INTRODUCTION

In chemistry, graph theory has been widely used to solve molecular problems. All structural formulas of covalently bonded compound are graph, namely molecular graphs. The molecular structure can be represented as a graph where the atoms represents the vertices and the bond between the atoms are the edges.

There are many applications of graph theory and group theory in chemistry. One of them is topological indices which represent the chemical structure with numerical value. Besides that, topological indices are useful to predict chemical and physical properties of the molecular structure.

In addition, various topological indices including the Wiener index, Zagreb index, Szeged index, Kirchoff index, Harary index, degree-distance index, and Hyper-Wiener index have been used to help chemists, scientists and biologist in solving problems related to chemistry and biology. For example, the Wiener index has been used to predict the boiling point of the alkanes known as paraffin.

This paper consists of three sections. The first section is the introduction section, followed by the second section, namely the preliminaries where some basic concepts, definitions and previous results on graph theory and group theory are stated. In the third section, the main results on the generalisation of Edge-Wiener index, First Zagreb index and Second Zagreb index of the non-commuting graph of dihedral groups are presented.

PRELIMINARIES

Group theory has many applications in various fields such as physics, chemistry, computer sciences and even in music. Groups occur as number systems or collections of matrices, in permutation theory, as the symmetries of geometrical objects or as sets of maps [1]. The following are some definitions in group theory that are used in this research.

Definition 1.1 [2] Conjugacy class
The conjugacy class of $g$ is the set $\text{cl}(g) = \{agag^{-1} | a \in G\}$ for all $a$ in $G$.

Many real world situations can be described as set of points and lines joining several points. The points could represent people, with lines joining pairs of friends or points represent communication center, with lines joining the communication link [3]. Those are some applications in graph theory. Following is the basic concept on graph theory which will be used in this paper.

Definition 1.2 [4] Non-commuting graph
Let $G$ be a finite group. The non-commuting graph of $G$, denoted by $\Gamma_G$, is the graph of vertex set $G - Z(G)$, whose vertices are non-central elements, in which $Z(G)$ is the center of $G$ and two distinct vertices $v_1$ and $v_2$ are joined by an edge if and only if $v_1v_2 \neq v_2v_1$. In this paper, some topological indices of the non-commuting graph, $\Gamma_G$ of the dihedral groups, $D_{2n}$ are presented.

Definition 1.3 [3] Wiener index
Let $v_i$ and $v_j$ be two distinct vertices where $i \neq j$ and $\Gamma$ be the connected graph with $n$ vertices. The Wiener index of a graph is defined as the sum of the half of the distances between every pair of vertices of $\Gamma$, written as,

\[ W(\Gamma) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i,v_j), \]

where $d(v_i,v_j)$ is the shortest distance of $v_i$ and $v_j$.

Definition 1.4 [6] The Edge-Wiener index
Let $\Gamma$ be a connected graph. Then, the Edge-Wiener index of $\Gamma$ is defined as the sum of the distances in the line graph between all pairs of edges of $\Gamma$, written as,
\[ W_e(\Gamma) = \sum_{(e,f) \in E(\Gamma)} d(e,f), \]

where \( E(\Gamma) \) is the set of edges in \( \Gamma \) and \( d(e,f) \) is the shortest distance between two edges. The distance between two edges is the distance between the corresponding vertices in the line graph of \( \Gamma \).

**Definition 1.5 [7] The First Zagreb index**

Let \( \Gamma \) be a connected graph. Then, the first Zagreb index is the sum of squares of the degrees of the vertices of \( \Gamma \), written as,

\[ M_1(\Gamma) = \sum_{u \in V(\Gamma)} \text{deg}(u)^2, \]

where \( \text{deg}(u) \) is the number of edges connected to vertex \( u \).

**Definition 1.6 [7] The Second Zagreb index**

Let \( \Gamma \) be a connected graph. Then, the second Zagreb index is the sum of the product of the degrees of pairs of adjacent vertices of \( \Gamma \), written as,

\[ M_2(\Gamma) = \sum_{u,v \in E(\Gamma)} \text{deg}(u) \text{deg}(v), \]

where \( u, v \) are the vertices on the edge connected them.

Now, some works related to group theory, graph theory and the topological indices of the non-commuting graph of finite groups are stated. The following propositions are some concepts that will be used in the later sections.

**Proposition 2.1 [8]** Let \( G \) be a dihedral group, \( D_{2n} \) of order \( 2n \) and \( k(G) \) be the number of the conjugacy classes of \( G \). Then,

\[ k(G) = \begin{cases} \frac{n+3}{2}, & n \text{ odd}, \\ \frac{n+6}{2}, & n \text{ even}, \end{cases} \]

where \( n = \frac{|D_{2n}|}{2} \).

**Proposition 2.2 [8]** Let \( G \) be a dihedral group, \( D_{2n} \equiv \langle a, b : a^n = 1, b^2 = 1, bab = a^{-1} \rangle \) where \( n \geq 3, n \in \mathbb{N} \) and \( Z(G) \) is the center of \( G \). Then,

\[ Z(G) = \begin{cases} \{1\}, & n \text{ odd,} \\ \{1, a^2\}, & n \text{ even.} \end{cases} \]

**Proposition 2.3 [9]** Let \( G \) be a finite group and \( \Gamma_G \) be the non-commuting graph of \( G \). Then,

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

where \( k(G) \) is the number of conjugacy classes of \( G \).

In 2015, Jahandideh et al. [10] has generalised the calculation of some topological indices of the non-commuting graph of a finite group based on the order of the group. The following are some related theorems and the proofs that can be found in [10].

**Theorem 2.1 [10]** Let \( G \) be a finite group and \( \Gamma_G \) be the non-commuting graph. Then, the Edge-Wiener index of \( \Gamma_G \) is,

\[ W_e(\Gamma_G) = |E(\Gamma_G)|^2 + |G|^2 \left( k(G) - \frac{1}{2}|Z(G)| - \frac{1}{2}|G| \right) - \frac{1}{2} \sum_{x \in D_G} |C_G(x)|^2, \]

where \( |E(\Gamma_G)| \) is the number of edges of graph, \( k(G) \) is the number of conjugacy classes, and \( C_G(x) \) is the centralizer of \( x \).

**Theorem 2.2 [10]** Let \( G \) be a finite group and \( \Gamma_G \) be the non-commuting graph. Then, the first Zagreb index of \( \Gamma_G \) is,

\[ M_1(\Gamma_G) = |G|^2(|G| + |Z(G)| - 2k(G)) - \sum_{x \in D_G} |C_G(x)|^2, \]

where \( k(G) \) is the number of conjugacy classes and \( C_G(x) \) is the centralizer of \( x \).

**Theorem 2.3 [11]** Let \( G \) be a finite group and \( \Gamma_G \) be the non-commuting graph. Then, the second Zagreb index of \( \Gamma_G \) is,

\[ M_2(\Gamma_G) = |E(\Gamma_G)| + |G|M_1(\Gamma_G) + \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)|. \]

**RESULTS AND DISCUSSION**

In this section, the edge-Wiener index, the first Zagreb index and the second Zagreb index of the non-commuting graph of dihedral group are determined. Lemma 3.1 and Lemma 3.2 show the summation of centralizers of an element in \( G - Z(G) \) that will be used in the main theorems.

**Lemma 3.1** Let \( G \) be a dihedral group, \( D_{2n} \equiv \langle a, b : a^n = 1, b^2 = 1, bab = a^{-1} \rangle > \text{order of } 2n \text{ where } n \geq 3, n \in \mathbb{N} \). Then,

\[ \sum_{x \in D_G - Z(G)} |C_G(x)|^2 = \frac{(2^n + n^2(n-1)}{2}, \] \text{odd,}

\[ \frac{(4^n + n^2(n-2))}{2}, \] \text{even},

where \( n = \frac{|D_{2n}|}{2} \) and \( C_G(x) \) is the centralizer of an element \( x \in G \).

**Proof** The centralizer of \( x \) in \( G, C_G(x) \) is the set of all elements in \( G \) that commute with element \( x \) in \( G \). We know that, \( a^i a^j = a^i a^j \) where \( i \neq j \).

For \( n \) is odd, there will be \( n \) elements which have \( |C_G(x)| = 2 \) since \( a^i b \) does not commute with \( b^j a^k \) where \( i = \{0,1,\ldots,n-1\} \) and \( j = \{1,2\} \). There will be \( n-1 \) elements which have \( |C_G(x)| = n \) since all \( a_i \) commute among each other where \( i = \{0,1,\ldots,n-1\} \) and \( |Z(G)| = 1 \). Then,

\[ \sum_{x \in D_G - Z(G)} |C_G(x)|^2 = 2^n + n^2(n-1). \]

For \( n \) is even, there will be \( n \) elements which have \( |C_G(x)| = 4 \) since it has two central elements which lead to having four elements that commute with \( x \). There will be \( n-2 \) elements which have \( |C_G(x)| = n \) since all \( a_i \) commute among each other where \( i = \{0,1,\ldots,n-1\} \) and \( |Z(G)| = 2 \). Then,

\[ \sum_{x \in D_G - Z(G)} |C_G(x)|^2 = 4^n + n^2(n-2). \]

Therefore,

\[ \sum_{x \in D_G - Z(G)} |C_G(x)|^2 = \frac{(2^n + n^2(n-1)}{2}, \] \text{odd,}

\[ \frac{(4^n + n^2(n-2))}{2}, \] \text{even,}

where \( n = \frac{|D_{2n}|}{2} \).

**Lemma 3.2** Let \( G \) be a dihedral group, \( D_{2n} \equiv \langle a, b : a^n = 1, b^2 = 1, bab = a^{-1} \rangle > \text{order of } 2n \text{ where } n \geq 3, n \in \mathbb{N} \). Then,
\[
\sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = \begin{cases} 
2n^2(n-1) + 2n(n-1), & \text{n odd}, \\
4n^2(n-2) + 8n(n-2), & \text{n even},
\end{cases}
\]

where \( n = |D_{2n}| \), \( \Gamma_G \) is the non-commuting graph of \( D_{2n} \) and \( C_G(x) \) is the centralizer of an element \( x \in G \).

**Proof** By Definition 1.2, the non-commuting graph is the graph of vertex set \( G - Z(G) \) and two distinct vertices \( x \) and \( y \) are joined by an edge whenever \( xy \neq yx \). So that, the non-commuting graph of the dihedral group consist an edge if and only if \( a^i b^j \neq b^j a^i \) where \( i = \{0,1,2,\ldots,n-1\} \) and \( j = \{1,2\} \). The centralizer of \( x \) in \( G \), \( C_G(x) \) is the set of all elements in \( G \) that commute with element \( x \) in \( G \).

For \( n \) is odd, there will be \( n(n-1) \) edges that connect two vertices \( x \) and \( y \) which have \( |C_G(x)| = 4 \) and \( |C_G(y)| = n \) while the other \( |E(\Gamma_G)| = n(n-1) \) edges connect two distinct vertices \( x \) and \( y \) which have \( |C_G(x)| = 4 \) and \( |C_G(y)| = 4 \). Then, after simplified,

\[
\sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = 2n^2(n-1) + 2n(n-1).
\]

For \( n \) is even, there will be \( n(n-2) \) edges that connect two vertices \( x \) and \( y \) which have \( |C_G(x)| = 4 \) and \( |C_G(y)| = n \) while the another \( |E(\Gamma_G)| = n(n-2) \) edges connect two distinct vertices \( x \) and \( y \) which have \( |C_G(x)| = 4 \) and \( |C_G(y)| = 4 \). Then, after simplified,

\[
\sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = 4n^2(n-2) + 8n(n-2).
\]

Therefore,

\[
\sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = \begin{cases} 
2n^2(n-1) + 2n(n-1), & \text{n odd}, \\
4n^2(n-2) + 8n(n-2), & \text{n even},
\end{cases}
\]

where \( n = \frac{|D_{2n}|}{2} \).

**Theorem 3.1** Let \( G \) be a dihedral group, \( D_{2n} \cong \langle a, b : a^n = 1, b^2 = 1, bab = a^{-1} \rangle \) of order \( 2n \) where \( n \geq 3, n \in \mathbb{N} \). Then, the Edge-Wiener index of the non-commuting graph, \( \Gamma_G \) of dihedral group is stated as follows:

\[
W_e(\Gamma_G) = \begin{cases} 
\frac{9}{4}n^2(n^2 + 3) - n(7n^2 + 2), & \text{n odd}, \\
\frac{9}{4}n^2(n^2 + 8) - n\left(\frac{23}{2}n^2 + 8\right), & \text{n even},
\end{cases}
\]

where \( n = \frac{|G|}{2} \).

**Proof** From Theorem 2.1,

\[
W_e(\Gamma_G) = |E(\Gamma_G)|^2 + |G|^2 \left(k(G) - \frac{1}{2}|Z(G)| - \frac{1}{2}|G|\right)
- \frac{1}{2} \sum_{x \in G - Z(G)} |C_G(x)|^2.
\]

For \( n \) is odd, by Proposition 2.1, \( k(G) = \frac{n+3}{2} \) by Proposition 2.2, we can see that \( |Z(G)| = 1 \) and by Proposition 2.3, the number of edges of the non-commuting graph, \( |E(\Gamma_G)| = \frac{|G|^2 - |N(G)|}{2} \). From Lemma 3.1,

\[
\sum_{x \in G - Z(G)} |C_G(x)|^2 = 2n^2 + n^2(n-1).
\]

Then,

\[
W_e(\Gamma_G) = \left|\frac{|G|^2 - k(G)|G|^2}{4} + |G|^2 \left(k(G) - \frac{1}{2}|Z(G)| - \frac{1}{2}|G|\right)\right|
- \frac{1}{2} \sum_{x \in G - Z(G)} |C_G(x)|^2
= \left(\frac{4n^2 - n + 3}{4}n\right)^2 + 4n\left(\frac{n + 3}{4} - \frac{1}{2}\right)^2
- \frac{1}{2} \left(4^2n + n^2(n-1)\right)
= \frac{9}{4}n^2(n^2 + 3) - n(7n^2 + 2).
\]

Therefore, the edge-wiener index of the non-commuting graph of dihedral group is as follows:

\[
W_e(\Gamma_G) = \begin{cases} 
\frac{9}{4}n^2(n^2 + 3) - n(7n^2 + 2), & \text{n odd}, \\
\frac{9}{4}n^2(n^2 + 8) - n\left(\frac{23}{2}n^2 + 8\right), & \text{n even},
\end{cases}
\]

where \( n = \frac{|G|}{2} \).

**Theorem 3.2** Let \( G \) be a dihedral group, \( D_{2n} \cong \langle a, b : a^n = 1, b^2 = 1, bab = a^{-1} \rangle \) of order \( 2n \) where \( n \geq 3, n \in \mathbb{N} \). Then, the first Zagreb index of the non-commuting graph, \( \Gamma_G \) of dihedral group is stated as follows:

\[
M_1(\Gamma_G) = \begin{cases} 
n(5n - 4)(n - 1), & \text{n odd}, \\
n(5n - 8)(n - 2), & \text{n even},
\end{cases}
\]

where \( n = \frac{|G|}{2} \).

**Proof** From Theorem 2.2,

\[
M_1(\Gamma_G) = |G|^2 - |Z(G)| - 2k(G) - \sum_{x \in G - Z(G)} |C_G(x)|^2.
\]

For \( n \) is odd, by Proposition 2.1, \( k(G) = \frac{n+3}{2} \) and by Proposition 2.2, we can see that \( |Z(G)| = 1 \). From Lemma 3.1,

\[
\sum_{x \in G - Z(G)} |C_G(x)|^2 = 2n^2 + n^2(n-1).
\]

Then,

\[
M_1(\Gamma_G) = |G|^2 - \frac{n+3}{2} - 2\frac{n+3}{2} - \frac{1}{2}\left(2n^2 + n^2(n-1)\right)
= \frac{9}{4}n^2(n^2 + 3) - n(7n^2 + 2).
\]
Then,
\[ M_1(\Gamma_G) = |G|^2(|G| + |Z(G)| - 2k(G)) - \sum_{x \in G - Z(G)} |C_G(x)|^2 \]
\[ = 4n^2 \left(2n + 1 - 2 \frac{n + 3}{2}\right) - 2^2n + n^2(n-1) \]
\[ = n(5n - 4)(n-1). \]

For \( n \) is even, by Proposition 2.1, \( k(G) = \frac{n+6}{2} \) and by Proposition 2.2, we can see that \(|Z(G)| = 2 \). From Lemma 3.1,
\[ \sum_{x \in G - Z(G)} |C_G(x)|^2 = 4^2n + n^2(2n-1). \]

Then,
\[ M_1(\Gamma_G) = |G|^2(|G| + |Z(G)| - 2k(G)) - \sum_{x \in G - Z(G)} |C_G(x)|^2 \]
\[ = 4n^2 \left(2n + 1 - 2 \frac{n + 6}{2}\right) - 4^2n + n^2(2n-1) \]
\[ = n(5n - 8)(n-2). \]

Therefore, the first Zagreb index of the non-commuting graph of the dihedral group is as follows:
\[ M_1(\Gamma_G) = \begin{cases} n(5n - 4)(n-1), & \text{if } n \text{ odd}, \\ n(5n - 8)(n-2), & \text{if } n \text{ even}, \end{cases} \]

where \( n = \frac{|G|}{2} \).

**Theorem 3.3** Let \( G \) be a dihedral group, \( D_{2n} \cong \langle a, b; a^n = 1, b^2 = 1, bab = a^{-1} \rangle \) of order \( 2n \) where \( n \geq 3, n \in \mathbb{N} \). Then, the second Zagreb index of the non-commuting graph, \( \Gamma_G \) of dihedral group is stated as follows:
\[ M_2(\Gamma_G) = \begin{cases} 2(n - 1)^2(2n - 1), & \text{if } n \text{ odd}, \\ 4(n - 2)^2(n - 1), & \text{if } n \text{ even}, \end{cases} \]

where \( n = \frac{|G|}{2} \).

**Proof** From Theorem 2.3,
\[ M_2(\Gamma_G) = -|G|^2[E(\Gamma_G)] + |G|M_1(\Gamma_G) + \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)|. \]

For \( n \) is odd, by Proposition 2.3, the number of edges of the non-commuting graph, \(|E(\Gamma_G)| = \frac{|G|^2-k(G)}{2} \) and from Theorem 3.2,
\[ M_1(\Gamma_G) = n(5n - 4)(n-1) \] and from Lemma 3.2,
\[ \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = 2n^2(n-1) + 2n(n-1). \]

Then,
\[ M_2(\Gamma_G) = -|G|^2 \left[ \frac{|G|^2-k(G)}{2} \right] + |G|M_1(\Gamma_G) \]
\[ + \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| \]
\[ = -2n^2 \left(4n^2 - 2n + (2n)(5n - 4)(n-1) \right) \]
\[ + 2n^2(n-1) + 2n(n-1) \]
\[ = 2n(n - 1)^2(2n - 1). \]

For \( n \) is even, the number of edges of the non-commuting graph, \(|E(\Gamma_G)| = \frac{|G|^2-k(G)}{2} \) and from Theorem 3.2,
\[ M_1(\Gamma_G) = n(5n - 8)(n-2) \] and from Lemma 3.2,
\[ \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| = 4n^2(n-2) + 8n(n-2). \]

Then,
\[ M_2(\Gamma_G) = -|G|^2 \left[ \frac{|G|^2-k(G)}{2} \right] + |G|M_1(\Gamma_G) \]
\[ + \sum_{x,y \in E(\Gamma_G)} |C_G(x)||C_G(y)| \]
\[ = -2n^2 \left(4n^2 - 2n \right) + (2n)(5n - 8)(n-2) \]
\[ + 4n^2(n-2) + 8n(n-2) \]
\[ = 4n(n - 2)^2(n - 1). \]

Therefore, the second Zagreb index of the non-commuting graph of the dihedral group is as follows:
\[ M_2(\Gamma_G) = \begin{cases} 2n(n - 1)^2(2n - 1), & \text{if } n \text{ odd}, \\ 4n(n - 2)^2(n - 1), & \text{if } n \text{ even}, \end{cases} \]

where \( n = \frac{|G|}{2} \).

**CONCLUSION**

In this paper, the Edge-Wiener index, the first Zagreb index and the second Zagreb index of the non-commuting graph of the dihedral groups have been generalised.

**ACKNOWLEDGEMENT**

This work was financially supported by the Universiti Teknologi Malaysia under the Research University Grant (GUP) Vote No. 13J82 and Ministry of Higher Education Malaysia. The first author is also indebted to Universiti Teknologi Malaysia (UTM) for her Zamalah Scholarship.

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