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THE FIRST MAX–MIN ZAGREB INDEX: STRUCTURAL IDENTITIES, SHARP BOUNDS AND NANOSTRUCTURE APPLICATIONS

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Abstract. The First Max–Min Zagreb index combines endpoint degrees with the minimum and maximum degrees of a graph. We establish an exact decomposition into the first Zagreb index and an extremal-degree term, leading to formulas for complements, subdivisions, line graphs, joins, Cartesian and strong products, and single-edge addition. Sharp bounds, equality cases, and a normalized regularity score are obtained, together with closed forms for eight graph families and three molecular nanostructures. Exact integer-arithmetic enumeration of 27,475 connected labelled graphs on two to six vertices verifies the principal identities, including 189,587 edge-addition tests. The cycle value is interpreted as a nominal carbon-skeleton mass contribution, not the complete cycloalkane molecular mass. The results provide a rigorous basis for this descriptor and clarify its discriminative limitations.

1. Introduction

Topological indices convert a molecular or abstract graph into numerical quantities that can be compared without preserving the full drawing. Classical examples include the distance-based Wiener index [27], the matching-based Hosoya index [13], and the highly discriminating Balaban index [2]. Degree-based descriptors are especially inexpensive to compute and have become standard tools in chemical graph theory, quantitative structure-property relationship analysis, and quantitative structure-activity relationship analysis [8]. Their value, however, depends on a clear mathematical definition, rigorous transformation rules, and an honest account of degeneracy: structurally different graphs may receive the same descriptor value.

The first and second Zagreb indices originated in the study of total π-electron energy [12]. Their development and mathematical properties are reviewed in [10, 18], while later work established useful bounds and extremal results [4, 11]. Numerous descendants and neighbouring constructions have since appeared. These include the reformulated Zagreb indices [16], the forgotten index [6], the Randić index [19], the geometric-arithmetic index [25], and the connectivity indices of Zhou and Trinajstić [29, 30]. Vukičević and Gašperov organized a broad family of

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Adriatic indices [26], within which the Max-min rodeg index was investigated separately [24]. More recently, the Sombor framework renewed interest in descriptors obtained from geometric combinations of endpoint degrees [9]. Its rapid theoretical development [3, 22] and chemical validation studies [21] also emphasize two expectations for any proposed descriptor: its relation to established indices should be explicit, and claims of chemical usefulness should not exceed the evidence supplied.

This paper considers the First Max-Min Zagreb index, denoted by $MM_1Z(G)$. For every edge, the index adds the two endpoint degrees and two copies of the sum of the global minimum and maximum degrees. This mixed local-global construction is simple, but simplicity does not make its behaviour automatic. In particular, graph operations can change the extremal degrees in ways that invalidate direct substitutions. Subdivision introduces vertices of degree two; a graph join shifts the degrees of both factors by different orders; and a line graph may increase, preserve, or decrease the index depending on the regular degree. These cases require exact treatment.

The central result is the decomposition

$$MM_1Z(G) = 2m\,(\delta(G) + \Delta(G)) + M_1(G).$$

It shows that MM_1Z is an affine extension of the first Zagreb index once the size and extremal degrees are fixed. Rather than concealing this dependence, the paper uses it systematically. Exact formulae are derived for benchmark families, complements, k-subdivisions, line graphs, joins, Cartesian products, and strong products. A strict increment formula under edge addition is proved. Two parameter-sensitive bounds are obtained from Cauchy's inequality and the degree interval, and their equality cases are characterized. A dimensionless score normalizes the descriptor by the largest possible edge contribution and supplies a regularity-oriented comparison across graph families.

The mathematical results are supported by exact computational verification. All connected labelled simple graphs of orders two through six are enumerated using integer arithmetic, and the identities, bounds, subdivision formulae, line-graph formula, complement formula, and edge-addition theorem are tested exhaustively within that range. The applications section then revisits a dendrimer nanostar, a carbon nanocone, and a carbon nanotori using edge partitions from the corresponding structural models [1, 7, 14, 17, 23]. The resulting formulae correct inconsistencies in the earlier draft and distinguish exact graph-theoretic statements from empirical chemical prediction.

Throughout, $G = (V(G), E(G))$ is a finite, simple, undirected, connected graph with at least one edge. Its order and size are $n = |V(G)|$ and $m = |E(G)|$. For $v \in V(G)$, the degree is $d_G(v)$, and the minimum and maximum degrees are $\delta(G)$ and $\Delta(G)$. The symbols $M_1(G)$, $M_2(G)$, and $F(G)$ denote the first Zagreb, second Zagreb, and forgotten indices. Standard graph operations follow the notation used in [5, 15], while subdivision and line-graph constructions follow [20, 28].

2. Preliminaries and the structural identity

The first Zagreb index has equivalent vertex- and edge-sum forms,

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} \left(d_G(u) + d_G(v)\right),$$

and the second Zagreb and forgotten indices are

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v), \qquad F(G) = \sum_{v \in V(G)} d_G(v)^3.$$

These forms will be used repeatedly because graph operations are most naturally analysed either through shifted vertex degrees or through endpoint-degree partitions.

Definition 2.1. For $v \in V(G)$, define its First Max-Min degree by

$$a_v = \delta(G) + \Delta(G) + d_G(v).$$

The First Max-Min Zagreb index of G is

$$MM_1Z(G) = \sum_{uv \in E(G)} \left(a_u + a_v\right).$$

Thus an edge uv contributes

$$2\left(\delta(G) + \Delta(G)\right) + d_G(u) + d_G(v).$$

The next identity is the organizing principle for all subsequent results.

Theorem 2.2. *If G has size m, then*

$$MM_1Z(G) = 2m\left(\delta(G) + \Delta(G)\right) + M_1(G).$$

Proof. Expanding Definition 2.1 edge by edge gives

$$\begin{aligned} MM_1Z(G) &= \sum_{uv \in E(G)} \left[2(\delta(G) + \Delta(G)) + d_G(u) + d_G(v)\right] \\ &= 2\left(\delta(G) + \Delta(G)\right) \sum_{uv \in E(G)} 1 + \sum_{uv \in E(G)} \left(d_G(u) + d_G(v)\right) \\ &= 2m\left(\delta(G) + \Delta(G)\right) + M_1(G). \end{aligned}$$

This proves the assertion. □

Corollary 2.3. *Let G and H satisfy $m_G = m_H$, $\delta(G) = \delta(H)$, and $\Delta(G) = \Delta(H)$. Then*

$$MM_1Z(G) - MM_1Z(H) = M_1(G) - M_1(H).$$

Consequently, within any class having fixed size and fixed extremal degrees, MM_1Z ranks graphs exactly as M_1 does and cannot distinguish two graphs that M_1 does not distinguish.

This conditional equivalence is important for interpreting the descriptor. Globally, the additional term reacts to changes in m, δ, and Δ; locally within a parameter class, the index contains no information beyond M_1. In particular, if G is r-regular of order n, then $m = nr/2$, $M_1 = nr^2$, and

$$MM_1Z(G) = 3nr^2.$$

All r-regular graphs of a fixed order therefore share the same value. This is a precise discriminative limitation, not an algebraic defect, and it motivates the normalized comparison introduced below.

3. Benchmark graph families and normalization

Closed forms for familiar graph families provide both reference values and unit tests for more elaborate formulae. We use $S_N = K_{1,N-1}$ for the star on N vertices, $W_{1,q} = K_1 \vee C_q$ for the wheel with q rim vertices, and F_k for the friendship graph formed from k triangles sharing a common vertex.

Theorem 3.1. *The following exact values hold for the indicated graph families:*

$$\begin{aligned} MM_1Z(P_N) &= 10N - 12, && N \geq 3, \\ MM_1Z(C_N) &= 12N, && N \geq 3, \\ MM_1Z(G_r) &= 3Nr^2, && G_r \text{ is } r\text{-regular}, \\ MM_1Z(K_N) &= 3N(N-1)^2, && N \geq 2, \end{aligned}$$

and

$$\begin{aligned} MM_1Z(K_{p,q}) &= 3pq(p+q), && p, q \geq 1, \\ MM_1Z(S_N) &= 3N(N-1), && N \geq 2, \\ MM_1Z(W_{1,q}) &= q(5q+21), && q \geq 3, \\ MM_1Z(F_k) &= 4k(4k+5), && k \geq 1. \end{aligned}$$

Proof. Each formula follows from Theorem 2.2 and the degree sequence of the family. For example, P_N has two vertices of degree one and $N-2$ vertices of degree two, so $M_1(P_N) = 4N - 6$ and $MM_1Z(P_N) = 6(N-1) + 4N - 6 = 10N - 12$. For $K_{p,q}$, one part has degree q and the other has degree p, giving $M_1 = pq(p+q)$ and $\delta + \Delta = p + q$; hence $MM_1Z = 3pq(p+q)$ without a separate balanced case. Finally, F_k has one vertex of degree $2k$ and $2k$ vertices of degree two. Therefore $M_1 = 4k^2 + 8k$, $m = 3k$, and

$$MM_1Z(F_k) = 12k(k+1) + 4k^2 + 8k = 16k^2 + 20k = 4k(4k+5).$$

□

Figure 1 separates the lower-growth path, cycle, and star families from the wheel and complete families so that all curves remain readable. The linear path and cycle formulae contrast with the quadratic star and wheel formulae and the cubic leading term of K_N. This scaling is a direct consequence of the size-extremal term in Theorem 2.2.

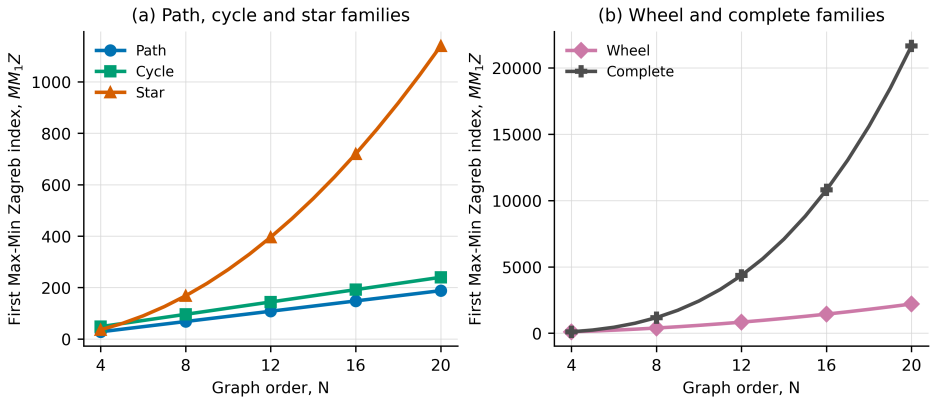


FIGURE 1. Exact growth of MM_1Z for five benchmark families of common order N. The wheel is $W_{1,N-1}$. Values are generated from Theorem 3.1; no fitted or simulated data are used.

To compare graphs of different orders and degree scales, define the normalized score

$$R_{MM}(G) = \frac{MM_1Z(G)}{6m\Delta(G)}.$$

The denominator is the value obtained if every edge contribution reached $6\Delta(G)$. It therefore provides a common dimensionless scale.

Proposition 3.2. *For every connected graph with at least one edge,*

$$\frac{2\delta + \Delta}{3\Delta} \leq R_{MM}(G) \leq \frac{\delta + 2\Delta}{3\Delta} \leq 1.$$

Moreover, $R_{MM}(G) = 1$ if and only if G is regular.

Proof. Every edge satisfies $2\delta \leq d(u)+d(v) \leq 2\Delta$. Adding $2(\delta+\Delta)$, summing over m edges, and dividing by $6m\Delta$ gives the displayed bounds. If $R_{MM} = 1$, every inequality used in the upper estimate is an equality, so $\delta = \Delta$ and G is regular. The converse follows from Corollary 2.3.

□

The score is regularity-oriented rather than a complete irregularity measure. It equals one for every regular graph and decreases as the edge contributions fall below the maximum-degree scale. Figure 2 also shows that normalization removes the strong size effect visible in Figure 1. It does not remove degeneracy: regular graphs with the same N and r still coincide, as required by the structural identity.

4. Exact formulae for graph operations

Graph operations are a stringent test of any descriptor that depends on extremal degrees. Let G and H have orders n_G, n_H, sizes m_G, m_H, and first Zagreb indices $M_1(G), M_1(H)$.

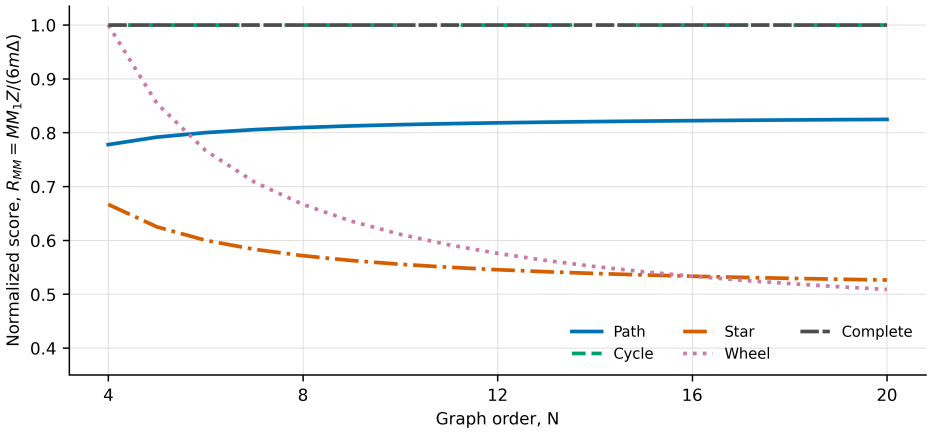


FIGURE 2. Normalized score R_{MM} for benchmark families of order N. The cycle and complete graph overlap at $R_{MM} = 1$ because both are regular; the wheel is $W_{1,N-1}$.

4.1. Complement.

Theorem 4.1. *If the complement $\overline{G}$ is connected, then*

$$\begin{aligned} MM_1Z\left(\overline{G}\right) = &[n(n-1)-2m]\,[2(n-1)-(\delta(G)+\Delta(G))] \\ &+ (n-1)\left(n^2-4m-n\right) + M_1(G). \end{aligned}$$

Proof. In $\overline{G}$,

$$\overline{m} = \frac{n(n-1)-2m}{2}, \quad \delta\left(\overline{G}\right) = n-1-\Delta(G), \quad \Delta\left(\overline{G}\right) = n-1-\delta(G).$$

Furthermore,

$$\begin{aligned} M_1\left(\overline{G}\right) &= \sum_{v\in V(G)} \left(n-1-d_G(v)\right)^2 \\ &= n(n-1)^2 - 4m(n-1) + M_1(G) \\ &= (n-1)\left(n^2-4m-n\right) + M_1(G). \end{aligned}$$

Substitution into Theorem 2.2 proves the formula.

□

4.2. Subdivision. Let $S_k(G)$ be the k-subdivision obtained by replacing each edge of G with a path of length $k+1$, where $k \geq 1$. The inserted vertices have degree two. Consequently, the extremal degrees are not generally inherited from G.

Theorem 4.2. *For $k \geq 1$,*

$$\begin{aligned} MM_1Z\left(S_k(G)\right) =& 2(k+1)m\left(\min\{\delta(G),2\}+\max\{\Delta(G),2\}\right) \\ &+ M_1(G)+4km. \end{aligned}$$

Proof. The subdivision has $(k+1)m$ edges. Original vertices retain their degrees, while the km inserted vertices have degree two. Hence

$$\delta\left(S_k(G)\right)=\min\{\delta(G),2\}, \qquad \Delta\left(S_k(G)\right)=\max\{\Delta(G),2\},$$

and

$$M_1\left(S_k(G)\right)=M_1(G)+4km.$$

The result follows from Theorem 2.2.

□

The minimum operation is essential when $\delta(G)>2$, while the maximum operation is essential for $G\cong K_2$. Thus a formula that simply preserves both extremal degrees is valid only when $\delta(G)\le 2\le\Delta(G)$.

4.3. Line graph. For an edge $uv\in E(G)$, the corresponding vertex of the line graph $L(G)$ has degree $d_G(u)+d_G(v)-2$. Define

$$\delta_L=\min_{uv\in E(G)}\{d_G(u)+d_G(v)-2\}, \qquad \Delta_L=\max_{uv\in E(G)}\{d_G(u)+d_G(v)-2\}.$$

Theorem 4.3. *The line graph satisfies*

$$\begin{aligned} MM_1Z\left(L(G)\right) =& \left(M_1(G)-2m\right)\left(\delta_L+\Delta_L\right) \\ &+ F(G)+2M_2(G)-4M_1(G)+4m. \end{aligned}$$

Proof. The size of the line graph is

$$\left|E\left(L(G)\right)\right|=\sum_{v\in V(G)}\binom{d_G(v)}{2}=\frac{M_1(G)-2m}{2}.$$

Its first Zagreb index is

$$\begin{aligned} M_1\left(L(G)\right) &= \sum_{uv\in E(G)}\left(d_G(u)+d_G(v)-2\right)^2 \\ &= F(G)+2M_2(G)-4M_1(G)+4m. \end{aligned}$$

Applying Theorem 2.2 to $L(G)$ gives the claim.

□

Corollary 4.4. *If G is r-regular of order n with $r\ge 2$, then*

$$MM_1Z\left(L(G)\right)=6nr(r-1)^2, \qquad \frac{MM_1Z\left(L(G)\right)}{MM_1Z(G)}=\frac{2(r-1)^2}{r}.$$

Thus $MM_1Z\left(L(G)\right)$ equals $MM_1Z(G)$ for $r=2$, whereas $MM_1Z\left(L(G)\right)>MM_1Z(G)$ for $r\ge 3$. A universal strict inequality for all line graphs is therefore false; cycles already provide equality.

4.4. Join. The join $G \vee H$ is obtained from disjoint copies of G and H by adding every edge between the two vertex sets. Put

$$\begin{aligned} m_\vee &= m_G + m_H + n_G n_H, \\ \delta_\vee &= \min\{\delta(G) + n_H, \delta(H) + n_G\}, \\ \Delta_\vee &= \max\{\Delta(G) + n_H, \Delta(H) + n_G\}. \end{aligned}$$

Theorem 4.5. *The First Max-Min Zagreb index of the join is*

$$\begin{aligned} MM_1Z(G \vee H) =& 2m_\vee (\delta_\vee + \Delta_\vee) + M_1(G) + M_1(H) \\ &+ 4m_G n_H + 4m_H n_G + n_G n_H^2 + n_H n_G^2. \end{aligned}$$

Proof. Vertices inherited from G have degree $d_G(u) + n_H$, and vertices inherited from H have degree $d_H(v) + n_G$. Therefore the displayed minimum and maximum are exact, without any comparison between the unshifted degrees of G and H. Squaring and summing the shifted degrees yields

$$\begin{aligned} M_1(G \vee H) =& M_1(G) + M_1(H) + 4m_G n_H + 4m_H n_G \\ &+ n_G n_H^2 + n_H n_G^2. \end{aligned}$$

The theorem follows from the structural identity.

□

4.5. Cartesian and strong products. The Cartesian product is denoted by $G \,\square\, H$, and the strong product by $G \boxtimes H$. In the Cartesian product, the degree of (u, v) is $d_G(u) + d_H(v)$. In the strong product it is

$$d_{G \boxtimes H}(u, v) = (d_G(u) + 1)\,(d_H(v) + 1) - 1.$$

Theorem 4.6. *The Cartesian product satisfies*

$$\begin{aligned} MM_1Z(G \,\square\, H) =& 2\,(m_G n_H + m_H n_G)\,[\delta(G) + \delta(H) + \Delta(G) + \Delta(H)] \\ &+ n_H M_1(G) + n_G M_1(H) + 8 m_G m_H. \end{aligned}$$

Proof. The product has $m_G n_H + m_H n_G$ edges, minimum degree $\delta(G) + \delta(H)$, and maximum degree $\Delta(G) + \Delta(H)$. Also,

$$M_1(G \,\square\, H) = n_H M_1(G) + n_G M_1(H) + 8 m_G m_H.$$

Substitution into Theorem 2.2 completes the proof.

□

For the strong product, define

$$\begin{aligned} m_\boxtimes &= m_G n_H + m_H n_G + 2 m_G m_H, \\ \delta_\boxtimes &= \delta(G) + \delta(H) + \delta(G)\delta(H), \\ \Delta_\boxtimes &= \Delta(G) + \Delta(H) + \Delta(G)\Delta(H). \end{aligned}$$

Theorem 4.7. *The strong product satisfies*

$$MM_1Z(G \boxtimes H) = 2m_{\boxtimes}\,(\delta_{\boxtimes} + \Delta_{\boxtimes}) + M_1(G \boxtimes H),$$

where

$$\begin{aligned} M_1(G \boxtimes H) =& n_H M_1(G) + n_G M_1(H) + M_1(G)M_1(H) \\ &+ 4m_H M_1(G) + 4m_G M_1(H) + 8m_G m_H. \end{aligned}$$

Proof. The strong-product degree formula is increasing in both factor degrees, so it gives the stated extremal degrees. Expanding

$$[d_G(u)d_H(v) + d_G(u) + d_H(v)]^2$$

and summing over $V(G) \times V(H)$ gives the expression for $M_1(G \boxtimes H)$. The structural identity then proves the result.

□

4.6. Addition of a single edge.

Theorem 4.8. *Let x and y be nonadjacent vertices of G, and let $G' = G + xy$. Write*

$$\eta = [\delta(G') + \Delta(G')] - [\delta(G) + \Delta(G)]\,.$$

Then $\eta \geq 0$ and

$$\begin{aligned} MM_1Z(G') - MM_1Z(G) =& 2\,[\delta(G) + \Delta(G)] + 2(m+1)\eta \\ &+ 2\,[d_G(x) + d_G(y) + 1] > 0. \end{aligned}$$

Proof. Adding xy increases the two endpoint degrees by one, and hence

$$M_1(G') - M_1(G) = 2\,[d_G(x) + d_G(y) + 1]\,.$$

Neither extremal degree can decrease, so $\eta \geq 0$. Subtracting the two forms supplied by Theorem 2.2 yields the formula, whose terms are strictly positive in total.

□

Thus MM_1Z is strictly monotone under edge addition on a fixed vertex set. The increment is piecewise governed by local endpoint degrees and jumps when the minimum or maximum degree changes.

5. Sharp bounds and equality cases

The structural identity transfers established degree inequalities to MM_1Z, but the equality conditions should be retained because they identify the extremal graph classes.

Theorem 5.1. *For a connected graph of order n and size m,*

$$2m(\delta + \Delta) + \frac{4m^2}{n} \leq MM_1Z(G) \leq 4m(\delta + \Delta) - n\delta\Delta.$$

The lower equality holds if and only if G is regular. The upper equality holds if and only if every vertex degree belongs to $\{\delta, \Delta\}$.

Proof. Cauchy's inequality and the handshaking lemma give

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \geq \frac{1}{n} \left(\sum_{v \in V(G)} d(v) \right)^2 = \frac{4m^2}{n},$$

with equality exactly for a regular graph. For each $d(v) \in [\delta, \Delta]$,

$$(d(v) - \delta)\,(d(v) - \Delta) \leq 0,$$

so

$$d(v)^2 \leq (\delta + \Delta) d(v) - \delta\Delta.$$

Summing gives $M_1(G) \leq 2m(\delta + \Delta) - n\delta\Delta$, with equality exactly when every degree is an endpoint of the interval. Adding $2m(\delta + \Delta)$ proves both estimates. □

Theorem 5.2. *Every connected graph with at least one edge satisfies*

$$2m(2\delta + \Delta) \leq MM_1Z(G) \leq 2m(\delta + 2\Delta).$$

Both equalities are attained precisely by regular graphs.

Proof. The edge form of M_1 gives $2m\delta \leq M_1(G) \leq 2m\Delta$. Add $2m(\delta + \Delta)$ and apply Theorem 2.2. In a connected graph, equality forces every incident vertex to have the same degree, hence regularity. □

A parameter-free consequence is

$$6m \leq MM_1Z(G) \leq 6m(n - 1).$$

The lower equality requires $\delta = \Delta = 1$ and therefore $G \cong K_2$. The upper equality requires every vertex to have degree $n-1$ and therefore $G \cong K_n$. A further comparison with the second Zagreb index follows from $d(u) + d(v) \leq 2d(u)d(v)$ on every edge of a connected graph:

$$MM_1Z(G) \leq 2\,[m(\delta + \Delta) + M_2(G)]\,,$$

with equality only for K_2. Together, these bounds locate the descriptor using either global graph parameters or established Zagreb quantities, and the equality cases provide quick consistency checks for symbolic or numerical calculations.

6. Computational validation and nanostructure applications

6.1. Exact finite-graph validation. The formulae above were checked independently using a deterministic integer-arithmetic enumeration. For each $n \in \{2, 3, 4, 5, 6\}$, every subset of the $\binom{n}{2}$ possible edges was generated, connectivity was tested by graph traversal, and the degree vector was calculated. The direct edge sum in Definition 2.1 was then compared with Theorem 2.2 and the bounds in Section 5. No floating-point tolerance was required.

In total, 27,475 connected labelled graphs were examined. The complement identity was checked in the 21,084 cases for which the complement remained connected. The subdivision formula was tested for $k = 1$ and $k = 2$, giving 54,950 checks. The line-graph first Zagreb expansion and Theorem 4.3 were checked 27,475 times. The join, Cartesian-product, and strong-product formulae were each checked on 1,849 ordered pairs drawn from all connected labelled graphs of orders two through four. Finally, every missing edge of every enumerated connected graph was inserted, resulting in 189,587 exact checks of Theorem 4.8. All comparisons returned equality where required and strict increase under edge addition.

To illustrate rather than merely count the edge-addition checks, start with P_{12} and insert its missing edges in lexicographic endpoint order until K_{12} is obtained. Selected exact states are

m	δ	Δ	M_1	MM_1Z	R_{MM}
11	1	2	42	108	0.818
20	1	10	186	626	0.522
30	3	11	388	1228	0.620
45	5	11	750	2190	0.737
55	6	11	1046	2916	0.803
66	11	11	1452	4356	1.000

The normalized score need not increase at every step because its denominator also changes with m and Δ. The selected states show that the early creation of a high-degree vertex lowers R_{MM} even though the unnormalized index increases strictly. The score later returns to one when the complete graph becomes regular.

6.2. Cycles and the carbon-skeleton interpretation. For C_N, every vertex has degree two, so $MM_1Z(C_N) = 12N$. Numerically, this equals the nominal carbon-12 mass contribution of a skeleton containing N carbon atoms. The interpretation must be stated carefully: a cycloalkane has formula C_NH_{2N}, so its full nominal molecular mass is approximately $14N$, not $12N$. The graph index records the carbon skeleton under the unweighted molecular-graph convention and does not include hydrogen atoms. The equality with $12N$ is therefore a transparent structural coincidence, not a fitted QSPR model. Empirical prediction would require a curated molecular dataset, comparison descriptors, and external validation of the type emphasized in [21].

6.3. Dendrimer nanostar. Consider the dendrimer nanostar $D_3[k]$ with the established endpoint-degree partition [1, 7]. Its vertices have degrees one, two, or three, so $\delta = 1$ and $\Delta = 3$. The edge classes are

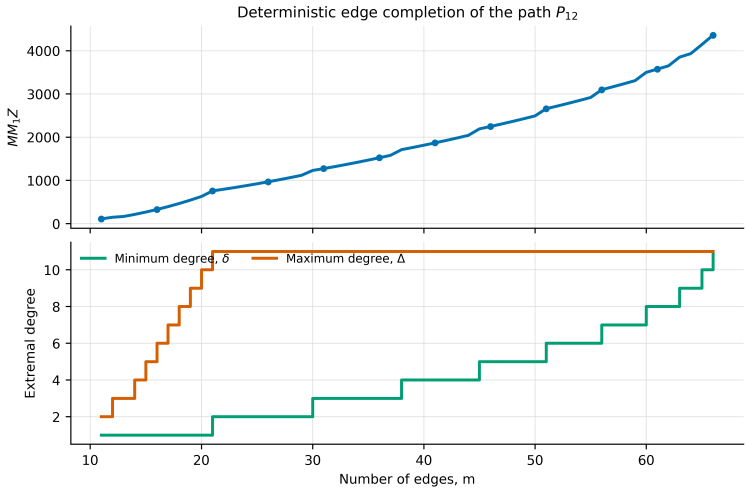


FIGURE 3. Exact change in MM_1Z, δ, and Δ during deterministic completion of P_{12}. The index increases at every insertion, while changes in the extremal degrees produce visible changes in the increment.

$$|E_{13}| = 3 \cdot 2^k, \qquad |E_{22}| = 12 \cdot 2^k - 6,$$
$$|E_{23}| = 24 \cdot 2^k - 12, \quad |E_{33}| = 9 \cdot 2^k - 6.$$

An edge in E_{13} or E_{22} contributes 12, an edge in E_{23} contributes 13, and an edge in E_{33} contributes 14.

Theorem 6.1. *For $k \geq 1$,*

$$MM_1Z\left(D_3[k]\right) = 618 \cdot 2^k - 312.$$

Proof. Direct summation over the four edge classes gives

$$\begin{aligned} MM_1Z\left(D_3[k]\right) =& 12\left(3 \cdot 2^k + 12 \cdot 2^k - 6\right) \\ &+ 13\left(24 \cdot 2^k - 12\right) + 14\left(9 \cdot 2^k - 6\right) \\ =& 618 \cdot 2^k - 312. \end{aligned}$$

The class sizes sum to $48 \cdot 2^k - 24$ edges, providing an independent partition check.

□

6.4. Carbon nanocone. Let $CNC_K(n)$ be the carbon nanocone model with Kn^2 vertices and $Kn(3n-1)/2$ edges [14, 17, 23]. Its vertices have degrees two or three, and its edge partition is

$$|E_{22}| = K, \qquad |E_{23}| = 2K(n-1), \qquad |E_{33}| = \frac{K}{2}(n-1)(3n-2).$$

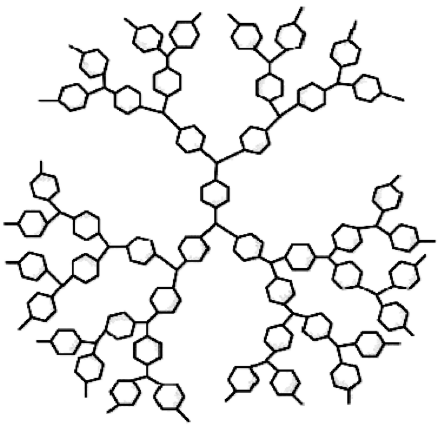


FIGURE 4. Structural motif of the dendrimer nanostar $D_3[k]$.

Because $\delta = 2$ and $\Delta = 3$, the three edge classes contribute 14, 15, and 16, respectively.

Theorem 6.2. *For the carbon nanocone $CNC_K(n)$,*

$$MM_1Z\left(CNC_K(n)\right) = Kn(24n - 10).$$

Proof. The edge partition gives

$$\begin{aligned} MM_1Z\left(CNC_K(n)\right) &= 14K + 30K(n-1) + 8K(n-1)(3n-2) \\ &= 24Kn^2 - 10Kn = Kn(24n-10). \end{aligned}$$

The factor K is present in both terms; this resolves the inconsistent factorization in the earlier expression.

□

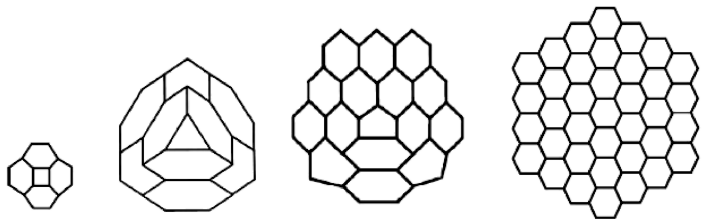
6.5. Carbon nanotori. The carbon nanotori $C_4C_6C_8(p,q)$ has $6pq + 4q + p$ vertices and $9pq + 2q$ edges [14]. Its endpoint-degree partition is

$$\begin{aligned} |E_{13}| &= 4q + p, \\ |E_{23}| &= 2p, \\ |E_{33}| &= 3p(3q-1) - 2q. \end{aligned}$$

Here $\delta = 1$ and $\Delta = 3$, so these classes contribute 12, 13, and 14.

Theorem 6.3. *For positive integers p and q,*

$$MM_1Z\left(C_4C_6C_8(p,q)\right) = 126pq - 4p + 20q.$$



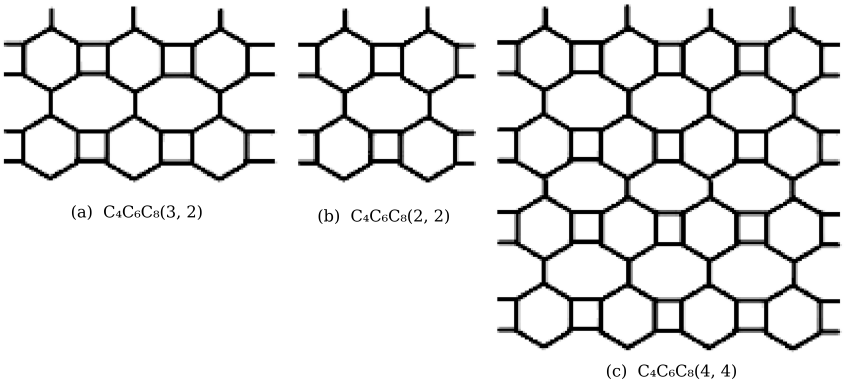
(a) $CNC_4(2)$ (b) $CNC_3(3)$ (c) $CNC_5(3)$ (d) $CNC_6(4)$

FIGURE 5. Structural representation of a carbon nanocone. The panels are labeled (a) $CNC_4(2)$, (b) $CNC_3(3)$, (c) $CNC_5(3)$, and (d) $CNC_6(4)$.

Proof. Using the three edge classes,

$$\begin{aligned} MM_1Z\left(C_4C_6C_8(p,q)\right) &= 12(4q+p) + 13(2p) + 14\left[3p(3q-1) - 2q\right] \\ &= 126pq - 4p + 20q. \end{aligned}$$

The edge counts sum to $9pq + 2q$, confirming that the partition is complete. □



(a) $C_4C_6C_8(3, 2)$ (b) $C_4C_6C_8(2, 2)$ (c) $C_4C_6C_8(4, 4)$

FIGURE 6. Structural representation of the carbon nanotori $C_4C_6C_8(p, q)$. The panels are labeled (a) $C_4C_6C_8(3, 2)$, (b) $C_4C_6C_8(2, 2)$, and (c) $C_4C_6C_8(4, 4)$.

7. Discussion and limitations

The exact decomposition of MM_1Z is both the main strength and the principal limitation of the descriptor. It makes computation, bounds, and graph-operation

formulae transparent, but it also proves that the index is not independent of M_1 once m, δ, and Δ are fixed. Regular graphs of the same order and degree cannot be distinguished. Similar degeneracy is common among degree-based descriptors and should be reported rather than obscured [21]. A future chemical study should therefore compare MM_1Z with M_1, Sombor-type indices, and at least one distance- or spectrum-based descriptor on constitutional isomers.

From a descriptor-design perspective, the global extremal term makes MM_1Z sensitive to degree-regime changes that may affect many edge contributions simultaneously. Theorem 4.8 isolates this effect through η: an inserted edge always changes the two endpoint degrees, but it can additionally raise δ, Δ, or both. This explains the slope changes in Figure 3 and distinguishes the index from a purely edge-local bond-additive expression. At the same time, sensitivity to extrema can make the descriptor respond strongly to a single exceptional hub or pendent vertex. Reporting MM_1Z together with $(n, m, \delta, \Delta, M_1)$ therefore makes comparisons auditable and prevents a large value from being attributed vaguely to "complexity." The normalized score helps separate scale from regularity, while the unnormalized index retains the absolute size and degree information needed for exact graph transformations.

The nanostructure results are exact for the stated unweighted graph models and endpoint-degree partitions. They do not by themselves establish prediction of thermal, electronic, or pharmacological properties. Such a claim would require experimental response variables, a prespecified modelling protocol, train-test separation, uncertainty estimates, and external validation. The present work instead supplies the graph-theoretic foundation needed before that empirical stage: corrected formulae, equality conditions, an edge-monotonicity theorem, and reproducible finite-graph checks.

The exhaustive verification is necessarily limited to small orders: the number of labelled simple graphs grows exponentially with the n(n - 1)/2 possible edges, and testing all candidate insertions adds a further quadratic factor. Direct enumeration therefore becomes prohibitive beyond order six; larger molecular graphs should be studied using canonical generation, symmetry reduction, parallel computation, or statistically controlled sampling.

The normalized score R_{MM} is useful for comparing degree scales, but it is not proposed as a universal irregularity index. Its value depends on size and degree distribution through MM_1Z, and different irregular graphs may coincide. More discriminating extensions could incorporate edge-degree variance, distance information, or spectral information while retaining the current index as an interpretable baseline.

8. Conclusion

The First Max-Min Zagreb index has been placed on a rigorous structural footing. Its exact relation to the first Zagreb index was used to derive closed forms for standard families, correct the effects of subdivision and graph join, characterize the line-graph behaviour of regular graphs, and obtain formulae for Cartesian and strong products. A single-edge increment formula proves strict monotonicity,

while sharp degree bounds identify regular and two-degree equality cases. The normalized score separates absolute growth from degree-scale effects.

The principal identities were verified by exact enumeration of all 27,475 connected labelled graphs through order six and by 189,587 edge-insertion tests. Corrected applications were obtained for a dendrimer nanostar, carbon nanocones, and carbon nanotori. The cycle value $12N$ was interpreted as a carbon-skeleton mass contribution, not the complete cycloalkane molecular mass. These results make the descriptor reproducible and mathematically transparent, while clearly defining the empirical validation still required before property-prediction claims can be made.

Viewed along successive edge-completion paths, the increment formula also defines a discrete response process that can be investigated asymptotically on graph sequences, linking the descriptor with broader questions of stability, limiting degree structure, and global graph behaviour.

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