symmetry

MDPI

Article

On the Topological Indices of Commuting Graphs for Finite Non-Abelian Groups

Fawad Ali [1,*], Bilal A. Rather [2], Nahid Fatima [3], Muhammad Sarfraz [4], Asad Ullah [5,*], Khalid Abdulkhaliq M. Alharbi [6] and Rahim Dad [7]

1 Institute of Numerical Sciences, Kohat University of Science & Technology, Kohat 26000, Khyber Pakhtunkhwa, Pakistan
2 Mathematical Sciences Department, College of Science, United Arab Emirate University, Al Ain 15551, Abu Dhabi, United Arab Emirates; bilalahmadrr@gmail.com
3 Department of Mathematics and Sciences, Prince Sultan University, Riyadh 11586, Saudi Arabia; nfatima@psu.edu.sa
4 Department of Mathematics, Sun Yat-sen University, Guangzhou 510275, China; sarfraz@mail2.sysu.edu.cn
5 Department of Mathematical Sciences, University of Lakki Marwat, Lakki Marwat 28420, Khyber Pakhtunkhwa, Pakistan
6 Mechanical Engineering Department, College of Engineering, Umm Al-Qura University, Makkah 24382, Saudi Arabia; kamharbi@uqu.edu.sa
7 Department of Mathematics, University of Science and Technology Bannu, Bannu 28100, Khyber Pakhtunkhwa, Pakistan; rahimdad498@gmail.com
* Correspondence: fawad_ali@kust.edu.pk (F.A.); asad@ulm.edu.pk (A.U.)

Abstract: A topological index is a number generated from a molecular structure (i.e., a graph) that indicates the essential structural properties of the proposed molecule. Indeed, it is an algebraic quantity connected with the chemical structure that correlates it with various physical characteristics. It is possible to determine several different properties, such as chemical activity, thermodynamic properties, physicochemical activity, and biological activity, using several topological indices, such as the geometric-arithmetic index, arithmetic-geometric index, Randić index, and the atom-bond connectivity indices. Consider $\mathcal{G}$ as a group and H as a non-empty subset of $\mathcal{G}$. The commuting graph $\mathcal{C}(\mathcal{G}, H)$, has H as the vertex set, where $h_1, h_2 \in H$ are edge connected whenever h_1 and h_2 commute in $\mathcal{G}$. This article examines the topological characteristics of commuting graphs having an algebraic structure by computing their atomic-bond connectivity index, the Wiener index and its reciprocal, the harmonic index, geometric-arithmetic index, Randić index, Harary index, and the Schultz molecular topological index. Moreover, we study the Hosoya properties, such as the Hosoya polynomial and the reciprocal statuses of the Hosoya polynomial of the commuting graphs of finite subgroups of $SL(2, \mathbb{C})$. Finally, we compute the Z-index of the commuting graphs of the binary dihedral groups.

Keywords: commuting graphs; chemical graphs; finite groups; molecular structure; topological indices; Hosoya index

check for updates

Citation: Ali, F.; Rather, B.A.; Fatima, N.; Sarfraz, M.; Ullah, A.; Alharbi, K.A.M.; Dad, R. On the Topological Indices of Commuting Graphs for Finite Non-Abelian Groups. *Symmetry* **2022**, *14*, 1266. https://doi.org/10.3390/sym14061266

Academic Editor: Alice Miller

Received: 22 May 2022
Accepted: 17 June 2022
Published: 19 June 2022

1. Introduction

The quantitative structure–property relationships (QSPR) studies are provided by the physicochemical characteristics (for example, the stability, boiling point, and strain energy) and the topological indices; namely, the geometric-arithmetic (GA) index, the atom-bond connectivity (ABC) index, as well as the Randić index to identify the biocompatibility of the chemical substances. In fact, a topological index is created by converting a chemical structure (i.e., a graph) to a numeric value. It is a numeric number that quantifies the symmetry of a molecular structure, defines its topology, and is unchangeable under a function that preserves the structure [1]. Certain aspects of chemical compounds with a molecular structure may be investigated using several kinds of topological indices. In

1947, Wiener developed the notion of the first topological index, which he termed the path number while exploring the boiling point of paraffin [2]. As a consequence, the Wiener index was made, which led to the idea of topological indices. Numerous degree-based and distance-based topological indices have been presented and deliberated in recent years, see for instance [3–6].

Well-known chemists utilized Pólya's [7] approach to calculating polynomials to determine the molecular orbital of unsaturated hydrocarbons. The spectrum of a graph has been widely investigated in this context. Hosoya [8] developed this concept in 1988 to calculate the polynomials of various important chemical graphs, referred to as the Hosoya polynomials. Sagan et al. [9] renamed the Hosoya polynomial the Wiener polynomial in 1996. However, most experts keep referring to it as the Hosoya polynomial. The Hosoya polynomial may be used to gain information on distance-based graph invariants. In [10], Cash identified a relationship between the hyper Wiener index and the Hosoya polynomial. Estrada et al. [11] focused on various innovative applications of the extended Wiener indices.

We discuss simple graphs in this article, that is, graphs that do not include loops or multiple edges. Consider $\mathcal{G}$ as a group and H as a non-empty subset of $\mathcal{G}$. The commuting graph $\mathcal{C}(\mathcal{G}, H)$ has H as the vertex set, where $h_1, h_2 \in H$ are edge connected whenever h_1 and h_2 commute in $\mathcal{G}$. Throughout the paper, we denote $\mathcal{C}(\mathcal{G})$ as the commuting graph $\mathcal{C}(\mathcal{G}, \mathcal{G})$ of a group $\mathcal{G}$. Many researchers have examined the commuting graphs in a variety of contexts, including groups of matrices [12,13], commutative rings with zero-divisors [14–17], the dihedral groups [18–21], and the authors of [22,23] discuss several characteristics of the automorphism groups and their associated commuting graphs.

Iranmanesh and Jafarzadeh presented [24] that, for the commuting graphs of $\mathrm{Alt}(n)$ and $\mathrm{Sym}(n)$, respectively, the alternating and symmetric groups of n letters are either disconnected or have a diameter of at most 5. They conjecture in the same paper that an absolute upper limit exists on the diameter of a connected commuting graph of a non-abelian finite group. This conjecture was disproved in [25], which demonstrated an endless collection of special two-groups having commuting graphs of increasing diameter. The central notion of the conjecture, on the other hand, is not far off the mark. Later on, in [26], the authors demonstrated that for every finite group $\mathcal{G}$ having a trivial centre, any connected component of the commuting graph of $\mathcal{G}$ has a diameter of no more than 10. Additionally, several researchers have explored the non-commuting graphs, the connectedness of the commuting graphs, and their metric dimensions, as shown by [27–29].

A matched or independent edge set is a group of edges that have no common vertices. The term "matched" refers to a vertex that is coincident with one of the matching edges. Otherwise, an unmatched vertex exists. The Z-index or the Hosoya index denotes the greatest number of matchings in a graph. Hosoya [30] proposed the Hosoya index in 1971 and later developed it as a general utensil for physical chemistry in [31]. It has now been shown to be effective in a wide range of molecular chemistry problems, including boiling point determination, entropy, and the heat of vaporization. The Hosoya index is a well-known case of a topological index that has considerable importance in combinatorial chemistry. Various researchers examined extremal difficulties relating to the Hosoya index while exploring a variety of graph structures. In [32–34], the extreme properties of various graphs, including unicyclic graphs and trees, were intensively examined.

As provided bounds, Bates et al. [35] examined the commuting involution graphs of special linear groups over fields of characteristic 2. The disc diameters of two and three-dimensional special linear groups are determined. They further presented examples of unbounded dimension commuting involution graphs. The authors of [36] studied the Hosoya characteristics of the non-commuting graphs, while the authors of [3] examined the Hosoya characteristics of the power graphs of finite non-abelian groups. Motivated by their work, we extended the work in [3,35] and focused our attention on the commuting graphs of finite subgroups of $\mathrm{SL}(2,\mathbb{C})$. This article investigates almost all of the topological properties of the commuting graphs of finite subgroups of $\mathrm{SL}(2,\mathbb{C})$ (as listed in Table 1). It is very challenging to calculate the (reciprocal) Hosoya polynomial, as well as the Hosoya index of the commuting graph of a group $\mathcal{G}$. In this regard, we provide both the Hosoya and the reciprocal statuses of Hosoya polynomials. We also discuss the Hosoya index of the commuting graph of a finite group $\mathcal{G}$.

There are still gaps in the current literature regarding the determination of several topological invariants, the Hosoya polynomials, the reciprocal status of Hosoya polynomials, and the Z-index (Hosoya index) of the commuting graphs of finite subgroups of $\mathrm{SL}(2,\mathbb{C})$. The obvious reason is that neither the structure of the commuting graphs is fully characterized nor is it possible to establish handy formulae for these graph invariants for general classes of graphs. In this article, we find all the indices of the commuting graphs as presented in Table 1. We further make an effort and look at one of these problems in this article.

The rest of the paper is organized as follows: Section 2 contains some relevant results and useful definitions for this paper. In Section 3, we explore the construction of vertex and edge partitions. In Section 4, we find numerous topological indices of the commuting graphs of the binary dihedral groups. Section 5 discusses the construction of finite subgroups of $\mathrm{SL}(2,\mathbb{C})$, and their Hosoya properties. The conclusion and future work of the paper is given in Section 7.

2. Basic Notions and Notations

This part reviews several fundamental graph-theoretic properties and well-known findings that will be important later in the article.

Suppose Γ is a simple finite undirected graph. The vertex and edge sets of Γ are represented by $V(\Gamma)$ and $E(\Gamma)$, respectively. The distance from u_1 to u_2 in a connected graph Γ represented by $dis(u_1,\ u_2)$ is the shortest distance between u_1 and u_2. The total number of vertices denoted by $|\Gamma|$ is the order of Γ. Two vertices, v_1 and v_2, are adjacent if there is an edge between them, and we denote them by $v_1 \sim v_2$; otherwise, $v_1 \nsim v_2$. The neighbourhood of u is a collection of all vertices in Γ that are connected to u is indicated by $N(u)$. The valency or degree represented by d_{u_1} of u_1 is the collection of vertices in Γ, which are adjacent to u_1, and $S_u = \sum_{u\in N(u)} d_u$ is the degree sum of u. A $u_1 - u_2$ path having $dis(u_1, u_2)$ length is known as a $u_1 - u_2$ geodesic. The largest distance between a vertex u_1 and any other vertex of Γ is known as the eccentricity, denoted by $ec(u_1)$. The diameter denoted by $diam(\Gamma)$ of Γ is the largest eccentricity among all the vertices of the graph Γ. Furthermore, the radius symbolized by $rad(\Gamma)$ of Γ has the lowest eccentricity among all the vertices of the graph Γ.

Suppose Γ_1 and Γ_2 are two connected graphs, then $\Gamma_1 \vee \Gamma_2$ is the join of Γ_1 and Γ_2 whose vertex and edge sets are $V(\Gamma_1) \cup V(\Gamma_2)$ and $E(\Gamma_1) \cup E(\Gamma_2) \cup \{y \sim z : y \in V(\Gamma_1),\ z \in V(\Gamma_2)\}$, respectively. A complete graph is a graph that has an edge between any single vertex in the graph, and K_n symbolizes it. A t-partite graph is one in which the vertices are or may be partitioned into t distinct independent sets, while a complete t-partite graph is one where any pair of vertices from distinct independent sets has an edge. Other unexplained terminologies and notations were taken from [37].

Table 1. A list of potential topological indices is shown below.

The Index's Name	Symbol	Formula
Wiener index [2]	$W(\Gamma)$	$\sum_{\{v,w\}\in V(\Gamma)} dis(v,w)$
Randić index [5]	$R_{-(\frac{1}{2})}(\Gamma)$	$\sum_{v\sim w} 1/(\sqrt{d_v \times d_w})$
Harary index [38,39]	$\mathcal{H}(\Gamma)$	$\sum_{\{v\neq w\}\in V(\Gamma)} 1/(dis(v,w))$
Harmonic index [40]	$\mathcal{H}_r(\Gamma)$	$\sum_{v\sim w} 2/(d_v + d_w)$
General Randić index [41]	$R_\alpha(\Gamma)$	$\sum_{v\sim w}(d_v \times d_w)^\alpha$
Schultz molecular topological index [42]	$MTI(\Gamma)$	$\sum_{\{v,w\}\in V(\Gamma)}(d_v + d_w)dis(v,w) + \sum_{w\in V(\Gamma)} d^{2/w}$
Reciprocal complementary Wiener index [43]	$RCW(\Gamma)$	$\sum_{\{v,w\}\in V(\Gamma)} 1/(diam(\Gamma) + 1 - dis(v,w))$
Atomic-bond connectivity (ABC) index [43]	$ABC(\Gamma)$	$\sum_{v\sim w} \sqrt{(d_v + d_w - 2)/(d_v \times d_w)}$
Fourth version of ABC index [1]	$ABC_4(\Gamma)$	$\sum_{v\sim w} \sqrt{(S_v + S_w - 2)/(S_v \times S_w)}$
Geometric-arithmetic (GA) index [44]	$GA(\Gamma)$	$\sum_{v\sim w}(2\sqrt{d_v \times d_w})/(d_v + d_w)$
Fifth version of GA index [4]	$GA_5(\Gamma)$	$\sum_{v\sim w}(2\sqrt{S_v \times S_w})/(S_v + S_w)$
Hosoya polynomial [8]	$\mathbb{H}(\Gamma,x)$	$\sum_{i\geq 0} dis(\Gamma,i)x^i$
Reciprocal status Hosoya polynomial [45]	$\mathbb{H}_{rs}(\Gamma,x)$	$\sum_{vw\in E(\Gamma)} x^{rs(v)+rs(w)}$, where $rs(w) = \sum_{v\in V(\Gamma),w\neq v} \frac{1}{dis(w,v)}$

Section 2 defines all of the notations used in formulae.

Definition 1. *The centre of a group $\mathcal{G}$ is specified is given as:*

$$Z(\mathcal{G}) = \{g_1 : g_1 \in \mathcal{G} \text{ and } g_1g_2 = g_2g_1, \text{ for all } g_2 \in \mathcal{G}\}.$$

The special linear group denoted by $\mathrm{SL}(2,\mathbb{C})$ of degree 2 over a field $\mathbb{C}$ is the set of 2×2 matrices whose determinant is 1. We represent the cyclic group of order n by $\mathbb{Z}_n$. Furthermore, the presentation of binary dihedral group BD_{4n} of order $4n$, where $n \in \mathbb{N}$, is shown as follows:

$$\mathrm{BD}_{4n} = \langle y, z \mid y^{2n} = e,\ y^n = z^2,\ zyz^{-1} = y^{-1}\rangle.$$

We now split BD_{4n} as follows:

$$\Omega = \{e, y^n\},\ X_1 = \langle y\rangle,\ X_2 = \bigcup_{i=0}^{n-1} X_2^i, \text{ where } X_2^i = \left\{y^i z,\ y^{n+i}z\right\} \text{ and } X_3 = X_1 \setminus \Omega.$$

Since X_1 is cyclic, its induced subgraph is complete, and it is denoted by K_{2n}. A remarkable feature of BD_{4n} is that the involution y^n and the identity e are adjacent to every other vertex in its commuting graph. Moreover,

$$\mathrm{BT}_{24} = \langle r, s, t \mid r^2 = s^3 = t^3 = rst\rangle,$$

$$\mathrm{BO}_{48} = \langle r, s, t \mid r^2 = s^3 = t^4 = rst\rangle,$$

$$\mathrm{BI}_{120} = \langle r, s, t \mid r^2 = s^3 = t^5 = rst\rangle,$$

are respectively the binary tetrahedral group of order 24, the binary octahedral group of order 48, and the binary icosahedral group of order 120. All these are the finite non-abelian subgroups of $\mathrm{SL}(2,\mathbb{C})$.

We will explore several properties of the aforementioned groups, but the commuting graph of BD_{4n} is our main focus.

Proposition 1 ([46])**.** *The structure of the commuting graphs of finite subgroups of* $\mathrm{SL}(2,\mathbb{C})$ *are:*

$$\mathcal{C}(\mathrm{BD}_{4n}) = K_2 \vee (K_{2n-2} \cup nK_2),$$
$$\mathcal{C}(\mathrm{BT}_{24}) = K_2 \vee (3K_2 \cup 4K_4),$$
$$\mathcal{C}(\mathrm{BO}_{48}) = K_2 \vee (6K_2 \cup 4K_4 \cup 3K_6),$$
$$\mathcal{C}(\mathrm{BI}_{120}) = K_2 \vee (15K_2 \cup 10K_4 \cup 6K_8),$$

where mK_ℓ represents the m copies of K_ℓ.

From the structure of the commuting graph of BD_{4n}, clearly it has $4n$ vertices, and the total number of edges of $\mathcal{C}(BD_{4n})$ is $\frac{n(n+4)}{2}$. The relevant vertex partition of $\mathcal{C}(BD_{4n})$ is shown in Table 2 depending on the sum distance number, reciprocal distance, degree and the distance numbers of any vertex. The usable edge partition for $\mathcal{C}(BD_{4n})$ is presented in Table 3. It is dependent on the degrees and their sum of the end vertices of every edge.

Table 2. Vertex partition of $\mathcal{C}(BD_{4n})$ for any vertex $u \in V(\mathcal{C}(BD_{4n}))$.

d_u	$ec(u)$	$D(u\|\mathcal{C}(BD_{4n}))$	$D_s(u\|\mathcal{C}(BD_{4n}))$	$D_r(u\|\mathcal{C}(BD_{4n}))$	Number of Vertices
$2n-1$	2	$6n-1$	$\frac{1}{2}(6n-1)$	$3n-1$	$2(n-1)$
$4n-1$	$4n-1$	$4n-1$	$\frac{1}{2}(4n-1)$	$4n-1$	2
3	$8n-5$	$8n-5$	$\frac{1}{2}(8n-5)$	$2n+1$	$2n$

Table 3. $\mathcal{C}(BD_{4n})$ is partitioned into edges based on their reciprocal statuses.

Type of Edge	Edge Set's Partition	Edges Count
$u \sim u$	$E_{u\sim u} = \{ab \in E(\mathcal{C}(BD_{4n})) : rs(a) = u, rs(b) = u\}$	$\|E_{u\sim u}\| = \binom{2(n-1)}{2}$
$u \sim v$	$E_{u\sim v} = \{ab \in E(\mathcal{C}(BD_{4n})) : rs(a) = u, rs(b) = v\}$	$\|E_{u\sim v}\| = 4(n-1)$
$v \sim v$	$E_{v\sim v} = \{ab \in E(\mathcal{C}(BD_{4n})) : rs(a) = v, rs(b) = v\}$	$\|E_{v\sim v}\| = 1$
$v \sim w$	$E_{v\sim w} = \{ab \in E(\mathcal{C}(BD_{4n})) : rs(a) = v, rs(b) = w\}$	$\|E_{v\sim w}\| = 4n$
$w \sim w$	$E_{w\sim w} = \{ab \in E(\mathcal{C}(BD_{4n})) : rs(a) = w, rs(b) = w\}$	$\|E_{w\sim w}\| = n$

3. Edge and Vertex Partitions

To begin, we create certain important factors that aid in the analysis of specified topological indices. These parameters are stated as follows for any vertex u of Γ:

1. The distance number of u in Γ is $\mathcal{D}(u|\Gamma) = \sum_{v\in V(\Gamma)} dis(v,u)$.
2. The u's reciprocal distance number in Γ is $\mathcal{D}_r(u|\Gamma) = \sum_{v\in V(\Gamma)} \frac{1}{dis(v,u)}$.
3. The total of u's distances in Γ is $\mathcal{D}_s(u|\Gamma) = \sum_{v\in V(\Gamma)\setminus\{u\}} \frac{1}{(diam(\Gamma)+1-dis(u,v))}$.

The distance-based topological indices mentioned in Table 1, become

$$W(\Gamma) = \frac{1}{2}\sum_{u\in V(\Gamma)} \mathcal{D}(u \mid \Gamma), \tag{1}$$

$$\mathrm{RCW}(\Gamma) = \frac{1}{2}\sum_{u\in V(\Gamma)} \mathcal{D}_s(u \mid \Gamma) + \frac{|\Gamma|}{diam(\Gamma)+1}, \tag{2}$$

$$\mathrm{MTI}(\Gamma) = \sum_{u\in V(\Gamma)} d(u)\mathcal{D}(u \mid \Gamma) + \sum_{u\in V(\Gamma)} (d(u))^2, \tag{3}$$

$$\mathcal{H}(\Gamma) = \frac{1}{2}\sum_{u\in V(\Gamma)} \mathcal{D}_r(u \mid \Gamma). \tag{4}$$

4. Topological Properties

Theorem 1. *The commuting graph $\mathcal{C}(BD_{4n})$ of BD_{4n} satisfies:*

$$W(\mathcal{C}(BD_{4n})) = 2n(7n-4).$$

Proof. We have obtained the Wiener index by using a vertex partition, as shown in Equation (1) and Table 2.

$$W(\mathcal{C}(BD_{4n})) = (n-1)(6n-1) + (4n-1) + n(8n-5).$$

After certain simplifications, the necessary Wiener index can be achieved. □

Theorem 2. *The commuting graph $\mathcal{C}(\mathrm{BD}_{4n})$ of BD_{4n} satisfies:*

$$RCW(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{n}{3}(21n-8).$$

Proof. Given that $\mathcal{C}(\mathrm{BD}_{4n})$ has a diameter of 2, we can get the reciprocal complementary Wiener index by applying the vertex partition described in Equation (2) and Table 2.

$$RCW(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{4n}{3} + \frac{1}{2}(n(8n-5) + (4n-1) + (n-1)(6n-1)).$$

By applying certain simplifications, the appropriate index can be simply determined. □

Theorem 3. *Assume that $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n}. Then*

$$MTI(\mathcal{C}(\mathrm{BD}_{4n})) = 8n(4n-1)(n+2).$$

Proof. By applying the vertex partition from Table 2, apply Equation (3) of the Schultz molecular topological index.

$$\begin{aligned} MTI(\mathcal{C}(\mathrm{BD}_{4n})) &= 2(n-1)(2n-1)^2 + 2(4n-1)^2 + 9n + 2(n-1)(2n-1)(6n-1) \\ &\quad + 2(4n-1)^2 + 6n(8n-5) \\ &= 8n(4n-1)(n+2). \end{aligned}$$

□

Theorem 4. *Let $\mathcal{C}(\mathrm{BD}_{4n})$ be the commuting graph of BD_{4n}. Then*

$$\mathcal{H}(\mathcal{C}(\mathrm{BD}_{4n})) = n(5n+1).$$

Proof. We may use the vertex partitions from Table 2, and in Equation (4) of the Harary index. Then

$$\mathcal{H}(\mathcal{C}(\mathrm{BD}_{4n})) = (n-1)(3n-1) + (4n-1) + n(2n+1).$$

Some straightforward simplifications result in the desired Harary index. □

Theorem 5. *Suppose $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n}. We have:*

$$R_\alpha(\mathcal{C}(\mathrm{BD}_{4n})) = \begin{cases} (2n-1)^2\left(2n^2-5n+3\right) + (4n-1)\left(8n^2+4n+3\right) + 9n, & \text{for } \alpha = 1, \\ \frac{4(4n-1)\left(8n^3-14n^2+5n+1\right)^2\left(16n^3+40n^2-11n+9\right)}{(2n-1)^2(4n-1)^2}, & \text{for } \alpha = -1, \\ (2n-1)(n-1)(2n-3) + (7n-1) + 4\sqrt{4n-1}\left((n-1)\sqrt{2n-1} + n\sqrt{3}\right), & \text{for } \alpha = \frac{1}{2}, \\ \frac{4n(2n-1)(4n-7)+6(5n-2)}{3(2n-1)(4n-1)} + \frac{4(n-1)\sqrt{3}+4n\sqrt{2n-1}}{\sqrt{3(4n-1)(2n-1)}}, & \text{for } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. We may get the general Randić index R_α for $\alpha = 1, -1, \frac{1}{2}, -(\frac{1}{2})$ by using the edge partition from Table 3.

$$\begin{aligned} R_1(\mathcal{C}(\mathrm{BD}_{4n})) &= (n-1)(2n-3)(2n-1)^2 + 4(n-1)(2n-1)(4n-1) + (4n-1)^2 + 12n(4n-1) + 9n; \\ R_{-1}(\mathcal{C}(\mathrm{BD}_{4n})) &= \frac{(n-1)(2n-3)}{(2n-1)^2} + \frac{4(n-1)}{(2n-1)(4n-1)} + \frac{1}{(4n-1)^2} + \frac{4n}{3(4n-1)} + \frac{n}{9}; \\ R_{\frac{1}{2}}(\mathcal{C}(\mathrm{BD}_{4n})) &= (n-1)(2n-3)(2n-1) + 4(n-1)\sqrt{(2n-1)(4n-1)} + (4n-1) + 4n\sqrt{3(4n-1)} + 3n; \\ R_{-(\frac{1}{2})}(\mathcal{C}(\mathrm{BD}_{4n})) &= \frac{(n-1)(2n-3)}{(2n-1)} + \frac{4(n-1)}{\sqrt{(2n-1)(4n-1)}} + \frac{1}{(4n-1)} + \frac{4n}{\sqrt{3(4n-1)}} + \frac{n}{3}. \end{aligned}$$

We get the desired result after minor simplification. □

Theorem 6. *Suppose that $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n}. We have:*

$$GA(\mathcal{C}(\mathrm{BD}_{4n})) = 2\left(n^2 - 2n + 2\right) + \frac{4(2n^2 - n - 1)\sqrt{8n^2 - 6n + 1} + 4n(3n-1)\sqrt{3(4n-1)}}{(2n+1)(3n-1)};$$
$$GA_5(\mathcal{C}(\mathrm{BD}_{4n})) = 2\left(n^2 - 2n + 2\right) + \frac{4(n-1)(2n+1)\sqrt{4n^2+1}}{4n^2+2n+1} + \frac{4n(2n+1)\sqrt{8n+1}}{2n^2+6n+1}.$$

Proof. By employing the geometric-arithmetic (GA) index formula, its fifth form, as well as the edge partition specified in Table 3, we obtain

$$GA(\mathcal{C}(\mathrm{BD}_{4n})) = (n-1)(2n-3) + \frac{4(n-1)\sqrt{(2n-1)(4n-1)}}{3n-1} + 1 + \frac{4n\sqrt{3(4n-1)}}{2n+1} + n;$$
$$GA_5(\mathcal{C}(\mathrm{BD}_{4n})) = (n-1)(2n-3) + \frac{4(n-1)\sqrt{(4n^2+1)(2n+1)^2}}{4n^2+2n+1} + 1 + \frac{4n\sqrt{(2n+1)^2(8n+1)}}{2n^2+6n+1} + n.$$

After some computations, the required values of GA and GA_5 can be derived. □

Theorem 7. *Assume that $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n}. Then*

$$ABC(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{2(n-1)(2n-3)\sqrt{n-1}}{(2n-1)} + \frac{8n\sqrt{2n^2-n} + 4(n-1)\sqrt{6(3n-2)}}{\sqrt{3(2n-1)(4n-1)}} + \frac{2\sqrt{2n-1}}{4n-1} + \frac{2n}{3};$$
$$ABC_4(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{2n(n-1)(2n-3)\sqrt{2}}{4n^2+1} + \frac{8(n-1)}{2n+1}\sqrt{\frac{2n^2+n}{4n^2+1}} + \frac{2\sqrt{2n^2+n}}{(2n+1)^2} + \frac{4n}{2n+1}\sqrt{\frac{4n(n+3)}{8n+1}} + \frac{4n\sqrt{n}}{8n+1}.$$

Proof. We have achieved this by including the edge partition, as specified in Table 3, into the ABC and ABC_4 index formulas.

$$ABC(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{2(n-1)(2n-3)\sqrt{n-1}}{2(n-1)} + 4(n-1)\sqrt{\frac{2(3n-2)}{(2n-1)(4n-1)}} + \frac{2n}{3} + \frac{2\sqrt{2n-1}}{(4n-1)} + 8n\sqrt{\frac{n}{3(4n-1)}};$$
$$ABC_4(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{(n-1)(2n-3)\sqrt{8n^2}}{(4n^2+1)} + \frac{4(n-1)}{2n+1}\sqrt{\frac{4n(2n+1)}{4n^2+1}} + \frac{\sqrt{8n(n+1)}}{(2n+1)^2} + \frac{4n}{2n+1}\sqrt{\frac{4n(n+3)}{8n+1}} + \frac{4n\sqrt{n}}{8n+1}.$$

By making a simple simplification, one may get the necessary formulae for both indices. □

Theorem 8. *Suppose $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n}. We have*

$$\mathcal{H}_r(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{(n-1)(6n^2-3n-1)}{(2n-1)(3n-1)} + \frac{3(2n+1) + n(4n-1)(2n+13)}{3(2n+1)(4n-1)}.$$

Proof. Using the harmonic index formula and the edge partition specified in Table 3, we obtain

$$\mathcal{H}_r(\mathcal{C}(\mathrm{BD}_{4n})) = \frac{1}{4n-1} + \frac{4(n-1)}{3n-1} + \frac{(n-1)(2n-3)}{(2n-1)} + \frac{4n}{2n+1} + \frac{n}{3}.$$

Certain computations resulting the necessary harmonic index. □

5. Hosoya Properties of Finite Subgroups of $\mathrm{SL}(2,\mathbb{C})$

The Hosoya polynomial and its reciprocal status of the commuting graphs $\mathcal{C}(\mathcal{G})$ are determined in this section.

The classification of the commuting graphs of finite subgroups of $\mathrm{SL}(2,\mathbb{C})$ have been given in [46] (see Proposition 1) using GAP [47] calculations.

5.1. Hosoya Polynomial

To establish certain results, we first prove some important results.

Proposition 2. *Suppose $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n} . Then*

$$dis(\mathcal{C}(\mathrm{BD}_{4n}),\ell) = \begin{cases} 4n, & for\ \ell = 0; \\ \frac{2n(2n+4)}{2}, & for\ \ell = 1; \\ \frac{6n(2n-2)}{2}, & for\ \ell = 2. \end{cases}$$

Proof. As we know that $diam(\mathcal{C}(\mathrm{BD}_{4n})) = 2$. We need to examine $dis(\mathcal{C}(\mathrm{BD}_{4n}),\ 0)$, $dis(\mathcal{C}(\mathrm{BD}_{4n}),\ 1)$ and $dis(\mathcal{C}(\mathrm{BD}_{4n}),\ 2)$. Suppose V_k is the collection of all pair of vertices of $\mathcal{C}(\mathrm{BD}_{4n})$, then

$$|V_k| = 2n(4n+1).$$

Suppose

$$\mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),\ell) = \{(j,k); j,k \in V(\mathcal{C}(\mathrm{BD}_{4n})) \mid dis(j,k) = \ell\},$$

and $dis(\mathcal{C}(\mathrm{BD}_{4n}),\ell) = |\mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),\ell)|$. Therefore:

$$V_k = \mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),0) \cup \mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),1) \cup \mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),2). \quad (5)$$

Since, $dis(j,j) = 0$, for any $j \in V(\mathcal{C}(\mathrm{BD}_{4n}))$, so

$$\mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),0) = \{(j,j); j \in V(\mathcal{C}(\mathrm{BD}_{4n}))\} = V(\mathcal{C}(\mathrm{BD}_{4n})).$$

Thus, $\mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),0) = 4n$. Using Proposition 1, and we have

$$V(K_2) = \{e, y^n\},\ V(K_{2n-2}) = X_3,\ \text{and}\ V(nK_2) = X_2 = \bigcup_{i=0}^{n-1} X_2^i.$$

Therefore,

$$\begin{aligned}\mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),1) = {} & \{(j,k); j \in \Omega, k \in X_2\} \cup \bigcup_{i=0}^{n-1} \Big\{(j,k); j,k \in X_2^i \text{ and } j \neq k\Big\} \\ & \cup \{(j,k); j \in \Omega, k \in X_3\} \cup \{(j,k); j,k \in X_3 \text{ and } j \neq k\} \\ & \cup \{(j,k); j,k \in \Omega \text{ and } j \neq k\}.\end{aligned}$$

Consequently,

$$\mathbb{S}(\mathcal{C}(\mathrm{BD}_{4n}),1) = 4n + n(1) + 2(2n-2) + \binom{2n-2}{2} + 1 = \frac{2n(2n+4)}{2}.$$

Using Equation (5), we get

$$|V_k| = dis(\mathcal{C}(\mathrm{BD}_{4n}),0) + dis(\mathcal{C}(\mathrm{BD}_{4n}),1) + dis(\mathcal{C}(\mathrm{BD}_{4n}),2).$$

Hence,

$$\begin{aligned} dis(\mathcal{C}(\mathrm{BD}_{4n}),2) &= |V_k| - dis(\mathcal{C}(\mathrm{BD}_{4n}),0) - dis(\mathcal{C}(\mathrm{BD}_{4n}),1) \\ &= 2n(2n+1) - 4n - \frac{2n(2n+4)}{2} \\ &= \frac{3n(2n-2)}{2}. \end{aligned}$$

□

The following results yield the Hosoya polynomials of the commuting graphs of finite subgroups of $\mathrm{SL}(2,\mathbb{C})$.

Theorem 9. *Assume that $\mathcal{C}(\mathrm{BD}_{4n})$ is the commuting graph of BD_{4n}. Then*

$$\mathbb{H}(\mathcal{C}(\mathrm{BD}_{4n}),x) = n\Big(6(n-1)x^2 + 2(n+2)x + 4\Big).$$

Proof. By substituting the coefficients $dis(\mathcal{C}(\mathrm{BD}_{4n}),\ell)$ derived in Proposition 2 into the formula for the Hosoya polynomial, we get.

$$\begin{aligned} \mathbb{H}(\mathcal{C}(\mathrm{BD}_{4n}),x) &= dis(\mathcal{C}(\mathrm{BD}_{4n}),2)x^2 + dis(\mathcal{C}(\mathrm{BD}_{4n}),1)x^1 + dis(\mathcal{C}(\mathrm{BD}_{4n}),0)x^0 \\ &= (6n(n-1))x^2 + (2n(n+2))x + (4n)x^0 \\ &= n\Big(6(n-1)x^2 + 2(n+2)x + 4\Big). \end{aligned}$$

We obtain the essential result. □

Theorem 10. *Suppose $\mathcal{C}(\mathcal{G})$ is the commuting graph of a group $\mathcal{G}$. Then*

$$\begin{aligned} &\text{If } \mathcal{G} = \mathrm{BT}_{24}, \text{ then } \mathbb{H}(\mathcal{C}(\mathcal{G}),x) = 204x^2 + 72x + 24. \\ &\text{If } \mathcal{G} = \mathrm{BO}_{48}, \text{ then } \mathbb{H}(\mathcal{C}(\mathcal{G}),x) = 960x^2 + 168x + 48. \\ &\text{If } \mathcal{G} = \mathrm{BI}_{120}, \text{ then } \mathbb{H}(\mathcal{C}(\mathcal{G}),x) = 6660x^2 + 480x + 120. \end{aligned}$$

Proof. Following GAP [47], Proposition 1 and using the similar computations as given in Theorem 9, we can prove the required result. □

5.2. Reciprocal Status Hosoya Polynomial

This section establishes the reciprocal status of the commuting graphs of certain finite subgroups of $\mathrm{SL}(2,\mathbb{C})$. As we know that $rs(w) = \sum_{v\in V(\Gamma), w\neq v} \frac{1}{dis(w,v)}$ is the reciprocal status of a vertex w. So we get the following proposition.

Proposition 3. *If z is a vertex of $\mathcal{C}(\mathrm{BD}_{4n})$, then:*

$$rs(z) = \begin{cases} 4n-1, & when\ \ z \in \Omega; \\ 2n+1, & when\ \ z \in X_2; \\ 3n-1, & when\ \ z \in X_3. \end{cases}$$

Proof. By applying Proposition 1, the vertex set of $\mathcal{C}(\mathrm{BD}_{4n})$ is $\Omega \cup X_2 \cup X_3$. Thus, when $v \in \Omega$, implies $ec(v) = 1$; additionally, we use the reciprocal status notion, then:

$$rs(v) = \left(\frac{1}{1}\right)\{2n + 1 + 2n - 2\} = 4n - 1.$$

When $v \in X_2$, implying $ec(v) = 2$, also, we use the reciprocal status concept, which results in the following:

$$rs(v) = 3\left(\frac{1}{1}\right) + \left(\frac{1}{2}\right)\left\{2n - 2 + \left(\frac{4n}{2} - 2\right)\right\} = 2n + 1.$$

When $v \in X_3$, then $ec(v) = 2$, further, we use the idea of reciprocal status, resulting in the following:

$$rs(v) = \left(\frac{1}{1}\right)\{2 - 3 + 2n\} + \left(\frac{1}{2}\right)(2n) = 3n - 1.$$

□

Theorem 11. *Let* $\mathcal{C}(\mathrm{BD}_{4n})$ *be the commuting graph of* BD_{4n}*, for* $n \geq 2$*. Then:*

$$\mathbb{H}_{rs}(\mathcal{C}(\mathrm{BD}_{4n})) = \binom{2(n-1)}{2} x^{2(3n-1)} + x^{2(4n-1)} + (n)x^{2(2n+1)} + 4(n-1)x^{7n-2} + (4n)x^{6n}.$$

Proof. Using Proposition 3, there are five different kinds of edges ($u \sim u, u \sim v, v \sim v, v \sim w, w \sim w$) in $\mathcal{C}(\mathrm{BD}_{4n})$. As a result, Table 3 illustrates the edge partitioning and the reciprocal status of its associated end vertices, when $u = \frac{6n}{2} - 1, v = 4n - 1, w = 2n + 1$.

By inserting the edge partition of $\mathcal{C}(\mathrm{BD}_{4n})$ presented in Table 3, we get the reciprocal status Hosoya polynomial.

$$\begin{aligned}
\mathbb{H}_{rs}(\mathcal{C}(\mathrm{BD}_{4n})) &= \sum_{E_{u\sim u}} x^{u+u} + \sum_{E_{v\sim v}} x^{v+v} + \sum_{E_{w\sim w}} x^{w+w} \sum_{E_{u\sim v}} x^{u+v} + \sum_{E_{v\sim w}} x^{v+w} \\
&= \binom{2(n-1)}{2} x^{2(3n-1)} + (1)x^{2(4n-1)} + (n)x^{2(2n+1)} \\
&+ 4(n-1)x^{(3n-1)+(4n-1)} + (4n)x^{(4n-1)+(2n+1)} \\
&= \binom{2(n-1)}{2} x^{2(3n-1)} + x^{2(4n-1)} + (n)x^{2(2n+1)} + 4(n-1)x^{7n-2} + (4n)x^{6n}.
\end{aligned}$$

□

Lemma 1. *Let* $\mathcal{C}(\mathcal{G})$ *be the commuting graph of* $\mathcal{G}$*. Then,*

$$\begin{aligned}
&\text{If } \mathcal{G} = \mathrm{BT}_{24}, \text{ then } \mathbb{H}_{rs}(\mathcal{C}(\mathrm{BT}_{24})) = x^{46} + 32x^{37} + 12x^{36} + 24x^{28} + 3x^{26}. \\
&\text{If } \mathcal{G} = \mathrm{BO}_{48}, \text{ then } \mathbb{H}_{rs}(\mathcal{C}(\mathrm{BO}_{48})) = x^{94} + 72x^{74} + 32x^{73} + 24x^{72} + 45x^{54} + 24x^{52} + 6x^{50}. \\
&\text{If } \mathcal{G} = \mathrm{BI}_{120}, \text{ then } \mathbb{H}_{rs}(\mathcal{C}(\mathrm{BI}_{120})) = x^{238} + 96x^{183} + 80x^{181} + 40x^{180} + 60x^{124} + 15x^{122}.
\end{aligned}$$

Proof. Following GAP [47], Proposition 1 and using the similar computations as given in Theorem 11, we can prove the required result. □

6. Hosoya Index

The Hosoya index of the commuting graphs is examined in this section. On a graph with n vertices, the complete graph K_n provides the maximum possible value of the Hosoya index [48]. The Hosoya index of K_n, where $n \geq 2$ is generally as follows:

$$1 + \sum_{i=1}^{\frac{n}{2}} \left(\frac{1}{i}\right) \prod_{k=0}^{i-1} \binom{n-2k}{2},$$

this may be observed concerning the whole set of non-void matchings stated in Table 4, whereas δ_i refers the cardinality of i matchings, where $1 \leq i \leq \frac{n}{2}$.

Table 4. The total number of non-void matchings in K_n.

K_n	δ_1	δ_2	δ_3	δ_4	$\cdots$	δ_i
K_2	$\binom{2}{2}$					
K_3	$\binom{3}{2}$					
K_4	$\binom{4}{2}$	$\frac{1}{2}\binom{4}{2}\binom{2}{2}$				
K_5	$\binom{5}{2}$	$\frac{1}{2}\binom{5}{2}\binom{3}{2}$				
K_6	$\binom{6}{2}$	$\frac{1}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{3}\binom{6}{2}\binom{4}{2}\binom{2}{2}$			
K_7	$\binom{7}{2}$	$\frac{1}{2}\binom{7}{2}\binom{5}{2}$	$\frac{1}{3}\binom{7}{2}\binom{5}{2}\binom{3}{2}$			
K_8	$\binom{8}{2}$	$\frac{1}{2}\binom{8}{2}\binom{6}{2}$	$\frac{1}{3}\binom{8}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{4}\binom{8}{2}\binom{6}{2}\binom{4}{2}\binom{2}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_n	$\binom{n}{2}$	$\frac{1}{2}\binom{n}{2}\binom{n-2}{2}$	$\frac{1}{3}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}$	$\frac{1}{4}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}\binom{n-6}{2}$	$\cdots$	$\frac{1}{i}\prod_{k=0}^{i-1}\binom{n-2k}{2}$

Theorem 12. *For $n \geq 2$, the Hosoya index of $\mathcal{C}(\mathrm{BD}_{4n})$ is given as:*

$$1+\sum_{i=1}^{n}\delta_i^1+\sum_{i=1}^{2}\delta_i^2+\sum_{i=1}^{n}\delta_i^3+\sum_{i=2}^{n+1}\delta_i^4+\delta_2^5+\sum_{i=2}^{n}\delta_i^6+\sum_{i=2}^{2n}\delta_i^7,$$

where

$$\begin{aligned}
\delta_i^1 &= \frac{1}{i}\prod_{k=0}^{i-1}\binom{2(n-k)}{2}, \quad \delta_1^2 = 4n, \quad \delta_2^2 = 4n(n-\frac{1}{2}),\\
\delta_i^3 &= \binom{n}{i}, \quad \delta_2^4 = 4n\binom{2(n-1)}{2},\\
\delta_i^4 &= 2n\left\{\frac{2}{i-1}\prod_{k=0}^{i-2}\binom{2(n-k-1)}{2}+\frac{2n-1}{i-2}\prod_{k=0}^{i-3}\binom{2(n-k-1)}{2}\right\},
\end{aligned}$$

where $3 \leq i \leq n$,

$$\begin{aligned}
\delta_{n+1}^4 &= \frac{4n(n-\frac{1}{2})}{i-2}\prod_{k=0}^{i-3}\binom{2(n-k-1)}{2}, \quad \delta_2^5 = 8n(n-\frac{1}{2}), \quad \delta_2^6 = 4n(n-1),\\
\delta_i^6 &= 2n\left\{2\binom{n-1}{i-1}+\binom{n-1}{i-2}+4(n-1)\binom{n-2}{i-2}\right\},
\end{aligned}$$

where $3 \leq i \leq n$,

$$\delta_i^7 = \sum_{j=1}^{i-1}\frac{1}{j}\prod_{k=0}^{j-1}\binom{2(n-k)}{2}\binom{n}{i-j}, \text{ where } 2 \leq i \leq 2n.$$

Proof. By applying Proposition 1, the vertex set of $\mathcal{C}(\mathrm{BD}_{4n})$ is $V(\mathcal{C}(\mathrm{BD}_{4n})) = \Omega \cup X_2 \cup X_3$, where $X_2 = \bigcup_{J=0}^{n-1} X_2^J$. Therefore, we have the subsequent kinds of edges in $\mathcal{C}(\mathrm{BD}_{4n})$:

Type-1: $v_1 \sim v_2$, for any $v_1, v_2 \in X_3$,

Type-2: $v_1 \sim v_2$, for any $v_1, v_2 \in \Omega$,

Type-3: $v_1 \sim v_2$, for any $v_1 \in X_3, v_2 \in \Omega$,

Type-4: $v_1 \sim v_2$, for any $v_1 \in X_2, v_2 \in \Omega$,

Type-5: $v_1 \sim v_2$, for any $v_1, v_2 \in X_2^j \subseteq X_2$, where $0 \leq j \leq n-1$.

Therefore, there are seven kinds of matchings among the edges of $\mathcal{C}(\mathrm{BD}_{4n})$, which may be classified into the categories listed as:

(δ^1) Matchings amongst the Type-1, -2 as well as Type-3 edges,
(δ^2) Matchings amongst the Type-4 edges,
(δ^3) Matchings amongst the Type-5 edges,
(δ^4) Matchings amongst the Type-1 and -4 edges,
(δ^5) Matchings amongst the Type-3 and -4 edges,
(δ^6) Matchings amongst the Type-4 and -5 edges,
(δ^7) Matchings amongst the Type-1, -2, -3 and Type-5 edges.

The preceding approach generates all of the above-mentioned forms of matchings:

(δ^1) As previously stated, the subgraph induced by X_1 is complete, i.e., K_{2n}. Thus, all Type-1, -2, and Type-3 edges are identical to K_{2n} edges, and all such matchings among these edges are shown in Table 5, whereas δ_i^1 means the total number of matchings having i order, where $1 \leq i \leq n$.

(δ^2) For $i = 1, 2$, suppose δ_i^2 denote the number of order i matchings.

For (δ_1^2)**:** The number of Type-4 edges, that is, $4n$, which is equal to the number of order 1 matchings. Therefore $(\delta_1^2) = 4n$.

For (δ_2^2)**:** Let $v_1 \sim v_2 = e$ be a Type-4 edge with $v_2 \in \Omega$ and $v_1 \in X_2^j$ for a fixed $0 \leq j \leq n-1$. Additionally, the edge e, any Type-4 edge with one end in $X_2 \setminus \{v_1\}$ while the other end in $\Omega \setminus \{v_2\}$ creates a matching of order 2. As a consequence,

$$(\delta_2^2) = \frac{1}{2} 8\left(n - \frac{1}{2}\right)(n) = 4n\left(n - \frac{1}{2}\right).$$

Hence, in this case, no order greater than two matchings.

(δ^3) Type-5 has n edges, none of which share a similar vertex. As a result, for each order i there is a match such that $1 \leq i \leq n$. Assume that (δ_i^3) denotes is the number of order i matchings. Then, $(\delta_i^3) = \binom{n}{i}$.

(δ^4) Suppose (δ_i^4) refers the number of order i matchings, where $1 \leq i \leq n+1$. Then, in this context, $(\delta_1^4) = 0$. There are no Type-1 edges connecting a vertex to any Type-4 edge in $\mathcal{C}(\mathrm{BD}_{4n})$. Hence, we may get a matching in this case by joining each matching of Type-1 edges to every matching of Type-4 edges. The edges of Type-1 are also the edges of K_{2n-2}, and there are (δ_ℓ^1) matchings of order ℓ between them. Every (δ_ℓ^1) can be determined in Table 5. Among the edges of Type-4, there are $(\delta_1^2) = 4n$ and $(\delta_2^2) = 4n(n - \frac{1}{2})$ matchings having orders of 1 and 2, respectively.

As a result of the product rule, we obtain:

$$\delta_2^4 = \delta_1^2 \times \delta_1^1 = 4n\delta_1^1.$$

When $3 \leq i \leq n$, then

$$\begin{aligned}\delta_i^4 &= \delta_1^2 \times \delta_{i-1}^1 + \delta_2^2 \times \delta_{i-2}^1, \\ &= 4n\delta_{i-1}^1 + 4n\left(n - \frac{1}{2}\right)\delta_{i-2}^1, \\ &= 2n\left(2\delta_{i-1}^1 + 2\left(n - \frac{1}{2}\right)\delta_{i-2}^1\right).\end{aligned}$$

Additionally, when $i = n+1$, then

$$\delta_i^4 = \delta_2^2 \times \delta_{i-2}^1 = 4n\left(n - \frac{1}{2}\right)\delta_{n-1}^1.$$

(δ^5) For $i = 1, 2$, (δ_i^5) denotes the total matchings of order i. Then $(\delta_1^5) = 0$. We can only use matchings of order 1 among Type-4 edges in this situation. Otherwise, we will be unable to use any Type-3 edge, since both types of edges often share vertices. So in this situation, we can only get matchings having orders of 2. Suppose $N = \{e = v_1 \sim v_2\}$ is the order 1 matching between the Type-4 edges with $v_1 \in X_2^j$, for $0 \leq j \leq n-1$. Then, any non-adjacent Type-3 edge to v_2 may result in the construction of an order 2 matching. Given the existence of $2n-2$ such Type-3 edges, any of which may be employed in any of the $4n$ order 1 matching among Type-4 edges, we get:

$$(\delta_2^5) = 8n(n-1).$$

(δ^6) For $1 \leq i \leq n$, (δ_i^6) represent the number of order i matchings. Then $(\delta_1^6) = 0$, to identify matching, both matchings of orders 1 and 2 among the edges of Type-4, and any matching of order ℓ among the edges of Type-5 will be evaluated, where $1 \leq \ell \leq n-1$. Thus by counting these matchings using the product rule, we obtain:

$$\delta_2^6 = 4 \times 1 \times n \times \binom{n-1}{1} = 4n(n-1),$$

and for $3 \leq i \leq n$:

$$\delta_i^6 = 2n\left\{2\binom{n-1}{i-1} + \binom{n-1}{i-2} + 4(n-1)\binom{n-2}{i-2}\right\}.$$

(δ^7) Considering that, the Type-1, -2, and Type-3 edges are also the K_{2n} edges generated by X_1, we can use them to detect matchings between the edges of Type-5 and K_{2n}. Suppose δ_i^7 is the number of order i matchings. Then, $\delta_i^7 = 0$. Due to the fact that no edge of Type-5 shares a vertex with an edge of K_{2n}, this equates to every pair of Type-5 edges matching. Thus, every matching of the edges of K_{2n} can also be used to find a match in this case. Since, there exist δ_κ^1 matchings of the cardinality $1 \leq \kappa \leq n$ amongst the K_{2n} edges, as listed in Table 5, also $\delta_j^3 = \binom{n}{j}$ matchings of order $1 \leq j \leq n$ amongst the Type-5 edges. Therefore, the highest order of a matching in this situation is $2n$. Consequently, we may determine δ_i^7, for $2 \leq i \leq 2n$ as follows:

$$\begin{aligned}
\delta_2^7 &= \delta_1^1\delta_1^3, \\
\delta_3^7 &= \delta_1^1\delta_2^3 + \delta_2^1\delta_1^3, \\
\delta_4^7 &= \delta_1^1\delta_3^3 + \delta_2^1\delta_2^3 + \delta_3^1\delta_1^3, \\
&\vdots \\
\delta_i^7 &= \sum_{j=1}^{i-1} \delta_j^1\delta_{i-j}^3.
\end{aligned}$$

As a result, by the sum rule, the Hosoya index of $\mathcal{C}(\mathrm{BD}_{4n})$ is as follows:

$$1 + \sum_{i=1}^{7}(\delta^i) = 1 + \sum_{i=1}^{n}\delta_i^1 + \sum_{i=1}^{2}\delta_i^2 + \sum_{i=1}^{n}\delta_i^3 + \sum_{i=2}^{n+1}\delta_i^4 + \delta_2^5 + \sum_{i=2}^{n}\delta_i^6 + \sum_{i=2}^{2n}\delta_i^7,$$

where

$$\delta_i^1 = \frac{1}{i}\prod_{k=0}^{i-1}\binom{2(n-k)}{2},\ \delta_1^2 = 4n,\ \delta_2^2 = 4n\left(n-\frac{1}{2}\right),\ \delta_i^3 = \binom{n}{i},\ \delta_2^4 = 4n\binom{2(n-1)}{2},$$

$$\delta_i^4 = 2n\left\{\frac{2}{i-1}\prod_{k=0}^{i-2}\binom{2(n-k-1)}{2} + \frac{2n-1}{i-2}\prod_{k=0}^{i-3}\binom{2(n-k-1)}{2}\right\},\ \text{for } 3 \le i \le n,$$

$$\delta_{n+1}^4 = \frac{2n(2n-1)}{i-2}\prod_{k=0}^{i-3}\binom{2(n-k-1)}{2},\quad \delta_2^5 = 8n(n-\frac{1}{2}),\quad \delta_2^6 = 4n(n-1),$$

$$\delta_i^6 = 2n\left\{2\binom{n-1}{i-1} + \binom{n-1}{i-2} + 4(n-1)\binom{n-2}{i-2}\right\},\ \text{for } 3 \le i \le n,$$

$$\delta_i^7 = \sum_{j=1}^{i-1}\frac{1}{j}\prod_{k=0}^{j-1}\binom{2(n-k)}{2}\binom{n}{i-j},\ \text{for } 2 \le i \le 2n.$$

□

Table 5. The total non-void matchings in K_{2n}.

K_{2n}	δ_1^1	δ_2^1	δ_3^1	δ_4^1	$\cdots$	δ_i^1
K_2	$\binom{2}{2}$					
K_4	$\binom{4}{2}$	$\frac{1}{2}\binom{4}{2}\binom{2}{2}$				
K_6	$\binom{6}{2}$	$\frac{1}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{3}\binom{6}{2}\binom{4}{2}\binom{2}{2}$			
K_8	$\binom{8}{2}$	$\frac{1}{2}\binom{8}{2}\binom{6}{2}$	$\frac{1}{3}\binom{8}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{4}\binom{8}{2}\binom{6}{2}\binom{4}{2}\binom{2}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_{2n-1}	$\binom{2n}{2}$	$\frac{1}{2}\binom{2n}{2}\binom{2n-2}{2}$	$\frac{1}{3}\binom{2n}{2}\binom{2n-2}{2}\binom{2n-4}{2}$	$\frac{1}{4}\binom{2n}{2}\binom{2n-2}{2}\binom{2n-4}{2}\binom{2n-6}{2}$	$\cdots$	$\frac{1}{i}\prod_{k=0}^{i-1}\binom{2(n-k)}{2}$

7. Conclusions

This paper aimed to investigate the structural features of the commuting graphs of the finite non-abelian subgroups of $SL(2,\mathbb{C})$. The special linear groups and their finite subgroups are well-known algebraic structures that have contributed significantly to the theory of molecular vibrations and electron structures. We studied an algebraic characteristic, specifically binary dihedral groups, and their related chemical structure (commuting graphs), in connection with the finite subgroups of $SL(2,\mathbb{C})$. The precise formulae of the reciprocal complementary Wiener index, Randić index, Harary index, harmonic index, geometric-arithmetic index and the arithmetic-geometric index, Schultz molecular topological index, the Hosoya polynomial and its reciprocal form, the Hosoya index, and the atomic-bond connectivity indices were used to obtain several degree-based and distance-based characteristics of the respective graphs.

In this study, we attempted to explore numerous topological indices of the commuting graphs of certain finite groups. Although, the problem of computing the topological indices of the commuting graph or the commuting involution graph of any finite group remains open and unsolved. In chemistry, an algebraic structure is critical for forming chemical structures and investigating different chemical characteristics of chemical compounds included inside these structures. All indices are numerical values, and this study contributes a novel chemical structure to the theory of topological indices. This could help predict the bioactive molecules using the physicochemical parameters examined in QSPR.

Author Contributions: Conceptualization, F.A., B.A.R. and M.S.; software, F.A., K.A.M.A., A.U., R.D. and N.F.; writing—original draft preparation, F.A., B.A.R. and M.S.; writing—review and editing, K.A.M.A., B.A.R., R.D., N.F., A.U. and F.A.; formal analysis, F.A., B.A.R. and A.U.; validation, F.A., M.S. and A.U.; methodology, F.A., B.A.R. and N.F.; investigation, F.A., B.A.R. and M.S.; resources, F.A. and B.A.R.; project administration, F.A., B.A.R. and A.U.; funding acquisition, N.F. and K.A.M.A. All authors have read and agreed to the published version of the manuscript.

Funding: The authors would like to thank the Deanship of Scientific Research, Umm Al-Qura University for supporting this work by Grant Code: (22UQU4310392DSR17).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data used to support the findings of this study are available within the article.

Acknowledgments: The author N.F. would like to thank Prince Sultan University for paying the publication fees (APC) for this work through TAS LAB. The authors would like to thank the Deanship of Scientific Research at Umm Al-Qura University for supporting this work by Grant Code: (22UQU4310392DSR17).

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Ghorbani, M.; Hosseinzadeh, M.A. Computing ABC_4 index of nanostar dendrimers. *Optoelectron. Adv. Mater.-Rapid Commun.* **2010**, *4*, 1419–1422.
2. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17–20. [CrossRef] [PubMed]
3. Ali, F.; Rather, B.A.; Din, A.; Saeed, T.; Ullah, A. Power Graphs of Finite Groups Determined by Hosoya Properties. *Entropy* **2022**, *24*, 213. [CrossRef] [PubMed]
4. Graovac, A.; Ghorbani, M.; Hosseinzadeh, M.A. Computing fifth geometric-arithmetic index for nanostar dendrimers. *J. Math. Nanosci.* **2011**, *1*, 33–42.
5. Hayat, S.; Imran, M.; Liu, J.B. An efficient computational technique for degree and distance based topological descriptors with applications. *IEEE Access* **2019**, *7*, 32276–32296. [CrossRef]
6. Hafeez, S.; Farooq, R. Inverse sum indeg energy of graphs. *IEEE Access* **2019**, *7*, 100860–100866. [CrossRef]
7. Pólya, G. Kombinatorische anzahlbestimmungen für gruppen, graphen und chemische verbindungen. *Acta Math.* **1937**, *68*, 145–254. [CrossRef]
8. Hosoya, H. On some counting polynomials in chemistry. *Discret. Appl. Math.* **1988**, *19*, 239–257. [CrossRef]
9. Sagan, B.E.; Yeh, Y.N.; Zhang, P. The Wiener polynomial of a graph. *Int. J. Quantum Chem.* **1996**, *60*, 959–969. [CrossRef]
10. Cash, G.G. Relationship between the Hosoya polynomial and the hyper-Wiener index. *Appl. Math. Lett.* **2002**, *15*, 893–895. [CrossRef]
11. Estrada, E.; Ivanciuc, O.; Gutman, I.; Gutierrez, A.; Rodríguez, L. Extended Wiener indices. A new set of descriptors for quantitative structure-property studies. *New J. Chem.* **1998**, *22*, 819–822. [CrossRef]
12. Bates, C.; Bundy, D.; Perkins, S.; Rowley, P. Commuting involution graphs for finite Coxeter groups. *J. Group Theory* **2003**, *6*, 461–476. [CrossRef]
13. Bates, C.; Bundy, D.; Perkins, S.; Rowley, P. Commuting involution graphs for symmetric groups. *J. Algebra* **2003**, *266*, 133–153. [CrossRef]
14. Jauhari, M.; Ali, F. Survey on topological indices and graphs associated with a commutative ring. *J. Phys. Conf. Ser.* **2020**, *1562*, 012008.
15. Anderson, D.F.; Livingston, P.S. The zero-divisor graph of a commutative ring. *J. Algebra* **1999**, *217*, 434–447. [CrossRef]
16. Rather, B.A.; Aijaz, M.; Ali, F.; Mlaiki, N.; Ullah, A. On distance signless Laplacian eigenvalues of zero divisor graph of commutative rings. *AIMS Math.* **2022**, *7*, 12635–12649. [CrossRef]
17. Pirzada, S.; Rather, B.A.; Chishti, T. On distance Laplacian spectrum of zero divisor graphs of the ring $\mathbb{Z}_n$. *Carpathian Math. Publ.* **2021**, *13*, 48–57. [CrossRef]
18. Ali, F.; Salman, M.; Huang, S. On the commuting graph of dihedral group. *Commun. Algebra* **2016**, *44*, 2389–2401. [CrossRef]
19. Chelvam, T.T.; Selvakumar, K.; Raja, S. Commuting graphs on dihedral group. *Turk. J. Math. Comput. Sci.* **2011**, *2*, 402–406. [CrossRef]
20. Woodcock, T.J. Commuting Graphs of Finite Groups. Ph.D. Thesis, University of Virginia, Charlottesville, VA, USA, 2010.
21. Ali, F.; Li, Y. The connectivity and the spectral radius of commuting graphs on certain finite groups. *Linear Multilinear Algebra* **2019**, *69*, 2945–2958. [CrossRef]
22. Ali, F.; Hayat, U.; Li, Y. Fixed points of automorphisms of certain finite groups. *Int. J. Algebra* **2019**, *13*, 167–183. [CrossRef]
23. Mirzargar, M.; Pach, P.P.; Ashrafi, A. The automorphism group of commuting graph of a finite group. *Bull. Korean Math. Soc.* **2014**, *51*, 1145–1153. [CrossRef]
24. Iranmanesh, A.; Jafarzadeh, A. On the commuting graph associated with the symmetric and alternating groups. *J. Algebra Its Appl.* **2008**, *7*, 129–146. [CrossRef]
25. Giudici, M.; Parker, C. There is no upper bound for the diameter of the commuting graph of a finite group. *J. Comb. Theory Ser. A* **2013**, *120*, 1600–1603. [CrossRef]

26. Morgan, G.; Parker, C. The diameter of the commuting graph of a finite group with trivial centre. *J. Algebra* **2013**, *393*, 41–59. [CrossRef]
27. Abdollahi, A.; Akbari, S.; Maimani, H. Non-commuting graph of a group. *J. Algebra* **2006**, *298*, 468–492. [CrossRef]
28. Ali, F.; Fatima, S.; Wang, W. On the power graphs of certain finite groups. *Linear Multilinear Algebra* **2020** , 1–15. [CrossRef]
29. Mirzargar, M.; Ashraf, A.R. Some Distance-Based Topological Indices of a Non-Commuting Graph. *Hacet. J. Math. Stat.* **2012**, *41*, 515–526.
30. Hosoya, H. Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn.* **1971**, *44*, 2332–2339. [CrossRef]
31. Hosoya, H. Topological index as a common tool for quantum chemistry, statistical mechanics, and graph theory. In *Mathematical and Computational Concepts in Chemistry*; Ellis Horwood Series in Mathematics and Its Applications; Ellis Horwood, Ltd.: Chichester, UK, 1986; pp. 110–123.
32. Deng, H.; Chen, S. The extremal unicyclic graphs with respect to Hosoya index and Merrifield-Simmons index. *MATCH Commun. Math. Comput. Chem.* **2008**, *59*, 171–190.
33. Wagner, S. Extremal trees with respect to Hosoya index and Merrifield-Simmons index. *MATCH Commun. Math. Comput. Chem.* **2007**, *57*, 221–233.
34. Yu, A.; Tian, F. A kind of graphs with minimal Hosoya indices and maximal Merrifield-Simmons indices. *MATCH Commun. Math. Comput. Chem.* **2006**, *55*, 103–118.
35. Bates, C.; Bundy, D.; Perkins, S.; Rowley, P. Commuting involution graphs in special linear groups. *Commun. Algebra* **2004**, *32*, 4179–4196. [CrossRef]
36. Salman, M.; Noreen, T.; Rehman, M.U.; Cao, J.; Abbas, M.Z. Non-commuting graph of the dihedral group determined by Hosoya parameters. *Alex. Eng. J.* **2022**, *61*, 3709–3717. [CrossRef]
37. Brouwer, A.E.; Haemers, W.H. *Spectra of Graphs*; Springer Science & Business Media: Berlin/Heidelberg, Germany, 2011.
38. Plavšić, D.; Nikolić, S.; Trinajstić, N.; Mihalić, Z. On the Harary index for the characterization of chemical graphs. *J. Math. Chem.* **1993**, *12*, 235–250. [CrossRef]
39. Ivanciuc, O.; Balaban, T.S.; Balaban, A.T. Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. *J. Math. Chem.* **1993**, *12*, 309–318. [CrossRef]
40. Liu, J.B.; Pan, X.F.; Hu, F.T.; Hu, F.F. Asymptotic Laplacian-energy-like invariant of lattices. *Appl. Math. Comput.* **2015**, *253*, 205–214. [CrossRef]
41. Hayat, S.; Wang, S.; Liu, J.B. Valency-based topological descriptors of chemical networks and their applications. *Appl. Math. Model.* **2018**, *60*, 164–178. [CrossRef]
42. Schultz, H.P.; Schultz, E.B.; Schultz, T.P. Topological organic chemistry. 1. Graph theory and topological indexes of heteronuclear systems. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1151–1157. [CrossRef]
43. Ivanciuc, O. QSAR comparative study of Wiener descriptors for weighted molecular graphs. *J. Chem. Inf. Comput. Sci.* **2000**, *40*, 1412–1422. [CrossRef]
44. Liu, J.B.; Wang, C.; Wang, S.; Wei, B. Zagreb indices and multiplicative Zagreb indices of Eulerian graphs. *Bull. Malays. Math. Sci. Soc.* **2019**, *42*, 67–78. [CrossRef]
45. Ramane, H.S.; Talwar, S.Y. Reciprocal transmission Hosoya polynomial of graphs. *Math. Comb.* **2019**, *3*, 70–79.
46. Hayat, U.; de Celis, Á.N.; Ali, F. Commuting graphs on coxeter groups, Dynkin diagrams and finite subgroups of SL(2, ℂ). *arXiv* **2017**, arXiv:1703.02480.
47. GAP Group. *Algorithms, and Programming, Version 4.11.1*; GAP—Groups: Glasgow, UK, 2021. Available online: http://www.gap-system.org (accessed on 2 March 2021).
48. Tichy, R.F.; Wagnerf, S. Extremal problems for topological indices in combinatorial chemistry. *J. Comput. Biol.* **2005**, *12*, 1004–1013. [CrossRef] [PubMed]