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Research Paper

On Vertex-Degree-Based Topological Indices of Cayley Digraphs of Rectangular Groups and Their Role as Molecular Descriptors

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Abstract
Let Cay(S,A) be the Cayley digraph of a finite rectangular group S with connection set A. We derive explicit formulas for several vertex-degree–based topological indices of these digraphs, including the Randić, Zagreb, sum-connectivity, geometric–arithmetic, atom–bond connectivity, and harmonic indices. The computations are reduced to Cayley digraphs of right groups, which simplifies the analysis. The underlying graphs are shown to be isomorphic to the hydrogen–included molecular graphs of cycloalkanes C_nH_{2n}. We prove that all considered indices depend linearly on the ring size n, exhibit stable growth, and differ only in their growth rates. Comparisons between related graph models illustrate the dependence of these indices on the underlying structure and support their interpretation as molecular descriptors, with possible relevance to QSAR/QSPR studies.

Keywords
Vertex Degree, Topological Indices, Cayley Digraphs, Rectangular Proups

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1. INTRODUCTION

Algebraic Graph Theory is an important branch of pure mathematics that applies algebraic methods to the study of graphs and digraphs. One main focus is the study of graph isomorphisms and graph invariants generated by algebraic constructions. In particular, graphs and digraphs defined by groups or semigroups have structures that depend directly on the algebraic operations used in their construction. As a result, many combinatorial and algebraic properties of these graphs can be analyzed through the associated algebraic structures.

Topological indices of graphs are numerical parameters that are widely used in graph theory and its applications, especially in chemistry. In chemical graph theory, molecular structures are studied using graph-theoretical models, where molecules are represented as graphs whose vertices represent atoms and edges represent chemical bonds (Trinajstić, 2018). Topological indices are important tools in Quantitative Structure Activity Relationships (QSAR) and Quantitative Structure–Property Relationships (QSPR), which aim to relate molecular structure to chemical, physical, and biological properties of compounds using graph-based descriptions (Devillers and Balaban, 2000; Emmert-Streib, 2012; Skvortsova et al., 1993).

A topological index, also called a molecular descriptor, is a numerical value that describes structural properties of a molecular graph. A molecular graph is an undirected graph derived from the structural formula of a chemical compound, where vertices represent atoms and edges indicate the presence of chemical bonds between atoms (Gutman, 2013). Various topological indices have been shown to correlate strongly with chemical properties such as boiling points, melting points, enthalpies of formation, vapor pressure, toxicity, and biological activity (ichi Aihara, 1996; Basak et al., 2002; Cioslowski, 1985; Garcia-Domenech et al., 2007; Guan et al., 2020; Khadikar et al., 2007; Liu et al., 2007; Pompe and Novic, 1999; Repnjak et al., 2018; Rouvray and Tatong, 1989; Rücker and Rücker, 1999; Sheridan et al., 2002; Zhou et al., 2015). Consequently, many new indices have been introduced and applied in QSAR and QSPR studies (Devillers and Balaban, 2000).

Among different classes of topological indices, vertex degree–based indices are particularly attractive due to their simple definitions and clear structural interpretation. These indices are defined in terms of vertex degrees and provide useful information about molecular size, branching, and connectivity (Gutman, 2013; Korinth et al., 2012). For example, the Randić connectivity index captures relationships between electron energy and hydrogen-carbon structures in benzene compounds (West, 1996), while other degree-based indices are related to skin permeability coefficients and octanol partition coefficients

(Basak et al., 1991; Lučić et al., 2009). The Zagreb indices are known to predict the total surface area of molecular isomers (Zhao et al., 2016). Recent studies have focused on developing new formulations and computational techniques, as well as investigating extremal properties of vertex degree–based indices (Cruz, 2024; Gao, 2024; Jeyaraj et al., 2023; Čomić, 2024). These indices are also applied to study the complexity and heat of formation of chemical compounds such as octane and heptane (Eliasi and Vukičević, 2013; Furtula et al., 2010).

From an algebraic perspective, Cayley graphs and Cayley digraphs provide a natural setting for studying vertex degree–based topological indices, since their adjacency structure is directly determined by the underlying algebraic system. Cayley graphs were first introduced by Arthur Cayley in 1878 and have been extensively studied for groups (Biggs, 1993; Kelarev and Praeger, 2003; Knauer, 2011). Cayley digraphs of semigroups have also received significant attention, as semigroups form a natural generalization of groups (Hao and Luo, 2010; Khosravi, 2009; Khosravi and Mahmoudi, 2010).

A particularly important class of semigroups in Algebraic Graph Theory is the class of rectangular groups. Several structural properties of Cayley digraphs associated with rectangular groups have been investigated in the literature (Hao and Luo, 2010; Khosravi, 2009; Khosravi and Mahmoudi, 2010; Meksawang and Panma, 2016; Panma, 2010; Panma et al., 2004; Ruangnai et al., 2012). A rectangular group can be expressed as a direct product $S = G \times L \times R$, where G is a group and L and R are left and right zero semigroups, respectively. An important result connecting Cayley digraphs of rectangular groups to those of right groups is given by the following theorem.

Theorem 1.1 *Nupo and Panma (2018) Let $S := G \times L \times R$ be a rectangular group and A a connection set of* $\mathrm{Cay}(S, A)$. *If*

$$\overline{A} = \{(a, \alpha) \in G \times R : (a, l, \alpha) \in A \text{ for some } l \in L\},$$

then $\mathrm{Cay}(S, A)$ *is the disjoint union of $|L|$ strong subdigraphs, each of which is isomorphic to the Cayley digraph* $\mathrm{Cay}(G \times R, \overline{A})$ *of the right group $G \times R$.*

This theorem shows that the Cayley digraph of a rectangular group can be decomposed into several isomorphic strong subdigraphs, each corresponding to a Cayley digraph of a right group. Consequently, the study of vertex degree based topological indices for Cayley digraphs of rectangular groups can be reduced to the study of such indices for Cayley digraphs of right groups. Therefore, in the research, we focus on Cayley digraphs of right groups of the form $\mathbb{Z}_n \times R$. Formulas for several vertex degree–based topological indices are derived, and their structural behavior is analyzed. By Theorem 1.1, these results can be directly extended to Cayley digraphs of rectangular groups. This provides a general structural description of vertex-degree–based topological indices of rectangular groups in chemical graph theory.

2. PRELIMINARIES

A digraph D (no loop) is a pair $((V(D), E(D))$ in which $V(D)$ is a nonempty set whose elements are called the *vertices* and $E(D)$ is the subset of the set of ordered pairs of elements in $V(D)$. The elements of $E(D)$ are called the *arcs* of D. The set $V(D)$ is called a *vertex set* of D and the set $E(D)$ is called an *arc set* of D. For any $v \in D$, the number of arcs incident to v is the *in-degree* of v which is denoted by d_v^-. The number of arcs incident from v is the *out-degree* of v, denoted by d_v^+. Furthermore, we define $N^-(v)$ and $N^+(v)$ by

$$N^-(v) = \{u \in V(D) : (u, v) \in E(D)\} \text{ and}$$
$$N^+(v) = \{u \in V(D) : (v, u) \in E(D)\}$$

We note that $d_v^- = |N^-(v)|$ and $d_v^+ = |N^+(v)|$. The *total degree* of v is $d_v = d_v^- + d_v^+$. A vertex v for which $d_v^+ = d_v^- = 0$ is called an *isolated vertex*.

In 2021, Monsalve and Rada (2021) introduced the concept of the vertex-degree based topological indices for digraphs. We had the idea to extend this research to investigate the values of vertex-degree based topological indices for Cayley digraphs of rectangular groups. These indices include the Randic index, Zagreb index, sum-connectivity index, geometric-arithmetic index, atom-bond connectivity index, and harmonic index, which are defined as follows :

Definition 2.1 Khosravi and Mahmoudi (2010) Let S be a semigroup and let A be a nonempty subset of S. *Denote by* $\Gamma = \mathrm{Cay}(S, A)$ *the* Cayley digraph *of S with* connection set *A. Then* Γ is the digraph with vertex set $V(\Gamma) = S$ *and arc set* $E(\Gamma) = \{(x, xa) : x \in S \text{ and } a \in A\}$.

Definition 2.2 Deng et al. (2022); Monsalve and Rada (2021) The *Zagreb index* of a digraph *D=((V(D), E(D))* without isolated vertices is a vertex-degree based topological index which is defined as follows :

$$ZI(D) = \frac{1}{2} \sum_{(u,v) \in E(D)} (d_u^+ + d_v^-).$$

Definition 2.3 Deng et al. (2022); Monsalve and Rada (2021) *The* Sum-Connectivity Index of a digraph $D = ((V(D), E(D))$ without isolated vertices is a vertex-degree based topological index which is defined as follows :

$$SCI(D) = \frac{1}{2} \sum_{(u,v) \in E(D)} (d_u^+ + d_v^-)^{-\frac{1}{2}}.$$

Definition 2.4 Deng et al. (2022); Monsalve and Rada (2021) The *Randic Index* of a digraph $D = ((V(D), E(D))$ without isolated vertices is a vertex-degree based topological index which is defined as follows :

$$RI(D) = \frac{1}{2} \sum_{(u,v) \in E(D)} (d_u^+ \cdot d_v^-)^{-\frac{1}{2}}.$$

Definition 2.5 Deng et al. (2022); Monsalve and Rada (2021) The *Geometric-Arithmetic index* of a digraph $D = ((V(D), E(D))$ without isolated vertices is a vertex-degree based topological index which is defined as follows :

$$GAI(D) = \frac{1}{2} \sum_{(u,v)\in E(D)} \frac{\sqrt{d_u^+ \cdot d_v^-}}{\frac{1}{2}(d_u^+ + d_v^-)}.$$

Definition 2.6 Deng et al. (2022); Monsalve and Rada (2021) The *Atom-Bond Connectivity Index* of a digraph $D = ((V(D), E(D))$ without isolated vertices is a vertex-degree based topological index which is defined as follows :

$$ABCI(D) = \frac{1}{2} \sum_{(u,v)\in E(D)} \sqrt{\frac{d_u^+ + d_v^- - 2}{d_u^+ \cdot d_v^-}}.$$

Definition 2.7 Deng et al. (2022); Monsalve and Rada (2021) The *Harmonic index* of a digraph $D = ((V(D), E(D))$ without isolated vertices is a vertex-degree based topological index which is defined as follows :

$$HI(D) = \frac{1}{2} \sum_{(u,v)\in E(D)} \frac{2}{d_u^+ + d_v^-}.$$

Definition 2.8 (Hao and Luo, 2010) A semigroup S is called a *left zero semigroup if* $xy = x$ *for all* $x, y \in S$ *and called a* right zero semigroup *if* $xy = y$ *for all* $x, y \in S$. Further, a semigroup S is a group whenever S contains the identity and each element of S has an inverse in S.

3. RESULTS AND DISCUSSION

This section presents the main results of the paper. We first study Cayley digraphs generated by right groups of the form $\mathbb{Z}_n \times R$, where $\mathbb{Z}_n$ is the cyclic group under addition and $R = \{r_1, r_2, \ldots, r_t\}$ is a right zero semigroup. For such digraphs, the out-degrees and in-degrees of vertices are determined by the connection set, which leads to closed-form expressions for several vertex-degree–based topological indices. By Theorem 1.1, the Cayley digraph of a rectangular group is the disjoint union of isomorphic strong subdigraphs, each isomorphic to a Cayley digraph of a right group. Hence, it suffices to derive the results for right groups, and the obtained formulas extend directly to Cayley digraphs of rectangular groups. Let $\Gamma = \mathrm{Cay}(\mathbb{Z}_n \times R, A)$. Define the projections of A by

$$p_1(A) = \{\, a \in \mathbb{Z}_n : (a, r) \in A \text{ for some } r \in R \,\},$$
$$p_2(A) = \{\, r \in R : (a, r) \in A \text{ for some } a \in \mathbb{Z}_n \,\},$$

and, for each $r_k \in R$, $A_k = \{\, a \in \mathbb{Z}_n : (a, r_k) \in A \,\}$. These sets are used to describe vertex degrees and to derive formulas for the indices ZI, SCI, RI, GAI, $ABCI$, and HI. We then relate the underlying graph of Γ to the hydrogen–included molecular graphs of cycloalkanes C_nH_{2n} and illustrate the resulting behavior of the indices using numerical tables and line charts.

3.1 Out-Degree and in-Degree of Vertices

Unlike studies on vertex-degree–based topological indices of general digraphs, this research focuses on Cayley digraphs generated by right groups of the form $\mathbb{Z}_n \times R$. The algebraic structure of these digraphs allows the out-degrees and in-degrees of vertices to be expressed directly in terms of the sets A_k associated with the connection set A. Such a description is not available for arbitrary digraphs, which are not based on an underlying algebraic construction. As a consequence, the vertex-degree–based topological indices considered in this paper admit closed-form expressions depending only on $|A|$, $|A_k|$, n, and t. We now determine the out-degree and in-degree of vertices in Cayley digraphs of right groups.

Lemma 3.1 *Let n be a positive integer such that $n \geq 2$ and Γ be the Cayley digraph of a right group $\mathbb{Z}_n \times R$ with respect to the connection set A. For each $(u, r_s) \in V(\Gamma)$,*

$$d^+_{(u,r_s)} = |A|. \tag{1}$$

Proof. Let $(u, r_s) \in V(\Gamma)$ and A a connection set of Γ. Consider
$N^+((u, r_s)) = \{(v, r_\delta) : ((u, r_s), (v, r_\delta)) \in E(\Gamma)\}$, and $(u, r_s)A = \{(u, r_s)(a, r) : (a, r) \in A\}$. It is clear that $N^+((u, r_s)) = (u, r_s)A$. Further, we prove $|A| = |(u, r_s)A|$. Define $f : (u, r_s)A \longrightarrow A$ by

$$f((u, r_s)(a, r)) = (a, r) \text{ for all } (a, r) \in A.$$

We first show that f is well-defined. Let (a, r), (a', r') be two distinct elements in A and assume that

$$(u, r_s)(a, r) = (u, r_s)(a', r').$$

Then $(u + a, r) = (u + a', r')$, which implies $(a, r) = (a', r')$. Hence $f((u, r_s)(a, r)) = f((u, r_s)(a', r'))$. Thus, f is well-defined. It is clear that f is injective and surjective. Therefore, f is bijective and $|(u, r_s)A| = |A|$. Consequently, (1) holds.

Lemma 3.2 *Let n be a positive integer such that $n \geq 2$ and let Γ be the Cayley digraph of a right group $\mathbb{Z}_n \times R$ with the connection set A. For each $(u, r_k) \in V(\Gamma)$,*

$$d^-_{(u,r_k)} = \begin{cases} |A_k||R|, & r_k \in p_2(A), \\ 0, & r_k \notin p_2(A). \end{cases} \tag{2}$$

Proof. Let $(u, r_k) \in V(\Gamma)$ and let A_k be as defined above. Assume $|A_k| = s$ and $|R| = t$.
Case 1: $r_k \in p_2(A)$.
We first show that

$$d^-_{(u,r_k)} \leq |A_k||R|. \tag{3}$$

For each $r \in R$, we have

$$(u, r_k) = (u - a_1, r)(a_1, r_k),$$
$$(u, r_k) = (u - a_2, r)(a_2, r_k),$$
$$\vdots$$
$$(u, r_k) = (u - a_s, r)(a_s, r_k),$$

where $(a_i, r_k) \in A_k$ for $i = 1, \ldots, s$. Since there are t choices for the second coordinate, it follows that $d^-_{(u,r_k)} \leq st = |A_k||R|$. Suppose, to the contrary, that $d^-_{(u,r_k)} < |A_k||R|$. Then there exist distinct $(a, r_k), (a', r_k) \in A_k$ and $r, r' \in R$ such that

$$(u, r_k) = (u - a, r)(a, r_k),$$
$$(u, r_k) = (u - a', r')(a', r_k),$$

with $(u-a, r) = (u-a', r')$. This implies $a = a'$, a contradiction. Hence,

$$d^-_{(u,r_k)} = |A_k||R|. \tag{4}$$

Case 2: $r_k \notin p_2(A)$.
Suppose $d^-_{(u,r_k)} > 0$. Then there exist $(u - a, r) \in V(\Gamma)$ and $(a, r') \in A$ such that
$(u, r_k) = (u - a, r)(a, r') = (u, r')$, which implies $r_k = r' \in p_2(A)$, a contradiction. Thus,

$$d^-_{(u,r_k)} = 0. \tag{5}$$

Theorem 3.3 *Let n be a positive integer such that $n \geq 2$ and let Γ be the Cayley digraph of the right group $\mathbb{Z}_n \times R$ with the connection set A, where $|R| = t$ and $|p_2(A)| = m$. Then*

$$(i)\ ZI(\Gamma) = \frac{nt}{2}\left(t\sum_{k=1}^{m}|A_k|^2 + |A|\sum_{k=1}^{m}|A_k|\right);$$

$$(ii)\ SCI(\Gamma) = \frac{nt}{2}\sum_{k=1}^{m}\frac{|A_k|}{\sqrt{|A| + |A_k|t}};$$

$$(iii)\ RI(\Gamma) = \frac{nt}{2}\sum_{k=1}^{m}\sqrt{\frac{|A_k|}{|A|t}};$$

$$(iv)\ GAI(\Gamma) = nt\sum_{k=1}^{m}\frac{\sqrt{|A_k|^3|A|t}}{|A_k|t + |A|};$$

$$(v)\ ABCI(\Gamma) = \frac{nt}{2}\sum_{k=1}^{m}\sqrt{\frac{|A_k|(|A| + |A_k|t - 2)}{|A|t}};$$

$$(vi)\ HI(\Gamma) = nt\sum_{k=1}^{m}\frac{|A_k|}{|A_k|t + |A|}.$$

Proof. Let $p_2(A) = \{r_1, \ldots, r_m\}$. By Lemmas 3.1 and 3.2, every vertex $(u, r) \in V(\Gamma)$ satisfies $d^+_{(u,r)} = |A|$, and for each $r_k \in p_2(A)$ every vertex (v, r_k) satisfies $d^-_{(v,r_k)} = |A_k|t$. Let $(u, r) \in V(\Gamma)$ and $k \in \{1, \ldots, m\}$. By the definition of A_k, there are exactly $|A_k|$ arcs from (u, r) to vertices of the form (v, r_k). Hence, $d^+_{(u,r)} + d^-_{(v,r_k)} = |A| + |A_k|t$, and therefore their sum equals $|A_k|(|A| + |A_k|t)$. Summing over $k = 1, \ldots, m$, we obtain the value

$$\sum_{k=1}^{m}|A_k|(|A| + |A_k|t)$$

for each vertex (u, r). Since $|V(\Gamma)| = nt$, summing over all vertices yields

$$2ZI(\Gamma) = nt\sum_{k=1}^{m}|A_k|(|A| + |A_k|t), \tag{6}$$

which gives the stated formula.

(ii) By the same counting argument,

$$SCI(\Gamma) = \frac{nt}{2}\sum_{k=1}^{m}\frac{|A_k|}{\sqrt{|A| + |A_k|t}}. \tag{7}$$

(iii)

$$RI(\Gamma) = \frac{nt}{2}\sum_{k=1}^{m}\sqrt{\frac{|A_k|}{|A|t}}. \tag{8}$$

(iv)

$$GAI(\Gamma) = nt\sum_{k=1}^{m}\frac{\sqrt{|A_k|^3|A|t}}{|A_k|t + |A|}. \tag{9}$$

(v)

$$ABCI(\Gamma) = \frac{nt}{2}\sum_{k=1}^{m}\sqrt{\frac{|A_k|(|A| + |A_k|t - 2)}{|A|t}}. \tag{10}$$

(vi)

$$HI(\Gamma) = nt\sum_{k=1}^{m}\frac{|A_k|}{|A_k|t + |A|}. \tag{11}$$

We now illustrate an example to present results of the topological indices of a finite Cayley digraph of a right group. The example shows, more clearly, the values of those topological indices according to the previous theorems.

Example 3.4 *Let n be a positive integer such that $n \geq 3$ and $\Gamma = \mathrm{Cay}(\mathbb{Z}_n \times \{r_1, r_2, r_3\}, \{(a, r_1)\})$ be the Cayley digraph for the right group $\mathbb{Z}_n \times \{r_1, r_2, r_3\}$ with respect to the connection set $\{(a, r_1)\}$ where a is a generator of $\mathbb{Z}_n$. Then*
$(i)\ ZI(\Gamma) = 6n$;
$(ii)\ SCI(\Gamma) = \frac{3n}{4}$;
$(iii)\ RI(\Gamma) = \frac{\sqrt{3}n}{2}$;
$(iv)\ GAI(\Gamma) = \frac{3\sqrt{3}n}{4}$;
$(v)\ ABCI(\Gamma) = \frac{\sqrt{6}n}{2}$;
$(vi)\ HI(\Gamma) = \frac{3n}{4}$.

Example 3.5 *Let $n \geq 5$ and $\Gamma = \mathrm{Cay}(\mathbb{Z}_n \times \{r_1, r_2, r_3\}, \{(a, r_1), (2a, r_1), (a, r_2)\})$ be the Cayley digraph for the right group $\mathbb{Z}_n \times \{r_1, r_2, r_3\}$ with respect to the connection set $\{(a, r_1), (2a, r_1), (a, r_2)\}$, where a is a generator of $\mathbb{Z}_n$. Then $|A_1| = 2$, $|A_2| = 1$, $|A| = 3$, $t = 3$, and $m = 2$. For instance, by Theorem 3.3 (i),*

$$ZI(\Gamma) = \frac{nt}{2}\left(t(|A_1|^2 + |A_2|^2) + |A|(|A_1| + |A_2|)\right) = \frac{3n}{2}(3(4+1)+3(3)) = 36n. \tag{12}$$

The remaining indices follow from Theorem 3.3 $(ii) - (vi)$. This example shows that the formulas apply to nontrivial connection sets.

3.2 Correspondence with Molecular Graphs of Cycloalkanes

For the following results, we denote by Γ' the underlying graph of the Cayley digraph Γ. Since chemical bonds are inherently undirected, the molecular graph of a cycloalkane corresponds naturally to the underlying graph Γ' rather than to the directed digraph Γ.

From a chemical perspective, Γ' is interpreted as the *hydrogen –included molecular graph* of the cycloalkane C_nH_{2n}. In this representation, each vertex corresponds to an atom (either carbon or hydrogen) and each edge corresponds to a covalent bond. Consequently, every carbon vertex has degree 4 (two C–C and two C–H bonds), while each hydrogen vertex has degree 1.

Although Γ' is constructed algebraically from the right group $\mathbb{Z}_n \times \{r_1, r_2, r_3\}$, its adjacency structure coincides exactly with that of the molecular graph of C_nH_{2n}, as shown in Lemma 3.6. Therefore, all vertex-degree–based topological indices computed on Γ' coincide with those of the molecular graph and are derived directly from the same degree structure.

Lemma 3.6 *Let $n \geq 3$ and let*

$$\Gamma = \mathrm{Cay}(\mathbb{Z}_n \times \{r_1, r_2, r_3\},\ \{(a, r_1)\})$$

be the Cayley digraph of the right group $\mathbb{Z}_n \times \{r_1, r_2, r_3\}$, where a is a generator of the cyclic group $\mathbb{Z}_n$. Let Γ' denote the underlying graph of Γ. Then the hydrogen–included molecular graph of the cycloalkane C_nH_{2n} is isomorphic to Γ'.

Proof. Let $n \geq 3$. We construct an explicit graph isomorphism.
Label the carbon atoms of C_nH_{2n} by $C_1, C_2, \ldots, C_n$ along the ring, and attach two hydrogen atoms $H_{i,1}, H_{i,2}$ to each carbon C_i. Define

$$\phi : V(C_nH_{2n}) \longrightarrow V(\Gamma')$$

by

$$\phi(C_i) = \{i, r_1\},\ \phi(H_{i,1}) = \{i-a, r_2\},\ \phi(H_{i,2}) = \{i-a, r_3\}.$$

It is immediate from the definition that ϕ is bijective. Since Γ' is the underlying graph of Γ, every arc of Γ induces an edge of Γ'. Hence, for each $i \in \mathbb{Z}_n$, the vertex (i, r_1) is adjacent to

$$(i-a, r_1),\ (i-a, r_2),\ (i-a, r_3),\ \text{and } (i+a, r_1),$$

so $\deg(i, r_1) = 4$.
For each $j \in \mathbb{Z}_n$, there is an arc $(j, r_2) \to (j+a, r_1)$ and no arc to (j, r_2). Hence (j, r_2) has exactly one neighbour in Γ'. Thus (j, r_2) is adjacent to exactly one vertex in Γ'. The same holds for (j, r_3), and therefore $\deg(j, r_2) = \deg(j, r_3) = 1$.
Finally, we show that ϕ preserves adjacency. Each carbon vertex C_i is adjacent in C_nH_{2n} to the two ring neighbors C_{i+a} and C_{i-a}, and to the two hydrogens $H_{i,1}$ and $H_{i,2}$. Consider

$$\{\phi(C_i), \phi(C_{i+a})\} = \{(i, r_1), (i+a, r_1)\},$$
$$\{\phi(C_i), \phi(C_{i-a})\} = \{(i, r_1), (i-a, r_1)\}.$$

and

$$\{\phi(C_i), \phi(H_{i,1})\} = \{(i, r_1), (i-a, r_2)\},$$
$$\{\phi(C_i), \phi(H_{i,2})\} = \{(i, r_1), (i-a, r_3)\}.$$

Therefore $\{u, v\} \in E(C_nH_{2n})$ if and only if $\{\phi(u), \phi(v)\} \in E(\Gamma')$,
so ϕ is a graph isomorphism and $C_nH_{2n} \cong \Gamma'$ as shown in Figure 1.

Theorem 3.7 *Let C_nH_{2n} with $n \geq 3$ be the hydrogen–included molecular graph of a cycloalkane, where each carbon has degree 4 (two C–C and two C–H bonds) and each hydrogen has degree 1. Then*

(i) $ZI(C_nH_{2n}) = 18n$;

(ii) $SCI(C_nH_{2n}) = \dfrac{n}{\sqrt{8}} + \dfrac{2n}{\sqrt{5}}$;

(iii) $RI(C_nH_{2n}) = \dfrac{5n}{4}$;

(iv) $GAI(C_nH_{2n}) = \dfrac{13n}{5}$;

(v) $ABCI(C_nH_{2n}) = \dfrac{n}{4}\left(\sqrt{6} + 4\sqrt{3}\right)$;

(vi) $HI(C_nH_{2n}) = \dfrac{21n}{20}$.

Proof. By Lemma 3.6, the underlying graph Γ' is isomorphic to the molecular graph of C_nH_{2n}. Hence all vertex-degree–based indices coincide. In C_nH_{2n}, there are n carbon vertices of degree 4 forming a cycle and $2n$ hydrogen vertices of degree 1. Thus the graph contains n C–C edges and $2n$ C–H edges.

(i)

$$\begin{aligned} ZI(C_nH_{2n}) &= \sum_{\{u,v\}\in E(C_nH_{2n})} \big(d(u) + d(v)\big) \\ &= n(4+4) + 2n(4+1) \\ &= 8n + 10n \\ &= 18n. \end{aligned} \tag{13}$$

(ii)

$$\begin{aligned} SCI(C_nH_{2n}) &= \sum_{\{u,v\}\in E(C_nH_{2n})} \frac{1}{\sqrt{d(u)+d(v)}} \\ &= n\,\frac{1}{\sqrt{4+4}} + 2n\,\frac{1}{\sqrt{4+1}} \\ &= \frac{n}{\sqrt{8}} + \frac{2n}{\sqrt{5}}. \end{aligned} \tag{14}$$

(iii)

$$\begin{aligned} RI(C_nH_{2n}) &= \sum_{\{u,v\}\in E(C_nH_{2n})} \frac{1}{\sqrt{d(u)\,d(v)}} \\ &= n\,\frac{1}{\sqrt{4\cdot 4}} + 2n\,\frac{1}{\sqrt{4\cdot 1}} \\ &= \frac{n}{4} + n \\ &= \frac{5n}{4}. \end{aligned} \tag{15}$$

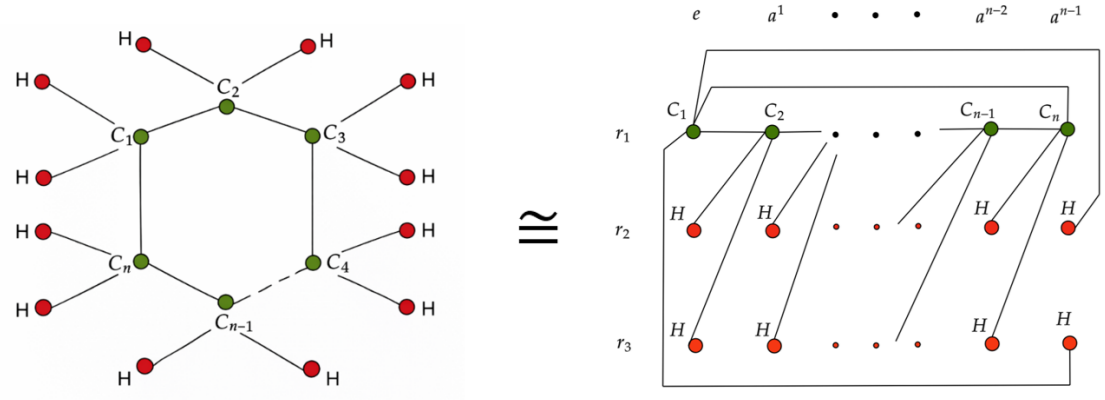

Figure 1. $C_nH_{2n} \cong \Gamma'$

n	$ZI(\Gamma)$	$ZI(\Gamma')$	$SCI(\Gamma)$	$SCI(\Gamma')$	$RI(\Gamma)$	$RI(\Gamma')$
1	6	18	0.75	1.247981	0.866025	1.25
2	12	36	1.5	2.495961	1.732051	2.5
3	18	54	2.25	3.743942	2.598076	3.75
4	24	72	3	4.991922	3.464102	5
5	30	90	3.75	6.239903	4.330127	6.25
6	36	108	4.5	7.487883	5.196152	7.5
7	42	126	5.25	8.735864	6.062178	8.75
8	48	144	6	9.983845	6.928203	10
9	54	162	6.75	11.23183	7.794229	11.25
10	60	180	7.5	12.47981	8.660254	12.5
11	66	198	8.25	13.72779	9.526279	13.75
12	72	216	9	14.97577	10.3923	15
13	78	234	9.75	16.22375	11.25833	16.25
14	84	252	10.5	17.47173	12.12436	17.5
15	90	270	11.25	18.71971	12.99038	18.75
16	96	288	12	19.96769	13.85641	20
17	102	306	12.75	21.21567	14.72243	21.25
18	108	324	13.5	22.46365	15.58846	22.5
19	114	342	14.25	23.71163	16.45448	23.75
20	120	360	15	24.95961	17.32051	25

n	$GAI(\Gamma)$	$GAI(\Gamma')$	$ABCI(\Gamma)$	$ABCI(\Gamma')$	$HI(\Gamma)$	$HI(\Gamma')$
1	1.299038	2.6	1.224745	2.344423	0.75	1.05
2	2.598076	5.2	2.44949	4.688846	1.5	2.1
3	3.897114	7.8	3.674235	7.03327	2.25	3.15
4	5.196152	10.4	4.898979	9.377693	3	4.2
5	6.495191	13	6.123724	11.72212	3.75	5.25
6	7.794229	15.6	7.348469	14.06654	4.5	6.3
7	9.093267	18.2	8.573214	16.41096	5.25	7.35
8	10.3923	20.8	9.797959	18.75539	6	8.4
9	11.69134	23.4	11.0227	21.09981	6.75	9.45
10	12.99038	26	12.24745	23.44423	7.5	10.5
11	14.28942	28.6	13.47219	25.78866	8.25	11.55
12	15.58846	31.2	14.69694	28.13308	9	12.6
13	16.8875	33.8	15.92168	30.4775	9.75	13.65
14	18.18653	36.4	17.14643	32.82193	10.5	14.7
15	19.48557	39	18.37117	35.16635	11.25	15.75
16	20.78461	41.6	19.59592	37.51077	12	16.8
17	22.08365	44.2	20.82066	39.8552	12.75	17.85
18	23.38269	46.8	22.04541	42.19962	13.5	18.9
19	24.68172	49.4	23.27015	44.54404	14.25	19.95
20	25.98076	52	24.4949	46.88846	15	21

Figure 2. The Data Tables of the Vertex-Degree Based Topological Indices of Γ and Γ'

(iv)

$$\begin{aligned} GAI(C_nH_{2n}) &= \sum_{\{u,v\}\in E(C_nH_{2n})} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)} \\ &= n\,\frac{2\sqrt{4\cdot 4}}{4+4} + 2n\,\frac{2\sqrt{4\cdot 1}}{4+1} \\ &= n + \frac{8n}{5} \\ &= \frac{13n}{5}. \end{aligned} \tag{16}$$

(v)

$$\begin{aligned} ABCI(C_nH_{2n}) &= \sum_{\{u,v\}\in E(C_nH_{2n})} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}} \\ &= n\sqrt{\frac{4+4-2}{4\cdot 4}} + 2n\sqrt{\frac{4+1-2}{4\cdot 1}} \\ &= \frac{n}{4}\left(\sqrt{6}+4\sqrt{3}\right). \end{aligned} \tag{17}$$

(*vi*)

$$\begin{aligned} HI(C_nH_{2n}) &= \sum_{\{u,v\}\in E(C_nH_{2n})} \frac{2}{d(u)+d(v)} \\ &= n\,\frac{2}{4+4} + 2n\,\frac{2}{4+1} \\ &= \frac{n}{4} + \frac{4n}{5} \\ &= \frac{21n}{20}. \end{aligned} \tag{18}$$

3.2.1 Quantitative Comparison with Existing Results

By Lemma 3.6, the underlying graph Γ' of the Cayley digraph Γ is isomorphic to the molecular graph of the cycloalkane C_nH_{2n}. Hence, both graphs have the same degree sequence and the same adjacency structure. Since all indices considered in Theorem 3.7 are vertex-degree–based topological indices, they are graph invariants. Consequently, their numerical values are identical on Γ' and on C_nH_{2n}.

For a direct quantitative comparison with existing results, we consider previously reported closed-form expressions for cycloalkane graphs. Maallah and Khalaf derived the Randić index of unicyclic (cycloalkane) graphs by a direct combinatorial analysis and obtained

$$R(U_n^{*2}) = \frac{n}{4} + \frac{2n}{2}. \tag{19}$$

In Theorem 3.7, we independently obtain

$$RI(C_nH_{2n}) = \frac{5n}{4}. \tag{20}$$

Thus both approaches yield exactly the same closed-form expression, providing a direct quantitative confirmation of the correctness of our formulas and showing that the Cayley digraph construction gives an alternative algebraic derivation of the same molecular descriptor.

Next, we present the vertex-degree based topological indices of Γ and Γ' using data tables. The tables presented in Figure 2 show the vertex-degree based topological indices of Γ and Γ' calculated using Example 3.4 and Theorem 3.7.

Next, we illustrate the trends for each of the vertex-degree based topological indices of Γ and Γ' using line charts which are shown in Figure 3.

Finally, we present line charts of every vertex-degree based topological index of Γ and Γ' as provided in Figure 4.

3.3 Quantitative Comparison and Discussion of Molecular Descriptors

In this section, we provide a comparative discussion of the vertex-degree–based topological indices of the molecular graphs Γ and Γ'. The analysis is supported by the numerical values reported in Figure 2 and the graphical trends shown in Figures 3 and 4. The observed behavior of these indices is interpreted from both graph-theoretic and chemical perspectives, with possible relevance to their use as molecular descriptors in QSAR/QSPR studies.

3.3.1 Linear Growth with Respect to the Ring Size n

From the explicit formulas given in Theorem 3.7 and the numerical values shown in Figure 2, all considered indices for the cycloalkane C_nH_{2n} increase linearly with the number of carbon atoms n. This linear trend is clearly visible in the straight-line plots presented in Figures 3 and 4. From a chemical point of view, increasing the ring size by one adds one carbon atom and two hydrogen atoms, which leads to a constant increment of each degree-based index. From a graph-theoretic point of view, the linear growth follows because the degree pattern is fixed (degree 4 for each carbon vertex and degree 1 for each hydrogen vertex), and the numbers of the two edge types grow linearly with n (namely, n C–C edges and $2n$ C–H edges).

3.3.2 Differences in Growth Rates of the Indices

Although all indices increase linearly with n, their growth rates are different. In particular, indices such as ZI, GAI, and $ABCI$ have steeper slopes than SCI, RI, and HI, as shown in Figures 3 and 4. This difference comes from the definitions of the indices, which weight the two edge types (C–C with degree pair (4, 4) and C–H with degree pair (4, 1)) in different ways. Consequently, the indices accumulate at different rates as n increases, even though the degree pattern and the edge-type counts follow the same linear scaling.

3.3.3 Comparison of Γ and Γ'

A direct comparison of the vertex-degree–based topological indices of Γ and Γ' shows a clear and consistent difference. For every index considered, the values associated with Γ' are larger than those of Γ, as shown in Figure 2. This means that the same pattern appears for all indices and for all values of n, and the difference is not accidental.

From a graph-theoretic point of view, this behavior is caused by the different adjacency structures of Γ and Γ'. Although both graphs represent the same molecular formula C_nH_{2n} and have the same number of vertices, the construction of Γ' results in a larger number of edges appearing in the index summations. Consequently, the total values of the indices for Γ' are consistently higher than those for Γ.

From a molecular perspective, these results indicate that vertex-degree–based topological indices depend on how the molecular graph is constructed, even when the chemical composition is unchanged. This shows that different graph models of the same molecule may describe structural characteristics in different ways, which should be considered when using such indices in QSAR/QSPR studies.

3.3.4 Stability of Linear Behavior for Large n

Figure 4 shows that all indices follow straight-line trends over a wide range of values of n, with no visible changes in their linear behavior. This shows that the dependence of each index on n remains the same as the ring size increases. As a result, the indices display stable behavior for larger cyclic systems, making them suitable for quantitative analysis without loss of interpretability.

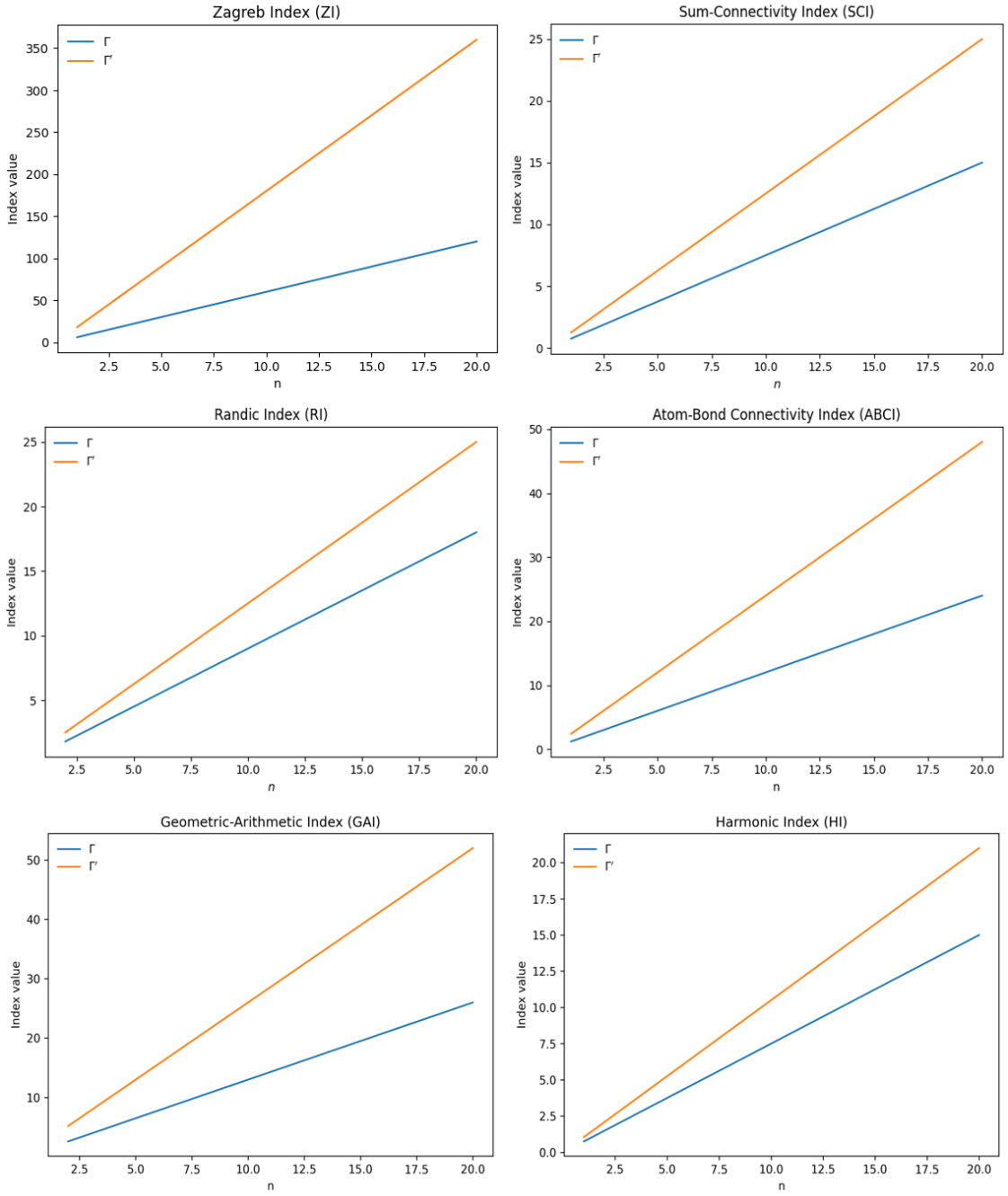

Figure 3. The Trends of Each of the Vertex-Degree Based Topological Indices of Γ and Γ′

3.3.5 Relevance to QSAR/QSPR Descriptors

The linear relationships and stable trends observed for all indices suggest that they may serve as vertex-degree–based molecular descriptors. Indices with steeper slopes show larger changes as the ring size increases, while those with smaller slopes change more slowly and provide more stable global measures.

Since all indices depend linearly on the ring size, they mainly describe the overall growth of the structure and may be less effective for distinguishing closely related cycloalkanes. Therefore, these indices may be considered together with other structural or physicochemical descriptors in practical applications.

Overall, these observations indicate that Cayley digraph models preserve the main growth behavior of degree-based topological indices and offer an alternative approach for analyzing structural properties.

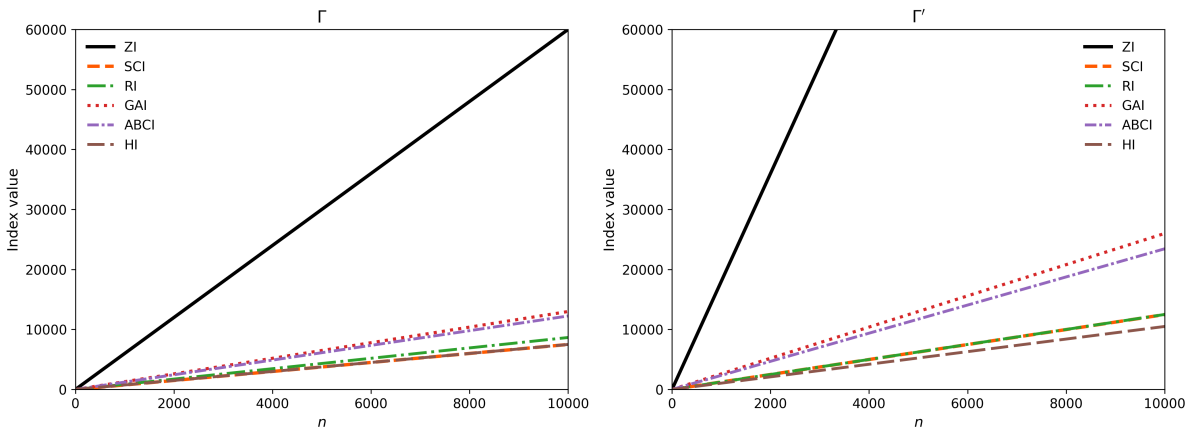

Figure 4. The Line Charts of Every Vertex-Degree Based Topological Index of Γ and Γ′

4. CONCLUSIONS

In this paper, we studied vertex-degree–based topological indices of Cayley digraphs associated with rectangular groups. By determining the in-degree and out-degree of vertices, we derived formulas for several indices. Using the decomposition of rectangular groups, the analysis was reduced to Cayley digraphs of right groups, which simplified the computations. For the Cayley digraph $\Gamma = \mathrm{Cay}(\mathbb{Z}_n \times \{r_1, r_2, r_3\}, \{(a, r_1)\})$, we showed that its underlying graph is isomorphic to the hydrogen–included molecular graph of the cycloalkanes C_nH_{2n}. A quantitative comparison showed that all considered indices grow linearly with the ring size n, remain linear for large n, and exhibit the same growth patterns for both Γ and its underlying graph, although their numerical values may differ. These results indicate that Cayley digraphs preserve the essential growth behavior of vertex-degree–based topological indices. Therefore, Cayley digraphs provide a natural graph-theoretic model for studying structural trends of cyclic molecules. From a QSAR/QSPR perspective, this suggests that degree-based indices derived from Cayley digraphs are suitable molecular descriptors, especially when combined with additional structural or physicochemical information.

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