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Generalization of Randić Index of the Non-commuting Graph for Some Finite Groups

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Abstract Randić index is one of the classical graph-based molecular structure descriptors in the field of mathematical chemistry. The Randić index of a graph is calculated by summing the reciprocals of the square root of the product of the degrees of two adjacent vertices in the graph. Meanwhile, the non-commuting graph is the graph of vertex set whose vertices are non-central elements and two distinct vertices are joined by an edge if and only if they do not commute. In this paper, the general formula of the Randić index of the non-commuting graph associated to three types of finite groups are presented. The groups involved are the dihedral groups, the generalized quaternion groups, and the quasi-dihedral groups. Some examples of the Randić index of the non-commuting graph related to a certain order of these groups are also given based on the main results.

Keywords: Randić index, Non-commuting graph, Dihedral group, Generalized quaternion group, Quasi-dihedral groups.

Introduction

A topological index is a numerical value that can be calculated from two-dimensional graph. It provides quantitative measures that can be used to correlate the topological characteristics of a molecular structure with its physical, chemical, or biological properties. The topological indices have become rapidly important especially in structural chemistry. Specifically, it can be used to code chemical information such as for the quantitative description of chemical structures in the analysis of relation between the structure of a molecule and its properties, in the theory of the atomic structure and reactivity of molecules and even in designing a chemical experiment [1].

The relationship between a topological index and the molecular structure lies in the fact that certain structural features or patterns can influence the properties or behavior of a molecule. By quantifying these features using topological indices, researchers can establish relationships or correlations between the index values and various molecular properties. This allows for the prediction or estimation of certain properties based solely on the structural information of a molecule [2].

Since 1947, the development of new concepts of topological indices is increasing, started with the first type of topological indices which is the Wiener index that has been introduced by Harold Wiener [3]. After that, many types of topological indices have been developed such as Szeged index [4-5], Zagreb index [6-8], Harary index [9-10], Randić index [11-13] and Gutman index [14-15]. Different topological indices focus on different aspects of a molecular structure. For example, the Randić index quantifies connectivity patterns and can provide information about reactivity or activity. Other indices may focus on measures of branching, symmetry, or distance-related properties within a molecule.

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In this paper, the general formulas of the Randić index of the non-commuting graph for the dihedral groups, the generalized quaternion groups, and the quasi-dihedral groups are determined. Then, some examples of each main result are given. Then, their general formulas are determined by using their definitions.

Preliminaries

In this section, some preliminaries are stated and are used to prove the main theorems. The following are the group presentations of the dihedral groups, generalized quaternion groups and the quasi-dihedral groups. This paper only focuses on these three types of groups since they belong to the same isomorphism classes.

Definition 1 [16] **Dihedral Group**

The dihedral group, D_{2n}, is the symmetry group of an n-sided regular polygon for $n \geq 1$ with order $2n$. The group presentation for the non-abelian dihedral group, D_{2n} , is as follows:

$$D_{2n} \cong \langle a, b | a^n = b^2 = 1,\ bab = a^{-1} \rangle,$$

where $n \geq 3$.

Definition 2 [16] **Generalized Quaternion Group**

The non-abelian generalized quaternion group is a group that has order $4n$ where $n \geq 2$. Its group presentation is as follows:

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

Definition 3 [16] **Quasi-dihedral Group**
The quasi-dihedral groups or also called semi-dihedral groups are certain non-abelian groups of order a power of 2 which is denoted as QD_{2^n}. The group presentation for the non-abelian quasi-dihedral group is as follows:

$$QD_{2^n} \cong \left\langle a, b \middle| a^{2^{n-1}} = b^2 = 1, bab = a^{2^{n-2}-1} \right\rangle,$$

where $n \geq 4$.

Next, some basic definitions and preliminaries are stated in the following definitions and propositions, respectively. These are used to prove the main results.

Definition 4 [17] **Conjugacy Class**

Let a and b be elements of G. The element of a and b are said to be conjugate if $xax^{-1} = b$ for some $x \in G$. The conjugacy class of a is the set $cl(a) = \{xax^{-1} | x \in G\}$ and the number of conjugacy classes of a is denoted by $k(G)$.

Definition 5 [18] **Center**
The center of a group G is the set of elements that commute with every element of G, denoted as $Z(G)$.

Proposition 1 [19] Let G be a dihedral group, D_{2n} of order $2n$ and $k(G)$ be the number of conjugacy classes of G. Then,

$$k(G) = \begin{cases} \dfrac{n+3}{2}, & \text{if } n \text{ is odd,} \\ \dfrac{n+6}{2}, & \text{if } n \text{ is even.} \end{cases}$$

Proposition 2 [20] Let G be the generalized quaternion group, Q_{4n} where $n \geq 2$ and the number of conjugacy classes of G is denoted by $k(G)$. Then, $k(G) = n + 3$.

Proposition 3 [21] Let G be a quasidihedral group, QD_{2^n} where $n \geq 4$ and the number of conjugacy classes of G is denoted by $k(G)$. Then,

$$k(G) = 2^{n-2} + 3.$$

Proposition 4 [19] Let G be a dihedral group, $D_{2n} = \langle a, b | a^n = b^2 = 1,\ bab = a^{-1} \rangle$ where $n \geq 3, n \in N$, and $Z(G)$ is the center of G. Then,

$$Z(G) = \begin{cases} \{1\}, & \text{if } n \text{ is odd,} \\ \left\{1, a^{\frac{n}{2}}\right\}, & \text{if } n \text{ is even.} \end{cases}$$

Proposition 5 [22] Let G be a generalized quaternion group, Q_{4n} and $Z(G)$ is the centre of G. Then, $Z(G) = \{1, a^n\}$ where $n \geq 2$.

Proposition 6 [23] Let G be a quasi-dihedral group, QD_{2^n}, and $Z(G)$ is the center of G. Then, $Z(G) = \left\{1, a^{2^{n-2}}\right\}$ where $n \geq 4$.

In graph theory, many types of graphs related to groups have been introduced and one of them is the non-commuting graph, which is defined in the following.

Definition 6 [24] **Non-commuting Graph**
A non-commuting graph of G defines as a set of vertices $G - Z(G)$ where two distinct vertices x and y are joined by an edge whenever $xy \neq yx$. The non-commuting graph of G is denoted as Γ_G^{NC}.

Definition 7 [26] **Complete Multipartite Graph**
A complete multipartite graph, which is denoted as $K_{n_1, n_2, \ldots, n_m}$ is a graph that has vertices partitioned into m subsets of $n_1, n_2, \ldots, n_m$ elements each, and vertices are adjacent if and only if they are in different subsets in the partition.

Proposition 7 [25] Let G be the dihedral groups of order $2n$ where $n \geq 3, n \in \mathbb{N}$ and let Γ_G^{NC} be the non-commuting graph of G. Then,

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

Proposition 8 [25] Let G be the generalized quaternion groups of order $4n$ where $n \geq 2, n \in \mathbb{N}$ and let Γ_G^{NC} be the non-commuting graph of G. Then,

$$\Gamma_G^{NC} = K_{\underbrace{2,2,\ldots,2}_{n \text{ times}}, n-2}.$$

Proposition 9 [25] Let G be the quasi-dihedral groups of order 2^n where $n \geq 4, n \in \mathbb{N}$ and let Γ_G^{NC} be the non-commuting graph of G. Then,

$$\Gamma_G^{NC} = K_{\underbrace{2,2,\ldots,2}_{2^{n-2} \text{ times}}, 2^{n-1}-2}.$$

Proposition 10 [24] Let G be a finite group and Γ_G be the non-commuting graph of G. Then,

$$2|E(\Gamma_G)| = |G|^2 - k(G)|G|,$$

where $E(\Gamma_G)$ is the set of edges in the graph and $k(G)$ is the number of conjugacy classes of G.

This paper focuses on finding the Randić index of the non-commuting graph for three types of groups. The Randić index is the degree-based topological index which has been introduced by Milan Randić that is used to measure the level of branching in the carbon-atom skeleton of saturated hydrocarbons [27]. The definition of the Randić index is given in the following.

Definition 8 [27] **Randić Index**
Let Γ be a connected graph. Then, the Randić index of Γ is given by

$$R(\Gamma) = \sum_{a,b \epsilon E(\Gamma)} \frac{1}{\sqrt{\deg(a)\deg(b)}},$$

where $E(\Gamma)$ is the set of edges in the graph, a, b are the vertices of the graph, and $\deg(a)$ is the degree of vertex of a while $\deg(b)$ is the degree of vertex b.

Results and Discussion

In this section, the Randić index of the non-commuting graph for three types of groups which are dihedral group, generalized quaternion group, and quasi-dihedral group are determined. The proofs are shown in the following theorems using their definitions and propositions stated in the preliminaries.

The Randić Index of the Non-commuting Graph for D_{2n}

Theorem 1 Let G be the dihedral group, $D_{2n} = \langle a, b | a^n = b^2 = 1, bab = a^{-1} \rangle$ where $n \geq 3$ and let Γ_G^{NC} be the non-commuting graph of the dihedral group. Then,

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

Proof

Case 1: n is odd.

By Proposition 7, $\Gamma_G^{NC} = K_{\underbrace{1,1,\dots,1}_{n \text{ times}},n-1}$. The non-central elements a^i do not adjacent to each other, where $i = \{1,2,\dots,n-1\}$, while they are always adjacent to elements $a^i b$. Thus, there are $n(n-1)$ edges that connect the vertices a^i and $a^i b$. The $\deg(a^i) = n$ and $\deg(a^i b) = 2n-2$. By Proposition 10 and Proposition 1, we have $|E(\Gamma_G^{NC})| = \frac{3}{2}n(n-1)$.

Hence, by Definition 8,

$$\begin{aligned} R(\Gamma_G^{NC}) &= \sum_{a,b \epsilon E(\Gamma)} \frac{1}{\sqrt{\deg(a)\deg(b)}} \\ &= n(n-1)\left[\frac{1}{\sqrt{n(2n-2)}}\right] + \left(|E(\Gamma_G^{NC})| - n(n-1)\right)\left[\frac{1}{\sqrt{(2n-2)^2}}\right] \\ &= \frac{n(n-1)}{\sqrt{n(2n-2)}} + \left(\frac{3}{2}n(n-1) - n(n-1)\right)\left[\frac{1}{(2n-2)}\right] \\ &= \frac{n\sqrt{2n(n-1)} + 4n(n-1)}{4\sqrt{2n(n-1)}}. \end{aligned}$$

Case 2: n is even.

By Proposition 7, $\Gamma_G^{NC} = K_{\underbrace{2,2,\dots,2}_{\frac{n}{2} \text{ times}},n-2}$. Then, there are $n(n-2)$ edges that connect the vertices a^i and $a^i b$, where $i = \{1,2,\dots,n-1\}$. The $\deg(a^i) = n$ and $\deg(a^i b) = 2n-4$. By Proposition 10 and Proposition 1, we have $|E(\Gamma_G^{NC})| = 3n\left(\frac{n}{2} - 1\right)$.

Hence, by Definition 8,

$$\begin{aligned} R(\Gamma_G^{NC}) &= \sum_{a,b \epsilon E(\Gamma)} \frac{1}{\sqrt{\deg(a)\deg(b)}} \\ &= n(n-2)\left[\frac{1}{\sqrt{n(2n-4)}}\right] + \left(|E(\Gamma_G^{NC})| - n(n-2)\right)\left[\frac{1}{\sqrt{(2n-4)^2}}\right] \\ &= \frac{n(n-2)}{\sqrt{n(2n-4)}} + \left(\frac{1}{2}n^2 - n\right)\left[\frac{1}{(2n-4)}\right] \end{aligned}$$

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

Example 1 Let G be the dihedral group of order six, D_6, which contains six elements and Γ_G^{NC} be the non-commuting graph of group G. By Theorem 3.1,

$$\begin{aligned} R(\Gamma_G^{NC}) &= \frac{n\sqrt{2n(n-1)} + 4n(n-1)}{4\sqrt{2n(n-1)}} \\ &= \frac{3\sqrt{2(3)(3-1)} + 4(3)(3-1)}{4\sqrt{2(3)(3-1)}} \\ &= 2.48. \end{aligned}$$

Example 2 Let G be a dihedral group of order eight, D_8, which contains eight elements and Γ_G^{NC} be the non-commuting graph of group G. By Theorem 3.1,

$$\begin{aligned} R(\Gamma_G^{NC}) &= \frac{n\sqrt{2n(n-2)} + 4n(n-2)}{4\sqrt{2n(n-2)}} \\ &= \frac{4\sqrt{2(4)(4-2)} + 4(4)(4-2)}{4\sqrt{2(4)(4-2)}} \\ &= 3. \end{aligned}$$

The Randić Index of the Non-commuting Graph for Q_{4n}

Theorem 2 Let G be the generalized quaternion group, $Q_{4n} = \langle a, b | a^n = b^2, a^{2n} = b^4 = 1, bab = a^{-1} \rangle$ where $n \geq 2$ and let Γ_G^{NC} be the non-commuting graph of the generalized quaternion group. Then, the Randić index of the non-commuting graph of the generalized quaternion group,

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

Proof

By Proposition 8, $\Gamma_G^{NC} = K_{\underbrace{2,2,\ldots,2}_{n\ \text{times}},n-2}$. Then, there are $2n(2n-2)$ edges that connect the vertices a^i and $a^i b$, where $i = \{1,2,\ldots,2n-1\}$. The $\deg(a^i) = 2n$ and $\deg(a^i b) = 4n-4$. By Proposition 10 and Proposition 1, we have $|E(\Gamma_G^{NC})| = 6n(n-1)$.

Hence, by Definition 8,

$$\begin{aligned} R(\Gamma_G^{NC}) &= \sum_{a,b \in E(\Gamma)} \frac{1}{\sqrt{\deg(a)\deg(b)}} \\ &= 2n(2n-2)\left[\frac{1}{\sqrt{2n(4n-4)}}\right] + \left(|E(\Gamma_G^{NC})| - 2n(2n-2)\right)\left[\frac{1}{\sqrt{(4n-4)^2}}\right] \\ &= \frac{4n(n-1)}{\sqrt{8n(n-1)}} + 2n(n-1)\left[\frac{1}{4(n-1)}\right] \\ &= \frac{4n(n-1)}{\sqrt{8n(n-1)}} + \frac{n}{2}. \qquad \blacksquare \end{aligned}$$

Example 3 Let G be the generalized quaternion group of order eight, Q_8, which contains eight elements and Γ_G^{NC} be the non-commuting graph of group G. By Theorem 2,

$$\begin{aligned} R(\Gamma_G^{NC}) &= \frac{4n(n-1)}{\sqrt{8n(n-1)}} + \frac{n}{2} \\ &= \frac{4(2)(2-1)}{\sqrt{8(2)(2-1)}} + \frac{2}{2} \\ &= 3. \end{aligned}$$

The Randić Index of the Non-commuting Graph for QD_{2^n}

Theorem 3 Let G be the quasi-dihedral group, $QD_{2^n} = \langle a, b | a^{2n-1} = b^2 = 1, bab = a^{2^{n-2}-1} \rangle$ where $n \geq 4$ and let Γ_G^{NC} be the non-commuting graph of quasi-dihedral group. Then, the Randić index of the non-commuting graph of quasi-dihedral group,

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

Proof

By Proposition 9, $\Gamma_G^{NC} = K_{\underbrace{2,2,\ldots,2}_{2^{n-2}\text{ times}},2^{n-1}-2}$. Then, there are $(2^{n-1}-2)(2^{n-1})$ edges that connect the vertices a^i and $a^i b$, where $i = \{1,2,\ldots,2^{n-1}-1\}$. The $\deg(a^i) = 2(2^{n-2})$ and $\deg(a^i b) = 2^n - 4$. By Proposition 10 and Proposition 1, we have $|E(\Gamma_G^{NC})| = 3(2^{n-1})(2^{n-2}-1)$.
Hence, by Definition 8,

$$\begin{aligned}
R(\Gamma_G^{NC}) &= \sum_{a,b \epsilon E(\Gamma)} \frac{1}{\sqrt{\deg(a)\deg(b)}} \\
&= (2^{n-1}-2)(2^{n-1}) \left[\frac{1}{\sqrt{2(2^{n-2})(2^n-4))}}\right] + \left(|E(\Gamma_G^{NC})| - (2^{n-1}-2)(2^{n-1})\right) \left[\frac{1}{\sqrt{(2^n-4)^2}}\right] \\
&= \frac{(2^{n-1}-2)(2^{n-1})}{\sqrt{2(2^{n-2})(2^n-4))}} + \left[\frac{2^{n-1}}{2^n-4}\right][3(2^{n-2}-1) - (2^{n-1}-2)] \\
&= \frac{2^{n-1}(2^{n-1}-2)}{\sqrt{(2^{n-1})(2^n-4)}} + \frac{2^{n-1}(2^{n-2}-1)}{2^n-4}.
\end{aligned}$$

■

Example 4 Let G be the generalized quaternion group of order eight, QD_{16}, which contains 16 elements and Γ_G^{NC} be the non-commuting graph of group G. By Theorem 3,

$$\begin{aligned}
R(\Gamma_G^{NC}) &= \frac{2^{n-1}(2^{n-1}-2)}{\sqrt{(2^{n-1})(2^n-4)}} + \frac{2^{n-1}(2^{n-2}-1)}{2^n-4} \\
&= \frac{2^{4-1}(2^{4-1}-2)}{\sqrt{(2^{4-1})(2^4-4)}} + \frac{2^{4-1}(2^{4-2}-1)}{2^4-4} \\
&= 6.90.
\end{aligned}$$

Based on the computation in Examples 1, 2, 3 and 4, the numerical values increases when the order of the graph and group increases. In order to predict the chemical properties of some molecules, the chemists need to develop a mathematical model which consists of the topological index as a variable. These numerical values computed will be substituted into the mathematical model after some analysis on the isomorphism of the graph and molecules are done.

Conclusion

In conclusion, the general formula of the Randić index of the non-commuting graph associated to three finite groups, which are the dihedral groups, the generalized quaternion groups and the quasi-dihedral groups are determined. Based on the results, it is found that the Randić index of the non-commuting graph for these groups are directly proportional to the order of the graph. These theoretical results can help chemists and biologists to predict the physical and chemical properties in a faster way, without involving any laboratory works. In future, the Randić index of different types of graphs and groups can be found and the results can be applied to some molecular structures by using point group of certain orders.

Conflicts of Interest

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper.

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