valuable for screening and prioritizing compounds in drug discovery and fabric technology. Topological indices contribute to QSAR studies, where the relationship between the structure of a molecule and its biological or chemical activity is investigated (Deviller et al., 1999). They aid in understanding how changes in molecular structure impact properties and activities. QSARs are predictive models that are created by applying statistical techniques to link the biological activity of chemicals (drugs, toxicants, and environmental pollutants) with characteristics that are indicative of their molecular structure and/or properties. This includes both desired therapeutic effect and undesirable side effects. In addition to drug discovery and lead optimization, QSARs are used in many other fields, such as risk assessment, toxicity prediction, and regulatory decisions (Dearden and John, 2003).

Literature Review.

The first time studied, the expanded new form of topological indices, such as the Silicate Network Graphs Arithmetic-Geometric Index (AG Index), SK Index, SK1 Index, and SK2 Index (Selvarani et al., 2021). Muhammad Javaid et al., (2017) for the first time studied For the rhombus silicate and rhombus oxide networks, we calculate the geometric arithmetic (GA), atom-bond connectivity (ABC), general Rancid, first general Zagreb, generalized Zagreb, multiplicative Zagreb, and geometric arithmetic indices. Furthermore, we calculate the most recent topological indices that have been constructed, including the enhanced Zagreb, Sanskruti, and fourth and fifth versions of ABC and GA, respectively. V. R. Kulli (2018) first time studied the polynomials for the first and second hyper-Revan indices of a certain family of networks, such as silicate networks. I Muhammad Javaid et al, (2019) for the first time studied, the relationships between quantitative structure and activity (QSAR) and quantitative structure and property (QSPR), The rhombus silicate's Randi's, geometric-arithmetic (GA), first general Zagreb, generalized Zagreb, multiplicative Zagreb, and atom-bond connectivity (ABC) indices In addition, topological indices, including the upgraded Zagreb and Sanskruti indices, the fifth edition of GA (GA5), and the fourth version of ABC (ABC4). Mondal et al (2019) for the first time studied The Zagreb index that is specific to a neighborhood is the neighborhood version of the forgotten topological index (FN), the neighborhood version of the second Zagreb index (M∗ 2), the neighborhood version of the hyper Zagreb index (HMN), and the modified neighborhood version of the forgotten topological index (F ∗ N). Hayat et al (2014) for the first time studied the ABC_4 and GA_5 indices for certain silicate networks. In [12], M. JAVAID el. at for the first time studied the M-polynomials of the oxide, silicate, and chain silicate networks. These polynomials are a recently developed tool that can be used to compute specific degree-based topological indices, including the augmented Zagreb, symmetric division, harmonic, inverse sum, and first, second, and second modified Zagreb's, as well as general and reciprocal Randi's. Mondal et al. (2019) studied the modified neighborhood version of the forgotten topological index, the neighborhood version of the second Zagreb index (M*2), the neighborhood version of the hyper Zagreb index (HMN), the neighborhood version of the second Zagreb index (MN), and the neighborhood version of the second Zagreb index (FN). Liu et al, (2017) the multiplicative Zagreb indices and sum-connectivity index for specific chemically significant networks, including silicate networks. Cancan et al. (2020) studied the article that calculates the topological indices of silicate networks using a specially devised approach called the M-polynomial. The Banhatti indices of different chemically interesting networks such as oxide, honeycomb, silicate, and chain silicate networks (Mirajkar et al., 2019, Kulli, 20218).

Methodology

Topological indices provide information about the shape of molecules. Understanding the topological features of a compound can help predict its behavior in chemical reactions and interactions. We are calculate some topological indices on type of silicate networks. These indices are calculate: The definition of the harmonic index and by previous research on topological indices. The Harmonic K-Banhatti Index of the graph G was introduced by Kulli.

The harmonic K-Banhatti index of a graph as

$$\mathrm{HKB}\ (\mathrm{G}) = \sum_{\theta,\varphi \epsilon G} \left(\frac{2}{\mathrm{d}(\theta) + \mathrm{d}(\varphi)}\right) \qquad (i)$$

The K-Banhatti Somber index of a graph as

$$\mathrm{KBS}\ (\mathrm{G}) = \sum_{\theta,\varphi \epsilon G} \sqrt{[\mathrm{d}(\theta)]^2 + [\mathrm{d}(\varphi)]^2} \qquad (ii)$$

The K-Banhatti Somber Reduced index of a graph as

$$\mathrm{KBSR}\ (\mathrm{G}) = \sum_{\theta,\varphi \epsilon G} \sqrt{[\mathrm{d}(\theta) - 1]^2 + [\mathrm{d}(\varphi) - 1]^2} \qquad (iii)$$

The entropy of the molecular structure is given as

$$ENT(G) = \log(TI) - \frac{1}{TI}\left[\sum f(du, dv) \times \log(du, dv)\right] \qquad (iv)$$

Main Results

We Computed the Harmonic K-Banhatti, K-Banhatti Somber, and K-Banhatti Somber Reduced, Degree-based topological indices for various networks such as 2-Dimensional silicate, Triangular Silicate and Rhombus Silicate networks.

Topological Indices results of 2-Dimensional Silicate

Metal carbonates or oxides are combined with sand to create silicates. A silicate network is represented by the symbol SL_k, where k is the number of hexagons that separate the network's perimeter and center.

$\theta, \varphi \in G$	$(6,6)$	$(6,3)$	$(3,3)$
Number of Edges	$6k$	$18k^2 + 6k$	$18k^2 - 12k$

Table 1: Edge Partitioning of 2-Dimensional Silicate Network

Let SL_k be the silicate networks. Then by using the equations (i), (ii) and (iii)

1) $HKB\ (G) = \sum_{\theta,\varphi \epsilon G}\left(\frac{2}{d(\theta)+d(\varphi)}\right) = \left[\frac{2}{(6+6)}6k + \frac{2}{(6+3)}(18k^2 + 6k) + \frac{2}{(3+3)}(18k^2 - 12k)\right]$

$= 10k^2 - 1.67k$

2) $KBS\ (G) = \sum_{u,v\epsilon G}\sqrt{[d(\theta)]^2 + [d(\varphi)]^2} = [\sqrt{(6)^2 + (6)^2}\,6k + \sqrt{(6)^2 + (3)^2}\,(18k^2 + 6) +$

$\sqrt{(3)^2 + (3)^2}\,(18k^2 - 12k)] = 197.11k^2 + 18k$

3). $KBSR\ (G) = \sum_{\theta,\varphi \epsilon G}\sqrt{[d(\theta) - 1]^2 + [d(\varphi) - 1]^2} = [\sqrt{(6-1)^2 + (6-1)^2}\,6k +$

$\sqrt{(6-1)^2 + (3-1)^2}\,(18\mathrm{k}^2 + 6k) + \sqrt{(3-1)^2 + (3-1)^2}\,(18k^2 - 12k)] = 147.84k^2 + 40.79k$

K	HKB(G)	KBS(G)	KBSR(G)
1	8.33	215.11	188.63
2	36.66	824.44	672.94
3	84.99	1827.99	1452.93
4	153.32	3225.76	2528.6
5	241.65	5017.75	3899.95
6	349.98	7203.96	5566.98
7	478.31	9784.39	7529.69
8	626.64	12759.04	9788.08
9	794.97	16127.91	12342.15
10	983.3	19891	15191.9

Table 2: Results of Topological Indices HKB, KBS and KBSR

The graph for HKB(G) has the form of a quadratic curve and increases steeply as 'k' increases. The term of -1.67k has a small influence compared to $10k^2$, resulting in the steepness of the curve changing more ask increases. The curve begins at a lower value and then increases faster with higher values of k. The slope of the KBS(G) graph is greater than that of HKB(G) and has a steeper slope which is the consequence of both of them having greater k^2 term coefficients. KBS's graph increases at a faster rate than HKB's ask increases. It is also worth noting that the linear term 18k raises the rate of increase of the curve when compared to HKB(G). The KBSR(G) graph is on the same upward trajectory with KBS(G), but is increasing at a rate smaller than KBS because of the smaller coefficient for the k^2 term. On the other hand, the 40.79k linear term increases the curve at a greater rate compared to KBS(G) for smaller values of k. In summary, while all three formulas exhibit quadratic growth, KBS(G) has the steepest rise, followed by KBSR(G), with HKB(G) growing at the slowest rate. This means that for small values of k, KBSR(G) is increasing at a greater rate. The behavior of these formulas suggests that KBS(G) and KBSR(G) have greater sensitivity to changes in k, especially k is large, which is consistent with their greater coefficients.

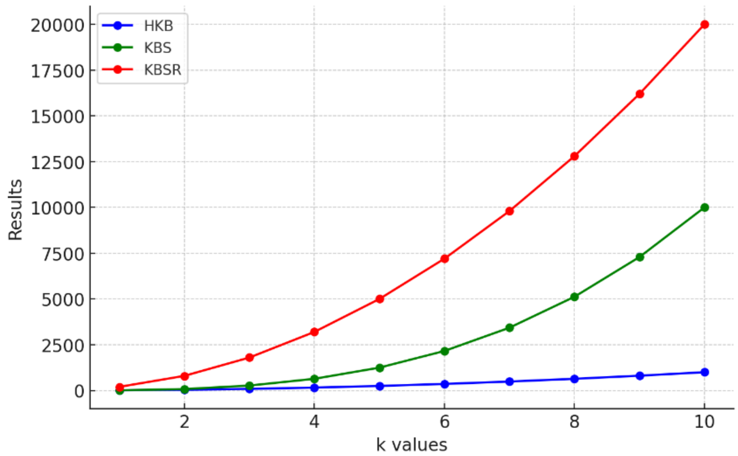


Figure 2: Comparison Graph of Topological Indices HKB, KBS and KBSR

Entropy of 2-Dimensional Silicate

Using equation (iv), we can compute the following

1) $ENT(HKB(\mathrm{SLk})) = \log\left(HKB(\mathrm{SLk})\right) - \frac{1}{HKB(\mathrm{SLk})}\left[\frac{1}{3}(18k^2 - 12)\log\left(\frac{1}{3}\right) + \frac{2}{9}(18k^2 + 8k)\log\left(\frac{2}{9}\right) + \frac{1}{6}(6k)\log\left(\frac{1}{6}\right)\right]$

2) $ENT(KBS(\mathrm{SLk})) = \log\left(KBS(\mathrm{SLk})\right) - \frac{1}{KBS(\mathrm{SLk})}\left[\sqrt{18}(18k^2 - 12)\log\left(\sqrt{18}\right) + \sqrt{45}(18k^2 + 8k)\log\left(\sqrt{45}\right) + \sqrt{72}(6k)\log\left(\sqrt{72}\right)\right]$

3) $ENT(KBSR(\mathrm{SLk})) = \log\left(KBSR(\mathrm{SLk})\right) - \frac{1}{KBSR(\mathrm{SLk})}\left[\sqrt{8}(18k^2 - 12)\log\left(\sqrt{8}\right) + \sqrt{29}(18k^2 + 8k)\log\left(\sqrt{29}\right) + \sqrt{50}(6k)\log\left(\sqrt{50}\right)\right]$

K	ENT_HKB	ENT_KBS	ENT_KBSR
1	3.641977	3.150793	3.456582
2	5.101109	4.641546	4.817165
3	5.883579	5.530029	5.645687
4	6.436101	6.15272	6.235741
5	6.866069	6.630214	6.692882
6	7.218774	7.016849	7.06565
7	7.518039	7.341448	7.380202
8	7.778049	7.621057	7.652204
9	8.007969	7.866574	7.891761
10	8.214072	8.085377	8.105772

Table 3: Entropy Value of 2-Dimensional silicate network

The entropy values calculated for polynomial s(2D) Silicate Networks are analyzed using the Harmonic k-Banhatti Index, K-Banhatti Somber Index, and K-Banhatti Somber Reduced Index of K-KBSR (k = 1,2,…). These indices show significant growth in structural complexity and information content ask increases. Orthogonal Silicate Somber indices behave similarly to the other two indices, but the growth of ENT(KBS) and ENT(KBSR) is more pronounced ask increases. The pattern of ENT(HKB) is almost linear upward, indicating that relationships based on the harmonic degree contribute to the total entropy. The gradual increase in ENT(HKB) indicates that high-degree nodes do not have a disproportionate influence on the value of harmonic indices, making them more consistent across network shapes and sizes. Conversely, ENT(KBS) is more aggressive in change rates, with shifts indicating the dominance of squared degree terms.

ENT(KBSR) reveals lower results than ENT(KBS) due to the reduced index accounting subtracting one degree terms of diminished high degree nodes. In smaller networks, the disparity among the entropy values is not significant, indicating that at lower values of k, there are little to no changes in the structure, leading to simpler topologies. However, when k is greater than 4, the discrepancies between entropy values become more distinct. The steep increase in ENT(KBS) and ENT(KBSR) suggests that larger networks tend to have more diverse interconnection patterns, resulting in relatively higher entropy. This highlights the responsiveness of Somber indices to more detailed topological alterations and changes.

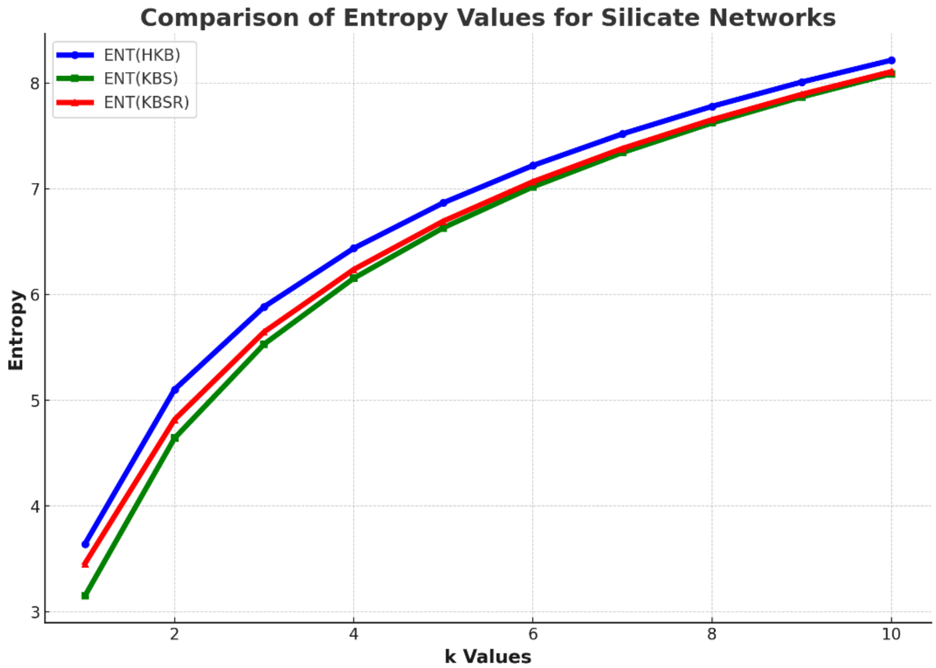


Figure 3: Entropy comparison of 2-dimensional silicate network

Topological Indices results of Triangular Silicate

Silicates are made by mixing sand with metal carbonates or oxides. The sign SL_k, where n is the number of hexagons separating the network's center and perimeter, is used to indicate silicate networks.

$\theta, \varphi \in G$	$(3,3)$	$(3,7)$	$(7,12)$	$(12,12)$	$(7,7)$	$(3,12)$
Number of Edges	3	$9k-3$	$6k-12$	$\frac{3(k-3)(k-2)}{2}$	$3(k-1)$	$\frac{6(k-2)(k-1)}{2}$

Table 4: Edge Partitioning Triangular Silicate Network

Let SL_k be the triangular silicate networks. Then by using equation (i), (ii) and (iii), we can easily compute the values of KBS(G) and KBSR(G).

1) $HKB\,(G) = \sum_{\theta,\varphi\epsilon G}\left(\frac{2}{d(\theta)+d(\varphi)}\right) = [\frac{2}{(3+3)}(3) + \frac{2}{(3+7)}\big(33+9(k-4)\big) + \frac{2}{(7+12)}\big(12+6(k-4)\big)$ $+ \frac{2}{(12+12)}(\frac{3(k-3)(k-2)}{2}) + \frac{2}{(7+7)}(3(k-1)) + \frac{2}{(3+12)}\left(\frac{6(k-2)(k-1)}{2}\right)] = 0.525k^2 + 1.035k + 0.25$

2) $KBS\,(G) = \sum_{\theta,\varphi\epsilon G}\sqrt{[d(\theta)]^2 + [d(\varphi)]^2} = [\sqrt{(3)^2+(3)^2}\,(3) + \sqrt{(3)^2+(7)^2}\,\big(33+9(k-4)\big)$ $+\sqrt{(7)^2+(12)^2}\,\big(12+6(k-4)\big) + \sqrt{(12)^2+(12)^2}\,(\frac{3(k-3)(k-2)}{2}) + \sqrt{(7)^2+(7)^2}\,\big(3(k-1)\big) +$ $\sqrt{(3)^2+(12)^2}\,\left(\frac{6(k-2)(k-1)}{2}\right)] = 62.563795k^2 - 57.007966k + 20.423756$

2) $KBSR\,(G) = \sum_{\theta,\varphi\epsilon G}\sqrt{[d(\theta)-1]^2 + [d(\varphi)-1]^2} = [\sqrt{(3-1)^2+(3-1)^2}\,(3) +$

$$\sqrt{(3-1)^2+(7-1)^2}\,\big(33+9(k-4)\big)+\sqrt{(7-1)^2+(12-1)^2}\,\big(12+6(k-4)\big)+\sqrt{(12-1)^2+(12-1)^2}\,\Big(\frac{3(k-3)(k-2)}{2}\Big)+\sqrt{(7-1)^2+(7-1)^2}\,(3(k-1))+\sqrt{(3-1)^2+(12-1)^2}\,\Big(\frac{6(k-2)(k-1)}{2}\Big)\Big]=65.875543k^2-59.739051k+20.785384$$

k	HKB(G)	KBS(G)	KBSR(G)
1	1.81	25.97958	26.92188
2	4.42	156.663	164.8095
3	8.08	412.474	434.4481
4	12.79	793.4126	835.8379
5	18.55	1299.479	1368.979
6	25.36	1930.673	2033.871
7	33.22	2686.994	2830.514
8	42.13	3568.443	3758.908
9	52.09	4575.019	4819.053
10	63.1	5706.724	6010.949

Table 5: Results of Topological Indices HKB, KBS and KBSR

Because of the lower coefficients in the quadratic and linear terms, HKB(G) is relatively slow growing. This suggests that it is more appropriate for cases in which the results need to increase but at a slower pace. In contrast KBS(G) and KBSR(G) have a relatively faster exponential growth curve compared to HKB(G). The same can be said to KBSR(G) where the growth rate exceeds that of KBS(G) because of the larger coefficients for both the quadratics and linear terms. Both KBS(G) and KBSR(G) formulas exhibit similarities which indicates that those are better suited for applications which require rapid increase in results as compared to the other formulas and the distinction between them is negligible for the values of k in question.

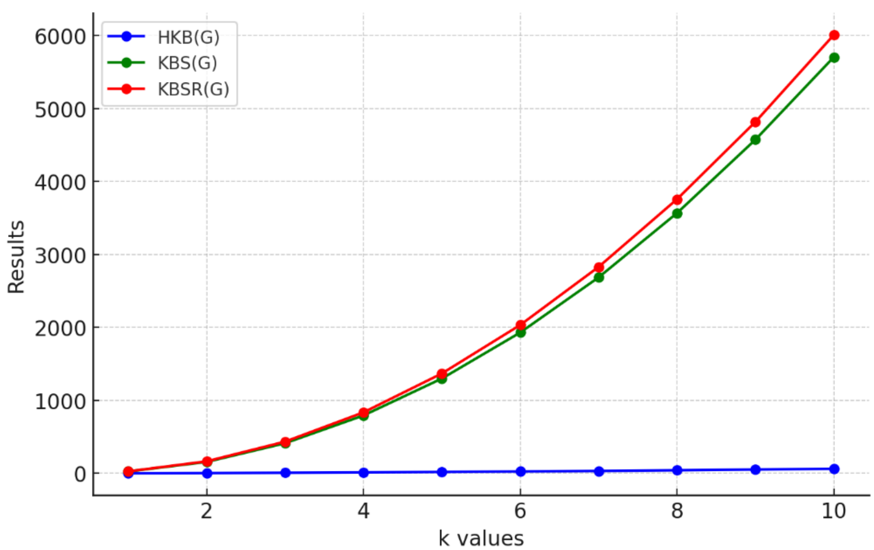


Figure 4: Comparison Graph of HKB, KBS and KBSR

Entropy of Triangular Silicate

Let SL_k be the triangular silicate networks. Then entropy measure of the triangular network is

(i) $ENT(G) = \log(\text{HKB(G)}) - \frac{1}{\text{HKB(G)}}\Big[\log\left(\frac{1}{3}\right) = \frac{1}{5}(9k-3)\log\left(\frac{1}{5}\right) + \frac{1}{12}\frac{(3(k-3)(k-2))}{2}\log\left(\frac{1}{12}\right) + \frac{2}{19}\,(6k-12)\log\left(\frac{2}{19}\right) + \frac{1}{7}(3k-3)\log\left(\frac{1}{7}\right) + \frac{2}{15}(3(k-2)(k-1))\log(\frac{2}{15})\Big]$

(ii) $ENT(G) = \log(\text{KBS(G)}) - \frac{1}{\text{KBS(G)}}\Big[\sqrt{18}(3)\log(\sqrt{18}) + \sqrt{58}(9k-3)\log(\sqrt{58}) + \sqrt{288}\frac{(3(k-3)(k-2))}{2}\log(\sqrt{288}) + \sqrt{193}\,(6k-12)\log(\sqrt{193}) + \sqrt{98}(3k-3)\log(\sqrt{98}) + \sqrt{153}(3(k-2)(k-1))\log(\sqrt{153})\Big]$

(iii) $ENT(G) = \log(\text{KBSR(G)}) - \frac{1}{\text{KBSR(G)}}\Big[\sqrt{8}(3)\log(\sqrt{8}) + \sqrt{40}(9k-3)\log(\sqrt{40}) + \sqrt{242}\frac{(3(k-3)(k-2))}{2}\log(\sqrt{242}) + \sqrt{158}\,(6k-12)\log(\sqrt{158}) + \sqrt{72}(3k-3)\log(\sqrt{72}) + \sqrt{125}(3(k-2)(k-1))\log(\sqrt{125})\Big]$

k	NT_G	ENT_G1	ENT_G2
1	1.218014	1.872185	2.699068
2	2.767197	3.021689	3.659276
3	3.627389	3.763495	4.346577
4	4.223793	4.312235	4.870644
5	4.680898	4.745204	5.289619
6	5.05179	5.102067	5.63748
7	5.364003	5.405341	5.934484
8	5.633662	5.668921	6.193444
9	5.87103	5.901946	6.422926
10	6.083047	6.110739	6.628916

Table 6: Entropy Measures of the Triangular silicate

The growth patterns and their sensitivities to structural changes of silicate networks can be analyzed through the comparison of the entropy metrics. ENT(HKB) has a more moderate growth rate as value k increases compared to its counterparts which means it is less sensitive to minor structural changes. This stability makes ENT(HKB) more ideal for analyzing networks that undergo gradual changes over a longer period. On the other side, ENT(KBS) has a sharper increase meaning it is more sensitive to topological changes which is common for complex networks with extensive branching. Therefore, this makes ENT(KBS) more useful for cases where small structural modifications have drastic effects on network behavior, such as in silicate reactive structures. ENT(KBSR) has a growth rate more aggressive than ENT(HKB) but less aggressive than ENT(KBS), which means it has a sensitivity ideal for networks of moderate complexity. The overwhelming quadratic terms that dominate ENT(KBS) and ENT(KBSR) push their entropy growth higher. Meanwhile, NT(G) with smaller coefficients delivers a more controlled progression. To summarize, ENT(HKB) can address stable network analyses, ENT(KBS) offers silicate structures with reactive environments, and ENT(KBSR) can tackle a network that needs both stability and reactivity.

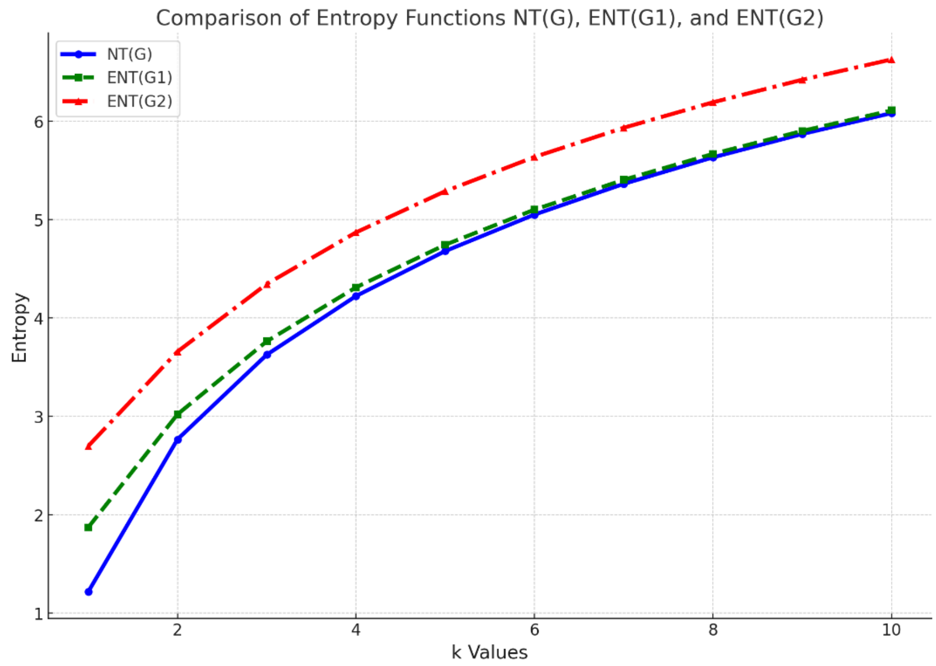


Figure 5: Entropy comparison of Triangular silicate network

Topological Indices results of Rhombus Silicate

Sand is combined with metal oxides or carbonates to create silicates. Silicate networks are denoted by the sign SL_k, where n is the number of hexagons that separate the network's perimeter and center.

$\theta, \varphi \in G$	$(3,3)$	$(3,6)$	$(6,6)$
Number of Edges	$4k+2$	$(6k^2+4k-4)$	$(6k^2-8k+2)$

Table 8: Edge Partitioning of Rhombus Silicate Network

Let SL_k be the rhombus silicate networks. Then entropy measure of the triangular network is

Let SL_k be Rhombus silicate networks. Then by suing equations (i), (ii) and (iii), we can easily compute the topological indices

1) $HKB\ (G) = \sum_{\theta,\varphi \epsilon G}\left(\frac{2}{d(\theta)+d(\varphi)}\right) = \frac{2}{(3+3)}(4k+2) + \frac{2}{(3+6)}(6k^2+4k-4) + \frac{2}{(6+6)} \times (6k^2-8k+2) = 2.33k^2 + 0.89k + 0.11$

2) $KBS\ (G) = \sum_{\theta,\varphi \epsilon G}\sqrt{[d(\theta)]^2+[d(\varphi)]^2} = \sqrt{(3)^2+(3)^2}(4k+2) + \sqrt{(3)^2+(6)^2} \times (6k^2+4k-4) + \sqrt{(6)^2+(6)^2}(6k^2-8k+2) = 91.160912k^2 - 24.078873k - 1.376972$

3) $KBSR\ (G) = \sum_{\theta,\varphi \epsilon G}\sqrt{[d(\theta)-1]^2+[d(\varphi)-1]^2} = \sqrt{(3-1)^2+(3-1)^2}(4k+2) + \sqrt{(3-1)^2+(6-1)^2}(6k^2+4k-4) + \sqrt{(6-1)^2+(6-1)^2}(6k^2-8k+2) = 74.737396k^2 - 23.714175k - 1.741669$

k	HKB(G)	KBS(G)	KBSR(G)
1	3.33	65.70507	49.28155
2	11.21	315.1089	249.7796
3	23.75	746.8346	599.7524
4	40.95	1360.882	1099.2
5	62.81	2157.251	1748.122
6	89.33	3135.943	2546.52
7	120.51	4296.956	3494.392
8	156.35	5640.29	4591.738
9	196.85	7165.947	5838.56
10	242.01	8873.925	7234.856

Table 9: Results of Topological Indices HKB, KBS and KBSR

HKB(G) is slower in terms of growth compared to KBS(G) and KBSR(G), implying that it could be more appropriate for uses where the outcome should be upper-limited or maximally reached slowly. The coefficients, mainly in the quadratic term, are higher, and as a consequence, KBS(G) and KBSR(G) increase at much faster rates. In addition, the gap between KBS(G) and KBSR(G) is minute. However, KBS(G) performs better and has a higher tendency to yield results than KBSR(G). HKB(G) seems more appropriate where slow or controlled growth is preferred in contrast with rapid growth which KBS(G) or KBSR(G) are deemed preferable.

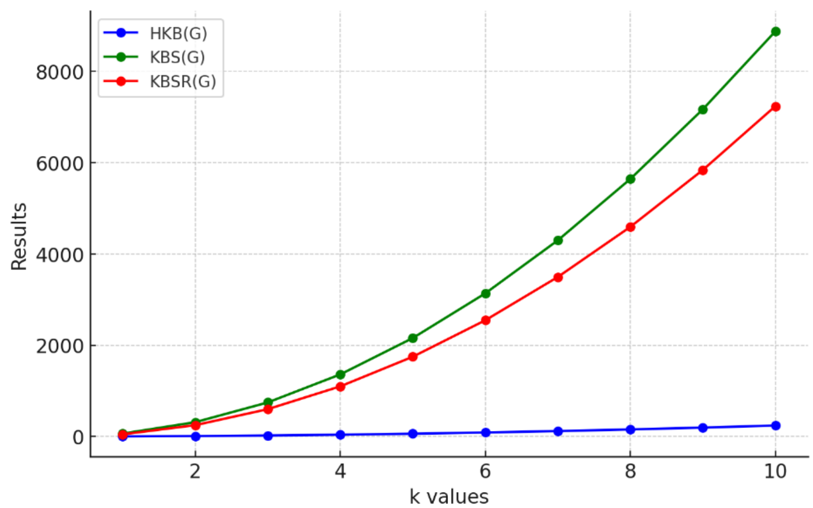


Figure 6: Comparison Graph of HKB, KBS and KBSR

Entropy of Triangular Silicate

Let SL_k be the rhombus silicate networks. Then entropy measure of the triangular network is

1) $ENT(HKB(\mathrm{SLk})) = \log(HKB(\mathrm{SLk})) - \frac{1}{HKB(\mathrm{SLk})}\left[\frac{1}{3}(4k+2)\log\left(\frac{1}{3}\right) + \frac{2}{9}(6k^2+4k-4)\log\left(\frac{2}{9}\right) + \frac{1}{6}(6k^2-8k+2)\log\left(\frac{1}{6}\right)\right]$

2) $ENT(KBS(\text{SLk})) = \log\big(KBS(\text{SLk})\big) - \frac{1}{KBS(\text{SLk})}\big[\sqrt{18}(4k+2)\log\big(\sqrt{18}\big) + \sqrt{45}(6k^2+4k-4)\log\big(\sqrt{45}\big) + \sqrt{72}\,(6k^2-8k+2)\log\big(\sqrt{72}\big)\big]$

3) $ENT(KBSR(\text{SLk})) = \log\big(KBSR(\text{SLk})\big) - \frac{1}{KBSR(\text{SLk})}\big[\sqrt{8}(4k+2)\log\big(\sqrt{8}\big) + \sqrt{29}(6k^2+4k-4)\log\big(\sqrt{29}\big) + \sqrt{50}\,(6k^2-8k+2)\log\big(\sqrt{50}\big)\big]$

k	ENT_HKB(SLk)	ENT_KBS(SLk)	ENT_KBSR(SLk)
1	2.465033	2.459342	2.435644
2	3.844729	3.847991	3.832743
3	4.658351	4.663509	4.652626
4	5.236134	5.241559	5.232877
5	5.684238	5.689554	5.682181
6	6.05025	6.055371	6.048862
7	6.359608	6.364526	6.358629
8	6.627507	6.632237	6.626796
9	6.86375	6.868312	6.863224
10	7.075029	7.079443	7.074636

The alteration of the k values for the indexes for ENT(HKB): ENT(KBS): ENT(KBSR) has resulted in different ranges in their growth trends, signifying how sensitive the index values are with respect to the changes in the size of the network. As the k increases, ENT(HKB) grows at a more moderate pace and keeps increasing consistently. This indicates that the structural complexity growth in the case of the Harmonic K-Banhatti index is proportional and uniform, thus it is not greatly affected by the changes occurring topologically within silicate networks.

Its growth trend can also show the contribution from both node degrees and edge multiplicity, which makes it preferable for controlled systems. However, the same twirls which above mentioned sank graphically system do increase their growth range having shown within greatly positive range of k scale. The K-Banhatti Somber index is more aggressive than K-banathi and seemingly weaker than other two. It's subclass range does respond as effectively summoning more than double powerful ranges. This growth can be made stronger and still accompanied by kbs to mark where complex network structures change Mabie even reduce down to point form to pinpoint signposts marking great structural alterations or even make KBS pinpoint irregular changes hidden within metamorphic densities of network systems.

In the same manner, ENT(KBSR) has a growth pattern similar to KBS, although it is less aggressive. The reduced form of the KBS index smoothens some of the changes that are carried in KBS, which suggests that it has some stabilizing function on the entropy fluctuations within the dense networks. Even in its moderated form, ENT(KBSR) is responsive to the size of the networks, which is indicative of sensitivity to the degree of connectivity. All in all, this comparison shows that while HKB gives an advanced access and controlled incremental progression of the entropy, KBS and KBSR are more responsive to shifts in architecture, especially KBS. These features differentiate the indices in the purposes of analysis gradual succession or acute forms within the silicate networks' topology.

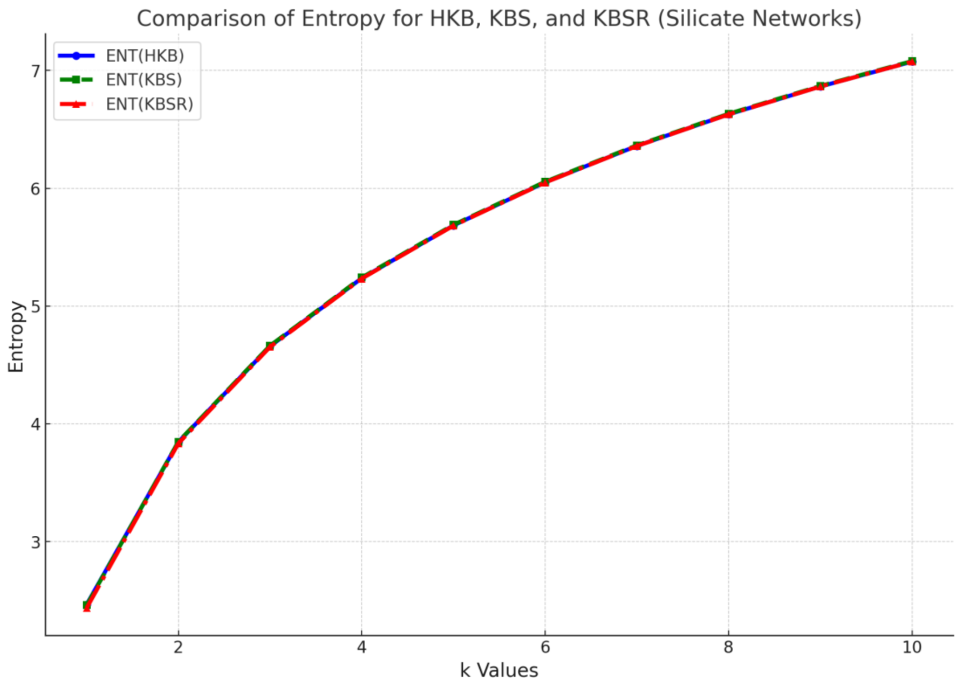


Figure 7: Entropy comparison of Rhombus silicate network

Conclusion

The paper presents a detailed investigation on degree-based topological indices and their application for the Harmonic K-Banhatti Index (HKB), K-Banhatti Somber Index (KBS) and K-Banhatti Somber Reduced Index (KBSR) of 2-D, Triangular, and Rhombus Silicate Networks. Our analysis shows that K-Banhatti indices capture the fluctuations of the topology more compared to the harmonic K-Banhatti index which HKB is best suited for stable network growth analyses. Overall entropy measures corroborate these findings stating the increased network size correlates with structural disorder increases. These results add more to the existing mathematical understanding of silicate networks and serves as a basis for developing further objectives towards studying new network forms, improving their predictive modeling of intricate materials systems in materials science and chemistry.

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