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THE *g*-NON-COMMUTING GRAPH FOR SOME FINITE GROUPS AND THEIR RANDIĆ INDEX

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Abstract

A molecular graph is an essentially non-numerical mathematical object, and to link molecular topology with molecular properties, its information is converted into a numerical characteristic called a topological index (TOI). The study on TOIs has grown significantly since 1947 and many types of topological indices have been developed until recently. The *g*-non-commuting graph is an extension of the non-commuting graph. For a finite group G and a fixed element $g \in G$, the g-non-commuting graph is defined with the vertex set G, where two distinct vertices x and y are adjacent if $[x, y] \neq g$ and $[x, y] \neq g^{-1}$. Meanwhile, the Randić index, a degree-based TOI, is defined as the sum of the reciprocal square roots of the product of the degrees of two adjacent vertices in a graph. In this study, the general form of the *g*-non-commuting graph associated to the dihedral, the generalized quaternion, and the quasidihedral groups, are introduced. Then, based on these graphs, their Randić indices are determined and some examples are also presented to illustrate the main theorems. These results can be beneficial to predict the physicochemical properties of the molecules.

1. Introduction

A topological index is a numerical descriptor that characterizes the structural properties from the molecular graph. In graph theory, a graph contains a set of vertices and a set of edges, where vertices and edges represent the atoms and bonds in a molecule, respectively. The study of graphs associated with finite groups has gained significant attention. Among these, the non-commuting graph is a significant construct in algebraic graph theory, offering a graphical representation of the non-commutative relationships within a group. According to [1], the non-commuting graph is a graph that contains the non-central elements of a group as a set of vertices wherein two vertices are adjacent if and only if they do not commute to each other.

The study of non-commuting graphs has gained considerable attention in algebraic graph theory due to its ability to encode group theoretic properties into a visual and analyzable graph structure. Earlier work by [1] and [5] demonstrated that properties such as group order and isomorphism types can be inferred from the non-commuting graph. Subsequent studies explored various topological indices such as the Wiener index, Zagreb indices, and graph energy which provide quantitative tools for comparing and analyzing their structural complexity [2, 11, 13, 14]. However, these non-commuting graphs focus solely on non-central elements of the group and treat all such elements uniformly, without accounting for the impact of specific elements on the graph's connectivity.

To address this limitation, Tolue et al. introduced the *g*-non-commuting graph, which considers adjacency based on the non-commutative elements with respect to a fixed group element [15]. While they established some basic graph-theoretical properties such as planarity and clique number, there remains a lack of systematic analysis on the structure of these graphs across various families of groups, and very limited exploration of topological indices in this context. This study fills that gap by developing general formulas for the Randić index of the *g*-non-commuting graph for dihedral, generalized quaternion, and quasidihedral groups, which are the classes of non-abelian finite groups with rich internal symmetries. By doing so, it not only extends the application of degree-based topological indices to a new class of algebraic graphs but also offers deeper insights into how group-specific features influence graph connectivity. This work contributes a novel intersection of group theory and chemical graph theory, laying a foundation for future investigations into more complex group types and alternative topological descriptors.

The aim of this study is to address these gaps by analyzing *g*-non-commuting graphs of some groups, introducing their general forms. Their *g*-

non-commuting graphs will be constructed by using Maple software. Then, the Randić index of g-non-commuting graph associated to the dihedral, generalized quaternion and quasidihedral groups will also be determined. The group presentations are stated as follows:

- Dihedral group

$$D_{2n} \cong \langle a, b \mid a^n = b^2 = 1, bab = a^{-1} \rangle, \quad n \geq 3.$$

- Generalized quaternion group

$$Q_{4n} \cong \langle a, b \mid a^n = b^2, a^{2n} = b^4 = 1, bab = a^{-1} \rangle, \quad n \geq 2.$$

- Quasidihedral group

$$QD_{2^n} \cong \langle a, b \mid a^{2^{n-1}} = b^2 = 1, bab = a^{2^{n-2}-1} \rangle, \quad n \geq 4.$$

Exploring the connection between group theory and graph theory helps us better understand the structure of groups. The g-non-commuting graph gives a clearer view of how group elements interact by focusing on how they relate to a fixed element, unlike the classical non-commuting graph which ignores central elements. This approach provides a more detailed picture of the group's structure. While previous studies have extensively explored various topological indices for non-commuting graphs, they often exclude central elements and do not account for the influence of a fixed group element on adjacency. This creates a gap in fully characterizing group structures through graphical means. By introducing the g-non-commuting graph and deriving general formulas for its Randić index across three classes of finite non-abelian groups, this study addresses that gap. It advances algebraic graph theory by providing a novel framework that links group-theoretic properties with graph connectivity patterns. Furthermore, the findings open up new directions for applying topological indices to analyse structural complexity in algebraic systems, with potential implications in mathematical chemistry, network analysis, and other interdisciplinary fields.

In addition to its theoretical contributions, this study holds significance for applied and industrial mathematics. The topological index, namely, Randić index was originally developed in chemical graph theory. It also demonstrates how algebraic structures can be leveraged to model and analyze real-world systems, such as molecular networks, communication systems, and data structures. By linking group properties to graph-based descriptors, the findings can support applications in areas like materials science, network security, and computational chemistry, where understanding complex relationships and connectivity patterns is essential. This highlights the broader relevance of algebraic graph theory in solving practical problems beyond pure mathematics.

2. Preliminaries

In this section, some important definitions on graph in general, graph of groups and topological indices are provided. These definitions are needed in order to determine the main results.

Definition 2.1 [15]**.** Let G be a group and $g \in G$ be a fixed element. Then a *g-non-commuting graph* of G, denoted as $NC\Gamma_G^g$, is a graph that consists all elements in G as vertices of the graph and two vertices x and y are adjacent if and only if $[x, y] \neq g$ and $[x, y] \neq g^{-1}$.

Note that $[x, y] = x^{-1}y^{-1}xy$.

Example 2.2. Let $NC\Gamma_G^g$ be the g-non-commuting graph of the dihedral groups of order six, $D_6 = \{e, a, a^2, b, ab, a^2b\}$. The identity element $g = e$ is self inverse. By Definition 2.1, the vertices x and y are adjacent if and only if $[x, y] \neq e$. Since $g = e$, $[x, y] \neq e$. That $[x, y] \neq e^{-1}$ means that the two vertices x and y do not commute. This is true for any pair of elements in D_6 except for e. Hence, $NC\Gamma_G^{g=e}$ is shown in the following:

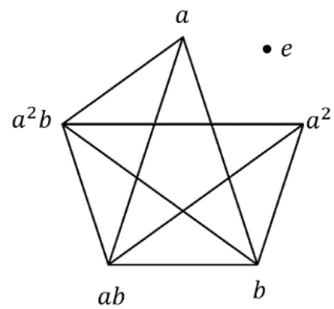

Figure 1. $NC\Gamma_G^{g=e}$.

Topological indices are widely used in drug design, molecular chemistry, and bioinformatics to predict properties, activities, and behaviors of compounds and biological networks. They also find applications in materials science, environmental studies, network analysis, and data science for structural analysis and optimization. One of the famous topological indices is the Wiener index, which is the first type of the topological indices that has been developed by Wiener [16]. In [16], the boiling point of a few types of alkanes is predicted by using the Wiener index. It is found that they are approximately the same as the experimental output. Its definition is stated in the following.

Definition 2.3 [16]**.** Let Γ be a connected graph with vertex set $V(\Gamma) = \{1, 2, ..., m\}$ and m is the total number of vertices. Then the *Wiener index* of Γ, denoted as $W(\Gamma)$, is defined as

$$W(\Gamma) = \frac{1}{2}\sum_{j=1}^{m}\sum_{i=1}^{m} d(i, j),$$

where $d(i, j)$ is the distance between two vertices *i* and *j*.

In 1971, a new distance-based topological index, namely, Hosoya index has been introduced in [10]. Then, Gutman and Trinajstić introduced the use of graph theory to calculate the total Π-electron energy of alternant hydrocarbons, bridging molecular chemistry and mathematics [7]. They demonstrated that the energy could be derived from the eigenvalues of the adjacency matrix of the molecular graph, providing a computationally efficient and insightful method for studying molecular stability and reactivity. This work laid the foundation for the development of degree-based topological indices, namely, first and second Zagreb indices.

A few years later, the article [12] introduced a Randić index, which is defined in Definition 2.4. It is used to study the molecular branching in the chemical graph theory. Recent studies have extensively explored the properties and applications of the Randić index. For instance, [8] examined its information-theoretic implications, highlighting its relevance in structural complexity analysis. In 2019, [4] explored the mathematical foundations, refining its computation for specific graph classes. The reference [3] provided a comprehensive overview, discussing novel properties and extensions of the index. Meanwhile, [6] investigated the relationships between the Randić index and other topological indices, including the Zagreb indices and the harmonic index. Their study identified specific mathematical bounds and correlations between these indices, demonstrating how the Randić index complements other descriptors in capturing structural properties of graphs. The article [9] focused on unicyclic graphs, identifying conditions for maximizing the Randić index, further extending its applicability in graph characterization.

Definition 2.4 [12]**.** Let Γ be a connected graph. The *Randić index* of Γ, denoted as $R(\Gamma)$, is defined as the sum of reciprocal of the square root of the product of the degree of two adjacent vertices, namely, u and v, written as

$$R(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\deg(u)\deg(v)}},$$

where $E(\Gamma)$ is the set of edges in Γ.

3. Results

This section states the general formulas of the g-non-commuting graph for the dihedral groups, generalized quaternion groups and the quasidihedral groups, denoted as $NC\Gamma^{g}_{D_{2n}}$, $NC\Gamma^{g}_{Q_{4n}}$ and $NC\Gamma^{g}_{QD_{2^n}}$, respectively. In this paper, g is fixed to be only e or $a^j b$. These results are presented in the following theorems. Lemma 3.1 is needed to prove the theorems. In this section, a g-non-commuting graph is denoted as a *gNC* graph.

Lemma 3.1. *Let* $NC\Gamma^{g=e}_{G}$ *be the gNC graph of the non-abelian group* G *with a fixed element* $g = e$. *Then e is not adjacent to all other vertices for all* $x \in G$.

Proof. It is obvious that $[e, x] = e^{-1}x^{-1}ex = e$ for all $x \in G$. Thus, by Definition 2.1, e is not adjacent to all other vertices of the graph.

Theorem 3.2. *Let* $NC\Gamma^{g=e}_{G}$ *be the gNC graph of the dihedral groups of order* $2n$, *where* $n \geq 3$ *for a fixed element e. Then*

$$NC\Gamma^{g=e}_{G} = \begin{cases} K_{\underbrace{1, 1, \ldots, 1}_{n \text{ times}}, n-1} \cup \{e\} & \text{if } n \text{ is odd}, \\ K_{\underbrace{2, 2, \ldots, 2}_{\frac{n}{2} \text{ times}}, n-2} \cup \{e\} \cup \{a^{\frac{n}{2}}\} & \text{if } n \text{ is even}. \end{cases}$$

Proof. Let $D_{2n} \cong \langle a, b \mid a^n = b^2 = 1, bab = a^{-1} \rangle$ be the dihedral groups of order $2n$, where $n \geq 3$. By Definition 2.1, the elements x and y are adjacent if and only if $[x, y] \neq e$. First, let n be odd. Elements x and $y \in a^i$ in D_{2n} are not adjacent to each other since $[x, y] = [a^i, a^j] = (a^i)^{-1}(a^j)^{-1}a^i a^j = e$, where $i, j = \{1, 2, \ldots, n-1\}$ and $i \neq j$. By Lemma 3.1, the vertex e is not adjacent to all other vertices in $NC\Gamma^{g=e}_{G}$. The vertices a^i are adjacent to the vertices $a^j b$, since

$$
\begin{aligned}
[a^i, a^j b] &= (a^i)^{-1}(a^j b)^{-1} a^i a^j b \\
&= a^{-1} b^{-1} a^{-j} a^i a^j b \\
&= a^{-i} b a^i b \\
&= a^{-i} a^{n-i} \\
&= a^{n-2i}.
\end{aligned}
$$

So, $a^{n-2i} \neq e$ since n is odd. Meanwhile, for the vertices $a^k b$ and $a^l b$,

$$
\begin{aligned}
[a^k b, a^l b] &= (a^k b)^{-1}(a^l b)^{-1} a^k a^l b \\
&= b^{-1} a^{-k} b^{-1} a^{-l} a^k b a^l b \\
&= (a^{n-k})^{-1} a^{k-l} a^{n-l} \\
&= a^{2(k-l)}.
\end{aligned}
$$

Since $k \neq l$, $[a^k b, a^l b] \neq e$. Hence, $a^k b$ is adjacent to $a^l b$, where $k, l = \{0, 1, 2, ..., n-1\}$. Therefore, $NC\Gamma_G^{g=e} = K_{\underbrace{1, 1, ..., 1}_{n \text{ times}}, n-1} \cup \{e\}$.

Next, let n be even. Then by Definition 2.1, the element $a^k b$ is not adjacent to $a^{k+\frac{n}{2}} b$ since

$$
\begin{aligned}
[a^k b, a^{k+\frac{n}{2}} b] &= (a^k b)^{-1}(a^{k+\frac{n}{2}} b)^{-1} a^k b a^{k+\frac{n}{2}} b \\
&= b^{-1} a^{-k} b^{-1} a^{-k-\frac{n}{2}} a^k b a^{k+\frac{n}{2}} b \\
&= b a^{-k} b a^{-k-\frac{n}{2}} a^k b a^{k+\frac{n}{2}} b
\end{aligned}
$$

$$= (a^{n-k})^{-1} a^{-\frac{n}{2}} a^{n-k-\frac{n}{2}}$$

$$= a^{-n}$$

$$= e.$$

Moreover, a^i and $a^j b$ are not adjacent to each other since $[a^i, a^j b] = a^{n-2i} = e$ when $i = \frac{n}{2}$, but for $i \neq \frac{n}{2}$, they are adjacent to each other. Two vertices $a^j b$ are adjacent to other $\frac{n}{2}$ set of vertices $a^j b$. Hence,

$$NC\Gamma_G^{g=e} = K_{\underbrace{2, 2, ..., 2}_{\frac{n}{2}\text{ times}}, n-2} \cup \{e\} \cup \{a^{\frac{n}{2}}\}.$$

Theorem 3.3. *Let* $NC\Gamma_G^{g=a^i b}$ *be the gNC graph of the dihedral groups of order* $2n$, *where* $n \geq 3$ *for a fixed element* $a^i b$, $i = \{1, 2, ..., n-1\}$. *Then* $NC\Gamma_G^{g=a^i b} = K_{2n}$, *which is a complete graph of* $2n$ *vertices.*

Proof. All elements in D_{2n} are the vertices of the *gNC* graph. For any two elements $x = a^i b$ and $y = a^j b$, where $i, j = \{0, 1, 2, ..., n-1\}$ and $i \neq j$,

$$[a^i b, a^j b] = (a^i b)^{-1} (a^j b)^{-1} a^i b a^j b$$

$$= b^{-1} a^{-i} b^{-1} a^{-j} a^i b a^j b$$

$$= (a^{n-1})^{-1} a^{-j+i} a^{n-j}$$

$$= a^{2(i-j)}$$

$$\neq a^i b.$$

For $x = a^i$ and $y = a^j b$,

$$[a^i, a^j b] = (a^i)^{-1}(a^j b)^{-1} a^i a^j b$$
$$= a^{n-2i}$$
$$\neq a^i b.$$

Obviously, a^i is adjacent to a^j since $[a^i, a^j] \neq a^i b.$ Hence, by Definition 2.1, they are adjacent to each other. Thus, $NC\Gamma_{D_{2n}}^{g=a^i b}$ is a complete graph of $2n$, K_{2n}.

Theorem 3.4. *Let* $NC\Gamma_{Q_{4n}}^{g=e}$ *be the gNC graph of the generalized quaternion groups of order* $4n$, *where* $n \geq 2$ *for a fixed element* e. *Then*

$$NC\Gamma_{Q_{4n}}^{g=e} = K_{\underbrace{2, 2, \ldots, 2}_{n \text{ times}}, 2n-2} \cup \{e\} \cup \{a^n\}.$$

Proof. The proof is similar to the proof of Theorem 3.2 in case n is even.

Theorem 3.5. *Let* $NC\Gamma_{Q_{4n}}^{g=a^i b}$ *be the gNC graph of the generalized quaternion groups of order* $4n$, *where* $n \geq 2$ *for a fixed element* $a^i b$, $i = \{0, 1, 2, \ldots, 2n-1\}$. *Then* $NC\Gamma_{Q_{4n}}^{g=a^i b} = K_{4n}$, *which is a complete graph of* $4n$ *vertices*.

Proof. All elements in Q_{4n} are the vertices of the *gNC* graph. The proof is similar to Theorem 3.3 for $i = \{0, 1, 2, \ldots, 2n-1\}$.

Theorem 3.6. *Let* $NC\Gamma_{QD_{2^n}}^{g=e}$ *be the gNC graph of the quasidihedral groups of order* 2^n, *where* $n \geq 4$ *for a fixed element* e. *Then*

$$NC\Gamma_{Q_{4n}}^{g=e} = K_{\underbrace{2, 2, ..., 2}_{2^{n-2} \text{ times}}, 2^{n-1}-2} \cup \{e\} \cup \{a^{2^{n-2}}\}.$$

Proof. The proof is similar to the proof of Theorem 3.2 in case n is even.

Theorem 3.7. *Let* $NC\Gamma_{QD_{2^n}}^{g=a^ib}$ *be the gNC graph of the quasidihedral groups of order* 2^n, *where* $n \geq 4$ *for a fixed element* a^ib, $i = \{0, 1, 2, ..., 2^{n-1} - 1\}$. *Then* $NC\Gamma_{QD_{2^n}}^{g=a^ib} = K_{2^n}$, *which is a complete graph of* 2^n *vertices*.

Proof. All elements in QD_{2^n} are the vertices of the *gNC* graph. The proof is similar to Theorem 3.3 for $i = \{0, 1, 2, ..., 2^{n-1} - 1\}$.

Next, the new theoretical results in terms of general expressions of the Randić index of the *gNC* graph for the graphs stated in the above theorems are determined. Note that the Randić index of a graph with an isolated vertex is zero. Hence, it will be omitted in the computation.

Theorem 3.8. *Let* $R(NC\Gamma_{D_{2n}}^{g=e})$ *be the Randić index of the gNC graph for the dihedral groups of order* $2n$, *where* $n \geq 3$ *for a fixed element* e. *Then*

$$R(NC\Gamma_G^{g=e}) = \begin{cases} \dfrac{n(n-1)}{\sqrt{2n(n-1)}} + \dfrac{n}{4}, & \text{if } n \text{ is odd}, \\ \dfrac{n(n-2)}{\sqrt{2n(n-2)}} + \dfrac{n}{4}, & \text{if } n \text{ is even}. \end{cases}$$

Proof. First, let n be odd. Based on Theorem 3.2, $NC\Gamma_{D_{2n}}^{g=e}$ is a multipartite graph which has $n + 1$ subsets with an isolated vertex. There are n subsets that have one vertex each, and only one subset that has $n - 1$ vertices. The elements a^i, where $i = \{1, 2, ..., n - 1\}$ are not adjacent to each other, but they are adjacent to all elements $a^j b$, where $j = \{1, 2, ..., n-1\}$. Meanwhile, the elements $a^j b$ are adjacent to each other since each of them contains in different subset. Therefore, $\deg(a^i) = n$ and $\deg(a^j b) = 2n - 2$.

Since there are $n(n-1)$ edges that connect the elements of degree n and degree $2n-2$, and there are $\frac{n(n-1)}{2}$ edges that connect the elements of degree $2n-2$, by Definition 2.4,

$$R(NC\Gamma_G^{g=e}) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}}$$

$$= \frac{n(n-1)}{\sqrt{\deg(a^i)\deg(a^j b)}} + \frac{n(n-1)}{2}\left[\frac{1}{\sqrt{\deg(a^j b)\deg(a^j b)}}\right]$$

$$= \frac{n(n-1)}{\sqrt{n(2n-2)}} + \frac{n(n-1)}{2}\left[\frac{1}{\sqrt{(2n-2)(2n-2)}}\right]$$

$$= \frac{n(n-1)}{\sqrt{2n(n-1)}} + \frac{n}{4}.$$

Next, let n be even. From Theorem 3.2, $NC\Gamma_{D_{2n}}^{g=e}$ is a multipartite graph which has $\frac{n}{2}$ subsets that contain two vertices each, and a subset of $n-2$ vertices. A subset of $n-2$ vertices contains the non-central elements a^i, where $i = \{1, 2, ..., n-1\}$ that are not adjacent to each other, but they are adjacent to all elements $a^j b$, where $j = \{0, 1, 2, ..., n-1\}$. Meanwhile, $\frac{n}{2}$ subsets have two elements $a^j b$ in each subset and they are adjacent to elements $a^j b$ in the other subsets. Therefore, $\deg(a^i) = 2\left(\frac{n}{2}\right) = n$ and $\deg(a^j b) = n - 2 + 2\left(\frac{n}{2} - 1\right) = 2n - 4$.

Since there are $n(n-2)$ edges that connect the elements of degree n and degree $2(n-4)$, and there are $|E(K_n)| - \frac{n}{2} = \frac{n(n-1)}{2} - \frac{n}{2} = \frac{n(n-2)}{2}$ edges that connect the elements of degree $2n-4$, by Definition 2.4,

$$R(NC\Gamma_G^{g=e}) = \sum_{uv\in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}}$$

$$= \frac{n(n-2)}{\sqrt{\deg(a^i)\deg(a^jb)}} + \frac{n(n-2)}{2}\left[\frac{1}{\sqrt{\deg(a^jb)\deg(a^jb)}}\right]$$

$$= \frac{n(n-2)}{\sqrt{n(2n-4)}} + \frac{n(n-2)}{2}\left[\frac{1}{\sqrt{(2n-4)(2n-4)}}\right]$$

$$= \frac{n(n-2)}{\sqrt{2n(n-2)}} + \frac{n}{4}.$$

Theorem 3.9. *Let* $R(NC\Gamma_{D_{2n}}^{g=a^ib})$ *be the Randić index of the gNC graph for the dihedral groups of order* $2n$, *where* $n \geq 3$ *for a fixed element* a^ib, $i = \{0, 1, 2, ..., n-1\}$. *Then* $R(NC\Gamma_{D_{2n}}^{g=a^ib}) = n$.

Proof. By Theorem 3.3, $NC\Gamma_{D_{2n}}^{g=a^ib}$ is a complete graph of $2n$ vertices that have degree $2n-1$. The number of edges is $n(2n-1)$. Thus,

$$R(NC\Gamma_{D_{2n}}^{g=e}) = \sum_{uv\in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}} = \frac{n(2n-1)}{\sqrt{(2n-1)(2n-1)}} = \frac{n(2n-1)}{(2n-1)} = n.$$

An example to illustrate Theorems 3.8 and 3.9 is presented in the following.

Example 3.10. Let $D_6 = \{e, a, a^2, b, ab, a^2b\}$, where $n = 3$ (odd). By Definition 2.1, $NC\Gamma_{D_6}^{g=e}$ and $NC\Gamma_{D_6}^{g=a^ib}$, where $i = \{0, 1, 2\}$ are shown in Figures 2 and 3, respectively.

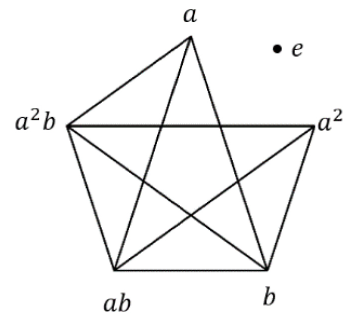

Figure 2. $NC\Gamma_{D_6}^{g=e}$.

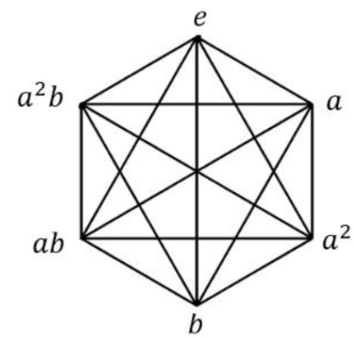

Figure 3. $NC\Gamma_{D_6}^{g=a^ib}$.

Based on Figure 2, $\deg(a) = \deg(a^2) = 3$ and $\deg(b) = \deg(ab) = \deg(a^2b) = 4$. By Definition 2.1, the Randić index of $NC\Gamma_{D_6}^{g=e}$ is

$$R(NC\Gamma_G^{g=e}) = \sum_{uv\in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}}$$

$$= \frac{1}{\sqrt{\deg(a)\deg(b)}} + \frac{1}{\sqrt{\deg(a)\deg(ab)}} + \frac{1}{\sqrt{\deg(a)\deg(a^2b)}}$$

$$+ \frac{1}{\sqrt{\deg(a^2)\deg(b)}} + \frac{1}{\sqrt{\deg(a^2)\deg(ab)}} + \frac{1}{\sqrt{\deg(a^2)\deg(a^2b)}}$$

$$+\frac{1}{\sqrt{\deg(b)\deg(ab)}}+\frac{1}{\sqrt{\deg(b)\deg(a^2b)}}+\frac{1}{\sqrt{\deg(ab)\deg(a^2b)}}$$

$$=\frac{1}{\sqrt{3(4)}}+\frac{1}{\sqrt{3(4)}}+\frac{1}{\sqrt{3(4)}}+\frac{1}{\sqrt{3(4)}}+\frac{1}{\sqrt{3(4)}}+\frac{1}{\sqrt{3(4)}}$$

$$+\frac{1}{\sqrt{4(4)}}+\frac{1}{\sqrt{4(4)}}+\frac{1}{\sqrt{4(4)}}$$

$$= 2.482.$$

Meanwhile, based on Figure 3, the degree of all vertices is five. Consider the edge number of a complete graph, $K_r = \frac{r(r-1)}{2}$. Then the number of edges for this graph is 15. Hence, by Definition 2.4,

$$R(NC\Gamma_{D_6}^{g=b}) = R(NC\Gamma_{D_6}^{g=ab}) = R(NC\Gamma_{D_6}^{g=a^2b}) = 15\left[\frac{1}{\sqrt{5(5)}}\right] = 3.$$

On the other hand, by using Theorems 3.8 and 3.9 for $n = 3$,

$$R(NC\Gamma_{D_6}^{g=e}) = \frac{n(n-1)}{\sqrt{2n(n-1)}} + \frac{n}{4} = \frac{3(3-1)}{\sqrt{2(3)(3-1)}} + \frac{3}{4} = 2.482,$$

$$R(NC\Gamma_{D_6}^{g=b}) = R(NC\Gamma_{D_6}^{g=ab}) = R(NC\Gamma_{D_6}^{g=a^2b}) = n = 3.$$

Therefore, it can be concluded that the Randić index of the *gNC* graph of D_6 computed manually is same that comes out from theorems.

In addition, the general formulas of the Randić index of the *gNC* graph for the generalized quaternion groups and the quasidihedral groups given in Theorems 3.11 to 3.14 are established in the following four theorems:

Theorem 3.11. *Let* $R(NC\Gamma_{Q_{4n}}^{g=e})$ *be the Randić index of the gNC graph for the generalized quaternion groups of order* $4n$, *where* $n \geq 2$ *with fixed element e. Then* $R(NC\Gamma_{Q_{4n}}^{g=e}) = \frac{4n(n-1)}{\sqrt{8n(n-1)}} + \frac{n}{2}$.

Proof. Based on Theorem 3.4, $NC\Gamma_{Q_{4n}}^{g=e}$ is a multipartite graph of $n+1$ subsets, in which n subsets have two vertices each, where the vertices are all elements of $a^j b$, $j = \{0, 1, 2, ..., 2n-1\}$, and a subset has $2n-2$ vertices which consists of non-central elements of a^i, $i = \{0, 1, 2, ..., 2n-1\}$. Hence, $\deg(a^i) = 2n$ and $\deg(a^j b) = 2n - 2 + 2(n-1) = 4n - 4$.

There are $(2n-2)(2n) = 4n(n-1)$ edges that connect the vertices of degree $4n-4$ and degree $2n$. Meanwhile, $|E(K_{2n})| - n = 2n(n-1)$ edges connect between two vertices of degrees $4n-4$. Therefore, by Definition 2.4,

$$R(NC\Gamma_G^{g=e}) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}}$$

$$= 4n(n-1)\left[\frac{1}{\sqrt{\deg(a^j b)\deg(a^i)}}\right]$$

$$+ 2n(n-2)\left[\frac{1}{\sqrt{\deg(a^j b)\deg(a^j b)}}\right]$$

$$= \frac{4n(n-1)}{\sqrt{(4n-4)(2n)}} + \frac{2n(n-1)}{\sqrt{(4n-4)(4n-4)}}$$

$$= \frac{4n(n-1)}{\sqrt{(8n)(n-1)}} + \frac{n}{2}.$$

Theorem 3.12. *Let* $R(NC\Gamma_{Q_{4n}}^{g=a^i b})$ *be the Randić index of the gNC graph for the generalized quaternion groups of order* $4n$, *where* $n \geq 2$ *with fixed element* $a^i b$, $i = \{0, 1, 2, ..., 2n-1\}$. *Then* $R(NC\Gamma_{Q_{4n}}^{g=a^i b}) = 2n$.

Proof. By Theorem 3.5, the $NC\Gamma_{Q_{4n}}^{g=a^i b}$ is a complete graph of $4n$ vertices. Then, obviously all vertices have degree $4n-1$. The number of edges is $2n(4n-1)$. Then

$$R(NC\Gamma_{Q_{4n}}^{g=a^i b}) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}} = \frac{2n(4n-1)}{\sqrt{(4n-1)(4n-1)}}$$

$$= \frac{2n(4n-1)}{(4n-1)} = 2n.$$

Theorem 3.13. *Let* $R(NC\Gamma_{QD_{2^n}}^{g=e})$ *be the Randić index of the gNC graph for the quasidihedral group of order* 2^n, *where* $n \geq 4$ *with fixed element e. Then* $R(NC\Gamma_{QD_{2^n}}^{g=e}) = \dfrac{2^{2n-2} - 2^n}{\sqrt{2^{n-1}(2^n - 4)}} + \dfrac{2^{2n-3} - 2^{n-1}}{2^n - 4}$.

Proof. Based on Theorem 3.6, $NC\Gamma_{QD_{2^n}}^{g=e}$ is a multipartite graph of $2^{n-2}+1$ subsets, in which 2^{n-2} subsets have two vertices each, where the vertices are all elements of $a^j b$, $j = \{0, 1, ..., 2^{n-1}-1\}$, and a subset has $2^{n-1}-2$ vertices which consists of non-central elements of a^i, $i = \{0, 1, ..., 2^{n-1}-1\}$. Hence, $\deg(a^i) = 2(2^{n-2}) = 2^{n-1}$ and $\deg(a^j b) = 2^{n-1} - 2 + 2(2^{n-2}-1) = 2^n - 4$.

There are $(2^{n-1}-2)(2 \times 2^{n-2}) = 2^{n-1}(2^{n-1}-2)$ edges that connect the vertices of degree 2^{n-1} and degree $2^n - 4$. Meanwhile, $|E(K_{2(2^{n-2})})| - 2^{n-2} = |E(K_{2^{n-1}})| - 2^{n-2} = \dfrac{2^{n-1}(2^{n-1}-1)}{2} - 2^{n-2}$ edges are connected between two vertices of degrees $2^n - 4$. Therefore, by Definition 2.4,

$$R(NC\Gamma^{g=e}_{QD_{2^n}}) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\deg u \deg v}}$$

$$= 2^{n-1}(2^{n-1} - 2)\left[\frac{1}{\sqrt{\deg(a^j b)\deg(a^i)}}\right]$$

$$+ \left(\frac{2^{n-1}(2^{n-1} - 1)}{2} - 2^{n-2}\right)\left[\frac{1}{\sqrt{\deg(a^j b)\deg(a^j b)}}\right]$$

$$= \frac{2^{n-1}(2^{n-1} - 2)}{\sqrt{2^{n-1}(2^n - 4)}} + \frac{1}{2^n - 4}\left[\frac{2^{n-1}(2^{n-1} - 1)}{2} - 2^{n-2}\right]$$

$$= \frac{2^{2n-2} - 2^n}{\sqrt{2^{n-1}(2^n - 4)}} + \frac{2^{2n-3} - 2^{n-1}}{2^n - 4}.$$

Theorem 3.14. *Let* $R(NC\Gamma^{g=a^i b}_{QD_{2^n}})$ *be the Randić index of the gNC graph for the quasidihedral groups of order* 2^n, *where* $n \geq 4$ *with fixed element* $a^i b$, $i = \{0, 1, ..., 2^{n-1} - 1\}$. *Then* $R(NC\Gamma^{g=a^i b}_{QD_{2^n}}) = 2^{n-1}$.

Proof. Based on Theorem 3.7, $NC\Gamma^{g=a^i b}_{QD_{2^n}}$ is a complete graph of 2^n vertices. By using the same proving method as Theorem 3.9, $R(NC\Gamma^{g=a^i b}_{QD_{2^n}})$ $= 2^{n-1}$.

This study distinguishes itself from prior work on non-commuting graphs and topological indices by focusing on the g-non-commuting graph, a recent extension of the classical non-commuting graph, which incorporates a fixed group element to refine adjacency relations. Unlike traditional non-commuting graphs that exclude central elements, a g-non-commuting graph includes them though as isolated vertices offering a more comprehensive view of the group's structure. By deriving general formulas for the Randić index of *g*-non-commuting graphs associated with dihedral, generalized quaternion, and quasidihedral groups, this work bridges algebraic properties and graph-theoretical measures in a novel way. The study introduces a fresh framework for understanding group connectivity through multipartite and complete graph structures, revealing how internal group symmetries translate into topological patterns. These contributions not only extend the scope of topological indices within algebraic graph theory but also provide new tools for analyzing group properties through graph connectivity which enable the applications beyond pure mathematics, such as in chemistry and network science.

4. Conclusion

The *g*-non-commuting graphs of the dihedral, generalized quaternion and quasidihedral groups with fixed g, namely e and $a^i b$ have been introduced. The graphs are found to be multipartite graph and complete graph, respectively. In addition, based on the general forms of the *g*-non-commuting graph for these three finite groups, each vertex degree in the graph is determined. Then, their general formulas of the Randić index in terms of n are established. Some examples are also given to illustrate the main theorem. The findings can be useful to the other disciplines to estimate the chemical and physical properties of molecules and they are also beneficial to those who also want to further this research to the other types of graphs of groups and different types of topological indices.

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