



# Reducing Degeneracy of Degree-Based Topological Indices via Reciprocal Composite Descriptors: Extremal Theory and Exhaustive Enumeration

**Hossein Faeq Hossein Akkal**

Razi University, Islamic Republic of Iran

\*Corresponding author email: [fayqh398@gmail.com](mailto:fayqh398@gmail.com)

تقليل التكرارية في المؤشرات الطوبولوجية القائمة على الدرجات باستخدام  
الواصفات المركبة التبادلية: النظرية القصوى والإحصاء الشامل

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## ABSTRACT

### Background:

Degree-based topological indices are important numerical descriptors of chemical graphs and are widely used in quantitative structure–property relationship *QSPR* and quantitative structure–activity relationship *QSAR* studies. However, many classical indices suffer from degeneracy, since non-isomorphic graphs may share the same descriptor value, thereby reducing their discriminative power.

### Materials and Methods:

This study investigates reciprocal composite descriptors of the form

$$\Xi(G) = TI(G) + RTI(G),$$

with particular emphasis on the reciprocal composite second Zagreb descriptor

$$\Xi_2(G) = Z_2(G) + RZ_2(G),$$

where

$$RZ_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u)d_G(v)}.$$

The work combines extremal graph theory, edge-transfer transformations, and exhaustive computational enumeration of connected non-isomorphic graphs up to order  $n = 9$ . Sharp lower and upper bounds are established for connected, unicyclic, and  $k$ -cyclic graph classes.

### Results:

The extremal analysis shows that minimum values are attained by paths and cycles, whereas maximum values are attained by graphs with high degree concentration. Exhaustive computational enumeration further shows that the reciprocal composite descriptor produces significantly more distinct values than the classical second Zagreb index. For graphs of order  $n = 9$ , the number of distinct values increases from 1,340 for  $Z_2$  to 46,418 for  $\Xi_2$ , and the degeneracy ratio is reduced by approximately 97.1%.

### Conclusion:

The proposed reciprocal composite descriptors reduce degeneracy while preserving analytical tractability and clear extremal structure. These results indicate that reciprocal structural correction enhances the discriminative power of degree-based topological indices and provides a promising direction for developing more sensitive graph descriptors in chemical graph theory.

**Keywords:** Chemical graph theory; topological indices; degeneracy reduction; reciprocal composite indices; Zagreb index; exhaustive enumeration.



## INTRODUCTION

One of the most powerful quantitative methods in chemical graph theory is the use of topological indices. In this framework, a molecule is represented as a simple connected graph

$$G = (V(G), E(G)),$$

where atoms correspond to vertices and chemical bonds correspond to edges. A topological index is a graph invariant, that is, a numerical value that remains unchanged under graph isomorphism. These numerical descriptors play an important role in quantitative structure–property relationship *QSPR* and quantitative structure–activity relationship *QSAR* studies, where statistically significant correlations between graph-based invariants and physicochemical or biological properties have frequently been reported [1-3].

One of the oldest and most widely studied degree-based descriptors is the class of Zagreb indices, which were proposed by Gutman and Trinajstić in 1972 in relation to the total  $\pi$ -electron energy of conjugated hydrocarbons [2]. They are defined by

$$Z_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} (d_G(u) + d_G(v)),$$

and

$$Z_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

These indices opened a wide research field devoted to degree-based graph invariants. Several related descriptors have subsequently been introduced, including the harmonic index [3-5], the forgotten index  $F$  [4], and the Sombor index [6-8]. Most of them can be represented within the unified edge-summation model

$$TI(G) = \sum_{uv \in E(G)} \Phi(d_G(u), d_G(v)),$$

where

$$\Phi: \mathbb{N} \times \mathbb{N} \rightarrow \mathbb{R}^+$$

is a symmetric function. The reciprocal variant of such a descriptor is defined by

$$RTI(G) = \sum_{uv \in E(G)} \frac{1}{\Phi(d_G(u), d_G(v))}.$$

Reciprocal variants have attracted attention because they may enhance sensitivity to local degree variations [6,7].

Although classical degree-based indices are mathematically elegant and chemically useful, they suffer from a fundamental structural drawback known as degeneracy. Degeneracy occurs when two non-isomorphic graphs have the same descriptor value. That is,



$$G_1 \cong G_2 \text{ while } TI(G_1) = TI(G_2).$$

Thus, degeneracy reduces the discriminative ability of the descriptor. This problem is especially clear for indices whose values depend only on degree sequences, since graphs with the same degree distribution may yield the same index value. Extensive degeneracy may weaken predictive reliability in QSPR/QSAR modeling because structurally different molecules can become indistinguishable with respect to a given descriptor [7-10].

Most previous studies have focused on extremal values, sharp bounds, and structural characterizations of degree-based indices within restricted graph classes, such as trees, unicyclic graphs, and molecular graphs [11], [12]. However, systematic theoretical approaches aimed at reducing degeneracy while retaining analytical tractability remain limited.

Motivated by recent extremal studies of composite indices and by the structural limitations caused by degeneracy, this paper proposes a reciprocal composite modification of degree-based topological indices. In general, we investigate descriptors of the form

$$\Xi(G) = TI(G) + RTI(G).$$

In particular, for the second Zagreb index, we define

$$RZ_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u)d_G(v)}.$$

Therefore, the reciprocal composite second Zagreb descriptor is defined as

$$\Xi_2(G) = Z_2(G) + RZ_2(G).$$

Equivalently,

$$\Xi_2(G) = \sum_{uv \in E(G)} \left( d_G(u)d_G(v) + \frac{1}{d_G(u)d_G(v)} \right).$$

Analogous reciprocal composite constructions are also considered for the Sombor index, the forgotten index, and the first Zagreb index.

The present paper has two complementary goals. First, we develop a unified extremal framework for reciprocal composite indices over connected,  $k$ -cyclic, unicyclic, and molecular graph classes. Sharp lower and upper bounds are established, together with complete extremal characterizations. In particular, minimum values are attained by paths and cycles, whereas maximum values are attained by graphs with maximum degree concentration  $\Delta(G) = n - 1$ .

Second, we quantitatively examine the effect of degeneracy reduction through reciprocal modification. By exhaustive computational enumeration of connected non-isomorphic graphs up to order  $n = 9$ , we show that the composite index  $\Xi_2$  generates significantly larger sets of distinct values than the classical second Zagreb index  $Z_2$ . For graphs of order  $n = 9$ , the degeneracy ratio decreases by approximately 97.1%, suggesting improved structural discriminative performance.



By combining extremal graph theory, edge-transfer transformations, and computational enumeration, this paper provides both theoretical and empirical support for the claim that reciprocal composite constructions can better capture the structural sensitivity of degree-based topological indices while preserving mathematical transparency. The findings contribute to the development of less degenerate graph descriptors and suggest a promising direction for designing more sensitive descriptors in chemical graph theory.

## 2. PRELIMINARIES AND AUXILIARY RESULTS

In this section, we define notation, review key definitions, and report useful structural and analytical facts needed for the analysis of extremes in Sections 3 and 4.

### 2.1 Basic Notation and Definitions

All graphs considered in this paper are finite, simple, and connected. For a graph

$$G = (V(G), E(G)),$$

we denote:

$|V(G)| = n$ — the order of  $G$ ,

$|E(G)| = m$ — the size of  $G$ ,  $d_G(v)$ , or simply  $d(v)$ , — the degree of a vertex  $v$ ,

$N_G(v) = \{u \in V(G) : uv \in E(G)\}$ — the neighborhood of  $v$ ,

$\Delta(G)$ — the maximum degree of  $G$ .

A graph of order  $n$  means that

$$|V(G)| = n.$$

A connected graph of order  $n$  and size

$$m = n + k - 1$$

is called a  $k$ -cyclic graph. In particular,

$$k = 0$$

corresponds to trees, while

$$k = 1$$

corresponds to unicyclic graphs.

We denote the path, cycle, and star graphs on  $n$  vertices by  $P_n$ ,  $C_n$ , and  $S_n$ , respectively. We also denote by  $S_n^+$  the unicyclic graph obtained from the star  $S_n$  by adding one edge between two pendant vertices.

Throughout the paper, we study edge-degree functionals of the general form

$$H(G) = \sum_{uv \in E(G)} h(d_G(u), d_G(v)), \quad \dots (1)$$



where

$$h: [1, \infty)^2 \rightarrow \mathbb{R}$$

is a symmetric function, that is,

$$h(x, y) = h(y, x).$$

Classical degree-based topological indices fit within this framework. In particular, the second Zagreb index is defined by

$$Z_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v),$$

the Sombor index is defined by

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2},$$

and the forgotten index is defined by

$$F(G) = \sum_{uv \in E(G)} (d_G(u)^2 + d_G(v)^2).$$

For a general degree-based topological index of the form

$$TI(G) = \sum_{uv \in E(G)} \Phi(d_G(u), d_G(v)),$$

where  $\Phi$  is a symmetric positive function, we define its reciprocal counterpart by

$$RTI(G) = \sum_{uv \in E(G)} \frac{1}{\Phi(d_G(u), d_G(v))}.$$

In particular, for the second Zagreb index, the reciprocal second Zagreb index is defined by

$$RZ_2(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u)d_G(v)}.$$

Therefore, the reciprocal composite second Zagreb descriptor is defined as

$$\mathbb{E}_2(G) = Z_2(G) + RZ_2(G).$$

Equivalently,

$$\mathbb{E}_2(G) = \sum_{uv \in E(G)} \left( d_G(u)d_G(v) + \frac{1}{d_G(u)d_G(v)} \right).$$

Similarly, we define the reciprocal Sombor index by

$$RSO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}},$$





$$G \cong P_n \text{ or } G \cong C_n.$$

The proof follows the classical transfer-inequality technique used in extremal degree-based analysis [7]. Full algebraic verification of the positivity condition for the generators considered in this paper is provided in Appendix A.

### 2.3 Maximum-Degree Concentration Principle

We next recall a structural concentration principle used to characterize extremal maximizers.

Maximum-degree concentration. Let

$$\hbar: [1, \infty)^2 \rightarrow \mathbb{R}$$

be symmetric and strictly increasing in each variable. Assume that, for all real numbers satisfying

$$2 \leq x_4 + 1 \leq x_3 \leq x_1, 1 \leq x_2 \leq x_1,$$

the following inequalities hold:

$$\hbar(x_1 + x_4, x_2) - \hbar(x_1, x_2) + \hbar(x_3 - x_4, x_2) - \hbar(x_3, x_2) \geq 0, \quad \dots (4)$$

and

$$\hbar(x_1 + x_4, x_3 - x_4) - \hbar(x_1, x_3) \geq 0. \quad \dots (5)$$

If  $G$  maximizes

$$\sum_{uv \in E(G)} \hbar(d_G(u), d_G(v))$$

over the class of connected  $n$ -order  $k$ -cyclic graphs, then

$$\Delta(G) = n - 1.$$

The proof relies on iterative edge-transfer operations. Under the monotonicity hypotheses, reassigning edges from lower-degree vertices to a vertex of maximum degree strictly increases the functional, unless the graph already satisfies

$$\Delta(G) = n - 1.$$

A complete derivation of the transfer inequality and the associated algebraic simplifications is given in Appendix A.

### 2.4 Analytic Properties of Reciprocal Generators

We now verify that the generators used later satisfy the hypotheses of the previous lemmas.

Let

$$f(x_1, x_2) = \sqrt{x_1^2 + x_2^2} + \frac{1}{\sqrt{x_1^2 + x_2^2}}, x_1, x_2 \geq 1.$$

Then  $f$  is strictly increasing in each variable.

**Proof.** A direct differentiation yields







$$\Delta(G^*) \leq n - 2,$$

then the previous lemma yields a strictly larger value, which contradicts the maximality of  $G^*$ . Hence,

$$\Delta(G^*) = n - 1.$$

The unique unicyclic graph with maximum degree  $n - 1$  is  $S_n^+$ . A direct computation gives

$$\Xi_2(S_n^+) = n^2 + \frac{13}{4} + \frac{n-2}{n-1} = \frac{4n^3 - 4n^2 + 17n - 21}{4(n-1)}.$$

### 3.2 Sharp Lower Bounds

We now derive best possible lower bounds for reciprocal composite indices. The proofs rely on the lower-bound framework of Section 2, together with the positivity verification given in Appendix A.

Sharp lower bound for  $\Xi_2$ . Let  $G$  be a connected graph of order  $n$  with  $m \geq 2$  edges. Then

$$\Xi_2(G) \geq \frac{31}{4}m - \frac{7}{2}n.$$

Equality holds if and only if

$$G \cong P_n \text{ or } G \cong C_n.$$

Proof. Apply the degree-sum framework with

$$\hbar(x_1, x_2) = x_1x_2 + \frac{1}{x_1x_2}.$$

Appendix A verifies that

$$\Phi(r_1, r_2) > 0$$

for all admissible pairs. Hence, the result follows directly.

Analogous arguments yield the following results.

Lower bound for  $SO + RSO$ . Let  $G$  be a connected graph of order  $n$  with  $m \geq 2$ . Then

$$SO(G) + RSO(G) \geq \frac{3}{20} [(45\sqrt{2} - 16\sqrt{5})m + (16\sqrt{5} - 30\sqrt{2})n].$$

Equality holds if and only if

$$G \cong P_n \text{ or } G \cong C_n.$$

Lower bound for  $F + RF$ . Let  $G$  be connected with  $m \geq 2$ . Then

$$F(G) + RF(G) \geq \frac{13}{40} (43m - 18n).$$

Equality holds if and only if



Let's start with equation  $G, G \cong P_n$  or  $G \cong C_n$ .

Lower bound for  $Z_1 + RZ_1$ . Let  $G$  be connected with  $m \geq 2$ . Then

$$Z_1(G) + RZ_1(G) \geq \frac{1}{12}(73m - 22n).$$

Equality holds if and only if

$$G \cong P_n \text{ or } G \cong C_n.$$

### 3.3 Extremal Characterization for General $k$ -Cyclic Graphs

The transfer principle extends beyond unicyclic graphs.

Maximum-degree concentration. If  $G$  maximizes any of the indices

$$SO + RSO, Z_1 + RZ_1, F + RF$$

over the class of  $n$ -order  $k$ -cyclic graphs, then

$$\Delta(G) = n - 1.$$

Proof. Each index is generated by a symmetric function satisfying the monotonicity and transfer inequalities of Section 2. Hence, the edge-transfer argument applies.

Among all  $n$ -order unicyclic graphs,  $S_n^+$  uniquely attains the maximum value for each reciprocal composite index considered above.

The results of this section establish a complete extremal dichotomy:

Minimum values occur precisely at graphs with maximal degree dispersion, namely  $P_n$  and  $C_n$ .

Maximum values occur at graphs with maximal degree concentration, namely  $\Delta(G) = n - 1$ .

This structural separation plays a central role in understanding the reduction in degeneracy observed in Section 4.

## 4. COMPUTATIONAL EXPERIMENTS AND DEGENERACY ANALYSIS

The theoretical results in Section 3 establish a clear extremal distinction between degree dispersion and degree concentration. However, extremal results alone are not sufficient to measure the discriminative power of a topological index. Therefore, exhaustive computational enumeration experiments were conducted to compare the classical second Zagreb index  $Z_2$  with the reciprocal composite descriptor  $\Xi_2$ .

### 4.1 Degeneracy Measure

Let  $\mathcal{G}_n$  denote the set of connected non-isomorphic graphs of order  $n$ . For a graph invariant  $TI$ , the degeneracy ratio is defined by

$$D_{TI}(n) = \frac{|\mathcal{G}_n|}{|\{TI(G): G \in \mathcal{G}_n\}|}$$



where  $|\cdot|$  denotes cardinality. The quantity  $D_{TI}(n)$  measures the average degeneracy level of the index. Larger values indicate lower discriminative power.

We also define the relative reduction factor by

$$R(n) = \frac{D_{Z_2}(n) - D_{\Xi_2}(n)}{D_{Z_2}(n)}.$$

## 4.2 Enumeration Methodology

All connected non-isomorphic graphs up to  $n=9$  were generated using the nauty/geng framework. For each graph, both the classical second Zagreb index

$$Z_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

and the reciprocal composite second Zagreb descriptor

$$\Xi_2(G) = Z_2(G) + RZ_2(G)$$

were computed, where

$$RZ_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}.$$

Equivalently,

$$\Xi_2(G) = \sum_{uv \in E(G)} \left( d(u)d(v) + \frac{1}{d(u)d(v)} \right).$$

The enumeration was exhaustive; no sampling was used.

## 4.3 Results

The results are summarized in Table 1.



Table 1: Degeneracy comparison for connected non-isomorphic graphs

$n$	Number of connected non-isomorphic graphs	Index	Distinct values	Degeneracy ratio $D_{TI}(n)$	Reduction vs. $Z_2$
5	21	$Z_2$	21	1.0000	–
5	21	$E_2$	21	1.0000	0.0%
6	112	$Z_2$	92	1.2174	–
6	112	$E_2$	100	1.1200	8.0%
7	853	$Z_2$	300	2.8433	–
7	853	$E_2$	594	1.4360	49.5%
8	11,117	$Z_2$	695	15.9957	–
8	11,117	$E_2$	4,606	2.4136	84.9%
9	261,080	$Z_2$	1,340	194.8358	–
9	261,080	$E_2$	46,418	5.6245	97.1%

#### 4.4 Quantitative Analysis

For  $n = 5$ , both  $Z_2$  and  $E_2$  produce 21 distinct values among 21 connected non-isomorphic graphs. Hence,

$$D_{Z_2}(5) = 1.0000, D_{E_2}(5) = 1.0000,$$

which gives

$$R(5) = 0.0\%.$$

For  $n = 6$ , we obtain

$$D_{Z_2}(6) = 1.2174, D_{E_2}(6) = 1.1200,$$

which gives

$$R(6) = 8.0\%.$$

For  $n = 7$ , we obtain

$$D_{Z_2}(7) = 2.8433, D_{E_2}(7) = 1.4360,$$

which gives

$$R(7) \approx 49.5\%.$$

For  $n = 8$ , we obtain

$$D_{Z_2}(8) = 15.9957, D_{E_2}(8) = 2.4136,$$

which gives



$$R(8) \approx 84.9\%.$$

For  $n = 9$ , we obtain

$$D_{Z_2}(9) = 194.8358, D_{\Xi_2}(9) = 5.6245,$$

which gives

$$R(9) \approx 97.1\%.$$

These results show that the reciprocal composite descriptor  $\Xi_2$  substantially reduces degeneracy compared with the classical second Zagreb index  $Z_2$ . The improvement becomes particularly strong for  $n = 8$  and  $n = 9$ . In particular, for  $n = 9$ , the number of distinct values increases from 1,340 for  $Z_2$  to 46,418 for  $\Xi_2$ , while the degeneracy ratio decreases from 194.8358 to 5.6245.

#### 4.5 Scalability Trend

The results indicate that the relative improvement increases with the graph's order. In particular,

$$R(9) > R(8) > R(7) > R(6) > R(5).$$

This confirms that the reciprocal composite modification becomes increasingly effective as graph order increases. The classical second Zagreb index  $Z_2$  depends only on products of vertex degrees, whereas  $\Xi_2$  includes an additional reciprocal correction term. This reciprocal term increases the numerical sensitivity of the descriptor and separates many graphs that share the same  $Z_2$  value.

For  $n = 9$ , the number of distinct values increases from 1,340 for  $Z_2$  to 46,418 for  $\Xi_2$ . Consequently, the degeneracy ratio decreases from 194.8358 to 5.6245, corresponding to an approximate 97.1% reduction. This provides strong computational evidence for the scalability of the proposed reciprocal composite descriptor.

#### 4.6 Interpretation

The computational results provide quantitative support for the theoretical conclusions of Section 3. In particular:

- The minimum extremal structures,  $P_n$  and  $C_n$ , are unique minimizers.
- Maximum-degree concentration structures are associated with extremal maximum values.
- Between these extremes, the values of  $\Xi_2$  are more widely distributed than those of  $Z_2$ .

Therefore, the reciprocal composite construction improves the descriptor's discriminative power while preserving analytical tractability.

Further work may extend the enumeration beyond  $n = 9$  and may also consider chemical datasets, such as QM9 or subsets of ZINC, to test the performance of the proposed descriptors under realistic QSPR conditions.



## 5. CONCLUSION

This paper addressed a fundamental limitation of classical degree-based topological indices, namely degeneracy. Degeneracy occurs when non-isomorphic graphs share the same descriptor value, thereby reducing the index's discriminative power. To reduce this limitation, reciprocal composite degree-based descriptors of the form

$$\Xi(G) = TI(G) + RTI(G)$$

were introduced and analyzed.

Theoretically, sharp lower and upper bounds were established for several reciprocal composite indices, including

$$\begin{aligned}\Xi_2(G) &= Z_2(G) + RZ_2(G), \\ SO(G) &+ RSO(G), \\ F(G) &+ RF(G),\end{aligned}$$

and

$$Z_1(G) + RZ_1(G),$$

over connected, unicyclic,  $k$ -cyclic, and molecular graph classes. The extremal characterisations show that paths and cycles attain the minimum values, whereas the maximum values are attained by graphs with maximum degree concentration. The edge-transfer method provides a unified structural explanation for this extremal dichotomy.

Computationally, exhaustive enumeration experiments were conducted for connected non-isomorphic graphs up to order  $n = 9$ . The results show that the reciprocal composite descriptor  $\Xi_2$  substantially reduces degeneracy compared with the classical second Zagreb index  $Z_2$ . In particular, for  $n = 9$ , the degeneracy ratio decreases from

$$D_{Z_2}(9) = 194.8358$$

to

$$D_{\Xi_2}(9) = 5.6245,$$

corresponding to an approximate reduction of 97.1%. Moreover, the number of distinct values increases from 1,340 for  $Z_2$  to 46,418 for  $\Xi_2$ , which provides strong computational evidence for the improved discriminative ability of the proposed descriptor.

Overall, the results indicate that reciprocal composite descriptors significantly enhance the structural sensitivity of degree-based topological indices while preserving analytical tractability and clear extremal structure. The proposed framework offers a promising direction for constructing less degenerate graph descriptors in chemical graph theory. Future work may extend the analysis beyond  $n = 9$ , consider weighted molecular graphs, and validate the proposed descriptors on large chemical datasets under realistic QSPR and QSAR conditions.



### Conflict of interests.

There are non-conflicts of interest.

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## Appendix A. Algebraic Verification of Auxiliary Conditions

This appendix provides the algebraic verification of the monotonicity and positivity conditions used in the extremal arguments of Sections 2 and 3.

### A.1 Verification for the Reciprocal Composite Second Zagreb Descriptor

For the reciprocal composite second Zagreb descriptor, the associated edge-degree generator is

$$\hbar_2(x, y) = xy + \frac{1}{xy}, x, y \geq 1.$$

Its partial derivatives are

$$\frac{\partial \hbar_2}{\partial x} = y - \frac{1}{x^2 y} = \frac{x^2 y^2 - 1}{x^2 y},$$

and

$$\frac{\partial \hbar_2}{\partial y} = x - \frac{1}{x y^2} = \frac{x^2 y^2 - 1}{x y^2}.$$

Since  $x, y \geq 1$ , both derivatives are non-negative, and they are positive whenever  $xy > 1$ . Hence,  $\hbar_2(x, y)$  is increasing in each variable on the admissible degree domain.

For the lower-bound framework, substituting

$$\hbar_2(x, y) = xy + \frac{1}{xy}$$

into the auxiliary function  $\Phi(r_1, r_2)$  gives

$$\Phi(r_1, r_2) = \frac{4r_1^2 r_2^2 - 31r_1 r_2 + 14r_1 + 14r_2 + 4}{4r_1 r_2}.$$

For all admissible integer pairs

$$n - 1 \geq r_2 \geq r_1 \geq 1, (r_1, r_2) \notin \{(1, 2), (2, 2)\},$$

the denominator is positive. The numerator is also positive over the admissible range. Therefore,

$$\Phi(r_1, r_2) > 0.$$

Thus, the lower-bound theorem applies to  $\Xi_2(G)$ .

### A.2 Verification for the Reciprocal Composite Sombor Descriptor

For the reciprocal composite Sombor descriptor, the generator is

$$\hbar_{SO}(x, y) = \sqrt{x^2 + y^2} + \frac{1}{\sqrt{x^2 + y^2}}.$$

Let

$$s = x^2 + y^2.$$



Then

$$\hbar_{SO}(x, y) = s^{1/2} + s^{-1/2}.$$

Differentiating with respect to  $x$ , we obtain

$$\frac{\partial \hbar_{SO}}{\partial x} = xs^{-1/2} - xs^{-3/2} = \frac{x(s-1)}{s^{3/2}}.$$

Similarly,

$$\frac{\partial \hbar_{SO}}{\partial y} = \frac{y(s-1)}{s^{3/2}}.$$

Since  $x, y \geq 1$ , we have

$$s = x^2 + y^2 \geq 2,$$

and therefore

$$s - 1 > 0.$$

Hence,

$$\frac{\partial \hbar_{SO}}{\partial x} > 0, \frac{\partial \hbar_{SO}}{\partial y} > 0.$$

Thus,  $\hbar_{SO}$  is strictly increasing in each variable.

### **A.3 Verification for the Reciprocal Forgotten Descriptor**

For the forgotten index, the reciprocal composite generator is

$$\hbar_F(x, y) = x^2 + y^2 + \frac{1}{x^2 + y^2}.$$

Let

$$s = x^2 + y^2.$$

Then

$$\hbar_F(x, y) = s + \frac{1}{s}.$$

Differentiating gives

$$\frac{\partial \hbar_F}{\partial x} = 2x - \frac{2x}{s^2} = 2x \left(1 - \frac{1}{s^2}\right),$$

and

$$\frac{\partial \hbar_F}{\partial y} = 2y \left(1 - \frac{1}{s^2}\right).$$

Since  $x, y \geq 1$ , we have  $s \geq 2$ , and hence

$$1 - \frac{1}{s^2} > 0.$$

Therefore,



$$\frac{\partial \hbar_F}{\partial x} > 0, \frac{\partial \hbar_F}{\partial y} > 0.$$

Thus,  $\hbar_F$  is strictly increasing in each variable.

#### **A.4 Verification for the Reciprocal First Zagreb Descriptor**

For the first Zagreb-type reciprocal composite descriptor, the generator is

$$\hbar_{Z_1}(x, y) = x + y + \frac{1}{x + y}.$$

Let

$$s = x + y.$$

Then

$$\hbar_{Z_1}(x, y) = s + \frac{1}{s}.$$

Differentiating gives

$$\frac{\partial \hbar_{Z_1}}{\partial x} = 1 - \frac{1}{s^2},$$

and

$$\frac{\partial \hbar_{Z_1}}{\partial y} = 1 - \frac{1}{s^2}.$$

Since  $x, y \geq 1$ , we have

$$s = x + y \geq 2.$$

Therefore,

$$1 - \frac{1}{s^2} > 0.$$

Hence,  $\hbar_{Z_1}$  is strictly increasing in each variable.

#### **A.5 Edge-Transfer Verification for $\Xi_2$**

In the proof of the edge-transfer improvement lemma, let

$$d_x = d_G(x), d_y = r + 2,$$

where  $r$  is the number of transferred edges. Define

$$\Theta = \Xi_2(G) - \Xi_2(G').$$

After collecting the local contributions of the affected edges, one obtains

$$\Theta = -\frac{r(d_x - 2)(rd_x + d_x - 1)}{(r + 1)d_x}.$$

Since

$$r \geq 1$$







**B.2 Summary of Computational Results**

The enumeration produced the following results:

<i>n</i>	Number of connected non-isomorphic graphs	Distinct $Z_2$ values	Distinct $\Xi_2$ values	$D_{Z_2}(n)$	$D_{\Xi_2}(n)$	Reduction
5	21	21	21	1.0000	1.0000	0.0%
6	112	92	100	1.2174	1.1200	8.0%
7	853	300	594	2.8433	1.4360	49.5%
8	11,117	695	4,606	15.9957	2.4136	84.9%
9	261,080	1,340	46,418	194.8358	5.6245	97.1%

These results confirm that the reciprocal composite descriptor  $\Xi_2$  produces a substantially larger number of distinct descriptor values than the classical second Zagreb index  $Z_2$ . The reduction in degeneracy becomes especially strong for larger graph orders.

**Appendix C. Additional Notes on Notation**

For clarity, the following reciprocal descriptors are used consistently throughout the paper:

$$\begin{aligned}
 RZ_2(G) &= \sum_{uv \in E(G)} \frac{1}{d_G(u)d_G(v)} \\
 RSO(G) &= \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)^2 + d_G(v)^2}} \\
 RF(G) &= \sum_{uv \in E(G)} \frac{1}{d_G(u)^2 + d_G(v)^2} \\
 RZ_1(G) &= \sum_{uv \in E(G)} \frac{1}{d_G(u) + d_G(v)}
 \end{aligned}$$

Therefore, the reciprocal composite descriptors considered in the paper are

$$\begin{aligned}
 \Xi_2(G) &= Z_2(G) + RZ_2(G), \\
 SO(G) &+ RSO(G), \\
 F(G) &+ RF(G),
 \end{aligned}$$

and

$$Z_1(G) + RZ_1(G).$$

These definitions remove the ambiguity caused by the earlier notation  $mZ_2(G)$  and ensure that all reciprocal composite descriptors are written consistently.