



Eccentric Connectivity Index of the Non-Commuting Graph Associated to the Dihedral Groups of Order at Most 12

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ABSTRACT

A topological index is a numerical value or invariant in mathematics that characterizes specific topological aspects of a space, manifold, or mathematical object. Topological indices are used to differentiate between topological spaces or to capture specific characteristics of their structure. Meanwhile, a non-commuting graph is a graph in which two unique vertices are adjacent if, and only if, they do not commute, meaning $xy \neq yx$ and it consists of the non-central elements set in a group as a vertex. In this paper, since there are lack of connecting the topological indices and the graphs related to finite groups, the eccentric connectivity index (ECI) of the non-commuting graph for certain order of dihedral groups, is computed. As a result, the eccentric connectivity index of non-commuting graphs for dihedral groups increases as the order of the groups increases. In real life, one of the eccentric connectivity index's effects is that it can be utilized as a chemical descriptor in drug discovery to predict biological activities such as binding affinities to target proteins or enzymes.

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1. Introduction

Graph theory is a branch of mathematics that studies graphs, which are mathematical structures that express relationships between objects. Objects are represented as vertices, also known as nodes in a graph, and relationships between them are represented as edges linking pairs of vertices. Graphs are frequently utilized to describe and evaluate a wide range of real-world and abstract situations, making graph theory a fundamental and flexible topic of study. It is a vital tool for modeling systems in physics, computer science, engineering, and other disciplines. On the other hand, a topological index is a numerical value that characterizes specific topological properties of a space, manifold, or mathematical object. Furthermore, topological indices serve a variety of uses in fields ranging from pure mathematics to chemistry, computer science, and beyond. Many types of topological indices, such as the Wiener index [1], [2], Harary index [3], and Zagreb index [4], provide insights into the structure, behavior, and interactions within mathematical objects, networks, and systems for future investigation.

Researchers in [5] developed the eccentric connectivity index (ECI) in 2004, presenting the concept of ECI and its significance in graph theory and chemical graph theory. The concept of the "First Zagreb Eccentricity Index" was also proposed by [5]. Then, researchers in [6] utilized the ECI as a feature vector in machine-learning models to predict anti-HIV activity. The tests described in the research suggest that topological indices based on k -eccentricity, such as the ECI, are useful in predicting anti-HIV activity. Many researchers have introduced many types of topological indices, and they provide a practical measure of the compactness of molecules that require different information from the graph.



Originating from the field of mathematical chemistry in the mid-20th century, topological indices have undergone significant development and refinement over the years, driven by advancements in computational chemistry, graph theory, and data analysis techniques. In graph theory, many researchers focus on the topological indices of graphs in general. Meanwhile, the graphs related to groups are important in understanding their algebraic and symmetrical properties, in which the properties are very useful in studying the properties of molecular graphs in chemistry. Hence, since there are lack of connecting the topological indices and the graphs related to finite groups, the eccentric connectivity index (ECI) of the non-commuting graph for certain order of dihedral groups, is computed. Beforehand, the their non-commuting graphs are constructed using Maple software. Based on the graphs obtained, some properties of the graphs are determined, including the degree of the vertex in a graph and the distance between two vertices.

2. Literature Review

This section presents fundamental concepts, definitions, and previous results in group theory, graph theory, and topological indices. This study's definition of the topological index involved is presented as follows.

Definition 1 : Eccentric Connectivity Index (ECI)

The eccentric connectivity index (ECI) [7], written as ξ , is defined as the sum of the product of eccentricity and degree of each vertex in a hydrogen-suppressed molecular graph with n total vertices,

$$\xi = \sum_{i=1}^n E(i)V(i) \quad (1)$$

where $E(i)$ is the eccentricity and $V(i)$ is the degree of vertex i .

The studies on ECI began to gain attention among researchers since 2004 and they started to develop many new concepts of ECI. Researchers in [8] determined the ECI of chemical trees and proposed a simple linear algorithm to compute the ECI. Meanwhile, in 2019, researchers in [9] determined the ECI of identity graph of cyclic group and finite commutative ring with unity. In 2020, researchers in [10] introduced the multiplicative version of ECI and investigated the behavior of various families of composite graphs. Then, paper [11] reported the sharp lower bound of multiplicative ECI. In addition, the definition of graph and the non-commuting graph are stated in Definition 2 and Definition 3, respectively.

Definition 2 : Graph

A graph Γ consists of a finite set V of objects known as vertices, a finite set E of objects known as edges, and a function f that assigns a subset $\{n_0, n_1\}$ to each edge, where n_0 and n_1 are vertices [12].

Definition 3 : Non-Commuting Graph

The non-commuting graph of a group G [13] is a graph in which the vertices are the elements of G except the center of G , $Z(G)$ and two different vertices x and y are connected by an edge if and only if $xy \neq yx$.

Definition 4 : Degree of a Vertex

A degree of a vertex, $\deg(v)$ is the number of edges that have that vertex as an end point [12].

Definition 5 : Distance Between Two Vertices

The distance between two vertices, $d(v_i, v_j)$, is the shortest path from the vertex v_i to vertex v_j , where i and j represent the number of vertices [12].

Definition 6 : Eccentricity of a Vertex

The eccentricity, $E(v)$ of a vertex, v is the distance between v and the vertex longest away from v , or defined as the maximum value of distance, $d(v_i, v_j)$ [14].

Definition 7 : Dihedral Groups

A dihedral group [15] is a group that describes both the rotation and reflections of an n -sided polygon. According to [15], its group presentation is given as follows:

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

where $n \in \mathbb{N}$.

3. Results and Discussion

This section shows the non-commuting graph of order six, eight, ten, and twelve in the following proposition. These graphs are used to prove the main theorems.

Proposition 1 : Let G be the dihedral group, D_{2n} where $3 \leq n \leq 6$. Then, the non-commuting graphs of G, Γ are stated in the following figures.

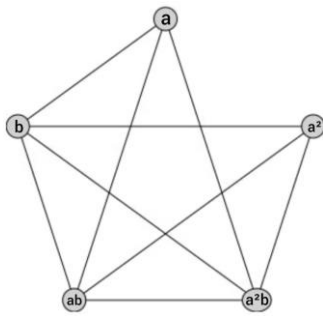


Figure 1. The non-commuting graph of D_6

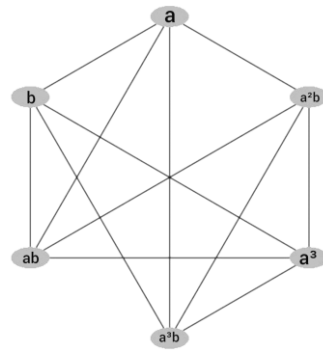


Figure 2. The non-commuting graph of D_8

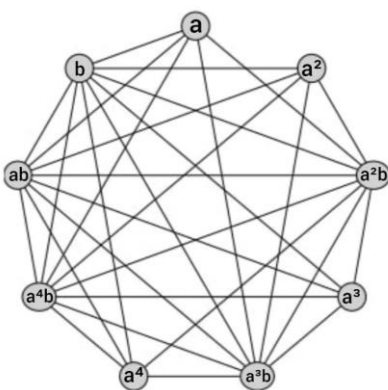


Figure 3. The non-commuting graph of D_{10}

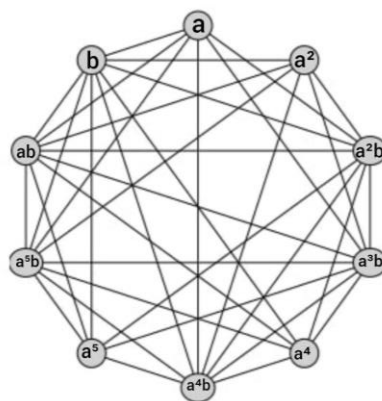


Figure 4. The non-commuting graph of D_{12}

Proof: The non-commuting graph is constructed by using Maple software.

Based on Proposition 1, the eccentric connectivity index of the non-commuting graph for a dihedral group of order at most 12 is given in the following theorems.

Theorem 1: Let G be a dihedral group of order 6, $D_6 = \langle a, b \mid a^3 = b^2 = 1, bab = a^{-1} \rangle$ where $n=3$ and Γ is the non-commuting graph of G . Then, the eccentric connectivity index of $\Gamma, \xi(\Gamma) = 24$.

Proof: Based on Proposition 1 and Figure 1, the distance, degree, and eccentricity of the non-commuting graph of D_6 are presented in the following Table 1 and Table 2.

Table 1. The degree of the non-commuting graph of D_6

Degree of an element	Number of edges
$deg(a)$	3
$deg(b)$	4
$deg(ab)$	4
$deg(a^2)$	3
$deg(a^2b)$	4

Table 2. The distance and eccentricity of the non-commuting graph of D_6

	a	b	ab	a^2b	a^2	$E(\Gamma)$
a	0	1	1	1	2	2
b	1	0	1	1	1	1
ab	1	1	0	1	1	1
a^2b	1	1	1	0	1	1
a^2	2	1	1	1	0	2

According to Tables 1 and 2, the eccentric connectivity index of the non-commuting graph of D_6 ,

$$\begin{aligned} \xi(\Gamma) &= \sum_{v \in V(G)} deg(v)ec(v) \\ &= deg(a)ec(a) + deg(b)ec(b) + deg(ab)ec(ab) + deg(a^2b)ec(a^2b) + deg(a^2)ec(a^2) \\ &= 2(3) + 1(4) + 1(4) + 1(4) + 2(3) \\ &= 24. \end{aligned}$$

Theorem 2 : Let G be a dihedral group of order 8, $D_8 = \langle a, b \mid a^4 = b^2 = 1, bab = a^{-1} \rangle$ where $n=4$ and Γ is the non-commuting graph of G . Then, the eccentric connectivity index of $\Gamma, \xi(\Gamma) = 48$.

Proof: Based on Proposition 1, Figure 2, the distance, degree, and eccentricity of the non-commuting graph of D_8 is presented in the following Table 3 and Table 4.

Table 3. The degree of the non-commuting graph of D_8

Degree of an element	Number of edges
$deg(a)$	4
$deg(b)$	4
$deg(ab)$	4
$deg(a^2b)$	4
$deg(a^3)$	4
$deg(a^3b)$	4

Table 4. The distance and eccentricity of the non-commuting graph of D_8

	a	b	ab	a^2b	a^3	a^3b	$E(\Gamma)$
a	0	1	1	1	2	1	2
b	1	0	1	2	1	1	2
ab	1	1	0	1	1	2	2
a^2b	1	2	1	0	1	1	2
a^3	2	1	1	1	0	1	2
a^3b	1	1	2	1	1	0	2

Based on Tables 3 and 4, the eccentric connectivity index of the non-commuting graph of D_8

$$\begin{aligned} \xi(\Gamma) &= \sum_{v \in V(G)} \text{deg}(v) \text{ec}(v) \\ &= \text{deg}(a) \text{ec}(a) + \text{deg}(b) \text{ec}(b) + \text{deg}(ab) \text{ec}(ab) + \text{deg}(a^2b) \text{ec}(a^2b) + \text{deg}(a^3) \text{ec}(a^3) + \text{deg}(a^3b) \text{ec}(a^3b) \\ &= 2(4) + 2(4) + 2(4) + 2(4) + 2(4) \\ &= 48. \end{aligned}$$

Theorem 3: Let G be a dihedral group of order 10, $D_{10} = \langle a, b \mid a^5 = b^2 = 1, bab = a^{-1} \rangle$, where $n = 5$ and Γ is the non-commuting graph of G . Then, the eccentric connectivity index of Γ , $\xi(\Gamma) = 80$.

Proof: Based on Proposition 1 and Figure 3., the distance, degree, and eccentricity of the non-commuting graph of D_{10} is presented in the following Table 5 and Table 6.

Table 5. The degree of the non-commuting graph of D_{10}

Degree of an element	Number of edges
$\text{deg}(a)$	5
$\text{deg}(b)$	8
$\text{deg}(ab)$	8
$\text{deg}(a^2)$	5
$\text{deg}(a^2b)$	8
$\text{deg}(a^3)$	5
$\text{deg}(a^3b)$	8

□

Table 6. The distance and eccentricity of the non-commuting graph of D_{10}

	a	b	ab	a^2	a^2b	a^3	a^3b	a^4	a^4b	$E(\Gamma)$
a	0	1	1	2	1	2	1	2	1	2
b	1	0	1	1	1	1	1	1	1	1
ab	1	1	0	1	1	1	1	1	1	1
a^2	2	1	1	0	1	2	1	2	1	2
a^2b	1	1	1	1	0	1	1	1	1	1
a^3	2	1	1	2	1	0	1	2	1	2
a^3b	1	1	1	1	1	1	0	1	1	1
a^4	2	1	1	2	1	2	1	0	1	2
a^4b	1	1	1	1	1	1	1	1	0	1

From Tables 5 and 6, the eccentric connectivity index of the non-commuting graph of D_{10} ,

$$\begin{aligned} \xi(\Gamma) &= \sum_{v \in V(G)} \text{deg}(v) \text{ec}(v) \\ &= \text{deg}(a) \text{ec}(a) + \text{deg}(b) \text{ec}(b) + \text{deg}(ab) \text{ec}(ab) + \text{deg}(a^2b) \text{ec}(a^2b) + \text{deg}(a^2) \text{ec}(a^2) + \\ &\quad \text{deg}(a^3) \text{ec}(a^3) + \text{deg}(a^3b) \text{ec}(a^3b) + \text{deg}(a^4) \text{ec}(a^4) + \text{deg}(a^4b) \text{ec}(a^4b) \\ &= 5(2) + 8(1) + 8(1) + 8(1) + 5(2) + 5(2) + 8(1) + 5(2) + 8(1) \\ &= 80. \end{aligned}$$

Theorem 4 : Let G be a dihedral group of order 10, $D_{10} = \langle a, b \mid a^5 = b^2 = 1, bab = a^{-1} \rangle$ where $n = 6$ and Γ is the non-commuting graph of G . Then, the eccentric connectivity index of Γ , $\xi(\Gamma) = 144$.

Proof: Based on Proposition 1 and Figure 4, the distance, degree, and eccentricity of the non-commuting graph of D_{12} is presented in the following Table 7 and Table 8.

Table 7. The degree of the non-commuting graph of D_{12}

Degree of an element	Number of edges
$\text{deg}(a)$	6
$\text{deg}(b)$	8
$\text{deg}(ab)$	8
$\text{deg}(a^2)$	6
$\text{deg}(a^2b)$	8
$\text{deg}(a^3b)$	8
$\text{deg}(a^4)$	6
$\text{deg}(a^4b)$	8
$\text{deg}(a^5)$	6
$\text{deg}(a^5b)$	8

□

Table 8. The distance and eccentricity of the non-commuting graph of D_{12}

	a	b	ab	a^2	a^2b	a^3b	a^4	a^4b	a^5	a^5b	$E(\Gamma)$
a	0	1	1	2	1	1	2	1	2	1	2
b	1	0	1	1	1	2	1	1	1	1	2
ab	1	1	0	1	1	1	1	2	1	1	2
a^2	2	1	1	0	1	1	2	1	2	1	2
a^2b	1	1	1	1	0	1	1	1	1	2	2
a^3b	1	2	1	1	1	0	1	1	1	1	2
a^4	2	1	1	2	1	1	0	1	2	1	2
a^4b	1	1	1	2	1	1	1	0	1	1	2
a^5	2	1	1	2	1	1	2	1	0	1	2
a^5b	1	1	1	1	2	1	1	1	1	0	2

Based on Tables 7 and 8, the eccentric connectivity index of the non-commuting graph of D_{12} ,

$$\begin{aligned}
\xi(\Gamma) &= \sum_{v \in V(G)} \deg(v) \text{ec}(v) \\
&= \deg(a) \text{ec}(a) + \deg(b) \text{ec}(b) + \deg(ab) \text{ec}(ab) + \deg(a^2b) \text{ec}(a^2b) + \deg(a^2) \text{ec}(a^2) + \\
&\quad \deg(a^3) \text{ec}(a^3) + \deg(a^4) \text{ec}(a^4) + \deg(a^4b) \text{ec}(a^4b) + \deg(a^5) \text{ec}(a^5) + \deg(a^5b) \text{ec}(a^5b) \\
&= 6(2) + 8(2) + 8(2) + 8(2) + 6(2) + 8(2) + 6(2) + 8(2) + 6(2) + 8(2) \\
&= 144.
\end{aligned}$$

4. Maple Coding for Constructing the Non-commuting Graph

This section provides the step-by-step to construct the non-commuting graph associated to the dihedral group of order eight by using Maple software. The Maple coding is shown in Figure 5.

- Step 1: Starts by calling 'with(GroupTheory)' and 'with(GraphTheory)'.
- Step 2: Write the group presentation of the dihedral group of order eight.
- Step 3: Draw the Cayley table.
- Step 4: Construct the non-commuting graph.

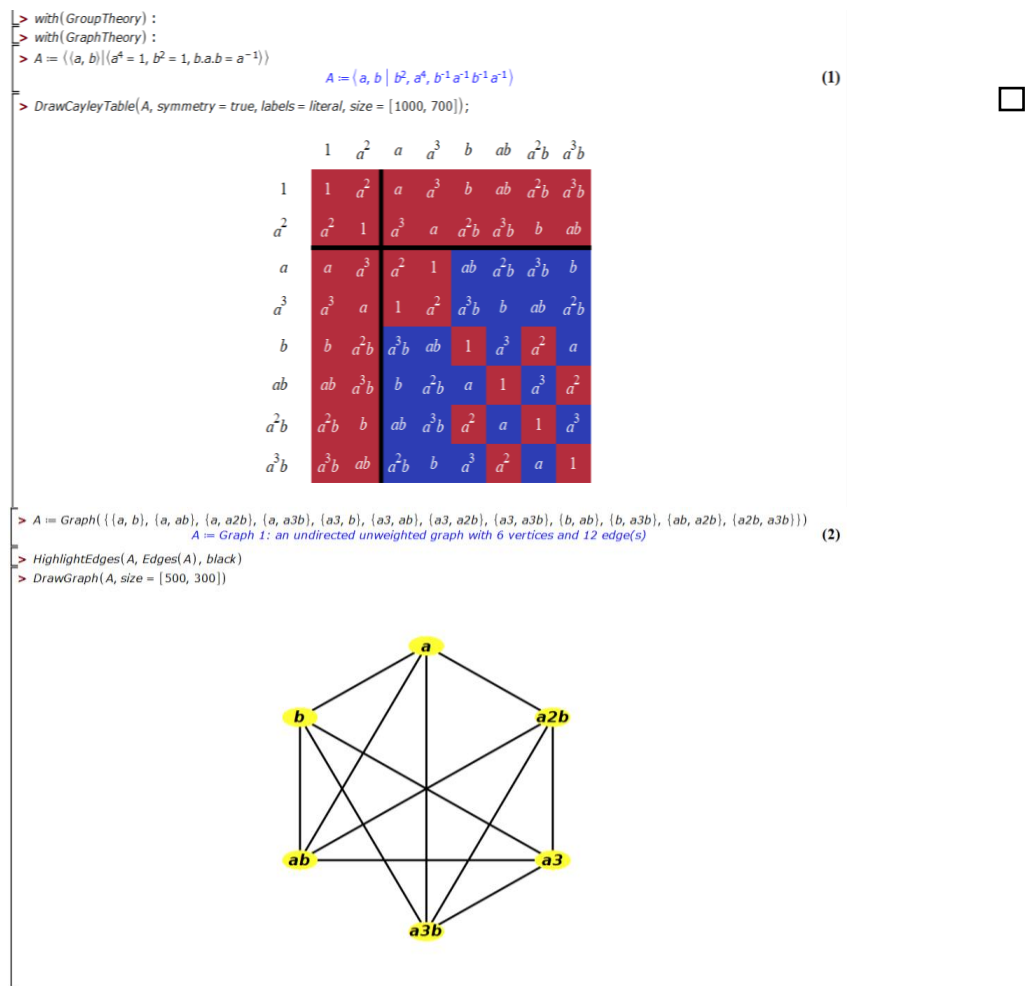


Figure 5. The maple coding for the non-commuting graph of D_8

5. Conclusion

The eccentric connectivity index of the non-commuting graph for dihedral groups of order at most 12 are computed. These findings help chemists and biologists to predict the physical and chemical properties of some molecular structures, where the mathematical modelling, which consists of the topological index as a variable, must be developed. The study contributed to exploring deeper links between group theory, graph theory, topological index, and mathematical chemistry. Hence, the general formula of the eccentric connectivity index of the non-commuting graph for dihedral groups can be determined. Research can be extended to other topological indices, such as the Hosoya Index and the Randic Index of other graphs.

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Conflict of Interest

The authors declare no conflict of interest in the subject matter or materials discussed in this manuscript.

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Biography of all authors

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	<p>Zulfazleen Natasha binti Zulkiflee is a third-year Bachelor of Mathematics student at Universiti Teknologi Malaysia (UTM) who is interested in mathematical theories. She is currently undertaking an enriching internship at Universiti Teknologi Mara (UiTM) Pasir Gudang under Dr. Nur Idayu binti Alimon's supervision. Zulfazleen's internship focuses on delving into the complexity of Topological Index research, which she plans to expand on for her final year project. Her internship is a step toward her goal of contributing to mathematics through study and discovery.</p>	<ul style="list-style-type: none"> • Compute the ECI of graph of groups. • Construct the non-commuting graph. • Writing the manuscript of journal.
	<p>Dr. Nur Idayu binti Alimon is a committed mathematician with a Ph.D. in Pure Mathematics who specializes in graph theory and group theory. Her current affiliation with Universiti Teknologi Mara (UiTM) Pasir Gudang displays her commitment to improving mathematical comprehension. She contributes significantly to academia and wider mathematical community through her teaching, research, and community involvement.</p>	<ul style="list-style-type: none"> • Supervised the research process and provided valuable guidance. • Reviewed methodology, results, and proofread.