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Research Article

Some Topological Invariants of Graphs Associated with the Group of Symmetries

Chang-Cheng Wei,[1] Muhammad Salman ,[2] Usman Ali ,[3,4] Masood Ur Rehman ,[5,6] Muhammad Aqeel Ahmad Khan,[7] Muhammad Hasanain Chaudary,[8] and Farooq Ahmad [8]

[1]*Department of Mathematics and Computer Science, Anhui TongLing University, Tongling 244061, China*
[2]*Department of Mathematics, The Islamia University of Bahawalpur, Bahawalpur, Pakistan*
[3]*Centre for Advanced Studies in Pure and Applied Mathematics (CASPAM), Bahauddin Zakaryia University, Multan, Pakistan*
[4]*Institut de Mathématiques de Jussieu-Paris Rive Gauche, Paris, France*
[5]*Department of Mathematics, Abbottabad University of Science and Technology, Abbottabad, Pakistan*
[6]*Department of Basic Sciences, Balochistan University of Engineering and Technology, Khuzdar, Balochistan, Pakistan*
[7]*Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore, Pakistan*
[8]*Department of Computer Science, COMSATS University Islamabad, Lahore Campus, Lahore, Pakistan*

Correspondence should be addressed to Usman Ali; uali@bzu.edu.pk and Masood Ur Rehman; masood@mail.ustc.edu.cn

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A topological index is a quantity that is somehow calculated from a graph (molecular structure), which reflects relevant structural features of the underlying molecule. It is, in fact, a numerical value associated with the chemical constitution for the correlation of chemical structures with various physical properties, chemical reactivity, or biological activity. A large number of properties like physicochemical properties, thermodynamic properties, chemical activity, and biological activity can be determined with the help of various topological indices such as atom-bond connectivity indices, Randić index, and geometric arithmetic indices. In this paper, we investigate topological properties of two graphs (commuting and noncommuting) associated with an algebraic structure by determining their Randić index, geometric arithmetic indices, atomic bond connectivity indices, harmonic index, Wiener index, reciprocal complementary Wiener index, Schultz molecular topological index, and Harary index.

1. Introduction

In quantitative structure-activity relationship (QSAR)/quantitative structure-property relationship (QSPR) study, physicochemical properties and topological indices such as Randić index, atom-bond connectivity (ABC) index, and geometric-arithmetic (GA) index are used to predict the bioactivity of chemical compounds. A topological index is actually designed by transforming a chemical structure into a numerical number. It correlates certain physicochemical properties such as boiling point, stability, and strain energy of chemical compounds of a molecular structure (graph). It is a numeric quantity associated with a chemical structure (graph), which characterizes the topology of the structure and is invariant under a structure-preserving mapping [1]. In 1947, Wiener [2] introduced the concept of (distance-based) topological index while working on the boiling point of paraffin. He named this index as the path number. Later on, the path number was renamed as the Wiener index [2], and then, the theory of topological indices started. Nowadays, a number of distance-based and degree-based topological indices have been introduced and computed (see for example [3–15], and the references therein).

We consider simple and connected graph (chemical structure) G with vertex set $V(G)$ and edge set $E(G)$. We denote the two adjacent vertices u and v in G as $u \sim v$ and nonadjacent vertices as $u \nsim v$. The number d_v denotes the degree of a vertex $v \in V(G)$ and $S_v = \sum_{u \in N(v)} d_u$ is the

Table 1: List of under consideration topological indices.

Name of the index	Notation	Formula
Wiener index [2]	$W(G)$	$\sum_{\{u,v\}\in V(G)} d(u,v)$
Reciprocal complementary Wiener index [21]	$\mathrm{RCW}(G)$	$\sum_{\{u,v\}\in V(G)} 1/(D(G)+1-d(u,v))$
Schultz molecular topological index [22]	$\mathrm{MTI}(G)$	$\sum_{\{u,v\}\in V(G)} (d_u+d_v)d(u,v)+\sum_{v\in V(G)} d^{2/v}$
Harary index [23, 24]	$H(G)$	$\sum_{\{u\neq v\}\in V(G)} 1/(d(u,v))$
Randić index [10]	$R_{-1/2}(G)$	$\sum_{u\sim v} 1/(\sqrt{d_u\times d_v})$
General Randić index [11, 12]	$R_\alpha(G)$	$\sum_{u\sim v} (d_u\times d_v)^\alpha$
Geometric arithmetic (GA) index [13]	$\mathrm{GA}(G)$	s
Fifth version of GA index [4]	$\mathrm{GA}_5(G)$	$\sum_{u\sim v} (2\sqrt{S_u\times S_v})/(S_u+S_v)$
Atomic bond connectivity (ABC) index [14]	$\mathrm{ABC}(G)$	$\sum_{u\sim v} \sqrt{(d_u+d_v-2)/(d_u\times d_v)}$
Fourth version of ABC index [5]	$\mathrm{ABC}_4(G)$	$\sum_{u\sim v} \sqrt{(S_u+S_v-2)/(S_u\times S_v)}$
Harmonic index [15]	$H_r(G)$	$\sum_{u\sim v} 2/(d_u+d_v)$

All the notations used in formulas are defined in Section 1.

degrees sum of v, where $N(v)=\{u\in V(G) \mid u\sim v \text{ in } G\}$ is the neighborhood of v. The number $d(u,v)$ denotes the length of a geodesic between u and v in G and is called the distance between u and v. The eccentricity of a vertex v in G, denoted by $\mathrm{ecc}(v)$, is the maximum distance between v and any other vertex of G. The minimum eccentricity amongst the vertices of G is called the radius of G, denoted by $\mathrm{rad}(G)$. The diameter of a graph G is the maximum eccentricity in G, denoted by $D(G)$. A vertex v in G is said to be a central vertex if $\mathrm{ecc}(v)=\mathrm{rad}(G)$, and the subgraph of G induced by central vertices of G is called the center of G. A vertex v in a graph G is called a peripheral vertex if $\mathrm{ecc}(v)=D(G)$, and the subgraph of G induced by peripheral vertices is called the periphery of G. The sum of two graphs G_1 and G_2, denoted by G_1+G_2, is a graph with vertex set $V(G_1)\cup V(G_2)$ and an edge set $E(G_1)\cup E(G_2)\cup\{u\sim v\colon u\in V(G_1)\wedge v\in V(G_2)\}$.

Let Γ be a group. The set $\zeta(\Gamma)=\{x\colon x\in\Gamma\wedge xy=yx\forall y\in\Gamma\}$ is called the center of the group Γ. Then, commuting and noncommuting graphs of Γ are defined as follows:

(i) The commuting graph of a nonabelian group Γ is denoted by $\Gamma_G=C(\Gamma,\Omega)$ with vertex set $\Omega\subseteq\Gamma$. For two distinct elements $x,y\in\Omega$, $x\sim y$ in Γ_G (x and y form an edge in Γ_G) if and only if $xy=yx$ in Γ. The concept of commuting graphs on noncentral elements of a group has been studied by various researchers (see [16, 17]).

(ii) The noncommuting graph of a nonabelian group G_Γ is a graph with vertex set $V(G_1)\cup V(G_2)$, and two distinct vertices u and v in G_Γ form an edge if $uv\neq vu$ in Γ. The study of noncommuting graphs of groups was initiated in 1975 by Neumann [18] who posed the problem regarding the clique number of a noncommuting graph. Noncommuting graphs on noncentral elements of a group have also been studied by various other researchers [19, 20].

The following useful property for a noncommuting graph was proposed in [19].

Proposition 1 (see [19]). *For any nonabelian group Γ, $D(G_\Gamma)=2$.*

A graph G is said to be self-centered if $\mathrm{rad}(G)=D(G)$. Since $\mathrm{ecc}(v)\leq 2$ for every $v\in G_\Gamma$, so we have the following straightforward proposition:

Proposition 2. *A noncommuting graph G_Γ of any nonabelian finite group Γ is self-centered if for each $v\in G_\Gamma$, $ecc(v)=2$. Otherwise, it is the sum of the center and the periphery of G_Γ.*

This paper aimed at investigating all the topological properties (listed in Table 1) of commuting and noncommuting graphs associated with the group of symmetries. The rest of the paper consists of five sections. In the next section, we illustrate the group of symmetries and associate commuting and noncommuting graphs to this group. In Section 3, some useful constructions to investigate our main results of Sections 4 and 5 are provided.

2. Group of Symmetries and Associated Graphs

Group of symmetries finds its remarkable use in the theory of electron structures and molecular vibrations. Due to their significant employment in chemical structures, in the context of topological indices, we consider the group of symmetries of a regular polygon (also called a regular n-gon for $n\geq 2$) in this paper. A regular n-gon is a geometrical figure all of whose sides have the same length and all the angles are of equal measurement. Each internal angle of a n-gon is of $\pi-(2\pi)/(n)$ radian. The group of symmetries of a n-gon consists of $2n$ elements, which are n rotations ($r_0=e, r_1, r_2, \ldots, r_{n-1}$ about its center through an angle of $(2k\pi)/n$ radian, where $k=0,1,\ldots,n-1$, either all clockwise or all anticlockwise) and n reflections (for even n, the reflections through a line joining the midpoints of the opposite sides or through a line joining two opposite vertices, and for odd n, the reflections through those lines which join a vertex with the midpoint of the opposite side). The group of symmetries is denoted by D_n and is called the dihedral group of order $2n$. If we denote a rotation by "a" and a reflection by "b," then $2n$ elements of D_n are $a, a^2, \ldots, a^{n-1}, a^n=e$ and $b, ab, a^2b, \ldots, a^{n-1}b$, where e is the identical rotation. The general representation of D_n is given by

Table 2: Vertex partition of Γ_G for each vertex $v \in V(\Gamma_G)$.

n is	d_v	$D(v\mid\Gamma_G)$	$D_s(v\mid\Gamma_G)$	$D_r(v\mid\Gamma_G)$	Number of vertices
Odd	$n-1$	$3n-1$	$(1/2)(3n-1)$	$(1/2)(3n-2)$	$n-1$
Odd	$2n-1$	$2n-1$	$(1/2)(2n-1)$	$2n-1$	1
Odd	1	$4n-3$	$(1/2)(4n-3)$	n	n
Even	$n-1$	$3n-1$	$(1/2)(3n-1)$	$(1/2)(3n-2)$	$n-2$
Even	$2n-1$	$2n-1$	$(1/2)(2n-1)$	$2n-1$	2
Even	3	$4n-5$	$(1/2)(4n-5)$	$n+1$	n

$$D_n = \langle a, b \mid a^n = b^2 = e, ab = ba^{-1}\rangle, \quad (1)$$

with the center

$$\zeta(D_n) = \begin{cases} \{e\}, & \text{when } n \text{ is odd}, \\ \{e, a^{n/2}\}, & \text{when } n \text{ is even}. \end{cases} \quad (2)$$

Let $\Omega_1 = \{e, a, a^2, \ldots, a^{n-1}\}$, $\Omega_2 = \{b, ab, a^2b, \ldots, a^{n-1}b\}$, and $\Omega_3 = \Omega_1 - \zeta(D_n)$. Then $|\Omega_1| = n = |\Omega_2|$ and

$$|\Omega_3| = \begin{cases} n-1, & \text{when } n \text{ is odd}, \\ n-2, & \text{when } n \text{ is even}. \end{cases} \quad (3)$$

In the case of even value of $n \geq 4$, we partitioned Ω_2 into $n/2$ two element subsets $\Omega_2^i = \{a^ib, a^{((n/2)+i)}b\}$, $0 \leq i \leq (n/2)-1$, so that $\Omega_2 = \cap_{i=0}^{(n/2)-1}\Omega_2^i$.

Remark 1. In the dihedral group D_n, we have

(i) $xy = yx$ for all $x, y \in D_2$
(ii) $a^ib = ba^{n-i}$ for $i = 1, 2, \ldots, n-1$
(iii) For odd values of $n \geq 3$, $xy \neq yx$ for distinct $x, y \in \Omega_2$
(iv) For even values of $n \geq 4$, and for any distinct $x, y \in \Omega_2$, $xy = yx$ if and only if $x, y \in \Omega_2^i$, $0 \leq i \leq (n/2)-1$
(v) For any distinct $x, y \in \Omega_3$, $xy = yx$
(vi) For each pair $(x, y) \in \Omega_2 \times \Omega_3$, $xy \neq yx$

According to Remark 1, the commuting graph on D_n is defined in the following result.

Proposition 3 (see [16]). *For all $n \geq 3$, let $\Gamma_G = \mathscr{C}(D_n, D_n)$ be a commuting graph on D_n, then*

$$\Gamma_G = \begin{cases} K_1 + \left(K_{|\Omega_3|} \cup N_{|\Omega_1|}\right), & \text{when } n \text{ is odd}, \\ K_2 + \left(K_{|\Omega_3|} \cup \frac{n}{2}K_2\right), & \text{when } n \text{ is even}. \end{cases} \quad (4)$$

Here, K_1 is the trivial graph, K_p is a complete graph on p vertices, N_t is a null (empty) graph on t vertices, and $(n/2)K_2$ is the union of $(n/2)$ copies of K_2.

Let $\Gamma = D_n, n \geq 3$, and G_Γ be the corresponding non-commuting graph. Then, according to Remark 1, we have the following points:

When $n \geq 3$ is odd, then

(1) For $u, v \in V(G_\Gamma), u \sim v$ whenever $u, v \in \Omega_2$.
(2) For $u, v \in V(G_\Gamma), u \sim v$ whenever $u, v \in \Omega_3$.
(3) For $u, v \in V(G_\Gamma), u \sim v$ whenever $u \in \Omega_2$ and $v \in \Omega_3$.
(4) In G_Γ, it can be seen that $\text{ecc}(v) = 1$ for all $v \in \Omega_2$, and $\text{ecc}(v) = 2$ for all $v \in \Omega_3$. It follows that Ω_2 induces the center of G_Γ, which is a complete graph $K_{|\Omega_2|}$ on $|\Omega_2|$ vertices, and Ω_3 induces the periphery of G_Γ, which is a null graph $N_{|\Omega_3|}$ on $|\Omega_3|$ vertices.

When $n \geq 4$ is even, then

(1) For $u, v \in V(G_\Gamma), u \nsim v$ whenever $u, v \in \Omega_2^i$ for any $0 \leq i \leq (n/2)-1$.
(2) For $u, v \in V(G_\Gamma), u \nsim v$ whenever $u, v \in \Omega_3$.
(3) For $u, v \in V(G_\Gamma), u \sim v$ whenever $u \in \Omega_2$ and $v \in \Omega_3$.
(4) For $u, v \in V(G_\Gamma), u \sim v$ whenever $u \in \Omega_2^i$ and $v \in \Omega_2^j$ with $0 \leq i, j \leq (n/2)-1$ and $i \neq j$.
(5) In G_Γ, it can be seen that $\text{ecc}(v) = 2$ for all $v \in \Omega_2 \cup \Omega_3$. It follows that G_Γ is a self-centered graph, which is a complete multipartite graph $K_{\underbrace{2, 2, \ldots, 2}_{(n/2)-\text{times}}, |\Omega_3|}$ with $n/2$ partite sets $\Omega_2^i, 0 \leq i \leq (n/2)-1$, and one partite set Ω_3.

Hence, by Proposition 2, we deduce the following result.

Proposition 4. *For $n \geq 3$, let $\Gamma = D_n$. Then, the non-commuting graph G_Γ of D_n is given by*

$$G_\Gamma = \begin{cases} K_{\Omega_2} + N_{\Omega_3}, & \text{when } n \text{ is odd}, \\ K_{\underbrace{2, 2, \ldots, 2}_{(n/2)-\text{times}}, |\Omega_3|}, & \text{when } n \text{ is even}. \end{cases} \quad (5)$$

3. Construction of Vertex and Edge Partitions

First we define some useful parameters, which support in the investigation of some predefined (in Table 1) topological indices. For any vertex v of G, these parameters are defined as follows:

(i) The distance number of v in G is $D(v \mid G) = \sum_{u \in V(G)} d(u, v)$
(ii) The sum distance number of v in G is $D_s(v \mid G) = \sum_{u \in V(G)-\{v\}} 1/(D(G) + 1 - d(u, v))$
(iii) The reciprocal distance number of v in G is $D_r(v \mid G) = \sum_{u \in V(G)} 1/(d(u, v))$

According to these parameters, the distance-based topological indices, listed in Table 1, become

Table 3: Edge partition of Γ_G for each edge $u \sim v \in E(\Gamma_G)$.

n is	(d_u, d_v) type edges	(S_u, S_v) type edges	Number of edges
Odd	$(n-1, n-1)$	(n^2-n+1, n^2-n+1)	$((n-1)(n-2))/2$
Odd	$(n-1, 2n-1)$	(n^2-n+1, n^2-n+1)	$n-1$
Odd	$(1, 2n-1)$	$(2n-n, n^2-n+1)$	n
Even	$(n-1, n-1)$	(n^2+1, n^2+1)	$((n-2)(n-3))/2$
Even	$(n-1, 2n-1)$	$(n^2+1, (n+1)^2)$	$2(n-2)$
Even	$(2n-1, 2n-1)$	$((n+1)^2, (n+1)^2)$	1
Even	$(2n-1, 3)$	$((n+1)^2, 4n+1)$	$2n$
Even	$(3, 3)$	$(4n+1, 4n+1)$	$n/2$

Note: (d_u, d_v) denotes the type of edge $u \sim v$ according to degrees of the end vertices, and (S_u, S_v) denotes the type of edge $u \sim v$ according to degrees sum of the end vertices.

Table 4: Vertex partition of G_Γ for each vertex $v \in V(G_\Gamma)$.

n is	d_v	$\mathrm{ecc}(v)$	$D(v \mid G_\Gamma)$	$D_s(v \mid G_\Gamma)$	$D_r(v \mid G_\Gamma)$	Number of vertices
Odd	$2n-2$	1	$2n-2$	$n-1$	$2n-2$	n
Odd	n	2	$3n-4$	$(1/2)(3n-4)$	$(1/2)(3n-1)$	$n-1$
Even	$2n-2$	2	$2n-2$	$n-1$	$(1/2)(4n-7)$	n
Even	n	2	$3n-6$	$(3/2)(n-2)$	$(3/2)(n-1)$	$n-2$

Table 5: Edge partition of G_Γ for each edge $u \sim v \in E(G_\Gamma)$.

n is	(d_u, d_v) type edges	(S_u, S_v) type edges	Number of edges
Odd	$(n, 2n-2)$	$(2n(n-1), (n-1)(3n-2))$	$n(n-1)$
Odd	$(2n-2, 2n-2)$	$((n-1)(3n-2), (n-1)(3n-2))$	$(n(n-1))/2$
Even	$(n, 2n-4)$	$(2n(n-2), (n-2)(3n-4))$	$n(n-2)$
Even	$(2n-4, 2n-4)$	$((n-2)(3n-4), (n-2)(3n-4))$	$(n(n-2))/2$

Note: (d_u, d_v) denotes the type of edge $u \sim v$ according to degrees of the end vertices, and (S_u, S_v) denotes the type of edge $u \sim v$ according to degrees sum of the end vertices.

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} D(v \mid G), \tag{6}$$

$$\mathrm{RCW}(G) = \frac{|G|}{D(G)+1} + \frac{1}{2} \sum_{v \in V(G)} D_s(v \mid G), \tag{7}$$

$$\mathrm{MTI}(G) = \sum_{v \in V(G)} (d(v))^2 + \sum_{v \in V(G)} d(v) D(v \mid G), \tag{8}$$

$$H(G) = \frac{1}{2} \sum_{v \in V(G)} D_r(v \mid G). \tag{9}$$

Let Γ_G be a commuting graph of the dihedral group D_n. In Γ_G, there are $2n$ vertices. The number of edges in Γ_G is $(n(n+1))/2$ when n is odd and is $(n(n+4))/2$ when n is even. Based on the degree, distance number, sum distance number, and reciprocal distance number of each vertex of Γ_G, the useful vertex partition is given in Table 2. Based on degrees and degrees sum of the end vertices of each edge of Γ_G, the useful edge partition is given in Table 3.

Let G_Γ be a non-commuting graph of the dihedral group D_n. In G_Γ,

(1) There are $2n-1$ vertices and $(3/2)n(n-1)$ edges when n is odd

(2) There are $2n-2$ vertices and $(3/2)n(n-2)$ edges when n is even

Based on the degree, eccentricity, distance number, sum distance number, and reciprocal distance number of each vertex of G_Γ, the useful vertex partition is given in Table 4. Based on degrees and degrees sum of the end vertices of each edge of G_Γ, the useful edge partition is given in Table 5.

4. Topological Properties of Commuting Graph Γ_G

In this section, we compute the Wiener, reciprocal complementary Wiener, MTI, Harary general Randić, ABC, ABC_4, GA, GA_5, and harmonic indices of Γ_G. Throughout this section, in each of the two-row equation arrays, the first row corresponds to odd values of n, while the second corresponds to even values of n.

Theorem 1. *For $n \geq 3$, let Γ_G be a commuting graph on D_n, then*

$$W(\Gamma_G) = \begin{cases} \dfrac{n}{2}(7n-5), & \text{when } n \text{ is odd}, \\ \dfrac{n}{2}(7n-8), & \text{when } n \text{ is even}. \end{cases} \quad (10)$$

Proof. Using the vertex partition, given in Table 2, in formula (6) of the Wiener index, we have

$$W(\Gamma_G) = \begin{cases} \dfrac{(n-1)(3n-1)+(2n-1)+n(4n-3)}{2}, & \text{when } n \text{ is odd}, \\ \dfrac{(n-2)(3n-1)+2(2n-1)+n(4n-5)}{2}, & \text{when } n \text{ is even}. \end{cases} \quad (11)$$

Now, the required Wiener index can be obtained after some simplifications. □

Theorem 2. *For $n \geq 3$, let Γ_G be a commuting graph on D_n, then*

$$\mathrm{RCW}(\Gamma_G) = \begin{cases} \dfrac{7n}{12}(3n-1), & \text{when } n \text{ is odd}, \\ \dfrac{n}{12}(21n-16), & \text{when } n \text{ is even}. \end{cases} \quad (12)$$

Proof. Since the diameter of G_Γ is 2, so by using the vertex partition, given in Table 4, in formula (7) of the reciprocal complimentary Wiener index, we have

$$\mathrm{RCW}(\Gamma_G) = \begin{cases} \dfrac{2n}{3} + \dfrac{1}{2}\left(\dfrac{n}{2}(4n-3) + \dfrac{1}{2}(2n-1) + \dfrac{1}{2}(n-1)(3n-1)\right), & \text{when } n \text{ is odd}, \\ \dfrac{2n}{3} + \dfrac{1}{2}\left(\dfrac{n}{2}(4n-5) + (2n-1) + \dfrac{1}{2}(n-2)(3n-1)\right), & \text{when } n \text{ is even}. \end{cases} \quad (13)$$

Now, the required index can be easily found by performing some simplifications. □

Theorem 3. *For $n \geq 3$, let Γ_G be a commuting graph on D_n, then*

$$\mathrm{MTI}(\Gamma_G) = \begin{cases} 2n(2n-1)(n+1), & \text{when } n \text{ is odd}, \\ 2n(2n-1)(n+4), & \text{when } n \text{ is even}. \end{cases} \quad (14)$$

Proof. By applying formula (8) of the Schultz molecular topological index using the vertex partition, given in Table 2, we have when n is odd

$$\begin{aligned} \mathrm{MTI}(\Gamma_G) &= (n-1)^3 + (2n-1)^2 + n + (n-1)^2(3n-1) \\ &\quad + (2n-1)^2 + n(4n-3) \\ &= 2n(2n-1)(n+1), \end{aligned} \quad (15)$$

and when n is even

$$\begin{aligned} \mathrm{MTI}(\Gamma_G) &= (n-2)(n-1)^2 + 2(2n-1)^2 + n(3)^2 \\ &\quad + (n-2)(n-1)(3n-1) + 2(2n-1)^2 \\ &\quad + 3n(4n-5) = 2n(2n-1)(n+4). \end{aligned} \quad (16)$$

□

Theorem 4. *For $n \geq 3$, let Γ_G be a commuting graph on D_n, then*

$$H(\Gamma_G) = \begin{cases} \dfrac{n}{4}(5n-1), & \text{when } n \text{ is odd}, \\ \dfrac{n}{4}(5n+2), & \text{when } n \text{ is even}. \end{cases} \quad (17)$$

Proof. Using the vertex partitions, given in Table 2, in formula (9) of the Harary index, we have

$$H(\Gamma_G) = \begin{cases} \frac{1}{2}\left(\frac{(n-1)(3n-2)}{2} + 2n - 1 + n^2\right), & \text{when } n \text{ is odd,} \\ \frac{1}{2}\left(\frac{(n-2)(3n-2)}{2} + 2(2n-1) + n(n+1)\right), & \text{when } n \text{ is even.} \end{cases} \quad (18)$$

Some easy simplifications yield the required Harary index. □

Theorem 5. *For $n \geq 3$, let Γ_G be a commuting graph of $\Gamma = D_n$. Then, for odd values of n,*

$$R_\alpha(\Gamma_G) = \begin{cases} \frac{n}{2}\left(n^3 - n^2 + 3n - 1\right), & \text{for } \alpha = 1, \\ \frac{n(4n-5)}{(2n-2)(2n-1)}, & \text{for } \alpha = -1, \\ \frac{(n-1)^2(n-2) + 2(n-1)\sqrt{(n-1)(2n-1)} + 2n\sqrt{2n-1}}{2}, & \text{for } \alpha = \frac{1}{2}, \\ \frac{n - 2\sqrt{2n-1} + 2\sqrt{n-1} + 2n}{2\sqrt{2n-1}}, & \text{for } \alpha = -\frac{1}{2}, \end{cases} \quad (19)$$

and for even values of n,

$$R_\alpha(\Gamma_G) = \begin{cases} \frac{1}{2}\left((n-1)^2\left(n^2 - 5n + 6\right) + 2(2n-1)\left(2n^2 + 2n + 3\right) + 9n\right), & \text{for } \alpha = 1, \\ \frac{9(2n-1)(2n^3 - 7n^2 + 5n + 2)^2(4n^3 + 20n^2 - 11n + 18)}{18(n-1)^2(2n-1)^2}, & \text{for } \alpha = -1, \\ \frac{(n-1)(n-2)(n-3) + 7n - 2 + 4\sqrt{2n-1}\,((n-2)\sqrt{n-1} + n\sqrt{3})}{2}, & \text{for } \alpha = \frac{1}{2}, \\ \frac{2n(n-1)(2n-7) + 3(5n-4)}{3(n-1)(2n-1)} + \frac{2(n-2)\sqrt{3} + 2n\sqrt{n-1}}{\sqrt{3(2n-1)(n-1)}}, & \text{for } \alpha = -\frac{1}{2}. \end{cases} \quad (20)$$

Proof. Using the edge partition, given in Table 3, in the formula of general Randić index R_α for $\alpha = 1, -1, (1/2), -(1/2)$, we have

$$R_1(\Gamma_G)=\begin{cases}\dfrac{(n-1)^3(n-2)}{2}+(n-1)^2(2n-1)+n(2n-1),\\[2ex] \dfrac{(n-2)(n-3)(n-1)^2}{2}+2(n-2)(n-1)(2n-1)+(2n-1)^2+6n(2n-1)+\dfrac{9n}{2},\end{cases}$$

$$R_{-1}(\Gamma_G)=\begin{cases}\dfrac{(n-2)}{2(n-1)}+\dfrac{1}{2n-1}+\dfrac{n}{2n-1},\\[2ex] \dfrac{(n-2)(n-3)}{2(n-1)^2}+\dfrac{2(n-2)}{(n-1)(2n-1)}+\dfrac{1}{(2n-1)^2}+\dfrac{2n}{3(2n-1)}+\dfrac{n}{18},\end{cases}$$

$$R_{1/2}(\Gamma_G)=\begin{cases}\dfrac{(n-1)(n-2)\sqrt{(n-1)^2}}{2}+(n-1)\sqrt{(n-1)(2n-1)}+n\sqrt{2n-1},\\[2ex] \dfrac{(n-2)(n-3)(n-1)}{2}+2(n-2)\sqrt{(n-1)(2n-1)}+2n-1+2n\sqrt{3(2n-1)}+\dfrac{3n}{2},\end{cases}\tag{21}$$

$$R_{-(1/2)}(\Gamma_G)=\begin{cases}\dfrac{(n-1)(n-2)}{2\sqrt{(n-1)(n-1)}}+\dfrac{(n-1)}{\sqrt{(n-1)(2n-1)}}+\dfrac{n}{\sqrt{2n-1}},\\[2ex] \dfrac{(n-2)(n-3)}{2(n-1)}+\dfrac{2(n-2)}{\sqrt{(n-1)(2n-1)}}+\dfrac{1}{2n-1}+\dfrac{2n}{\sqrt{3(2n-1)}}+\dfrac{n}{6}.\end{cases}$$

After a minor simplification, we get our required result. □

Theorem 6. *For $n \geq 3$, let Γ_G be a commuting graph of $\Gamma = D_n$, then*

$$GA(\Gamma_G)=\begin{cases}\dfrac{(n-1)(n-2)}{2}+\dfrac{2(n-1)\sqrt{(n-1)(2n-1)}}{3n-2}+\sqrt{2n-1},\\[2ex] \dfrac{n^2-4n+8}{2}+\dfrac{4(n^2-n-2)\sqrt{2n^2-3n+1}+2n(3n-2)\sqrt{3(2n-1)}}{(n+1)(3n-2)},\end{cases}$$

$$GA_5(\Gamma_G)=\begin{cases}\dfrac{n(n^2-1)+4\sqrt{n^3+(n-1)^3}}{2(n+1)},\\[2ex] \dfrac{n^2-4n+8}{2}+\dfrac{2(n-2)(n+1)\sqrt{n^2+1}}{n^2+n+1}+\dfrac{4n(n+1)\sqrt{4n+1}}{n^2+6n+2}.\end{cases}\tag{22}$$

Proof. Applying formulas of the geometric arithmetic index and its fifth version, using the edge partition given in Table 3, we have

$$\mathrm{GA}(\Gamma_G) = \begin{cases} \dfrac{2(n-1)^2(n-2)}{2(2n-2)} + \dfrac{2(n-1)\sqrt{(n-1)(2n-1)}}{3n-2} + \dfrac{2n\sqrt{2n-1}}{2n}, \\ \dfrac{(n-2)(n-3)}{2} + \dfrac{4(n-2)\sqrt{(n-1)(2n-1)}}{3n-2} + 1 + \dfrac{2n\sqrt{3(2n-1)}}{n+1} + \dfrac{n}{2}, \end{cases}$$

$$\mathrm{GA}_5(\Gamma_G) = \begin{cases} \dfrac{2n(n-1)\sqrt{(n^2-n+1)^2}}{4(n^2-n+1)} + \dfrac{2n\sqrt{(n^2-n+1)(2n-1)}}{n(n+1)}, \\ \dfrac{(n-2)(n-3)}{2} + \dfrac{4(n-2)\sqrt{(n^2+1)(n+1)^2}}{2n^2+2n+2} + 1 + \dfrac{4n\sqrt{(n+1)^2(4n+1)}}{n^2+6n+2} + \dfrac{n}{2}. \end{cases} \quad (23)$$

The required values of the geometric arithmetic index and its fifth version can be obtained after some simplifications. □

Theorem 7. *For $n \geq 3$, let Γ_G be a commuting graph of $\Gamma = D_n$, then*

$$\mathrm{ABC}(\Gamma_G) = \begin{cases} \dfrac{(n-2)\sqrt{(n-2)(2n-1)} + \sqrt{2(n-1)(3n-4)} + 2n\sqrt{n-1}}{\sqrt{2(2n-1)}}, \\ \dfrac{(n-2)(n-3)\sqrt{2(n-2)}}{2(n-1)} + \dfrac{2\sqrt{n-1}}{(2n-1)} + \dfrac{n}{3} + \dfrac{2n\sqrt{2n(n-1)} + 2(n-2)\sqrt{3(3n-4)}}{\sqrt{3(n-1)(2n-1)}}, \end{cases}$$

$$\mathrm{ABC}_4(\Gamma_G) = \begin{cases} \dfrac{n(n-1)\sqrt{2n(n-1)}}{2(n^2-n+1)} + n\sqrt{\dfrac{n^2+n-2}{(2n-1)(n^2-n+1)}}, \\ \dfrac{n(n-2)(n-3)\sqrt{2}}{2(n^2+1)} + \dfrac{2(n-2)}{n+1}\sqrt{\dfrac{2n(n+1)}{n^2+1}} + \dfrac{\sqrt{2n(n+2)}}{(n+1)^2} + \dfrac{2n}{n+1}\sqrt{\dfrac{n(n+6)}{4n+1}} + \dfrac{n\sqrt{2n}}{4n+1}. \end{cases} \quad (24)$$

Proof. By using the edge partition, given in Table 3, in formulas of ABC and ABC_4 indices, we have

$$\mathrm{ABC}(\Gamma_G) = \begin{cases} \dfrac{(n-2)\sqrt{2(n-2)}}{2} + (n-1)\sqrt{\dfrac{3n-4}{(n-1)(2n-1)}} + n\sqrt{\dfrac{2(n-1)}{2n-1}}, \\ \dfrac{(n-2)(n-3)\sqrt{2(n-2)}}{2(n-1)} + 2(n-2)\sqrt{\dfrac{3n-4}{(n-1)(2n-1)}} + \dfrac{2\sqrt{n-1}}{2n-1} + \dfrac{n}{3} + 2n\sqrt{\dfrac{2n}{3(2n-1)}}. \end{cases} \quad (25)$$

Also, for odd values of n, we have

$$\mathrm{ABC}_4(\Gamma_G) = \frac{n(n-1)}{2}\sqrt{\frac{(n^2-n+1)+(n^2-n+1)-2}{(n^2-n+1)(n^2-n+1)}} + n\sqrt{\frac{(n^2-n+1)+(2n-1)-2}{(n^2-n+1)(2n-1)}}, \quad (26)$$

and for even values of n, we have

$$\mathrm{ABC}_4(\Gamma_G) = \frac{(n-2)(n-3)\sqrt{2n^2}}{2(n^2+1)} + \frac{2(n-2)}{n+1}\sqrt{\frac{2n^2+2n}{n^2+1}} + \frac{\sqrt{2n^2+4n}}{(n+1)^2} + \frac{2n}{n+1}\sqrt{\frac{n^2+6n}{4n+1}} + \frac{n\sqrt{8n}}{2(4n+1)}. \quad (27)$$

The required formulas for both the indices one can get by performing an easy simplification. □

Theorem 8. *For $n \geq 3$, let Γ_G be a commuting graph of $\Gamma = D_n$, then*

$$H_r(\Gamma_G) = \begin{cases} \dfrac{3n^2+2n-4}{2(3n-2)}, \\ \dfrac{(n-2)(3n^2-3n-2)}{2(n-1)(3n-2)} + \dfrac{6(n+1)+n(2n-1)(n+13)}{6(n+1)(2n-1)}. \end{cases} \tag{28}$$

Proof. By applying the formula of the harmonic index, using the edge partition given in Table 3, we have

$$H_r(\Gamma_G) = \begin{cases} \dfrac{(n-1)(n-2)}{2(n-1)} + \dfrac{2(n-1)}{3n-2} + 1, \\ \dfrac{(n-2)(n-3)}{2(n-1)} + \dfrac{4(n-2)}{3n-2} + \dfrac{1}{2n-1} + \dfrac{2n}{n+1} + \dfrac{n}{6}. \end{cases} \tag{29}$$

Some simplifications yield the required values of the harmonic index. □

5. Topological Properties of Noncommuting Graph G_Γ

In this section, we compute the reciprocal complementary Wiener, Harary, general Randić, ABC, ABC_4, GA, GA_5, and harmonic indices of G_Γ.

Theorem 9. *For $n \geq 3$, let G_Γ be a noncommuting graph of $\Gamma = D_n$, then*

$$\mathrm{RCW}(G_\Gamma) = \begin{cases} \dfrac{1}{12}\left(15n^2-19n+4\right), & \text{when } n \text{ is odd}, \\ \dfrac{1}{12}\left(15n^2-34n+28\right), & \text{when } n \text{ is even}. \end{cases} \tag{30}$$

Proof. Since the diameter of G_Γ is 2, so by sing the vertex partition, given in Table 4, in formula (7) of the reciprocal complimentary Wiener index, we have

$$\mathrm{RCW}(G_\Gamma) = \begin{cases} \dfrac{2n-1}{3} + \dfrac{n(n-1)}{2} + \dfrac{(n-1)(3n-4)}{4}, & \text{when } n \text{ is odd}, \\ \dfrac{2n-2}{3} + \dfrac{n(n-1)}{2} + \dfrac{3(n-2)(n-2)}{4}, & \text{when } n \text{ is even}. \end{cases} \tag{31}$$

Exact values for this index are due to some easy calculations. □

Theorem 10. *For $n \geq 3$, let G_Γ be a noncommuting graph of $\Gamma = D_n$, then*

$$H(G_\Gamma) = \begin{cases} \dfrac{1}{4}\left(7n^2-8n+1\right), & \text{when } n \text{ is odd}, \\ \dfrac{1}{4}\left(7n^2-16n+6\right), & \text{when } n \text{ is even}. \end{cases} \tag{32}$$

Proof. By sing the vertex partition, given in Table 4, in formula (9) of the Harary index, we have

$$H(G_\Gamma) = \begin{cases} \dfrac{n(2n-2)}{2} + \dfrac{(n-1)(3n-1)}{4}, & \text{when } n \text{ is odd}, \\ \dfrac{n(4n-7)}{4} + \dfrac{3(n-2)(n-1)}{4}, & \text{when } n \text{ is even}. \end{cases} \tag{33}$$

By performing some algebraic computations, one can obtain the required Harary index. □

Theorem 11. *For $n \geq 3$, let G_Γ be a noncommuting graph of $\Gamma = D_n$. Then, for odd values of n,*

$$R_\alpha(G_\Gamma) = \begin{cases} 2n(n-1)^2(2n-1), & \text{for } \alpha = 1, \\ \dfrac{5n-4}{8(n-1)}, & \text{for } \alpha = -1, \\ n(n-1)\sqrt{2n(n-1)} + n - 1, & \text{for } \alpha = \dfrac{1}{2}, \\ \sqrt{\dfrac{n(n-1)}{2}} + \dfrac{n}{4}, & \text{for } \alpha = -\dfrac{1}{2}, \end{cases} \tag{34}$$

and for even values of n,

$$R_\alpha(G_\Gamma) = \begin{cases} 4n(n-2)^2(n-1), & \text{for } \alpha = 1, \\ \dfrac{10n-16}{16n-32}, & \text{for } \alpha = -1, \\ n(n-2)\sqrt{n(2n-4)} + n(n-2)^2, & \text{for } \alpha = \dfrac{1}{2}, \\ \dfrac{4n(n-2) + n\sqrt{2n(n-2)}}{4\sqrt{2n(n-2)}}, & \text{for } \alpha = -\dfrac{1}{2}. \end{cases} \tag{35}$$

Proof. Using the edge partition, given in Table 5, in the formula of general Randić index R_α for $\alpha = 1, -1, 1/2, -(1/2)$, we have

$$\begin{aligned} R_1(G_\Gamma) &= \begin{cases} n^2(n-1)(2n-2) + \dfrac{n(n-1)(2n-2)^2}{2}, & \text{when } n \text{ is odd}, \\ n^2(n-2)(2n-4) + \dfrac{n(n-2)(2n-4)^2}{2}, & \text{when } n \text{ is even}, \end{cases} \\ R_{-1}(G_\Gamma) &= \begin{cases} \dfrac{n(n-1)}{n(2n-2)} + \dfrac{n(n-1)}{2(2n-2)^2}, & \text{when } n \text{ is odd}, \\ \dfrac{n(n-2)}{n(2n-4)} + \dfrac{n(n-2)}{2(2n-4)^2}, & \text{when } n \text{ is even}, \end{cases} \\ R_{1/2}(G_\Gamma) &= \begin{cases} n(n-1)\sqrt{n(2n-2)} + \dfrac{n(n-1)(2n-2)}{2}, & \text{when } n \text{ is odd}, \\ n(n-2)\sqrt{n(2n-4)} + \dfrac{n(n-2)(2n-4)}{2}, & \text{when } n \text{ is even}, \end{cases} \\ R_{-(1/2)}(G_\Gamma) &= \begin{cases} \dfrac{n(n-1)}{\sqrt{n(2n-2)}} + \dfrac{n(n-1)}{2(2n-2)}, & \text{when } n \text{ is odd}, \\ \dfrac{n(n-2)}{\sqrt{n(2n-4)}} + \dfrac{n(n-2)}{2(2n-4)}, & \text{when } n \text{ is even}. \end{cases} \end{aligned} \tag{36}$$

By performing some simplifications, we get the required results. □

Theorem 12. *Let G_Γ be a noncommuting graph of $\Gamma = D_n$, for $n \geq 3$, then*

$$\mathrm{GA}(G_\Gamma)=\begin{cases}\dfrac{2(2n(n-1))^{3/2}+n(n-1)(3n-2)}{2(3n-2)}, & \text{when } n \text{ is odd},\\[2ex] \dfrac{2(2n(n-2))^{3/2}+n(n-2)(3n-4)}{2(3n-4)}, & \text{when } n \text{ is even},\end{cases}$$
$$\mathrm{GA}_5(G_\Gamma)=\begin{cases}\dfrac{4n\sqrt{2n(n-1)^2(3n-2)}+n(n-1)(5n-2)}{10n-4}, & \text{when } n \text{ is odd},\\[2ex] \dfrac{n(n-2)(5n-4+\sqrt{32n(3n-4)})}{10n-8}, & \text{when } n \text{ is even}.\end{cases} \quad (37)$$

Proof. Applying formulas of the geometric arithmetic index and its fifth version, using the edge partition given in Table 5, we have

$$\mathrm{GA}(G_\Gamma)=\begin{cases}\dfrac{2n(n-1)\sqrt{n(2n-2)}}{3n-2}+\dfrac{n(n-1)}{2}, & \text{when } n \text{ is odd},\\[2ex] \dfrac{2n(n-2)\sqrt{n(2n-4)}}{3n-4}+\dfrac{n(n-2)}{2}, & \text{when } n \text{ is even},\end{cases}$$
$$\mathrm{GA}_5(G_\Gamma)=\begin{cases}\dfrac{2n(n-1)\sqrt{2n(n-1)^2(3n-2)}}{2n(n-1)+(n-1)(3n-2)}+\dfrac{n(n-1)}{2}, & \text{when } n \text{ is odd},\\[2ex] \dfrac{2n(n-2)\sqrt{2n(n-2)^2(3n-4)}}{2n(n-2)+(n-2)(3n-4)}+\dfrac{n(n-2)}{2}, & \text{when } n \text{ is even}.\end{cases} \quad (38)$$

The required values of the geometric arithmetic index and its fifth version can be obtained after some simplifications. □

Theorem 13. *For $n \geq 3$, let G_Γ be a noncommuting graph of $\Gamma = D_n$, then*

$$\mathrm{ABC}(G_\Gamma)=\begin{cases}\sqrt{\dfrac{n(n-1)(3n-4)}{2}}+\sqrt{\dfrac{n^2(2n-3)}{8}}, & \text{when } n \text{ is odd},\\[2ex] \sqrt{\dfrac{n(n-2)(3n-6)}{2}}+\dfrac{n\sqrt{4n-10}}{4}, & \text{when } n \text{ is even},\end{cases}$$
$$\mathrm{ABC}_4(G_\Gamma)=\begin{cases}\sqrt{\dfrac{n^2(n-1)^2(5n^2-7n)}{6n^4-16n^3+14n^2-4n}}+\dfrac{\sqrt{n^2(6n^2-10n+2)}}{2(3n-2)}, & \text{when } n \text{ is odd},\\[2ex] \sqrt{\dfrac{5n^3-14n^2+6n}{3n-4}}+\dfrac{\sqrt{2n^2(n-1)(3n-7)}}{2(3n-4)}, & \text{when } n \text{ is even}.\end{cases} \quad (39)$$

Proof. By using the edge partition, given in Table 5, in formulas of ABC and ABC_4 indices, we have

$$\mathrm{ABC}\left(G_\Gamma\right)=\begin{cases} n(n-1)\sqrt{\dfrac{3n-4}{2n(n-1)}}+\dfrac{n(n-1)\sqrt{4n-6}}{2(2n-2)}, & \text{when } n \text{ is odd,}\\[2ex] n(n-2)\sqrt{\dfrac{3n-6}{n(2n-4)}}+\dfrac{n(n-2)\sqrt{4n-10}}{2(2n-4)}, & \text{when } n \text{ is even.}\end{cases} \quad (40)$$

Also, for odd values of n, we have

$$\mathrm{ABC}_4\left(G_\Gamma\right)=n(n-1)\sqrt{\frac{2n(n-1)+(n-1)(3n-2)-2}{2n(n-1)^2(3n-2)}}+\frac{n(n-1)}{2}\sqrt{\frac{2(n-1)(3n-2)-2}{((n-1)(3n-2))^2}}, \quad (41)$$

and for even values of n, we have

$$\mathrm{ABC}_4\left(G_\Gamma\right)=n(n-2)\sqrt{\frac{2n(n-2)+(n-2)(3n-4)-2}{2n(n-2)^2(3n-4)}}+\frac{n(n-2)\sqrt{2(n-2)(3n-4)-2}}{2(n-2)(3n-4)}. \quad (42)$$

The required formulas for both the indices one can get by performing an easy simplification. □

Theorem 14. *For $n \geq 3$, let G_Γ be a noncommuting graph of $\Gamma = D_n$, then*

$$H_r\left(G_\Gamma\right)=\begin{cases}\dfrac{n(11n-10)}{4(3n-2)}, & \text{when } n \text{ is odd,}\\[2ex] \dfrac{n(11n-20)}{4(3n-4)}, & \text{when } n \text{ is even.}\end{cases} \quad (43)$$

Proof. By applying the formula of the harmonic index, using the edge partition given in Table 5, we have

$$H_r\left(G_\Gamma\right)=\begin{cases}\dfrac{2n(n-1)}{3n-2}+\dfrac{n(n-1)}{2(2n-2)}, & \text{when } n \text{ is odd,}\\[2ex] \dfrac{2n(n-2)}{3n-4}+\dfrac{n(n-2)}{2(2n-4)}, & \text{when } n \text{ is even.}\end{cases} \quad (44)$$

Some simplifications yield the required values of the harmonic index. □

6. Concluding Remarks

An algebraic structure plays a vital role in chemistry to form chemical compound structures and in investigating various chemical properties of chemical compounds in these structures. Here, we considered a very well-known algebraic structure, called the group of symmetries of regular gons (the dihedral group), which has remarkable contribution in the theory of electron structures and molecular vibrations. We considered one algebraic property, namely, commutation property, on the dihedral group and associated two graphs (chemical structure) with the group of symmetries. We computed some distance-based and degree-based topological properties of these associated graphs by computing the exact formulae of the Wiener index, reciprocal complementary Wiener index, Schultz molecular topological index, Harary index, Randić index, geometric arithmetic indices, atomic bond connectivity indices, and harmonic index. All the indices are numeric quantities and, in fact, this work is a theoretical contribution in the theory of topological indices with the unique algebraic structure, and it can be very helpful to predict the bioactivity of chemical compounds using physicochemical properties in QSAR/QSPR studied.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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