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Research Article

Some Topological Invariants of Graphs Associated with the Group of Symmetries

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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 $u \not\sim v$. 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)     | \( \sum_{x \in V(G)} d(x,v) \) |
| Reciprocal complementary Wiener index [21] | RCW(G) | \( \sum_{x \in V(G)} d(x,v)^2 \) |
| Schultz molecular topological index [22] | MTI(G) | \( \frac{1}{\sqrt{\sum_{x \in V(G)} d(x,v)}} \) |
| Harary index [23, 24] | H(G) | \( \sum_{x \in V(G)} d(x,v) \) |
| Randić index [10] | \( R_{-\alpha}(G) \) | \( \sum_{x \in V(G)} d(x,v)^{-\alpha} \) |
| General Randić index [11, 12] | \( R_{\alpha}(G) \) | \( \sum_{x \in V(G)} d(x,v)^\alpha \) |
| Geometric arithmetic (GA) index [13] | GA(G) | \( \sum_{x \in V(G)} (d(x,v)^2)^{1/2} \) |
| Fifth version of GA index [4] | GA\(_s\)(G) | \( \sum_{x \in V(G)} (d(x,v)^2)^{1/2} \) |
| Fourth version of ABC index [5] | ABC\(_s\)(G) | \( \sum_{x \in V(G)} (d(x,v)^2)^{1/2} \) |
| Harmonic index [15] | \( H_r(G) \) | \( \sum_{x \in V(G)} (d(x,v)^2)^{1/2} \) |

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 \( ecc(v) \), 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 \( rad(G) \).

The diameter of a graph \( G \) is the maximum eccentricity in \( G \), denoted by \( diam(G) \). A vertex \( v \) in a graph \( G \) is a peripheral vertex if \( ecc(v) = diam(G) \), 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 a central vertex if \( d(u,v) = diam(G) \), and the subgraph of \( G \) induced by central vertices is called the periphery of \( G \). The sum of two graphs \( G_1 \) and \( G_2 \), denoted by \( G_1 \oplus G_2 \), is a graph with vertex set \( V(G_1) \cup V(G_2) \) and an edge set \( E(G_1) \cup E(G_2) \cup \{ u \sim v : u \in V(G_1) \land v \in V(G_2) \} \).

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

(i) The commuting graph of a nonabelian group \( \Gamma \) is denoted by \( C(\Gamma, \Omega) \) with vertex set \( \Omega \subseteq \Gamma \). For two distinct elements \( x, y \in \Gamma \), \( x \sim y \) in \( \Gamma \) if and only if \( xy = yx \in \Gamma \). 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 \( \Gamma \) is a graph with vertex set \( V(G_1) \cup V(G_2) \), and two distinct vertices \( u \) and \( v \) in \( G_2 \) form an edge if \( uv \neq vu \) in \( \Gamma \). 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 \( \Gamma \), \( D(G_\Gamma) = 2 \).

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

Proposition 2. A noncommuting graph \( G_\Gamma \) of any nonabelian finite group \( \Gamma \) 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 \( G_\Gamma \).

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 \( r_k = e, r_1, r_2, \ldots, r_{n-1} \) 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 $\Gamma _v$ for each vertex $v \in V(\Gamma _v)$.

| $n$ is | $d_v$ | $D(v|\Gamma _v)$ | $D_i(v|\Gamma _v)$ | $D_r(v|\Gamma _v)$ | Number of vertices |
|-------|-------|-----------------|-----------------|-----------------|------------------|
| Odd   | $n - 1$ | $3n - 1$ | $\frac{1}{2}(3n - 1)$ | $\frac{1}{2}(3n - 2)$ | $n - 1$ |
| Odd   | $2n - 1$ | $2n - 1$ | $\frac{1}{2}(2n - 1)$ | $2n - 1$ | $1$ |
| Odd   | $1$ | $4n - 3$ | $n$ | $n$ | $n$ |
| Even  | $n - 1$ | $3n - 1$ | $\frac{1}{2}(3n - 1)$ | $\frac{1}{2}(3n - 2)$ | $n - 2$ |
| Even  | $2n - 1$ | $2n - 1$ | $\frac{1}{2}(2n - 1)$ | $2n - 1$ | $2$ |
| Even  | $3$ | $4n - 5$ | $\frac{1}{2}(4n - 5)$ | $n + 1$ | $n$ |

(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) For $u \in V(G_\Gamma ), u \sim v$ whenever $u \in \Omega _2$.
(5) For $u, v \in V(G_\Gamma ), u \sim v$ whenever $u \in \Omega _2$.

In the case of even value of $n \geq 4$, let $\Omega _3$ be a commuting graph on $n/2$ two element subsets. Let $\Omega _3 = \{ a, b, a^2, \ldots, a^{n-1} b \}$, and $\Delta _3 = \Delta _2 - \zeta (\Delta _n)$. Then $\Omega _1 = n - \Omega _3$ and

$$|\Omega _3| = \begin{cases} n - 1, & \text{when } n \text{ is odd,} \\ n - 2, & \text{when } n \text{ is even.} \end{cases}$$

In the case of even value of $n \geq 4$, we partitioned $\Omega _3$ into $n/2$ two element subsets. $\Omega _3 = \{ a, b, a^{(n+2i)+1} \}, 0 \leq i \leq (n/2) - 1$, so that $\Omega _2 = \cap_{i=0}^{(n/2)-1} \Omega _2$.

Remark 1. In the dihedral group $D_n$, we have

(i) $xy = yx$ for all $x, y \in D_2$
(ii) $a^i b = ba^{i-1}$ 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 $x, y \in \Omega _2$, $0 \leq i \leq (n/2) - 1$
(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 $\Gamma _G = \mathcal{C}(D_n, D_n)$ be a commuting graph on $D_n$, then

$$\Gamma _G = \begin{cases} K_1 + \left( K_{|\Omega _1|} \cup N_{|\Omega _1|} \right), & \text{when } n \text{ is odd,} \\ K_2 + \left( K_{|\Omega _1|} \cup \frac{n}{2} K_2 \right), & \text{when } n \text{ is even.} \end{cases}$$

Here, $K_1$ is the trivial graph, $K_n$ is a complete graph on $n$ vertices, $N_1$ 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 $G_\Gamma$ be the corresponding non-commuting graph. Then, according to Remark 1, we have the following points:

When $n \geq 3$ is odd, then

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

with the center

$$\zeta (D_n) = \begin{cases} \{ e \}, & \text{when } n \text{ is odd,} \\ \{ e, a^{n/2} \}, & \text{when } n \text{ is even.} \end{cases}$$  \hspace{1cm} (2)

Let $\Omega _1 = \{ e, a, a^2, \ldots, a^{n-1} \}, \Omega _2 = \{ b, ab, a^2b, \ldots, a^{n-1}b \}$, and $\Omega _3 = \Omega _2 - \zeta (\Delta _n)$. Then $\Omega _1 = n - \Omega _3$ and

$$|\Omega _3| = \begin{cases} n - 1, & \text{when } n \text{ is odd,} \\ n - 2, & \text{when } n \text{ is even.} \end{cases}$$

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

According to these parameters, the distance-based topological indices, listed in Table 1, become
Table 3: Edge partition of $\Gamma_G$ 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    | $(n - 1, 2n - 1)$       | $(n^2 - n + 1, n^2 + n - 1)$ | $3/2$                        |
| Odd    | $(1, 2n - 1)$           | $(2n - n, n^2 - n + 1)$   | $n$                          |
| Even   | $(n - 1, n - 1)$        | $(n^2 + 1, n^2 + n + 1)$ | $((n - 2)(n - 3))/2$         |
| 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   | $(2n - 1, 1, 3)$        | $(n + 1)^2, 4n + 1$      | $2n$                         |
| 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 $G_t$ for each vertex $v \in V(G_t)$.

| $n$ is  | $d_v$ | ecc($v$) | $D(v | G_t)$ | $D_2(v | G_t)$ | $D_4(v | G_t)$ | 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        | $3n - 6$ | $(3/2)(n - 2)$ | $(3/2)(n - 1)$ | $n - 2$ |

Note: $d_v$ 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 5: Edge partition of $G_t$ for each edge $u \sim v \in E(G_t)$.

| $n$ 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.

\[
W(G) = \frac{1}{2} \sum_{v \in V(G)} D(v | G), \quad (6)
\]

\[
RCW(G) = \frac{|G|}{D(G) + 1} + \frac{1}{2} \sum_{v \in V(G)} D_2(v | G), \quad (7)
\]

\[
MTI(G) = \sum_{v \in V(G)} (d(v))^2 + \sum_{v \in V(G)} d(v)D(v | G), \quad (8)
\]

\[
H(G) = \frac{1}{2} \sum_{v \in V(G)} D_4(v | G). \quad (9)
\]

Let $\Gamma_G$ be a commuting graph of the dihedral group $D_n$. In $\Gamma_G$, there are $2n$ vertices. The number of edges in $\Gamma_G$ 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 $\Gamma_G$, the useful vertex partition is given in Table 2. Based on degrees and degrees sum of the end vertices of each edge of $\Gamma_G$, the useful edge partition is given in Table 3.

Let $G_t$ be a non-commuting graph of the dihedral group $D_n$. In $G_t$, $n$.

(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 $G_t$, the useful vertex partition is given in Table 4. Based on degrees and degrees sum of the end vertices of each edge of $G_t$, the useful edge partition is given in Table 5.

4. Topological Properties of Commuting Graph $\Gamma_G$

In this section, we compute the Wiener, reciprocal complementary Wiener, MTI, Harary general Randić, ABC, ABC4, GA, Gα, and harmonic indices of $\Gamma_G$. 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 $\Gamma_G$ be a commuting graph on $D_n$, then
Theorem 2. For $n \geq 3$, let $\Gamma_G$ be a commuting graph on $D_n$, then

$$W(\Gamma_G) = \begin{cases} \frac{n}{2} (7n - 5), & \text{when } n \text{ is odd,} \\ \frac{n}{2} (7n - 8), & \text{when } n \text{ is even.} \end{cases}$$ \hspace{1cm} (10)$$

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

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

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

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

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

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

and when $n$ is even

$$MTI(\Gamma_G) = (n-2)(n-1)^2 + 2(2n-1)^2 + n(3)^2 + (n-2)(n-1)(3n-1) + 2(2n-1)^2 + 3n(4n-5) = 2n(2n-1)(n+4).$$ \hspace{1cm} (16)$$

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

$$MTI(\Gamma_G) = \begin{cases} \frac{n}{4} (5n-1), & \text{when } n \text{ is odd,} \\ \frac{n}{4} (5n+2), & \text{when } n \text{ is even.} \end{cases}$$ \hspace{1cm} (17)$$

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

$$H(\Gamma_G) = \begin{cases} \frac{n}{4} (5n-1), & \text{when } n \text{ is odd,} \\ \frac{n}{4} (5n+2), & \text{when } n \text{ is even.} \end{cases}$$ \hspace{1cm} (18)$$
Some easy simplifications yield the required Harary index.

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

Theorem 5. For \( n \geq 3 \), let \( \Gamma_G \) be a commuting graph of \( \Gamma = D_n \). Then, for odd values of \( n \),

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

and for even values of \( n \),

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

Proof. Using the edge partition, given in Table 3, in the formula of general Randić index \( R_\alpha \) for \( \alpha = 1, -1, (1/2), -(1/2) \), we have
After a minor simplification, we get our required result.

\[ R_1(\Gamma_G) = \frac{(n-1)^3(n-2)}{2} + (n-1)^2(2n-1) + n(2n-1), \]

\[ R_{-1}(\Gamma_G) = \frac{(n-2)(n-3)(n-1)^2}{2} + 2(n-2)(n-1)(2n-1) + (2n-1)^2 + 6n(2n-1) + \frac{9n}{2}, \]

\[ R_{1/2}(\Gamma_G) = \frac{(n-2)(n-3)(n-1)}{2} + 2(n-2)\sqrt{(n-1)(2n-1)} + 2n - 1 + 2n\sqrt{3(2n-1)} + \frac{3n}{2}, \]

\[ R_{-1/2}(\Gamma_G) = \frac{(n-2)(n-3)(n-1)}{2\sqrt{(n-1)(2n-1)}} + \frac{(n-1)}{\sqrt{(n-1)(2n-1)}} + \frac{n}{\sqrt{2n-1}}, \]

\[ R_{-1/3}(\Gamma_G) = \frac{(n-2)(n-3)}{2(n-1)} + \frac{2(n-2)}{\sqrt{(n-1)(2n-1)}} + \frac{1}{2n-1} + \frac{2n}{\sqrt{3(2n-1)}} + \frac{n}{6}. \]

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

\[ \text{GA}(\Gamma_G) = \begin{cases} 
\frac{(n-1)(n-2)}{2} + \frac{2(n-1)\sqrt{(n-1)(2n-1)}}{3n-2} + \sqrt{2n-1}, \\
\frac{n^2 - 4n + 8}{2} + \frac{4(n^2 - n - 2)\sqrt{2n^2 - 3n + 1} + 2n(3n-2)\sqrt{3(2n-1)}}{(n+1)(3n-2)}, \\
\frac{n(n^2 - 1) + 4\sqrt{n^3 + (n-1)^3}}{2(n+1)} \\
\frac{n^2 - 4n + 8}{2} + \frac{2(n-2)(n+1)\sqrt{n^2 + 1}}{n^2 + n + 1} + \frac{4n(n+1)\sqrt{4n+1}}{n^2 + 6n + 2}. 
\end{cases} \]

**Proof.** Applying formulas of the geometric arithmetic index and its fifth version, using the edge partition given in Table 3, we have
\[
\text{GA}(\Gamma_G) = \begin{cases} 
\frac{2(n-1)^2(n-2)}{2(2n-2)} + \frac{2(n-1)\sqrt{(n-1)(2n-1)}}{3n-2} + \frac{2n\sqrt{2n-1}}{2n} , \\
\frac{(n-2)(n-3)}{2} + \frac{4(n-2)\sqrt{(n-1)(2n-1)}}{3n-2} + 1 + \frac{2n\sqrt{3(2n-1)}}{n+1} + \frac{n}{2}, \\
\end{cases}
\]
\[
\text{GA}_3(\Gamma_G) = \begin{cases} 
\frac{2(n-1)\sqrt{(n^2-n+1)^2}}{4(n^2-n+1)} + \frac{2n\sqrt{(n^2-n+1)(2n-1)}}{n(n+1)} , \\
\frac{(n-2)(n-3)}{2} + \frac{4(n-2)\sqrt{(n^2+1)(n+1)^2}}{2n^2+2n+2} + 1 + \frac{4n\sqrt{(n+1)^2(4n+1)}}{n^2+6n+2} + \frac{n}{2}, \\
\end{cases}
\]

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

\[\text{Theorem 7.} \text{ For } n \geq 3, \text{ let } \Gamma_G \text{ be a commuting graph of } \Gamma = D_n, \text{ then}\]

\[\text{ABC}(\Gamma_G) = \begin{cases} 
\frac{(n-2)\sqrt{(n-2)(2n-1)}}{\sqrt{2(2n-1)}} + \frac{2\sqrt{n-1}}{2n-1} + \frac{n\sqrt{2n-1}}{2n-1}, \\
\frac{(n-2)(n-3)\sqrt{2(n-2)}}{2(n-1)} + \frac{2\sqrt{n-1}}{2(n-1)} + \frac{n\sqrt{2n(n-1)} + 2(n-2)\sqrt{3(2n-4)}}{\sqrt{3(n-1)(2n-1)}}, \\
\end{cases}\]

\[\text{ABC}_4(\Gamma_G) = \begin{cases} 
\frac{n(n-1)\sqrt{2n(n-1)}}{2(n^2-n+1)} + \frac{n\sqrt{n^2+n-2}}{2(n-1)(n^2-n+1)}, \\
\frac{n(n-2)(n-3)\sqrt{2(n-2)}}{2(n^2+1)} + \frac{2\sqrt{n(n+1)}}{n^2+1} + \frac{\sqrt{2n(n+2)}}{(n+1)^2} + \frac{2n}{n+1} + \frac{n\sqrt{2n}}{4n+1} + \frac{n\sqrt{2n}}{4n+1}, \\
\end{cases}\]

Proof. By using the edge partition, given in Table 3, in formulas of ABC and ABC\(_4\) indices, we have

\[\text{ABC}(\Gamma_G) = \begin{cases} 
\frac{(n-2)\sqrt{2(n-2)}}{2} + (n-1)\sqrt{\frac{3n-4}{(n-1)(2n-1)}} + n\sqrt{\frac{2(n-1)}{2n-1}}, \\
\frac{(n-2)(n-3)\sqrt{2(n-2)}}{2(n-1)} + 2(n-2)\sqrt{\frac{3n-4}{(n-1)(2n-1)}} + \frac{2\sqrt{n-1}}{2n-1} + \frac{n\sqrt{2n}}{2n-1}, \\
\end{cases}\]

Also, for odd values of \(n\), we have

\[\text{ABC}_4(\Gamma_G) = \begin{cases} 
\frac{n(n-1)}{2} \sqrt{\frac{n^2-n+1 + n^2-n+1 - 2}{(n^2-n+1)(n^2-n+1)}} + n\sqrt{\frac{2(n-1)}{2n-1}}, \\
\frac{n(n-2)(n-3)\sqrt{2(n-2)}}{2(n^2+1)} + \frac{2\sqrt{n-1}}{n+1} + \frac{n\sqrt{2n}}{2n^2 + 2n} + \frac{n\sqrt{2n}}{n^2+1}, \\
\end{cases}\]

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

and for even values of \(n\), we have

\[\text{ABC}(\Gamma_G) = \begin{cases} 
\frac{n(n-1)}{2} \sqrt{\frac{n^2-n+1 + n^2-n+1 - 2}{(n^2-n+1)(n^2-n+1)}} + n\sqrt{\frac{2(n-1)}{2n-1}}, \\
\frac{n(n-2)(n-3)\sqrt{2(n-2)}}{2(n^2+1)} + \frac{2\sqrt{n-1}}{n+1} + \frac{n\sqrt{2n}}{2n^2 + 2n} + \frac{n\sqrt{2n}}{n^2+1}, \\
\end{cases}\]

(26)
Theorem 8. For \( n \geq 3 \), let \( \Gamma_G \) be a commuting graph of \( \Gamma = D_n \), then

\[
H_r(\Gamma_G) = \begin{cases} 
\frac{3n^2 + 2n - 4}{2(3n - 2)} \\
\frac{(n - 2)(3n^2 - 3n - 2)}{2(n - 1)(3n - 2)} + \frac{6(n + 1) + n(2n - 1)(n + 13)}{6(n + 1)(2n - 1)}.
\end{cases}
\]  

\hspace{1cm} (28)

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

\[
H_r(\Gamma_G) = \begin{cases} 
\frac{(n - 1)(n - 2)}{2(n - 1)} + \frac{2(n - 1)}{3n - 2} + 1, \\
\frac{(n - 2)(n - 3)}{2(n - 1)} + \frac{4(n - 2)}{3n - 2} + \frac{1}{2n - 1} + \frac{2n}{n + 1} + \frac{n}{6}
\end{cases}
\]  

\hspace{1cm} (29)

Some simplifications yield the required values of the harmonic index.

5. Topological Properties of Noncommuting Graph \( G_T \)

In this section, we compute the reciprocal complementary Wiener, Harary, general Randić, ABC, ABC₄, GA, GA₅, and harmonic indices of \( G_T \).

Theorem 9. For \( n \geq 3 \), let \( G_T \) be a noncommuting graph of \( \Gamma = D_n \), then

\[
\text{RCW}(G_T) = \begin{cases} 
\frac{1}{12}(15n^2 - 19n + 4), & \text{when } n \text{ is odd,} \\
\frac{1}{12}(15n^2 - 34n + 28), & \text{when } n \text{ is even.}
\end{cases}
\]  

\hspace{1cm} (30)

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

\[
\text{RCW}(G_T) = \begin{cases} 
\frac{2n - 1}{3} + \frac{n(n - 1)}{2} + \frac{(n - 1)(3n - 4)}{4}, & \text{when } n \text{ is odd,} \\
\frac{2n - 2}{3} + \frac{n(n - 1)}{2} + \frac{3(n - 2)(n - 2)}{4}, & \text{when } n \text{ is even.}
\end{cases}
\]  

\hspace{1cm} (31)

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

Theorem 10. For \( n \geq 3 \), let \( G_T \) be a noncommuting graph of \( \Gamma = D_n \), then

\[
H(G_T) = \begin{cases} 
\frac{1}{4}(7n^2 - 8n + 1), & \text{when } n \text{ is odd,} \\
\frac{1}{4}(7n^2 - 16n + 6), & \text{when } n \text{ is even.}
\end{cases}
\]  

\hspace{1cm} (32)

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

\[
H(G_T) = \begin{cases} 
\frac{n(2n - 2)}{2} + \frac{(n - 1)(3n - 1)}{4}, & \text{when } n \text{ is odd,} \\
\frac{n(4n - 7)}{4} + \frac{3(n - 2)(n - 1)}{4}, & \text{when } n \text{ is even.}
\end{cases}
\]  

\hspace{1cm} (33)

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

Theorem 11. For \( n \geq 3 \), let \( G_T \) be a noncommuting graph of \( \Gamma = D_n \). Then, for odd values of \( n \),
By performing some simplifications, we get the required results.

**Theorem 12.** Let $G_\Gamma$ be a noncommuting graph of $\Gamma = D_n$, for $n \geq 3$, then
Proof. Applying formulas of the geometric arithmetic index and its fifth version, using the edge partition given in Table 5, we have

\[
\begin{align*}
\text{GA}(G_I) &= \begin{cases} 
\frac{2(2n(n-1))^{3/2} + n(n-1)(3n-2)}{2(3n-2)}, & \text{when } n \text{ is odd,} \\
\frac{2(2n(n-2))^{3/2} + n(n-2)(3n-4)}{2(3n-4)}, & \text{when } n \text{ is even,}
\end{cases} \\
\text{GA}_5(G_I) &= \begin{cases} 
\frac{4n\sqrt{2n(n-1)^2(3n-2)} + n(n-1)(5n-2)}{10n-4}, & \text{when } n \text{ is odd,} \\
\frac{n(n-2)(5n-4 + \sqrt{32n(3n-4)})}{10n-8}, & \text{when } n \text{ is even.}
\end{cases}
\end{align*}
\]

(37)

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 \(G_I = D_n\), then

\[
\begin{align*}
\text{ABC}(G_I) &= \begin{cases} 
\sqrt{\frac{n(n-1)(3n-4)}{2} + \frac{n^2(2n-3)}{8}}, & \text{when } n \text{ is odd,} \\
\sqrt{\frac{n(n-2)(3n-6)}{2} + \frac{n\sqrt{4n-10}}{4}}, & \text{when } n \text{ is even,}
\end{cases} \\
\text{ABC}_4(G_I) &= \begin{cases} 
\sqrt{\frac{n^2(n-1)^2(5n^2-7n)}{6n^4-16n^3+14n^2-4n} + \frac{n^2(6n^2-10n+2)}{2(3n-2)}}, & \text{when } n \text{ is odd,} \\
\sqrt{\frac{5n^3-14n^2+6n}{3n-4} + \frac{2n^2(n-1)(3n-7)}{2(3n-4)}}, & \text{when } n \text{ is even.}
\end{cases}
\end{align*}
\]

(39)

Proof. By using the edge partition, given in Table 5, in formulas of ABC and ABC\(_4\) indices, we have
Also, for odd values of \( n \), we have
\[
ABC_4(G_T) = n(n - 1) \sqrt{\frac{2n(n - 1) + (n - 1)(3n - 2) - 2}{2n(n - 1)^2(3n - 2)}} + \frac{n(n - 1)}{2} \sqrt{\frac{2(n - 1)(3n - 2) - 2}{((n - 1)(3n - 2))^2}},
\]
and for even values of \( n \), we have
\[
ABC_4(G_T) = n(n - 2) \sqrt{\frac{2n(n - 2) + (n - 2)(3n - 4) - 2}{2n(n - 2)^2(3n - 4)}} + \frac{n(n - 2)}{2} \sqrt{\frac{2(n - 2)(3n - 4) - 2}{2(n - 2)(3n - 4)}}.
\]

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

**Theorem 14.** For \( n \geq 3 \), let \( G_T \) be a noncommuting graph of \( \Gamma = D_4 \), then
\[
H_r(G_T) = \begin{cases} 
\frac{n(11n - 10)}{4(3n - 2)} & \text{when } n \text{ is odd,} \\
\frac{n(11n - 20)}{4(3n - 4)} & \text{when } n \text{ is even.}
\end{cases}
\]

**Proof.** By applying the formula of the harmonic index, using the edge partition given in Table 5, we have
\[
H_r(G_T) = \begin{cases} 
\frac{2n(n - 1)}{3n - 2} + \frac{n(n - 1)}{2(2n - 2)} & \text{when } n \text{ is odd,} \\
\frac{2n(n - 2)}{3n - 4} + \frac{n(n - 2)}{2(2n - 4)} & \text{when } n \text{ is even.}
\end{cases}
\]

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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