



Research article**Topological irregularity and entropy signatures of generalized silicate cage networks via generalized M -polynomials****Duyu Zhang¹, Xiaohong Dong^{2,*}, Hongjie Zhang³ and Haoyu Kong⁴**¹ School of Mathematics, Hefei University of Technology, Hefei 230601, China² College of Civil Engineering, Anhui Jianzhu University, Hefei 230601, China³ School of Electronics and Information Engineering, Anhui Jianzhu University, Hefei 230601, China⁴ Faculty of Science, The University of Melbourne, Melbourne 3000, Australia*** Correspondence:** Email: mmbbdxh999@163.com.

Abstract: Silicate cage frameworks, assembled from interconnected Si–O units, combine chemically relevant porosity and connectivity with structural motifs that are naturally amenable to graph-theoretical characterization. First, the parity-dependent structures of the generalized silicate cage network $SLC_{\mu}(\nu)$ were distinguished through degree partitions and generalized M -polynomials for even- and odd-layer configurations. The inherited partitions were checked by both edge totals and degree sums, and the degree-5 boundary corrections of the odd case were made explicit. Second, differential and spectral operators yielded exact closed-form expressions for twelve degree-based irregularity indices from the common M -polynomial representation. Third, exact parameter-sensitivity relations quantified the parity-preserving layer increments, the proportional effect of replication, and the common quadratic leading behavior under layer expansion. Representative exact surfaces illustrated distinct absolute, squared, normalized, and logarithmic weighting mechanisms without redundant graphical displays. Finally, descriptor-weighted Shannon entropy formulas were established for both parity classes; positive-scale invariance reduced the twelve descriptor entropies to eleven distinct expressions, while the new scaling law gave logarithmic replication growth and universal large-layer behavior. These results retained the exact structural information of both parity classes and isolated how local degree heterogeneity, cage replication, and layer number jointly organize the network, condensing the numerical presentation while preserving the mathematical distinctions needed for interpreting parity-dependent structural complexity. The resulting framework supplies exact structural fingerprints for comparison and classification, as well as candidate structural variables for future property-oriented modeling when verified physicochemical data become available.

Keywords: generalized M -polynomial; silicate cage network; topological descriptor; irregularity index; descriptor-weighted Shannon entropy

1. Introduction

In chemical graph theory, molecular structures are abstracted as mathematical graphs, where atoms are represented by vertices and chemical bonds by edges [1–3]; standard graph-theoretical treatments include [4, 5]. This graph-theoretical representation provides a compact yet informative framework that preserves the essential topological connectivity of a molecule while omitting complex quantum mechanical details. Such molecular graphs enable the quantitative modeling of chemical structures through topological indices [6–8]. Such indices correlate molecular connectivity with various physicochemical, biological, and thermodynamic properties [9–11].

Topological indices are numerical invariants that quantify essential molecular features such as symmetry, branching, and atomic bonding environments. Since the introduction of the Hosoya index [1] and the Zagreb indices [2], degree-based descriptors have become central tools in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) modeling [8, 12, 13]. Over time, numerous variants have been proposed to enhance structural sensitivity and correlation performance in high-throughput materials discovery and virtual drug-screening pipelines [9, 14, 15]. While traditional degree-based indices (such as Zagreb, Randić, and sum-connectivity indices) effectively capture global network connectivity, they often exhibit limited sensitivity toward local degree variations and structural non-uniformity [2, 15, 16]. To address this limitation, a diverse family of *irregularity indices* has been developed. Based on the degree difference $|d_u - d_v|$ between adjacent atoms, these indices systematically measure non-uniformity, topological disorder, and local symmetry breaking. This local-degree sensitivity makes irregularity descriptors useful for parameterized networks whose growth redistributes heterogeneous edges.

To unify the evaluation of degree-based descriptors, Deutsch and Klavžar [17] introduced the M -polynomial framework. The M -polynomial is a bivariate generating function, $M(G; s, t) = \sum_{n \leq p} m_{np}(G) s^n t^p$, that compactly encodes edge-degree distributions. Its differential and integral operators generate numerous invariants from one expression for large periodic nanostructures [18–20]. A related M -polynomial application is reported in [21]. Descriptor-weighted Shannon entropy links these topological weights to information-theoretic complexity [22–24], while recent work combines topological and spectral viewpoints in fractal, polygonal, and asymmetric networks [25–27].

Recent degree-based topological studies extend to parameterized and random chain-like chemical graph families. Random polyomino, polygonal, spiro, and related chains have been analyzed through degree-based and resistance-distance invariants [28–30]. A related chain analysis is reported in [31]. Their exact or expected values, parameter dependence, and asymptotic behavior show that degree-based descriptors form a common analytical language for structured and stochastic chemical graph families. In contrast, the present work concerns a parity-dependent silicate cage architecture and its exact irregularity and entropy characteristics.

Silicate cage and related zeolitic frameworks are prominent inorganic architectures built from tetrahedral units and cage-like motifs [32–34]; related silsesquioxane cage materials are discussed in [35]. Related zeolitic and polyhedral oligomeric silsesquioxane (POSS) cage frameworks are

valued for their porous architectures, catalytic applications, and thermal stability [36–38]. Graph-theoretically, silicon and oxygen atoms form degree-four and degree-two or higher connectivity nodes, allowing structural regularity to be parameterized in terms of layer count (ν) and unit replication (μ). Graph-theoretical and M -polynomial approaches have been applied to silicate and related cage frameworks [39], whereas a systematic parity-resolved algebraic treatment of this family of irregularity descriptors together with descriptor-weighted entropy remains unavailable for the generalized silicate cage setting. Crucially, existing studies frequently neglect the fundamental boundary disparities between even-layer ($\nu \equiv 0 \pmod{2}$) and odd-layer ($\nu \equiv 1 \pmod{2}$) cage architectures.

The generalized silicate cage construction and the generalized M -polynomial framework used here were established in Ref. [39]. Accordingly, this paper does not claim the network family, the M -polynomial idea, or its inherited degree-based partition as new. Its contribution is a systematic parity-dependent treatment of twelve irregularity descriptors, a unified differential/spectral-operator representation, descriptor-weighted Shannon entropy, positive-scale invariance, and exact sensitivity, scaling, and asymptotic results.

To address these gaps, this work presents a unified algebraic and information-theoretic analysis of the generalized silicate cage network $SLC_\mu(\nu)$. We construct exact M -polynomials for both even- and odd-layer configurations, derive closed-form expressions for twelve degree-based irregularity indices, and establish their corresponding descriptor-weighted Shannon entropy formulas. We prove that positive-scale invariance reduces the twelve descriptor entropies to eleven distinct functional expressions per parity class and derive exact parameter-sensitivity and entropy-scaling laws. These quantities are intended as mathematically defined structural fingerprints for future structure–property studies, rather than as presently validated property-prediction models.

2. Construction of generalized silicate cage networks

2.1. Structural description of the silicate cage

A silicate cage network can be represented in the language of chemical graph theory by a finite simple graph in which the atomic sites are identified with vertices and the chemical connections between adjacent sites are represented by edges [5, 10, 11]. In the present study, the generalized silicate cage network is denoted by $SLC_\mu(\nu)$, with the vertex set $V(SLC_\mu(\nu))$ and the edge set $E(SLC_\mu(\nu))$. The degree of a vertex describes the number of adjacent vertices and therefore records the local connectivity of the corresponding site within the molecular network. This graph-theoretical representation preserves the essential bonding pattern of the cage structure and provides a convenient basis for the computation of degree-dependent structural descriptors.

The network $SLC_\mu(\nu)$ forms a two-parameter family of periodically repeated cage structures. The parameter ν controls the number of structural layers in each cage unit, whereas μ specifies the number of replicated units included in the generalized construction. Consequently, variation in ν enlarges the internal layered arrangement of the network, while variation in μ extends the repeated cage architecture. These two parameters make it possible to describe an entire class of silicate cage networks through a single symbolic model and to investigate their structural growth without reconstructing every graph separately [34, 35].

An important feature of this family is that its local connectivity depends on the parity of the layer

parameter. For an even number of layers, the network is considered under the conditions

$$\nu \geq 2, \quad \nu \equiv 0 \pmod{2}, \quad \mu \geq 2,$$

and its vertices occurring in the degree partition have degrees 3, 4, and 6. For an odd number of layers, the admissible range is

$$\nu \geq 3, \quad \nu \equiv 1 \pmod{2}, \quad \mu \geq 3,$$

and degree 5 appears in addition to degrees 3, 4, and 6. The appearance of this additional degree class changes the associated edge-degree partition and introduces new local connection types in the odd-layer configuration.

Accordingly, the even- and odd-layer networks are treated separately throughout the subsequent analysis. Their parity-dependent edge partitions lead to different M -polynomials, different closed forms of the twelve irregularity indices, and different descriptor-weighted entropy expressions. Nevertheless, both cases belong to the same parameterized network family $SLC_\mu(\nu)$, which enables the influence of layer growth and structural replication to be examined within a unified mathematical framework. This parity separation is therefore structural rather than merely notational and must be preserved in all subsequent counting and descriptor calculations.

2.2. Even-layer silicate cage networks

The first structural configuration is the generalized silicate cage network with an even number of layers, defined for

$$\nu \geq 2, \quad \nu \equiv 0 \pmod{2}, \quad \mu \geq 2,$$

where ν and μ denote the number of silicate layers and repeated cage units, respectively.

In the even-layer configuration, the central vertices of one layer are connected systematically to their corresponding vertices in the neighboring layers, preserving interlayer symmetry and connectivity during network expansion.

The network contains vertices of degrees 3, 4, and 6, yielding five degree-based edge pairs: (3, 4), (3, 6), (4, 4), (4, 6), and (6, 6). The heterogeneous edge classes (3, 4), (3, 6), and (4, 6) are precisely the classes that carry nonzero irregularity weights. In contrast, the homogeneous edges (4, 4) and (6, 6) contribute to network size and the M -polynomial but carry zero weight for irregularity measures.

This structural regularity allows degree-pair multiplicities to be expressed directly in terms of ν and μ , providing the foundation for the exact M -polynomials and irregularity descriptors derived in Section 4.

2.3. Odd-layer silicate cage networks

The second configuration considers an odd number of layers, defined under

$$\nu \geq 3, \quad \nu \equiv 1 \pmod{2}, \quad \mu \geq 3,$$

where at least three layers and three repeated cage units are required.

Unlike the even-layer structure, the regular central vertex correspondence is shifted in the central region, modifying local degree distributions and creating a richer topology.

The vertex degree partition includes degrees 3–6, resulting in eight degree-based edge pairs: (3, 4), (3, 5), (3, 6), (4, 4), (4, 6), (5, 5), (5, 6), and (6, 6). The presence of degree 5 introduces new edge types (3, 5), (5, 5), and (5, 6). Here, heterogeneous edges (3, 4), (3, 5), (3, 6), (4, 6), and (5, 6) yield nonzero contributions to the twelve irregularity indices, whereas homogeneous edges (4, 4), (5, 5), and (6, 6) have zero irregularity weight but remain in the complete M -polynomial.

Thus, the odd-layer architecture represents a distinct parity-dependent topology whose modified connectivity alters the edge partition and subsequent analytical expressions for M -polynomials, irregularity indices, and entropy measures.

3. Mathematical preliminaries

3.1. Generalized M -polynomial

Let G be a finite simple graph. For each edge $uv \in E(G)$, we write

$$n = \min\{d_u, d_v\}, \quad p = \max\{d_u, d_v\},$$

so that $n \leq p$. Let $m_{n,p}(G)$ denote the number of edges whose endpoint degrees form the pair (n, p) . The generalized M -polynomial of G is defined by

$$M(G; s, t) = \sum_{n \leq p} m_{n,p}(G) s^n t^p,$$

$$M(G; 1, 1) = |E(G)|.$$

Thus, evaluation at $s = t = 1$ provides an immediate consistency check for every degree-based edge partition used below.

The main advantage of the generalized M -polynomial framework is that a large family of degree-dependent indices can be obtained from a single polynomial through suitable operators. Let X be an edge-based topological descriptor with single-edge weight $f_X(n, p)$. If an operator T_X acts diagonally on the monomial basis according to

$$T_X(s^n t^p) = f_X(n, p) s^n t^p,$$

then applying T_X to the M -polynomial and subsequently setting $s = t = 1$ produces the corresponding topological index.

The extraction principle needed throughout Sections 4–6 is summarized in the following theorem.

Theorem 3.1 (M -polynomial extraction principle). *Let*

$$M(G; s, t) = \sum_{n \leq p} m_{n,p}(G) s^n t^p$$

be the M -polynomial of a finite simple graph G . Suppose that an edge-based descriptor X has the single-edge weight $f_X(n, p)$, and let T_X be an operator satisfying

$$T_X(s^n t^p) = f_X(n, p) s^n t^p.$$

Then

$$X(G) = T_X M(G; s, t) \Big|_{s=t=1} = \sum_{n \leq p} m_{n,p}(G) f_X(n, p).$$

Proof. By the linearity of T_X ,

$$\begin{aligned} T_X M(G; s, t) &= T_X \left(\sum_{n \leq p} m_{n,p}(G) s^n t^p \right) \\ &= \sum_{n \leq p} m_{n,p}(G) T_X (s^n t^p) \\ &= \sum_{n \leq p} m_{n,p}(G) f_X(n, p) s^n t^p. \end{aligned}$$

Evaluating the resulting expression at $s = t = 1$ gives

$$T_X M(G; s, t) \big|_{s=t=1} = \sum_{n \leq p} m_{n,p}(G) f_X(n, p),$$

which is exactly the degree-partition representation of $X(G)$. $\square$

Theorem 3.1 establishes the mathematical link between the degree-based edge partition and the twelve irregularity descriptors considered in this work. Once the parity-dependent M -polynomial of $SLC_\mu(v)$ is obtained, the corresponding index formulas can be derived by selecting the appropriate edge-weight operator. The same M -polynomial also supplies the edge multiplicities required for the descriptor-weighted entropy calculations developed later.

For the generalized silicate cage family, the even- and odd-layer configurations possess different edge partitions and therefore lead to two distinct M -polynomials. These parity-dependent polynomials will be constructed explicitly in Sections 4 and 5, and will serve as the common algebraic input for the exact descriptor, sensitivity, and entropy calculations that follow.

3.2. Differential and spectral operators

To extract the twelve irregularity descriptors from the generalized M -polynomial, we introduce differential and spectral operators acting on the monomial basis $s^n t^p$, where $n \leq p$ are the endpoint degrees of an edge.

We define the Euler operators by

$$D_s = s \frac{\partial}{\partial s}, \quad D_t = t \frac{\partial}{\partial t}.$$

Their actions on a monomial are

$$D_s(s^n t^p) = n s^n t^p, \quad D_t(s^n t^p) = p s^n t^p.$$

The degree-difference and degree-sum operators are defined as

$$\Delta = D_t - D_s, \quad \Sigma = D_s + D_t,$$

so that

$$\Delta(s^n t^p) = (p - n) s^n t^p, \quad \Sigma(s^n t^p) = (n + p) s^n t^p.$$

Since $n \leq p$, the eigenvalue $p - n$ equals the absolute endpoint-degree difference.

For every real number α , the spectral powers of the Euler operators are defined by

$$D_s^\alpha(s^n t^p) = n^\alpha s^n t^p, \quad D_t^\alpha(s^n t^p) = p^\alpha s^n t^p.$$

In particular,

$$D_s^{-1}(s^n t^p) = \frac{1}{n} s^n t^p, \\ D_s^{-1/2}(s^n t^p) = \frac{1}{\sqrt{n}} s^n t^p, \quad D_t^{-1/2}(s^n t^p) = \frac{1}{\sqrt{p}} s^n t^p,$$

and

$$\Sigma^{-1}(s^n t^p) = \frac{1}{n+p} s^n t^p.$$

For the logarithmic descriptors, we define

$$L_s = \ln D_s, \quad L_t = \ln D_t,$$

with

$$L_s(s^n t^p) = (\ln n) s^n t^p, \quad L_t(s^n t^p) = (\ln p) s^n t^p.$$

Here, logarithms and fractional powers of the operators are understood spectrally on the monomial basis.

The identity operator I satisfies

$$I(s^n t^p) = s^n t^p.$$

All these operators act diagonally on the monomial basis and therefore commute whenever their compositions are defined. In each subsequent calculation, the required operator is first applied to the complete M -polynomial, after which the transformed expression is evaluated at $s = t = 1$. In this way, the monomial exponents preserve the endpoint-degree information during the calculation, while the final evaluation converts the transformed polynomial into the corresponding numerical topological descriptor.

3.3. Twelve irregularity descriptors

Let $uv \in E(G)$ be an edge of a finite simple graph G , and write

$$n = \min\{d_u, d_v\}, \quad p = \max\{d_u, d_v\}, \quad n \leq p.$$

An edge-based irregularity descriptor X can then be expressed in the general form

$$X(G) = \sum_{uv \in E(G)} f_X(n, p) = \sum_{n \leq p} m_{n,p}(G) f_X(n, p),$$

where $f_X(n, p)$ is the single-edge weight associated with X . The twelve descriptors considered in this study are listed in Table 1.

Table 1. Mathematical definitions and single-edge weights of the twelve irregularity indices.

Index	Definition	Single-edge weight $f_X(n, p)$
AL [40, 41]	$AL(G) = \sum_{uv \in E(G)} d_u - d_v $	$p - n$
IRR_t [42]	$IRR_t(G) = \frac{1}{2} \sum_{uv \in E(G)} d_u - d_v $	$\frac{1}{2}(p - n)$
$IRLU$	$IRLU(G) = \sum_{uv \in E(G)} \frac{ d_u - d_v }{\min\{d_u, d_v\}}$	$\frac{p - n}{n}$
$IRDIF$	$IRDIF(G) = \sum_{uv \in E(G)} \left(\frac{p}{n} - \frac{n}{p} \right)$	$\frac{p}{n} - \frac{n}{p}$
IRL	$IRL(G) = \sum_{uv \in E(G)} \ln\left(\frac{p}{n}\right)$	$\ln\left(\frac{p}{n}\right)$
$IRLF$	$IRLF(G) = \sum_{uv \in E(G)} \frac{p - n}{\sqrt{np}}$	$\frac{p - n}{\sqrt{np}}$
IRF [41, 43]	$IRF(G) = \sum_{uv \in E(G)} (p - n)^2$	$(p - n)^2$
$IRLA$	$IRLA(G) = \sum_{uv \in E(G)} \frac{2(p - n)}{n + p}$	$\frac{2(p - n)}{n + p}$
$IRD1$	$IRD1(G) = \sum_{uv \in E(G)} \ln(1 + p - n)$	$\ln(1 + p - n)$
IRA	$IRA(G) = \sum_{uv \in E(G)} \left(n^{-1/2} - p^{-1/2} \right)^2$	$\left(n^{-1/2} - p^{-1/2} \right)^2$
$IRGA$	$IRGA(G) = \sum_{uv \in E(G)} \ln\left(\frac{n + p}{2\sqrt{np}}\right)$	$\ln\left(\frac{n + p}{2\sqrt{np}}\right)$
IRB	$IRB(G) = \sum_{uv \in E(G)} (\sqrt{p} - \sqrt{n})^2$	$(\sqrt{p} - \sqrt{n})^2$

The table also makes clear that all twelve weights vanish on equal-degree endpoint pairs. For all twelve descriptors considered in this study,

$$f_X(n, n) = 0.$$

Hence, same-degree edges are retained in the complete M -polynomial but do not contribute to the irregularity indices.

3.4. Operator formulas for the irregularity indices

Table 2 collects the operator representation of each edge weight, so that all descriptors can be generated from the same M -polynomial without repeating the edge partition.

The following theorem establishes that the operators in Table 2 generate exactly the required irregularity weights.

Table 2. Generalized M -polynomial operators for the twelve irregularity indices.

Index	Single-edge weight $f_X(n, p)$	Operator T_X
AL	$p - n$	Δ
IRR_t	$\frac{1}{2}(p - n)$	$\frac{1}{2}\Delta$
$IRLU$	$\frac{p - n}{n}$	$D_s^{-1}\Delta$
$IRDIF$	$\frac{p}{n} - \frac{n}{p}$	$D_t D_s^{-1} - D_s D_t^{-1}$
IRL	$\ln\left(\frac{p}{n}\right)$	$L_t - L_s$
$IRLF$	$\frac{p - n}{\sqrt{np}}$	$(D_s D_t)^{-1/2}\Delta$
IRF	$(p - n)^2$	Δ^2
$IRLA$	$\frac{2(p - n)}{n + p}$	$2\Delta\Sigma^{-1}$
$IRD1$	$\ln(1 + p - n)$	$\ln(I + \Delta)$
IRA	$(n^{-1/2} - p^{-1/2})^2$	$(D_s^{-1/2} - D_t^{-1/2})^2$
$IRGA$	$\ln\left(\frac{n + p}{2\sqrt{np}}\right)$	$\ln \Sigma - (\ln 2)I - \frac{1}{2}(L_s + L_t)$
IRB	$(\sqrt{p} - \sqrt{n})^2$	$(D_t^{1/2} - D_s^{1/2})^2$

Theorem 3.2 (Unified operator representation). *Let*

$$M(G; s, t) = \sum_{n \leq p} m_{n,p}(G) s^n t^p$$

be the generalized M -polynomial of a finite simple graph G . Then the twelve irregularity descriptors are obtained as follows:

- (1) $AL(G) = \Delta M(G; s, t)|_{s=t=1}$.
- (2) $IRR_t(G) = \frac{1}{2}\Delta M(G; s, t)|_{s=t=1}$.
- (3) $IRLU(G) = D_s^{-1}\Delta M(G; s, t)|_{s=t=1}$.
- (4) $IRDIF(G) = (D_t D_s^{-1} - D_s D_t^{-1}) M(G; s, t)|_{s=t=1}$.
- (5) $IRL(G) = (L_t - L_s) M(G; s, t)|_{s=t=1}$.
- (6) $IRLF(G) = (D_s D_t)^{-1/2} \Delta M(G; s, t)|_{s=t=1}$.
- (7) $IRF(G) = \Delta^2 M(G; s, t)|_{s=t=1}$.
- (8) $IRLA(G) = 2\Delta\Sigma^{-1} M(G; s, t)|_{s=t=1}$.
- (9) $IRD1(G) = \ln(I + \Delta) M(G; s, t)|_{s=t=1}$.

$$(10) \quad IRA(G) = \left(D_s^{-1/2} - D_t^{-1/2}\right)^2 M(G; s, t) \Big|_{s=t=1}.$$

$$(11) \quad IRGA(G) = \left[\ln \Sigma - (\ln 2)I - \frac{1}{2}(L_s + L_t) \right] M(G; s, t) \Big|_{s=t=1}.$$

$$(12) \quad IRB(G) = \left(D_t^{1/2} - D_s^{1/2}\right)^2 M(G; s, t) \Big|_{s=t=1}.$$

Proof. For an arbitrary monomial $s^n t^p$, the operators act as

$$(1) \quad \Delta(s^n t^p) = (p - n)s^n t^p.$$

$$(2) \quad \frac{1}{2}\Delta(s^n t^p) = \frac{p - n}{2}s^n t^p.$$

$$(3) \quad D_s^{-1}\Delta(s^n t^p) = \frac{p - n}{n}s^n t^p.$$

$$(4) \quad (D_t D_s^{-1} - D_s D_t^{-1})(s^n t^p) = \left(\frac{p}{n} - \frac{n}{p}\right)s^n t^p.$$

$$(5) \quad (L_t - L_s)(s^n t^p) = \ln\left(\frac{p}{n}\right)s^n t^p.$$

$$(6) \quad (D_s D_t)^{-1/2}\Delta(s^n t^p) = \frac{p - n}{\sqrt{np}}s^n t^p.$$

$$(7) \quad \Delta^2(s^n t^p) = (p - n)^2 s^n t^p.$$

$$(8) \quad 2\Delta\Sigma^{-1}(s^n t^p) = \frac{2(p - n)}{n + p}s^n t^p.$$

$$(9) \quad \ln(I + \Delta)(s^n t^p) = \ln(1 + p - n)s^n t^p.$$

$$(10) \quad \left(D_s^{-1/2} - D_t^{-1/2}\right)^2 (s^n t^p) = \left(n^{-1/2} - p^{-1/2}\right)^2 s^n t^p.$$

$$(11) \quad \left[\ln \Sigma - (\ln 2)I - \frac{1}{2}(L_s + L_t) \right] (s^n t^p) = \ln\left(\frac{n + p}{2\sqrt{np}}\right)s^n t^p.$$

$$(12) \quad \left(D_t^{1/2} - D_s^{1/2}\right)^2 (s^n t^p) = (\sqrt{p} - \sqrt{n})^2 s^n t^p.$$

Each operator therefore has the required single-edge eigenvalue on $s^n t^p$. Linearity and evaluation at $s = t = 1$ then yield all twelve descriptor identities. $\square$

Theorem 3.2 shows that the same generalized M -polynomial can generate a broad collection of irregularity measures through different operator choices. The linear difference operators recover absolute and normalized degree differences, the generalized powers produce reciprocal and square-root forms, and the logarithmic spectral operators recover the logarithmic descriptors. This unified construction avoids separate edge-by-edge derivations and provides the analytical framework used for the even- and odd-layer silicate cage networks in Sections 4 and 5.

3.5. Descriptor-weighted entropy methodology

Descriptor-weighted graph entropy extends Shannon's information measure [44] to edge-probability distributions induced by structural weights. Degree-based and weighted graph-entropy formulations closely related to the present construction are given in [45, 46].

Let X be an irregularity descriptor with nonnegative single-edge weight $w_X(n, p)$. Its total positive edge weight is

$$T_X = \sum_{\substack{n \leq p \\ w_X(n, p) > 0}} m_{n,p}(G) w_X(n, p) = X(G).$$

Thus, the normalizing constant of the induced probability distribution is exactly the corresponding irregularity-index total.

For each positive-weight edge uv , define

$$P_X(uv) = \frac{w_X(d_u, d_v)}{T_X}.$$

Since every degree pair (n, p) occurs $m_{n,p}(G)$ times,

$$\sum_{\substack{uv \in E(G) \\ w_X(uv) > 0}} P_X(uv) = 1.$$

The descriptor-weighted Shannon entropy is

$$H_X(G) = - \sum_{\substack{uv \in E(G) \\ w_X(uv) > 0}} P_X(uv) \log_2 P_X(uv).$$

Define

$$C_X = \sum_{\substack{n \leq p \\ w_X(n, p) > 0}} m_{n,p}(G) w_X(n, p) \log_2 w_X(n, p).$$

Theorem 3.3. *For every descriptor satisfying $T_X > 0$,*

$$H_X(G) = \log_2 T_X - \frac{C_X}{T_X}.$$

Proof. Grouping the positive-weight edges by degree pair gives

$$\begin{aligned} H_X(G) &= - \sum_{\substack{n \leq p \\ w_X(n, p) > 0}} m_{n,p}(G) \frac{w_X(n, p)}{T_X} \log_2 \left(\frac{w_X(n, p)}{T_X} \right) \\ &= \log_2 T_X - \frac{1}{T_X} \sum_{\substack{n \leq p \\ w_X(n, p) > 0}} m_{n,p}(G) w_X(n, p) \log_2 w_X(n, p) \\ &= \log_2 T_X - \frac{C_X}{T_X}. \end{aligned}$$

□

Here, $m_{n,p}(G)$ counts individual edges carrying the same weight; it is not included in the weight of a single edge.

The entropy is invariant under positive rescaling. If

$$\widetilde{w}(e) = c w(e), \quad c > 0,$$

then

$$\frac{\widetilde{w}(e)}{\sum_f \widetilde{w}(f)} = \frac{w(e)}{\sum_f w(f)},$$

and therefore

$$H_{\widetilde{w}}(G) = H_w(G).$$

Since the edge weights of IRR_t and AL satisfy

$$w_{IRR_t}(n, p) = \frac{1}{2} w_{AL}(n, p),$$

it follows that

$$H_{IRR_t}(G) = H_{AL}(G).$$

Hence, the two descriptors differ in magnitude but not in their normalized edge-probability distribution.

The natural logarithm $\ln$ occurs in the definitions of several irregularity descriptors, whereas the Shannon entropy is calculated using the base-two logarithm $\log_2$.

4. Topological modeling of even-layer silicate cage networks

4.1. Edge partition and generalized M -polynomial

For the even-layer silicate cage network, the structural parameters satisfy

$$\nu \geq 2, \quad \nu \equiv 0 \pmod{2}, \quad \mu \geq 2.$$

For the even-layer architecture in Figure 1, the admissible degree set is $\{3, 4, 6\}$, giving the five edge classes summarized in Table 3.

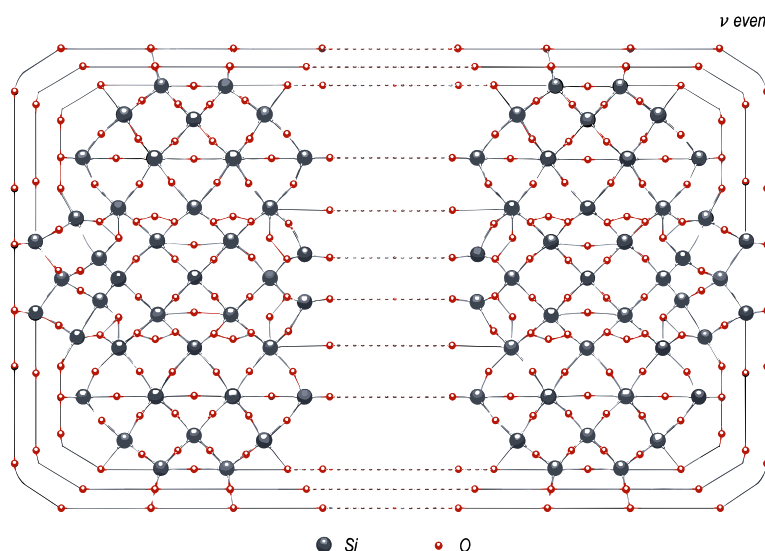


Figure 1. Schematic even-layer generalized silicate cage network $SLC_{\mu}(\nu)$, illustrating the repeated Si–O connectivity pattern used in the degree-partition analysis.

Table 3. Degree-based edge partition of the even-layer generalized silicate cage network $SLC_\mu(\nu)$.

Degree pair (n, p)	(3, 4)	(3, 6)	(4, 4)	(4, 6)	(6, 6)
$m_{n,p}$	$6\nu\mu$	$(18\nu^2 - 6\nu)\mu$	$3\nu\mu$	$12\nu\mu$	$(18\nu^2 - 12\nu)\mu$

Proposition 4.1 (Degree-based edge partition for the even-layer network). *For $\nu \geq 2$ with $\nu \equiv 0 \pmod{2}$, the degree-based edge partition of $SLC_\mu(\nu)$ is the one in Table 3; namely,*

$$\begin{aligned} m_{3,4} &= 6\nu\mu, & m_{3,6} &= (18\nu^2 - 6\nu)\mu, & m_{4,4} &= 3\nu\mu, \\ m_{4,6} &= 12\nu\mu, & m_{6,6} &= (18\nu^2 - 12\nu)\mu. \end{aligned}$$

Proof. The generalized construction and its complete layer-by-layer degree partition are inherited from Ref. [39]; they are recalled here because every subsequent irregularity calculation depends on them. In the inherited decomposition, one cage unit is separated into boundary bookkeeping and layer-interior/interlayer bookkeeping. The boundary blocks occur at each of the ν layer positions, and their accumulated record is 6ν edges of type (3, 4), 3ν of type (4, 4), and 12ν of type (4, 6). The complementary interior/interlayer record, accumulated over the repeated layer connections, is $18\nu^2 - 6\nu$ edges of type (3, 6) and $18\nu^2 - 12\nu$ edges of type (6, 6). Thus the linear boundary terms and quadratic interior/interlayer terms have distinct structural origins; replication by μ identical cage units multiplies every entry by μ . This proof records that inherited partition and verifies it independently below, rather than claiming a new geometric derivation.

First, summing the disjoint edge classes gives

$$\sum_{n \leq p} m_{n,p} = [6\nu + (18\nu^2 - 6\nu) + 3\nu + 12\nu + (18\nu^2 - 12\nu)]\mu = (36\nu^2 + 3\nu)\mu,$$

which is $|E(SLC_\mu(\nu))|$. Second, the degree incidences supplied by the same construction are

$$N_3 = 6\nu^2\mu, \quad N_4 = 6\nu\mu, \quad N_6 = (9\nu^2 - 3\nu)\mu.$$

Hence the degree-sum identity gives

$$\sum_{v \in V} d(v) = 3N_3 + 4N_4 + 6N_6 = (72\nu^2 + 6\nu)\mu = 2|E(SLC_\mu(\nu))|.$$

The agreement of the independent edge-total and degree-sum checks confirms the consistency of the inherited partition before it is used in the irregularity calculations. $\square$

The multiplicities in Table 3 give

$$|E(SLC_\mu(\nu))| = (36\nu^2 + 3\nu)\mu.$$

Accordingly, the generalized M -polynomial of the even-layer network is

$$\begin{aligned} g_e(s, t) &= M(SLC_\mu(\nu); s, t) \\ &= 6\nu\mu s^3 t^4 + (18\nu^2 - 6\nu)\mu s^3 t^6 + 3\nu\mu s^4 t^4 \\ &\quad + 12\nu\mu s^4 t^6 + (18\nu^2 - 12\nu)\mu s^6 t^6. \end{aligned}$$

Although all five degree classes are required to construct the complete M -polynomial, the same-degree classes (4, 4) and (6, 6) are retained in the complete M -polynomial but contribute zero to the twelve irregularity descriptors. Hence, their active degree-pair support is

$$\mathcal{A}_e = \{(3, 4), (3, 6), (4, 6)\}.$$

For an arbitrary irregularity descriptor X with single-edge weight $f_X(n, p)$,

$$\begin{aligned} X(SLC_\mu(\nu)) &= 6\nu\mu f_X(3, 4) + (18\nu^2 - 6\nu)\mu f_X(3, 6) + 12\nu\mu f_X(4, 6) \\ &= \mu[18f_X(3, 6)\nu^2 + (6f_X(3, 4) - 6f_X(3, 6) + 12f_X(4, 6))\nu]. \end{aligned}$$

Thus, every even-layer irregularity descriptor is linear in μ and at most quadratic in ν . Combining $g_e(s, t)$ with the operators introduced in Section 3 yields the twelve exact expressions derived in the following subsection.

4.2. Exact expressions of the twelve irregularity indices

The operator framework of Section 3 now converts the even-layer M -polynomial into the following closed forms.

Theorem 4.1 (Twelve irregularity indices for even layers). *Let $SLC_\mu(\nu)$ be a generalized silicate cage network satisfying*

$$\nu \geq 2, \quad \nu \equiv 0 \pmod{2}, \quad \mu \geq 2.$$

Then the twelve irregularity indices of the even-layer network are as follows:

- (1) $AL(SLC_\mu(\nu)) = \mu(54\nu^2 + 12\nu).$
- (2) $IRR_i(SLC_\mu(\nu)) = \mu(27\nu^2 + 6\nu).$
- (3) $IRLU(SLC_\mu(\nu)) = \mu(18\nu^2 + 2\nu).$
- (4) $IRDIF(SLC_\mu(\nu)) = \mu(27\nu^2 + \frac{9}{2}\nu).$
- (5) $IRL(SLC_\mu(\nu)) = \mu(18\nu^2 \ln 2 + 6\nu \ln \frac{3}{2}).$
- (6) $IRLF(SLC_\mu(\nu)) = \mu[9\sqrt{2}\nu^2 + (\sqrt{3} - 3\sqrt{2} + 2\sqrt{6})\nu].$
- (7) $IRF(SLC_\mu(\nu)) = 162\mu\nu^2.$
- (8) $IRLA(SLC_\mu(\nu)) = \mu(12\nu^2 + \frac{88}{35}\nu).$
- (9) $IRD1(SLC_\mu(\nu)) = \mu(36\nu^2 \ln 2 + 6\nu \ln \frac{9}{2}).$
- (10) $IRA(SLC_\mu(\nu)) = \mu[(9 - 6\sqrt{2})\nu^2 + (\frac{11}{2} + 2\sqrt{2} - 2\sqrt{3} - 2\sqrt{6})\nu].$
- (11) $IRGA(SLC_\mu(\nu)) = \mu[18\nu^2 \ln(\frac{3}{2\sqrt{2}}) + 6\nu \ln(\frac{175\sqrt{6}}{432})].$
- (12) $IRB(SLC_\mu(\nu)) = \mu[(162 - 108\sqrt{2})\nu^2 + (108 + 36\sqrt{2} - 24\sqrt{3} - 48\sqrt{6})\nu].$

Proof. Applying the corresponding generalized M -polynomial operators to the even-layer polynomial $g_e(s, t)$ gives the following identities.

- (1) $AL(SLC_\mu(\nu)) = \Delta g_e(s, t)|_{s=t=1} = \mu(54\nu^2 + 12\nu).$
- (2) $IRR_t(SLC_\mu(\nu)) = \frac{1}{2}\Delta g_e(s, t)|_{s=t=1} = \mu(27\nu^2 + 6\nu).$
- (3) $IRLU(SLC_\mu(\nu)) = D_s^{-1}\Delta g_e(s, t)|_{s=t=1} = \mu(18\nu^2 + 2\nu).$
- (4) $IRDIF(SLC_\mu(\nu)) = (D_t D_s^{-1} - D_s D_t^{-1})g_e(s, t)|_{s=t=1} = \mu(27\nu^2 + \frac{9}{2}\nu).$
- (5) $IRL(SLC_\mu(\nu)) = (L_t - L_s)g_e(s, t)|_{s=t=1} = \mu(18\nu^2 \ln 2 + 6\nu \ln \frac{3}{2}).$
- (6) $IRLF(SLC_\mu(\nu)) = (D_s D_t)^{-1/2}\Delta g_e(s, t)|_{s=t=1} = \mu[9\sqrt{2}\nu^2 + (\sqrt{3} - 3\sqrt{2} + 2\sqrt{6})\nu].$
- (7) $IRF(SLC_\mu(\nu)) = \Delta^2 g_e(s, t)|_{s=t=1} = 162\mu\nu^2.$
- (8) $IRLA(SLC_\mu(\nu)) = 2\Delta\Sigma^{-1}g_e(s, t)|_{s=t=1} = \mu(12\nu^2 + \frac{88}{35}\nu).$
- (9) $IRD1(SLC_\mu(\nu)) = \ln(I + \Delta)g_e(s, t)|_{s=t=1} = \mu(36\nu^2 \ln 2 + 6\nu \ln \frac{9}{2}).$
- (10) $IRA(SLC_\mu(\nu)) = (D_s^{-1/2} - D_t^{-1/2})^2 g_e(s, t)|_{s=t=1} = \mu[(9 - 6\sqrt{2})\nu^2 + (\frac{11}{2} + 2\sqrt{2} - 2\sqrt{3} - 2\sqrt{6})\nu].$
- (11) $IRGA(SLC_\mu(\nu)) = [\ln \Sigma - (\ln 2)I - \frac{1}{2}(L_s + L_t)]g_e(s, t)|_{s=t=1} = \mu[18\nu^2 \ln(\frac{3}{2\sqrt{2}}) + 6\nu \ln(\frac{175\sqrt{6}}{432})].$
- (12) $IRB(SLC_\mu(\nu)) = (D_t^{1/2} - D_s^{1/2})^2 g_e(s, t)|_{s=t=1}$
 $= \mu[(162 - 108\sqrt{2})\nu^2 + (108 + 36\sqrt{2} - 24\sqrt{3} - 48\sqrt{6})\nu].$

□

These formulas show that the replication parameter enters multiplicatively, whereas the layer parameter governs the dominant quadratic growth. Theorem 4.1 provides a unified analytical characterization of the even-layer silicate cage network. Its dominant layer dependence is governed by the (3, 6)-edge class, whose multiplicity is

$$(18\nu^2 - 6\nu)\mu.$$

The obtained expressions provide the exact basis for the sensitivity analysis below.

4.3. Exact parameter sensitivity for even layers

4.3.1. Layer sensitivity

For every even-layer descriptor, we write

$$X^{(e)}(\mu, \nu) = \mu(A_X \nu^2 + B_X \nu).$$

Because admissible layer numbers in the same parity class differ by two, we define

$$\Delta_\nu X^{(e)} = X^{(e)}(\mu, \nu + 2) - X^{(e)}(\mu, \nu).$$

Direct substitution into the exact quadratic formula gives

$$\Delta_\nu X^{(e)} = \mu(4A_X\nu + 4A_X + 2B_X).$$

For fixed μ , this increment is linear in ν ; hence the index itself has accelerated layer growth. The exact finite difference describes layer sensitivity directly from the analytical formulas, without introducing an additional empirical approximation. The twelve sensitivities are collected compactly in Table 4.

Table 4. Exact parity-preserving layer sensitivities for the even-layer descriptors.

Index	$\Delta_\nu X^{(e)}$
<i>AL</i>	$\mu(216\nu + 240)$
<i>IRR_t</i>	$\mu(108\nu + 120)$
<i>IRLU</i>	$\mu(72\nu + 76)$
<i>IRDIF</i>	$\mu(108\nu + 117)$
<i>IRL</i>	$\mu[72\nu \ln 2 + 72 \ln 2 + 12 \ln(3/2)]$
<i>IRLF</i>	$\mu[36\sqrt{2}\nu + 30\sqrt{2} + 2\sqrt{3} + 4\sqrt{6}]$
<i>IRF</i>	$\mu(648\nu + 648)$
<i>IRLA</i>	$\mu(48\nu + 1856/35)$
<i>IRD1</i>	$\mu[144\nu \ln 2 + 144 \ln 2 + 12 \ln(9/2)]$
<i>IRA</i>	$\mu[(36 - 24\sqrt{2})\nu + 47 - 20\sqrt{2} - 4\sqrt{3} - 4\sqrt{6}]$
<i>IRGA</i>	$\mu\{72\nu \ln(3/(2\sqrt{2})) + 72 \ln(3/(2\sqrt{2})) + 12 \ln(175\sqrt{6}/432)\}$
<i>IRB</i>	$\mu[(648 - 432\sqrt{2})\nu + 864 - 360\sqrt{2} - 48\sqrt{3} - 96\sqrt{6}]$

All entries are linear in ν , confirming that the increment itself grows systematically as additional even layers are introduced.

4.3.2. Replication sensitivity and asymptotic behavior

Writing $X^{(e)}(\mu, \nu) = \mu F_X^{(e)}(\nu)$ gives the exact replication increment

$$X^{(e)}(\mu + 1, \nu) - X^{(e)}(\mu, \nu) = F_X^{(e)}(\nu).$$

Moreover,

$$X^{(e)}(\mu, \nu) \sim A_X \mu \nu^2, \quad \nu \rightarrow \infty.$$

Hence, replication produces exact proportional scaling, while layer enlargement controls the asymptotically dominant quadratic contribution.

4.4. Parameter-dependent structural behavior for even layers

4.4.1. Exact computed values

The exact values in Table 5 are retained to illustrate the joint dependence on ν and μ ; they are evaluated directly from Theorem 4.1.

Table 5. Computed values of twelve irregularity indices for $SLC_{\mu}(\nu)$ with $\mu \geq 3$ and even $\nu \geq 2$.

ν	μ	AL	IRR_t	$IRLU$	$IRDIF$	IRL	$IRLF$	IRF	$IRLA$	$IRD1$	IRA	$IRGA$	IRB
2	3	720	360	228.00	351.00	164.32	167.07	1944	159.09	353.59	5.97	12.44	109.78
2	4	960	480	304.00	468.00	219.09	222.75	2592	212.11	471.45	7.96	16.59	146.37
2	5	1200	600	380.00	585.00	273.86	278.44	3240	265.14	589.31	9.95	20.74	182.97
2	6	1440	720	456.00	702.00	328.63	334.13	3888	318.17	707.17	11.94	24.88	219.56
4	3	2736	1368	888.00	1350.00	628.07	639.60	7776	606.17	1306.05	24.29	50.32	441.92
4	4	3648	1824	1184.00	1800.00	837.43	852.80	10368	808.23	1741.40	32.39	67.10	589.23
4	5	4560	2280	1480.00	2250.00	1046.79	1066.00	12960	1010.29	2176.75	40.48	83.87	736.53
4	6	5472	2736	1776.00	2700.00	1256.15	1279.20	15552	1212.34	2612.10	48.58	100.65	883.84
6	3	6048	3024	1980.00	2997.00	1391.27	1417.61	17496	1341.26	2857.40	54.97	113.65	996.42
6	4	8064	4032	2640.00	3996.00	1855.02	1890.14	23328	1788.34	3809.86	73.29	151.53	1328.56
6	5	10080	5040	3300.00	4995.00	2318.78	2362.68	29160	2235.43	4762.33	91.61	189.41	1660.70
6	6	12096	6048	3960.00	5994.00	2782.54	2835.21	34992	2682.51	5714.79	109.93	227.29	1992.84
8	3	10656	5328	3504.00	5292.00	2453.90	2501.08	31104	2364.34	5007.62	97.99	202.41	1773.27
8	4	14208	7104	4672.00	7056.00	3271.87	3334.78	41472	3152.46	6676.83	130.66	269.88	2364.37
8	5	17760	8880	5840.00	8820.00	4089.84	4168.47	51840	3940.57	8346.03	163.32	337.35	2955.46
8	6	21312	10656	7008.00	10584.00	4907.81	5002.16	62208	4728.69	10015.24	195.99	404.82	3546.55

4.4.2. Graphical interpretation of exact structural trends

Figures 2–5 present the exact surfaces of AL , IRF , $IRLA$, and $IRGA$, respectively, for the even-layer configuration. Together they display the exact linear dependence on μ and quadratic dependence on ν without reproducing twelve closely related surfaces. The selected surfaces are therefore representative of distinct weighting mechanisms rather than an exhaustive graphical catalogue.

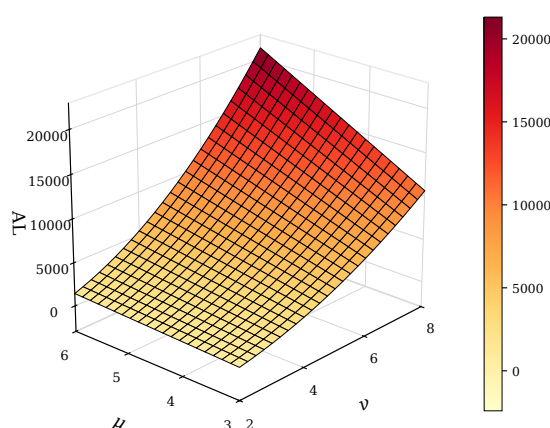


Figure 2. Exact AL surface for even layers.

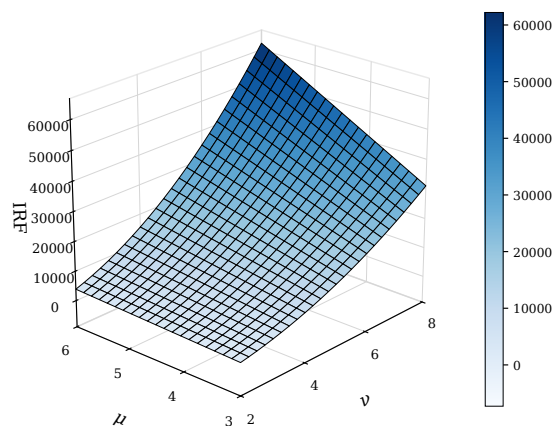


Figure 3. Exact *IRF* surface for even layers.

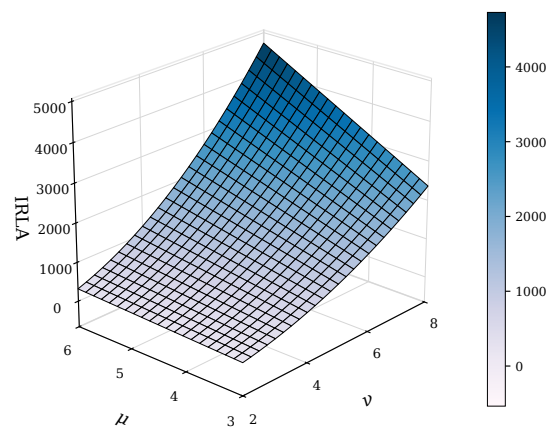


Figure 4. Exact *IRLA* surface for even layers.

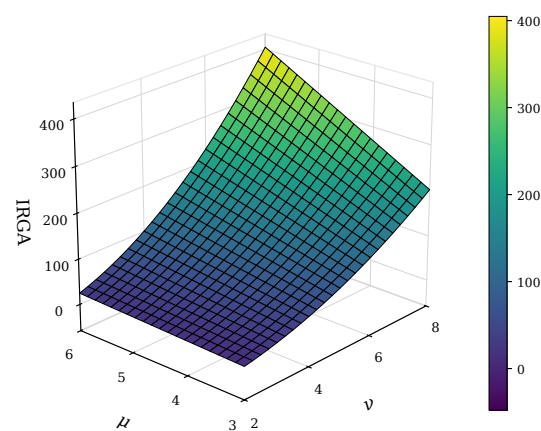


Figure 5. Exact *IRGA* surface for even layers.

5. Topological modeling of odd-layer silicate cage networks

5.1. Edge partition and generalized M -polynomial

The odd-layer case requires a separate degree partition because the modified central boundary introduces degree-5 vertices. Throughout this section, the structural parameters satisfy

$$\nu \geq 3, \quad \nu \equiv 1 \pmod{2}, \quad \mu \geq 3.$$

The vertex degrees occurring in the odd-layer network are 3–6, and the degree-5 vertices produce additional edge types in the degree-based partition.

For an ordered degree pair $n \leq p$, let $m_{n,p}$ denote the number of edges whose endpoints have degrees n and p . The edge set of the odd-layer network is divided into the eight pairwise disjoint classes $E_{3,4}$, $E_{3,5}$, $E_{3,6}$, $E_{4,4}$, $E_{4,6}$, $E_{5,5}$, $E_{5,6}$, and $E_{6,6}$.

The resulting eight edge multiplicities are summarized in Table 6 and justified below.

Table 6. Degree-based edge partition of the odd-layer generalized silicate cage network $SLC_\mu(\nu)$.

Degree pair (n, p)	(3, 4)	(3, 5)	(3, 6)	(4, 4)	(4, 6)	(5, 5)	(5, 6)	(6, 6)
$m_{n,p}$	$(6\nu - 2)\mu$	2μ	$(18\nu^2 - 6\nu)\mu$	$(3\nu - 1)\mu$	$(12\nu - 4)\mu$	2μ	4μ	$(18\nu^2 - 12\nu)\mu$

Proposition 5.1 (Degree-based edge partition for the odd-layer network). *For $\nu \geq 3$ with $\nu \equiv 1 \pmod{2}$, the eight degree-based edge multiplicities of $SLC_\mu(\nu)$ are*

$$\begin{aligned} m_{3,4} &= (6\nu - 2)\mu, & m_{3,5} &= 2\mu, & m_{3,6} &= (18\nu^2 - 6\nu)\mu, & m_{4,4} &= (3\nu - 1)\mu, \\ m_{4,6} &= (12\nu - 4)\mu, & m_{5,5} &= 2\mu, & m_{5,6} &= 4\mu, & m_{6,6} &= (18\nu^2 - 12\nu)\mu. \end{aligned}$$

Proof. The structural partition follows the generalized construction introduced in Ref. [39]; its complete layer-by-layer degree bookkeeping is inherited here, and the present proof supplies direct consistency checks for the subsequent irregularity analysis. The odd central boundary is the only local component that contains degree-5 vertices. It occurs once per repeated cage unit, so the inherited central-boundary record contributes exactly two (3, 5) edges, two (5, 5) edges, and four (5, 6) edges, independently of ν . The same central closure replaces the corresponding boundary incidences, producing the corrections -2 , -1 , and -4 in the (3, 4), (4, 4), and (4, 6) records, respectively. All (3, 6) and (6, 6) edges belong to the recurring layer-interior/interlayer pattern, which is unaffected by this localized central-boundary modification; hence their terms $18\nu^2 - 6\nu$ and $18\nu^2 - 12\nu$ remain unchanged. Replication by μ identical units then gives the claimed partition. This records the inherited construction without asserting a new geometric derivation.

The edge-total check is

$$\sum_{n \leq p} m_{n,p} = (36\nu^2 + 3\nu + 1)\mu = |E(SLC_\mu(\nu))|.$$

For the independent degree-sum check, the construction gives the degree incidences

$$N_3 = 6\nu^2\mu, \quad N_4 = (6\nu - 2)\mu, \quad N_5 = 2\mu, \quad N_6 = (9\nu^2 - 3\nu)\mu.$$

Consequently,

$$\sum_{v \in V} d(v) = 3N_3 + 4N_4 + 5N_5 + 6N_6 = (72v^2 + 6v + 2)\mu = 2|E(SLC_\mu(v))|.$$

Thus, the odd-layer correction is localized at the central boundary, while the dominant interior/interlayer terms retain the same quadratic structure as in the even case. $\square$

Thus,

$$E(SLC_\mu(v)) = E_{3,4} \cup E_{3,5} \cup E_{3,6} \cup E_{4,4} \cup E_{4,6} \cup E_{5,5} \cup E_{5,6} \cup E_{6,6}.$$

Summing the multiplicities in Table 6 gives

$$\begin{aligned} |E(SLC_\mu(v))| &= (6v - 2)\mu + 2\mu + (18v^2 - 6v)\mu + (3v - 1)\mu \\ &\quad + (12v - 4)\mu + 2\mu + 4\mu + (18v^2 - 12v)\mu \\ &= (36v^2 + 3v + 1)\mu. \end{aligned}$$

This result agrees with the odd-layer size formula obtained earlier.

Using the degree-pair multiplicities, the generalized M -polynomial of the odd-layer silicate cage network is

$$\begin{aligned} g_o(s, t) &= M(SLC_\mu(v); s, t) \\ &= (6v - 2)\mu s^3 t^4 + 2\mu s^3 t^5 + (18v^2 - 6v)\mu s^3 t^6 \\ &\quad + (3v - 1)\mu s^4 t^4 + (12v - 4)\mu s^4 t^6 \\ &\quad + 2\mu s^5 t^5 + 4\mu s^5 t^6 + (18v^2 - 12v)\mu s^6 t^6. \end{aligned}$$

Each monomial represents one endpoint-degree class, and its coefficient gives the number of edges belonging to that class. Hence, $g_o(s, t)$ completely records the degree-pair structure of the odd-layer network.

Evaluating the polynomial at $s = t = 1$ yields

$$\begin{aligned} g_o(1, 1) &= (6v - 2)\mu + 2\mu + (18v^2 - 6v)\mu \\ &\quad + (3v - 1)\mu + (12v - 4)\mu + 2\mu + 4\mu \\ &\quad + (18v^2 - 12v)\mu \\ &= (36v^2 + 3v + 1)\mu = |E(SLC_\mu(v))|, \end{aligned}$$

which provides a direct consistency check for the edge partition.

Although all eight edge classes are required in the complete M -polynomial, the same-degree classes (4, 4), (5, 5), and (6, 6) make no contribution to the twelve irregularity descriptors because their single-edge weights vanish when the endpoint degrees are equal. Therefore, the active degree-pair support is

$$\mathcal{A}_o = \{(3, 4), (3, 5), (3, 6), (4, 6), (5, 6)\}.$$

For an arbitrary irregularity descriptor X with single-edge weight $f_X(n, p)$, the corresponding odd-layer index is therefore expressed as

$$\begin{aligned} X(SLC_\mu(v)) &= (6v - 2)\mu f_X(3, 4) + 2\mu f_X(3, 5) \\ &\quad + (18v^2 - 6v)\mu f_X(3, 6) + (12v - 4)\mu f_X(4, 6) \\ &\quad + 4\mu f_X(5, 6). \end{aligned}$$

Equivalently,

$$\begin{aligned} X(SLC_{\mu}(\nu)) = & \mu \left[18f_X(3, 6)\nu^2 \right. \\ & + (6f_X(3, 4) - 6f_X(3, 6) + 12f_X(4, 6))\nu \\ & \left. - 2f_X(3, 4) + 2f_X(3, 5) - 4f_X(4, 6) + 4f_X(5, 6) \right]. \end{aligned}$$

The odd-layer expression therefore differs from its even-layer counterpart only through descriptor-dependent boundary corrections of lower order in ν .

The polynomial $g_o(s, t)$ will now be combined with the operators introduced in Section 3 to derive the twelve exact irregularity indices for the odd-layer configuration.

5.2. Exact expressions of the twelve irregularity indices

Applying the same operators to $g_o(s, t)$ yields the parity-corrected closed forms below.

Theorem 5.1 (Twelve irregularity indices for odd layers). *Let $SLC_{\mu}(\nu)$ be an odd-layer generalized silicate cage network satisfying*

$$\nu \geq 3, \quad \nu \equiv 1 \pmod{2}, \quad \mu \geq 3.$$

Then the twelve irregularity indices are as follows:

- (1) $AL(SLC_{\mu}(\nu)) = \mu(54\nu^2 + 12\nu - 2).$
- (2) $IRR_i(SLC_{\mu}(\nu)) = \mu(27\nu^2 + 6\nu - 1).$
- (3) $IRLU(SLC_{\mu}(\nu)) = \mu(18\nu^2 + 2\nu - \frac{8}{15}).$
- (4) $IRDIF(SLC_{\mu}(\nu)) = \mu(27\nu^2 + \frac{9}{2}\nu - \frac{9}{10}).$
- (5) $IRL(SLC_{\mu}(\nu)) = \mu(18\nu^2 \ln 2 + 6\nu \ln \frac{3}{2} + \ln \frac{16}{25}).$
- (6) $IRLF(SLC_{\mu}(\nu)) = \mu[9\sqrt{2}\nu^2 + (\sqrt{3} - 3\sqrt{2} + 2\sqrt{6})\nu - \frac{\sqrt{3}}{3} - \frac{2\sqrt{6}}{3} + \frac{4\sqrt{15}}{15} + \frac{2\sqrt{30}}{15}].$
- (7) $IRF(SLC_{\mu}(\nu)) = \mu(162\nu^2 - 6).$
- (8) $IRLA(SLC_{\mu}(\nu)) = \mu(12\nu^2 + \frac{88}{35}\nu - \frac{171}{385}).$
- (9) $IRD1(SLC_{\mu}(\nu)) = \mu(36\nu^2 \ln 2 + 6\nu \ln \frac{9}{2} + \ln \frac{4}{9}).$
- (10) $IRA(SLC_{\mu}(\nu)) = \mu[(9 - 6\sqrt{2})\nu^2 + (\frac{11}{2} + 2\sqrt{2} - 2\sqrt{3} - 2\sqrt{6})\nu - \frac{3}{10} + \frac{2\sqrt{3}}{3} + \frac{2\sqrt{6}}{3} - \frac{4\sqrt{15}}{15} - \frac{4\sqrt{30}}{15}].$
- (11) $IRGA(SLC_{\mu}(\nu)) = \mu[18\nu^2 \ln(\frac{3}{2\sqrt{2}}) + 6\nu \ln(\frac{175\sqrt{6}}{432}) + 2 \ln(\frac{1936}{875\sqrt{5}})].$
- (12) $IRB(SLC_{\mu}(\nu)) = \mu[(162 - 108\sqrt{2})\nu^2 + (108 + 36\sqrt{2} - 24\sqrt{3} - 48\sqrt{6})\nu + 6 + 8\sqrt{3} + 16\sqrt{6} - 4\sqrt{15} - 8\sqrt{30}].$

Proof. Applying the corresponding generalized M -polynomial operators to $g_o(s, t)$ gives the following identities.

- (1) $AL(SLC_\mu(\nu)) = \Delta g_o(s, t)|_{s=t=1} = \mu(54\nu^2 + 12\nu - 2).$
- (2) $IRR_t(SLC_\mu(\nu)) = \frac{1}{2}\Delta g_o(s, t)|_{s=t=1} = \mu(27\nu^2 + 6\nu - 1).$
- (3) $IRLU(SLC_\mu(\nu)) = D_s^{-1}\Delta g_o(s, t)|_{s=t=1} = \mu(18\nu^2 + 2\nu - \frac{8}{15}).$
- (4) $IRDIF(SLC_\mu(\nu)) = (D_t D_s^{-1} - D_s D_t^{-1})g_o(s, t)|_{s=t=1} = \mu(27\nu^2 + \frac{9}{2}\nu - \frac{9}{10}).$
- (5) $IRL(SLC_\mu(\nu)) = (L_t - L_s)g_o(s, t)|_{s=t=1} = \mu(18\nu^2 \ln 2 + 6\nu \ln \frac{3}{2} + \ln \frac{16}{25}).$
- (6) $IRLF(SLC_\mu(\nu)) = (D_s D_t)^{-1/2}\Delta g_o(s, t)|_{s=t=1}$
 $= \mu[9\sqrt{2}\nu^2 + (\sqrt{3} - 3\sqrt{2} + 2\sqrt{6})\nu - \frac{\sqrt{3}}{3} - \frac{2\sqrt{6}}{3} + \frac{4\sqrt{15}}{15} + \frac{2\sqrt{30}}{15}].$
- (7) $IRF(SLC_\mu(\nu)) = \Delta^2 g_o(s, t)|_{s=t=1} = \mu(162\nu^2 - 6).$
- (8) $IRLA(SLC_\mu(\nu)) = 2\Delta\Sigma^{-1}g_o(s, t)|_{s=t=1} = \mu(12\nu^2 + \frac{88}{35}\nu - \frac{171}{385}).$
- (9) $IRD1(SLC_\mu(\nu)) = \ln(I + \Delta)g_o(s, t)|_{s=t=1} = \mu(36\nu^2 \ln 2 + 6\nu \ln \frac{9}{2} + \ln \frac{4}{9}).$
- (10) $IRA(SLC_\mu(\nu)) = (D_s^{-1/2} - D_t^{-1/2})^2 g_o(s, t)|_{s=t=1}$
 $= \mu[(9 - 6\sqrt{2})\nu^2 + (\frac{11}{2} + 2\sqrt{2} - 2\sqrt{3} - 2\sqrt{6})\nu - \frac{3}{10} + \frac{2\sqrt{3}}{3} + \frac{2\sqrt{6}}{3} - \frac{4\sqrt{15}}{15} - \frac{4\sqrt{30}}{15}].$
- (11) $IRGA(SLC_\mu(\nu)) = [\ln \Sigma - (\ln 2)I - \frac{1}{2}(L_s + L_t)]g_o(s, t)|_{s=t=1}$
 $= \mu[18\nu^2 \ln(\frac{3}{2\sqrt{2}}) + 6\nu \ln(\frac{175\sqrt{6}}{432}) + 2\ln(\frac{1936}{875\sqrt{5}})].$
- (12) $IRB(SLC_\mu(\nu)) = (D_t^{1/2} - D_s^{1/2})^2 g_o(s, t)|_{s=t=1}$
 $= \mu[(162 - 108\sqrt{2})\nu^2 + (108 + 36\sqrt{2} - 24\sqrt{3} - 48\sqrt{6})\nu$
 $+ 6 + 8\sqrt{3} + 16\sqrt{6} - 4\sqrt{15} - 8\sqrt{30}].$

□

The odd-layer expressions retain the same leading quadratic and linear dependence on ν as the even-layer formulas, while the additional degree-5 edge types contribute descriptor-dependent finite-size constants that distinguish the two parity classes.

5.3. Parameter sensitivity and structural trends for odd layers

5.3.1. Exact computed values and sensitivity

Table 7 reports only representative exact values, since the full parameter dependence is already determined analytically by Theorem 5.1.

Table 7. Representative exact values for odd-layer descriptors.

ν	μ	AL	IRF	$IRLA$	$IRGA$
3	3	1560	4356	345.30	28.14
5	3	4224	12132	936.38	78.74
7	3	8184	23796	1815.47	154.79
9	3	13440	39348	2982.55	256.27

For an odd-layer descriptor,

$$X^{(o)}(\mu, \nu) = \mu(A_X \nu^2 + B_X \nu + C_X).$$

The parity-preserving layer difference is therefore

$$X^{(o)}(\mu, \nu + 2) - X^{(o)}(\mu, \nu) = \mu(4A_X \nu + 4A_X + 2B_X),$$

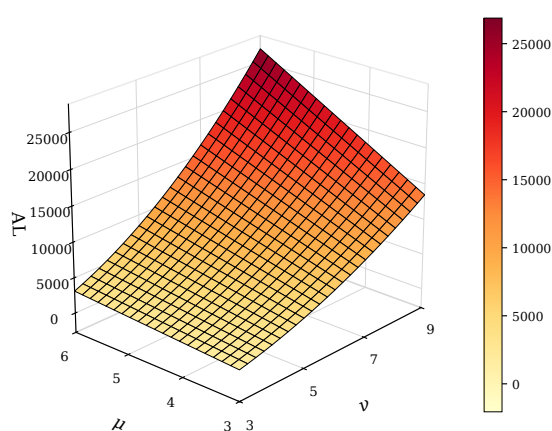
where the finite-size correction C_X cancels. Likewise,

$$X^{(o)}(\mu + 1, \nu) - X^{(o)}(\mu, \nu) = F_X^{(o)}(\nu), \quad X^{(o)}(\mu, \nu) \sim A_X \mu \nu^2.$$

The degree-5 corrections affect finite-size values, whereas even- and odd-layer configurations share the same dominant quadratic scaling structure.

5.3.2. Graphical interpretation of exact structural trends

Figures 6–9 present the corresponding exact surfaces for the odd-layer configuration. This reduced graphical set preserves the contrast among weighting mechanisms while avoiding repetitive surfaces with identical qualitative growth.

**Figure 6.** Exact AL surface for the odd-layer configuration.

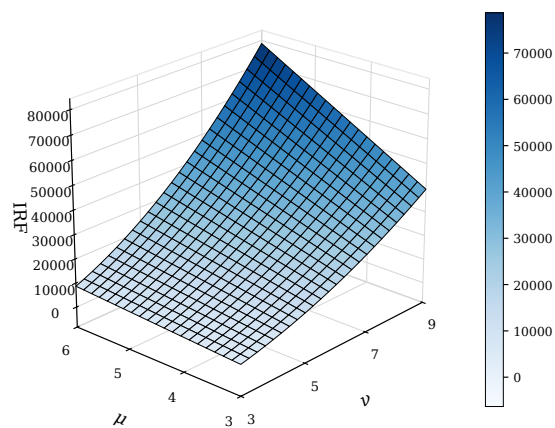


Figure 7. Exact *IRF* surface for the odd-layer configuration.

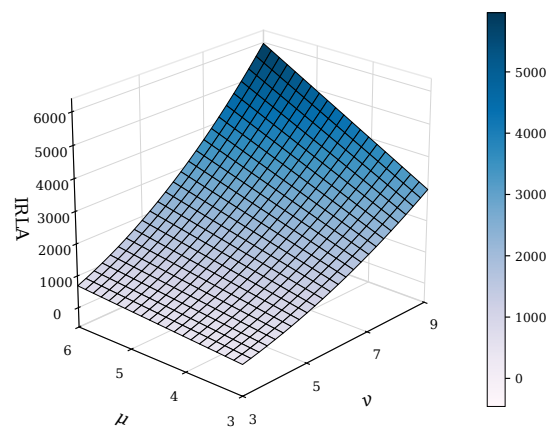


Figure 8. Exact *IRLA* surface for the odd-layer configuration.

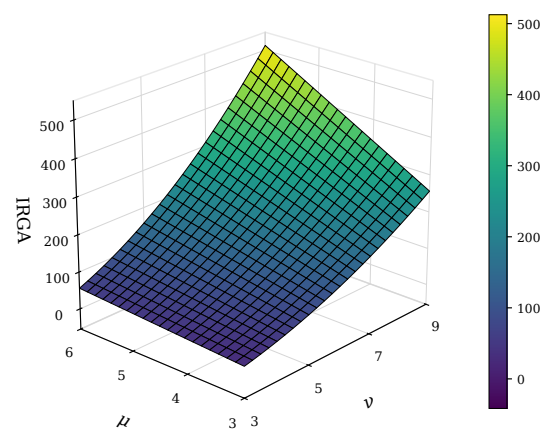


Figure 9. Exact *IRGA* surface for the odd-layer configuration.

6. Descriptor-weighted entropy measures

Having established the exact descriptor totals and their parameter sensitivity, we now examine how the corresponding edge weights are distributed probabilistically.

6.1. Exact entropy formulas for even layers

The irregularity indices derived in Sections 4 and 5 measure the total degree heterogeneity of the generalized silicate cage networks. The corresponding descriptor-weighted entropies provide an additional characterization by measuring the distribution of each irregularity contribution over the positive-weight edges.

For compactness, write $\Phi(x) = x \log_2 x$.

For the even-layer network, the active degree-pair support is $\mathcal{A}_e$.

Using the three active even-layer degree pairs, define

$$a_e = 6\nu\mu, \quad b_e = (18\nu^2 - 6\nu)\mu, \quad c_e = 12\nu\mu.$$

These quantities are the multiplicities of the active degree pairs (3, 4), (3, 6), and (4, 6), respectively. Thus, for every descriptor X ,

$$T_X^{(e)} = a_e w_X(3, 4) + b_e w_X(3, 6) + c_e w_X(4, 6) \quad (6.1)$$

and

$$C_X^{(e)} = a_e \Phi(w_X(3, 4)) + b_e \Phi(w_X(3, 6)) + c_e \Phi(w_X(4, 6)). \quad (6.2)$$

The entropy associated with X is then obtained from

$$H_X^{(e)} = \log_2 T_X^{(e)} - \frac{C_X^{(e)}}{T_X^{(e)}}.$$

The exact expressions are summarized in the following theorem.

Theorem 6.1 (Entropy formulas for even layers). *Let $SLC_\mu(\nu)$ be an even-layer generalized silicate cage network satisfying*

$$\nu \geq 2, \quad \nu \equiv 0 \pmod{2}, \quad \mu \geq 2.$$

For every descriptor X ,

$$H_X^{(e)} = \log_2 T_X^{(e)} - \frac{C_X^{(e)}}{T_X^{(e)}},$$

where the corresponding normalizing totals and logarithmic correction terms are as follows.

$$(1) \quad T_{AL}^{(e)} = \mu(54\nu^2 + 12\nu),$$

$$C_{AL}^{(e)} = a_e \Phi(1) + b_e \Phi(3) + c_e \Phi(2).$$

$$(2) \quad T_{IRR_t}^{(e)} = \frac{1}{2} T_{AL}^{(e)} = \mu(27\nu^2 + 6\nu),$$

$$C_{IRR_t}^{(e)} = a_e \Phi\left(\frac{1}{2}\right) + b_e \Phi\left(\frac{3}{2}\right) + c_e \Phi(1),$$

and

$$H_{IRR_t}^{(e)} = H_{AL}^{(e)}.$$

$$(3) \quad T_{IRLU}^{(e)} = \mu(18\nu^2 + 2\nu),$$

$$C_{IRLU}^{(e)} = a_e \Phi\left(\frac{1}{3}\right) + b_e \Phi(1) + c_e \Phi\left(\frac{1}{2}\right).$$

$$(4) \quad T_{IRDIF}^{(e)} = \mu\left(27\nu^2 + \frac{9}{2}\nu\right),$$

$$C_{IRDIF}^{(e)} = a_e \Phi\left(\frac{7}{12}\right) + b_e \Phi\left(\frac{3}{2}\right) + c_e \Phi\left(\frac{5}{6}\right).$$

$$(5) \quad T_{IRL}^{(e)} = \mu\left(18\nu^2 \ln 2 + 6\nu \ln \frac{3}{2}\right),$$

$$C_{IRL}^{(e)} = a_e \Phi\left(\ln \frac{4}{3}\right) + b_e \Phi(\ln 2) + c_e \Phi\left(\ln \frac{3}{2}\right).$$

$$(6) \quad T_{IRLF}^{(e)} = \mu\left[9\sqrt{2}\nu^2 + (\sqrt{3} - 3\sqrt{2} + 2\sqrt{6})\nu\right],$$

$$C_{IRLF}^{(e)} = a_e \Phi\left(\frac{1}{\sqrt{12}}\right) + b_e \Phi\left(\frac{1}{\sqrt{2}}\right) + c_e \Phi\left(\frac{1}{\sqrt{6}}\right).$$

$$(7) \quad T_{IRF}^{(e)} = 162\mu\nu^2,$$

$$C_{IRF}^{(e)} = a_e \Phi(1) + b_e \Phi(9) + c_e \Phi(4).$$

$$(8) \quad T_{IRLA}^{(e)} = \mu\left(12\nu^2 + \frac{88}{35}\nu\right),$$

$$C_{IRLA}^{(e)} = a_e \Phi\left(\frac{2}{7}\right) + b_e \Phi\left(\frac{2}{3}\right) + c_e \Phi\left(\frac{2}{5}\right).$$

$$(9) \quad T_{IRD1}^{(e)} = \mu\left(36\nu^2 \ln 2 + 6\nu \ln \frac{9}{2}\right),$$

$$C_{IRD1}^{(e)} = a_e \Phi(\ln 2) + b_e \Phi(\ln 4) + c_e \Phi(\ln 3).$$

$$(10) \quad T_{IRA}^{(e)} = \mu\left[(9 - 6\sqrt{2})\nu^2 + \left(\frac{11}{2} + 2\sqrt{2} - 2\sqrt{3} - 2\sqrt{6}\right)\nu\right],$$

$$C_{IRA}^{(e)} = a_e \Phi\left(\frac{7}{12} - \frac{\sqrt{3}}{3}\right) + b_e \Phi\left(\frac{1}{2} - \frac{\sqrt{2}}{3}\right) + c_e \Phi\left(\frac{5}{12} - \frac{\sqrt{6}}{6}\right).$$

$$(11) \quad T_{IRGA}^{(e)} = \mu\left[18\nu^2 \ln\left(\frac{3}{2\sqrt{2}}\right) + 6\nu \ln\left(\frac{175\sqrt{6}}{432}\right)\right],$$

$$C_{IRGA}^{(e)} = a_e \Phi\left(\ln\left(\frac{7}{4\sqrt{3}}\right)\right) + b_e \Phi\left(\ln\left(\frac{3}{2\sqrt{2}}\right)\right) + c_e \Phi\left(\ln\left(\frac{5}{2\sqrt{6}}\right)\right).$$

$$(12) \quad T_{IRB}^{(e)} = \mu\left[(162 - 108\sqrt{2})\nu^2 + (108 + 36\sqrt{2} - 24\sqrt{3} - 48\sqrt{6})\nu\right],$$

$$C_{IRB}^{(e)} = a_e \Phi(7 - 4\sqrt{3}) + b_e \Phi(9 - 6\sqrt{2}) + c_e \Phi(10 - 4\sqrt{6}).$$

Proof. The active even-layer edge multiplicities are a_e , b_e , and c_e . Substituting the three single-edge descriptor weights associated with (3, 4), (3, 6), and (4, 6) into Eqs (6.1) and (6.2) gives the twelve expressions listed above. The values of $T_X^{(e)}$ coincide with the exact irregularity-index totals established in Theorem 4.1. Applying Theorem 3.3 then gives $H_X^{(e)} = \log_2 T_X^{(e)} - \frac{C_X^{(e)}}{T_X^{(e)}}$.

Moreover, $w_{IRR_i}(n, p) = \frac{1}{2}w_{AL}(n, p)$, so the positive-scale invariance established above gives $H_{IRR_i}^{(e)} = H_{AL}^{(e)}$. $\square$

Thus, the twelve even-layer descriptors induce eleven distinct entropy distributions, with AL and IRR_i forming the unique positive-scale-equivalent pair.

6.2. Exact entropy formulas for odd layers

The odd-layer architecture contains a larger positive-weight degree-pair support than the even-layer configuration because the modified central connectivity introduces degree-5 vertices. The active degree pairs are $\mathcal{A}_o$. The enlarged support modifies the finite entropy corrections but leaves the replication structure unchanged.

For compactness, define

$$a_o = (6\nu - 2)\mu, \quad b_o = 2\mu, \quad c_o = (18\nu^2 - 6\nu)\mu, \quad d_o = (12\nu - 4)\mu, \quad e_o = 4\mu.$$

These quantities are the respective multiplicities of the five active degree pairs. Thus, for every irregularity descriptor X ,

$$T_X^{(o)} = a_o w_X(3, 4) + b_o w_X(3, 5) + c_o w_X(3, 6) + d_o w_X(4, 6) + e_o w_X(5, 6) \quad (6.3)$$

and

$$C_X^{(o)} = a_o \Phi(w_X(3, 4)) + b_o \Phi(w_X(3, 5)) + c_o \Phi(w_X(3, 6)) + d_o \Phi(w_X(4, 6)) + e_o \Phi(w_X(5, 6)). \quad (6.4)$$

The corresponding descriptor-weighted entropy is

$$H_X^{(o)} = \log_2 T_X^{(o)} - \frac{C_X^{(o)}}{T_X^{(o)}}.$$

The exact odd-layer entropy expressions are stated in the following theorem.

Theorem 6.2 (Entropy formulas for odd layers). *Let $SLC_\mu(\nu)$ be an odd-layer generalized silicate cage network satisfying*

$$\nu \geq 3, \quad \nu \equiv 1 \pmod{2}, \quad \mu \geq 3.$$

For every descriptor X ,

$$H_X^{(o)} = \log_2 T_X^{(o)} - \frac{C_X^{(o)}}{T_X^{(o)}},$$

where the normalizing totals and logarithmic correction terms are as follows.

$$(1) \quad T_{AL}^{(o)} = \mu(54v^2 + 12v - 2),$$

$$C_{AL}^{(o)} = a_o\Phi(1) + b_o\Phi(2) + c_o\Phi(3) + d_o\Phi(2) + e_o\Phi(1).$$

$$(2) \quad T_{IRR_t}^{(o)} = \frac{1}{2}T_{AL}^{(o)} = \mu(27v^2 + 6v - 1),$$

$$C_{IRR_t}^{(o)} = a_o\Phi\left(\frac{1}{2}\right) + b_o\Phi(1) + c_o\Phi\left(\frac{3}{2}\right) + d_o\Phi(1) + e_o\Phi\left(\frac{1}{2}\right),$$

and

$$H_{IRR_t}^{(o)} = H_{AL}^{(o)}.$$

$$(3) \quad T_{IRLU}^{(o)} = \mu\left(18v^2 + 2v - \frac{8}{15}\right),$$

$$C_{IRLU}^{(o)} = a_o\Phi\left(\frac{1}{3}\right) + b_o\Phi\left(\frac{2}{3}\right) + c_o\Phi(1) + d_o\Phi\left(\frac{1}{2}\right) + e_o\Phi\left(\frac{1}{5}\right).$$

$$(4) \quad T_{IRDF}^{(o)} = \mu\left(27v^2 + \frac{9}{2}v - \frac{9}{10}\right),$$

$$C_{IRDF}^{(o)} = a_o\Phi\left(\frac{7}{12}\right) + b_o\Phi\left(\frac{16}{15}\right) + c_o\Phi\left(\frac{3}{2}\right) + d_o\Phi\left(\frac{5}{6}\right) + e_o\Phi\left(\frac{11}{30}\right).$$

$$(5) \quad T_{IRL}^{(o)} = \mu\left(18v^2 \ln 2 + 6v \ln \frac{3}{2} + \ln \frac{16}{25}\right),$$

$$C_{IRL}^{(o)} = a_o\Phi\left(\ln \frac{4}{3}\right) + b_o\Phi\left(\ln \frac{5}{3}\right) + c_o\Phi(\ln 2) + d_o\Phi\left(\ln \frac{3}{2}\right) + e_o\Phi\left(\ln \frac{6}{5}\right).$$

$$(6) \quad T_{IRLF}^{(o)} = \mu\left[9\sqrt{2}v^2 + \left(\sqrt{3} - 3\sqrt{2} + 2\sqrt{6}\right)v - \frac{\sqrt{3}}{3} - \frac{2\sqrt{6}}{3} + \frac{4\sqrt{15}}{15} + \frac{2\sqrt{30}}{15}\right],$$

$$C_{IRLF}^{(o)} = a_o\Phi\left(\frac{1}{\sqrt{12}}\right) + b_o\Phi\left(\frac{2}{\sqrt{15}}\right) + c_o\Phi\left(\frac{1}{\sqrt{2}}\right) + d_o\Phi\left(\frac{1}{\sqrt{6}}\right) + e_o\Phi\left(\frac{1}{\sqrt{30}}\right).$$

$$(7) \quad T_{IRF}^{(o)} = \mu(162v^2 - 6),$$

$$C_{IRF}^{(o)} = a_o\Phi(1) + b_o\Phi(4) + c_o\Phi(9) + d_o\Phi(4) + e_o\Phi(1).$$

$$(8) \quad T_{IRLA}^{(o)} = \mu\left(12v^2 + \frac{88}{35}v - \frac{171}{385}\right),$$

$$C_{IRLA}^{(o)} = a_o\Phi\left(\frac{2}{7}\right) + b_o\Phi\left(\frac{1}{2}\right) + c_o\Phi\left(\frac{2}{3}\right) + d_o\Phi\left(\frac{2}{5}\right) + e_o\Phi\left(\frac{2}{11}\right).$$

$$(9) \quad T_{IRD1}^{(o)} = \mu\left(36v^2 \ln 2 + 6v \ln \frac{9}{2} + \ln \frac{4}{9}\right),$$

$$C_{IRD1}^{(o)} = a_o\Phi(\ln 2) + b_o\Phi(\ln 3) + c_o\Phi(\ln 4) + d_o\Phi(\ln 3) + e_o\Phi(\ln 2).$$

$$(10) \quad T_{IRA}^{(o)} = \mu[(9 - 6\sqrt{2})v^2 + (\frac{11}{2} + 2\sqrt{2} - 2\sqrt{3} - 2\sqrt{6})v - \frac{3}{10} + \frac{2\sqrt{3}}{3} + \frac{2\sqrt{6}}{3} - \frac{4\sqrt{15}}{15} - \frac{4\sqrt{30}}{15}],$$

$$C_{IRA}^{(o)} = a_o\Phi\left(\frac{7}{12} - \frac{\sqrt{3}}{3}\right) + b_o\Phi\left(\frac{8}{15} - \frac{2\sqrt{15}}{15}\right) + c_o\Phi\left(\frac{1}{2} - \frac{\sqrt{2}}{3}\right) \\ + d_o\Phi\left(\frac{5}{12} - \frac{\sqrt{6}}{6}\right) + e_o\Phi\left(\frac{11}{30} - \frac{\sqrt{30}}{15}\right).$$

$$(11) \quad T_{IRGA}^{(o)} = \mu[18v^2 \ln\left(\frac{3}{2\sqrt{2}}\right) + 6v \ln\left(\frac{175\sqrt{6}}{432}\right) + 2 \ln\left(\frac{1936}{875\sqrt{5}}\right)],$$

$$C_{IRGA}^{(o)} = a_o\Phi\left(\ln\left(\frac{7}{4\sqrt{3}}\right)\right) + b_o\Phi\left(\ln\left(\frac{4}{\sqrt{15}}\right)\right) + c_o\Phi\left(\ln\left(\frac{3}{2\sqrt{2}}\right)\right) \\ + d_o\Phi\left(\ln\left(\frac{5}{2\sqrt{6}}\right)\right) + e_o\Phi\left(\ln\left(\frac{11}{2\sqrt{30}}\right)\right).$$

$$(12) \quad T_{IRB}^{(o)} = \mu[(162 - 108\sqrt{2})v^2 + (108 + 36\sqrt{2} - 24\sqrt{3} - 48\sqrt{6})v + 6 + 8\sqrt{3} + 16\sqrt{6} - 4\sqrt{15} - 8\sqrt{30}],$$

$$C_{IRB}^{(o)} = a_o\Phi(7 - 4\sqrt{3}) + b_o\Phi(8 - 2\sqrt{15}) + c_o\Phi(9 - 6\sqrt{2}) \\ + d_o\Phi(10 - 4\sqrt{6}) + e_o\Phi(11 - 2\sqrt{30}).$$

Proof. The active odd-layer edge multiplicities are a_o , b_o , c_o , d_o , and e_o . Substitution of the five positive single-edge weights of each descriptor into Eqs (6.3) and (6.4) gives the expressions listed above. The normalizing totals $T_X^{(o)}$ coincide with the exact odd-layer irregularity indices established in Theorem 5.1. Therefore, Theorem 3.3 gives $H_X^{(o)} = \log_2 T_X^{(o)} - \frac{C_X^{(o)}}{T_X^{(o)}}$.

Since $w_{IRR_i}(n, p) = \frac{1}{2}w_{AL}(n, p)$, the positive-scale invariance established above further gives $H_{IRR_i}^{(o)} = H_{AL}^{(o)}$. $\square$

Hence, the odd-layer descriptors again produce eleven distinct entropy distributions. The additional degree-5 classes alter the nonproportional weights but preserve the equality $H_{IRR_i}^{(o)} = H_{AL}^{(o)}$; all resulting probability distributions satisfy normalization.

6.3. Scaling and asymptotic behavior of descriptor-weighted entropy

Theorem 6.3 (Scaling law for descriptor-weighted entropy). *For either parity class and any descriptor X , suppose*

$$T_X(\mu, \nu) = \mu F_X(\nu), \quad C_X(\mu, \nu) = \mu G_X(\nu).$$

Then

$$H_X(\mu, \nu) = \log_2 \mu + \log_2 F_X(\nu) - \frac{G_X(\nu)}{F_X(\nu)}.$$

Consequently, for admissible μ_1, μ_2 ,

$$H_X(\mu_2, \nu) - H_X(\mu_1, \nu) = \log_2 \left(\frac{\mu_2}{\mu_1} \right).$$

Moreover, for fixed admissible μ and along the corresponding parity subsequence,

$$H_X(\mu, \nu) = 2 \log_2 \nu + \log_2(18\mu) + o(1), \quad \nu \rightarrow \infty.$$

Proof. Substitution of the common factor μ into $H_X = \log_2 T_X - C_X/T_X$ gives the first identity, and subtracting the two replication cases gives the second. For large ν , the (3,6)-edge class has multiplicity $(18\nu^2 - 6\nu)\mu$ and supplies the dominant positive contribution to both T_X and C_X . Its single-edge weight cancels between $\log_2 T_X$ and C_X/T_X , which yields the stated asymptotic formula. $\square$

The theorem isolates two universal effects: replication contributes exactly $\log_2 \mu$, whereas layer enlargement contributes the leading term $2 \log_2 \nu$.

7. Conclusions

This study establishes a parity-resolved algebraic framework for the irregularity and descriptor-weighted entropy of generalized silicate cage networks $SLC_\mu(\nu)$.

(1) The even- and odd-layer configurations have distinct degree partitions because degree-5 vertices occur only in the odd-layer structure; the inherited partitions were directly checked by edge totals and degree sums.

(2) The twelve irregularity descriptors have exact closed forms. Their parity-preserving layer differences and replication increments make the respective roles of ν and μ explicit: ν produces quadratic leading growth, whereas μ produces exact proportional amplification.

(3) Exact descriptor-weighted entropy formulas were obtained for both parity classes. Positive-scale invariance gives identical entropy distributions for AL and IRR_t , leaving eleven distinct entropy expressions in each configuration.

(4) The new entropy-scaling theorem shows that replication changes entropy logarithmically and that both parity classes share the universal large-layer leading term $2 \log_2 \nu$.

These topological fingerprints provide candidate structural variables for comparing, classifying, and conducting future property-oriented modeling of silicate frameworks. Future work may combine them with verified experimental or computational physicochemical data to develop genuine QSPR or machine-learning models.

Author contributions

Duyu Zhang: Conceptualization; Methodology; Formal analysis; Investigation; Software; Validation; Visualization; Writing-original draft; Writing-review and editing. Xiaohong Dong: Supervision; Project administration; Writing-review and editing. Hongjie Zhang: Writing-original draft; Writing-review and editing. Haoyu Kong: Supervision; Project administration; Writing-review and editing. All authors have read and approved the final version of the manuscript.

Data availability

All data used in this study are generated analytically from the degree partitions and generalized M -polynomials of the considered silicate cage networks. The exact formulas, parameter settings, and numerical results required to reproduce the findings are contained within this article.

Use of Generative-AI tools declaration

Generative-AI tools were used to assist with language refinement, manuscript organization, and graphical preparation. All mathematical derivations, numerical results, scientific interpretations, and final manuscript content were independently checked and approved by the authors. The authors take full responsibility for the accuracy and integrity of the work.

Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this article.

References

1. H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.*, **44** (1971), 2332–2339. <https://doi.org/10.1246/bcsj.44.2332>
2. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17** (1972), 535–538. [https://doi.org/10.1016/0009-2614\(72\)85099-1](https://doi.org/10.1016/0009-2614(72)85099-1)
3. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69** (1947), 17–20. <https://doi.org/10.1021/JA01193A005>
4. A. T. Balaban, Highly discriminating distance-based topological index, *Chem. Phys. Lett.*, **89** (1982), 399–404. [https://doi.org/10.1016/0009-2614\(82\)80009-2](https://doi.org/10.1016/0009-2614(82)80009-2)
5. N. Trinajstić, *Chemical graph theory*, Boca Raton: CRC Press, 1983.
6. A. R. Khan, S. A. Bhatti, F. Tawfiq, M. K. Siddiqui, S. Hussain, M. A. Ali, On degree-based operators and topological descriptors of molecular graphs and their applications to QSPR analysis of carbon derivatives, *Sci. Rep.*, **14** (2024), 21543. <https://doi.org/10.1038/s41598-024-72621-7>
7. T. Nair A., D. Antony Xavier, A. Baby, Enhanced molecular descriptors using degree-distance invariants and their efficacy in QSPR quadratic modelling of chemical compounds, *J. Mol. Struct.*, **1314** (2024), 138730. <https://doi.org/10.1016/j.molstruc.2024.138730>
8. I. Haider, M. Li, M. K. Jamil, A. Li, A graph-based machine learning framework for predicting physicochemical properties of antiviral drugs via topological indices, *J. Chem. Inf. Model.*, **65** (2025), 12038–12057. <https://doi.org/10.1021/acs.jcim.5c01125>
9. M. W. Rasheed, A. Mahboob, I. Hanif, Uses of degree-based topological indices in QSPR analysis of alkaloids with poisonous and healthful nature, *Front. Phys.*, **12** (2024), 1381887. <https://doi.org/10.3389/fphy.2024.1381887>
10. R. Todeschini, V. Consonni, *Handbook of molecular descriptors*, Weinheim: Wiley-VCH, 2000. <https://doi.org/10.1002/9783527613106>
11. J. Devillers, A. T. Balaban, *Topological indices and related descriptors in QSAR and QSPR*, Amsterdam: Gordon and Breach, 1999. <https://doi.org/10.1201/9781482296945>

12. I. Gutman, B. Furtula, *Novel molecular structure descriptors—theory and applications I*, Kragujevac: University of Kragujevac, 2010.
13. X. Li, I. Gutman, *Mathematical aspects of randić-type molecular structure descriptors*, Kragujevac: University of Kragujevac and Faculty of Science, 2006.
14. B. Furtula, A. Graovac, D. Vukicević, Augmented zagreb index, *J. Math. Chem.*, **48** (2010), 370–380. <https://doi.org/10.1007/s10910-010-9677-3>
15. B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.*, **53** (2015), 1184–1190. <https://doi.org/10.1007/s10910-015-0480-z>
16. M. Randić, Characterization of molecular branching, *J. Am. Chem. Soc.*, **97** (1975), 6609–6615. <https://doi.org/10.1021/ja00856a001>
17. E. Deutsch, S. Klavžar, *M*-polynomial and degree-based topological indices, *Iran. J. Math. Chem.*, **6** (2015), 93–102. <https://doi.org/10.22052/ijmc.2015.10106>
18. S. Mondal, M. K. Siddiqui, N. De, A. Pal, Neighborhood *M*-polynomial of crystallographic structures, *Biointerface Res. Appl. Chem.*, **11** (2021), 9372–9381. <https://doi.org/10.33263/BRIAC112.93729381>
19. Z. Raza, M. E. K. Sukaiti, *M*-polynomial and degree based topological indices of some nanostructures, *Symmetry*, **12** (2020), 831. <https://doi.org/10.3390/sym12050831>
20. M. Javaid, J. Cao, Computing topological indices of probabilistic neural network, *Neural Comput. Appl.*, **30** (2018), 3869–3876. <https://doi.org/10.1007/s00521-017-2972-1>
21. M. Imran, M. K. Siddiqui, A. A. E. Abunamous, D. Adi, S. H. Rafique, A. Q. Baig, Eccentricity based topological indices of an oxide network, *Mathematics*, **6** (2018), 126. <https://doi.org/10.3390/math6070126>
22. M. U. Ghani, S. Ali, M. Imran, H. Karamti, F. Sultan, M. Y. Almusawa, Hex-derived molecular descriptors via generalized valency-based entropies, *IEEE Access*, **11** (2023), 42052–42068. <https://doi.org/10.1109/ACCESS.2023.3248507>
23. N. Rashevsky, Life, information theory, and topology, *Bull. Math. Biophys.*, **17** (1955), 229–235. <https://doi.org/10.1007/BF02477860>
24. M. Dehmer, Information-theoretic concepts for the analysis of complex networks, *Appl. Artif. Intell.*, **22** (2008), 684–706. <https://doi.org/10.1080/08839510802164101>
25. J. B. Liu, K. Wang, X. Zhai, Statistical analysis and topological property of a class of fractal networks, *Fractals*, **34** (2026), 2640001. <https://doi.org/10.1142/S0218348X26400013>
26. J. B. Liu, F. Zou, G. J. Cai, J. Cao, Network coherence and robustness analysis of extended polygonal networks, *Circuits Syst. Signal Process.*, **45** (2026), 6881–6901. <https://doi.org/10.1007/s00034-026-03526-1>
27. J. B. Liu, M. Y. Yu, J. Cao, Laplacian spectra and coherence analysis of asymmetric networks under noise disturbance, *J. Complex Netw.*, **14** (2026), cnag009. <https://doi.org/10.1093/comnet/cnag009>
28. S. C. Sigarreta, S. M. Sigarreta, H. Cruz-Suárez, On degree-based topological indices of random polyomino chains, *Math. Biosci. Eng.*, **19** (2022), 8760–8773. <https://doi.org/10.3934/mbe.2022406>

29. P. Agarwal, A. Bharali, Degree-based topological indices in random polygonal and spiro chains, *South East Asian J. Math. Math. Sci.*, **21** (2025), 1–24. <https://doi.org/10.56827/SEAJMMS.2025.2102.1>
30. W. Zhang, L. You, H. Liu, X. Fang, The expected values and variances for degree-based topological indices in three random chains, *Filomat*, **38** (2024), 6563–6580. <https://doi.org/10.2298/FIL2418563Z>
31. Y. Ahmad, X. F. Pan, U. Ali, Z. Diao, Computing the expected value of invariants based on resistance distance for random spiro-polynomio chains, *Discrete Appl. Math.*, **361** (2025), 111–120. <https://doi.org/10.1016/j.dam.2024.09.026>
32. A. Gandhi, M. M. F. Hasan, A graph theoretic representation and analysis of zeolite frameworks, *Comput. Chem. Eng.*, **155** (2021), 107548. <https://doi.org/10.1016/j.compchemeng.2021.107548>
33. D. Paul, M. Arockiaraj, S. Tigga, K. Balasubramanian, Zeolite AST: relativistic degree and distance based topological descriptors, *Comput. Theor. Chem.*, **1218** (2022), 113933. <https://doi.org/10.1016/j.comptc.2022.113933>
34. K. Jacob, J. Clement, Zeolite ATN: topological characterization and predictive analysis on potential energies using entropy measures, *J. Mol. Struct.*, **1299** (2024), 137101. <https://doi.org/10.1016/j.molstruc.2023.137101>
35. Y. Du, H. Liu, Cage-like silsesquioxanes-based hybrid materials, *Dalton Trans.*, **49** (2020), 5396–5405. <https://doi.org/10.1039/D0DT00587H>
36. M. M. Levitsky, A. I. Yalymov, A. N. Kulakova, A. A. Petrov, A. N. Bilyachenko, Cage-like metallasilsesquioxanes in catalysis: a review, *J. Mol. Catal. A: Chem.*, **426** (2017), 297–304. <https://doi.org/10.1016/j.molcata.2016.06.016>
37. Y. Qian, P. Wei, X. Zhao, P. Jiang, H. Yu, Flame retardancy and thermal stability of polyhedral oligomeric silsesquioxane nanocomposites, *Fire Mater.*, **37** (2013), 1–16. <https://doi.org/10.1002/fam.1126>
38. H. Zhou, Q. Ye, J. Xu, Polyhedral oligomeric silsesquioxane-based hybrid materials and their applications, *Mater. Chem. Front.*, **1** (2017), 212–230. <https://doi.org/10.1039/C6QM00062B>
39. Z. Yan, M. Salman, S. Shahzaib, I. Khalid, H. Karamti, Generalized M -polynomial and graphical invariants of silicate cage networks with applications to property prediction, *AIMS Math.*, **11** (2026), 21743–21780. <https://doi.org/10.3934/math.2026880>
40. M. O. Albertson, The irregularity of a graph, *Ars Comb.*, **46** (1997), 219–225.
41. I. Gutman, Topological indices and irregularity measures, *Bull. Int. Math. Virtual Inst.*, **8** (2018), 469–475. <https://doi.org/10.7251/BIMVII803469G>
42. T. Réti, R. Sharafadini, A. Drágelyi-Kiss, H. Haghbin, Graph irregularity indices used as molecular descriptors in QSPR studies, *MATCH Commun. Math. Comput. Chem.*, **79** (2018), 509–524.
43. H. Abdo, D. Dimitrov, I. Gutman, Graph irregularity and its measures, *Appl. Math. Comput.*, **357** (2019), 317–324. <https://doi.org/10.1016/j.amc.2019.04.013>
44. C. E. Shannon, A mathematical theory of communication, *Bell Syst. Tech. J.*, **27** (1948), 379–423. <https://doi.org/10.1002/j.1538-7305.1948.tb01338.x>

-
45. S. Cao, M. Dehmer, Y. Shi, Extremality of degree-based graph entropies, *Inf. Sci.*, **278** (2014), 22–33. <https://doi.org/10.1016/j.ins.2014.03.133>
 46. Z. Chen, M. Dehmer, F. Emmert-Streib, Y. Shi, Entropy of weighted graphs with Randić weights, *Entropy*, **17** (2015), 3710–3723. <https://doi.org/10.3390/e17063710>



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