Jurnal
Teknologi

Full Paper

ON THE SZEGED INDEX AND ITS NON-COMMUTING GRAPH

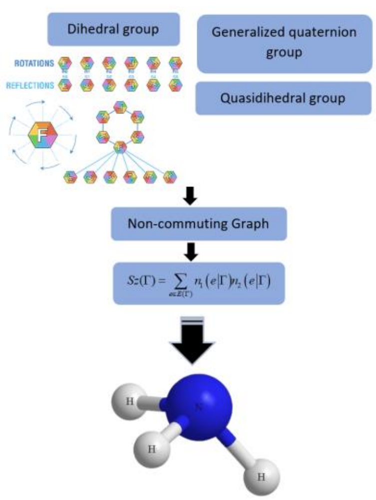
Nur Idayu Alimon[a]*, Nor Haniza Sarmin[b], Ahmad Erfanian[c]

[a]Faculty of Computer and Mathematical Sciences, Universiti Teknologi MARA (UiTM), Johor Branch, Pasir Gudang Campus, Bandar Sri Alam 81750 Masai, Johor, Malaysia
[b]Department of Mathematical Sciences, Faculty of Science, Universiti Teknologi Malaysia (UTM), 81310 Johor Bahru, Johor, Malaysia
[c]Faculty of Mathematical Sciences, Ferdowsi University of Mashhad, Mashhad, Iran

Article history
Received
21 September 2022
Received in revised form
27 February 2023
Accepted
23 March 2023
Published Online
19 April 2023

*Corresponding author
idayualimon@uitm.edu.my

Graphical abstract



Abstract

In chemistry, the molecular structure can be represented as a graph. Based on the information from the graph, its characterization can be determined by computing the topological index. Topological index is a numerical value that can be computed by using some algorithms and properties of the graph. Meanwhile, the non-commuting graph is a graph, in which two distinct vertices are adjacent if and only if they do not commute, where it is made up of the non-central elements in a group as a vertex set. In this paper, the Szeged index of the non-commuting graph of some finite groups are computed. This paper focuses on three finite groups which are the quasidihedral groups, the dihedral groups, and the generalized quaternion groups. The construction of the graph is done by using Maple software. In finding the Szeged index, some of the previous results and properties of the graph for the quasidihedral groups, the dihedral groups, and the generalized quaternion groups are used. The generalisation of the Szeged index of the non-commuting graph is then established for the aforementioned groups. The results are then applied to find the Szeged index of the non-commuting graph of ammonia molecule.

Keywords: Szeged index, non-commuting graph, dihedral groups, generalized quaternion groups, quasidihedral groups

Abstrak

Suatu nombor yang boleh dikira daripada graf yang boleh mewakili penciriannya dinamai indeks topologi. Sebuah graf mewakili struktur molekul dalam kimia dan pengiraan dalam mencari indeks topologi melibatkan beberapa maklumat yang diperoleh daripada graf. Sementara itu, graf kalis bertukar-tertib ialah suatu graf yang mana dua bucu berbeza bersebelahan jika dan hanya jika ia tidak bertukar-tertib, di mana ia terdiri daripada unsur-unsur bukan pusat dalam kumpulan sebagai set bucu. Dalam makalah ini, indeks Szeged bagi graf kalis bertukar-tertib bagi beberapa kumpulan terhingga dikira. Kertas kerja ini memfokuskan kepada tiga kumpulan terhingga iaitu kumpulan kuasidihedral, kumpulan dihedral, dan kumpulan kuaternion teritlak. Pembinaan graf dilakukan dengan menggunakan perisian Maple. Dalam mencari indeks Szeged, beberapa hasil dan sifat graf sebelumnya untuk kumpulan kuasidihedral, kumpulan dihedral dan kumpulan kuaternion teritlak digunakan. Generalisasi indeks Szeged bagi graf kalis bertukar-tertib kemudiannya diwujudkan untuk kumpulan yang disebutkan di atas. Hasilnya kemudian digunakan untuk mencari indeks Szeged bagi graf kalis bertukar-tertib molekul ammonia.

Kata kunci: Indeks Szeged, graf kalis bertukar-tertib, kumpulan kuaternion teritlak, kumpulan dihedral, kumpulan kuasidihedral

1.0 INTRODUCTION

In molecular graph theory, specifically in chemistry, a graph made up of a collection of vertices and edges is used to illustrate the chemical structure of a covalent bond molecule. The atoms represent the vertices and the bond between the atoms represent the edges [1].

Topological indices have a wide application in chemistry especially in predicting the physicochemical properties such as the boiling point, the melting point, the density, and the polarisability. The topological indices have been applied in various model in chemistry such as the quantitative structure-activity relationship (QSAR) to estimate the properties or activities of the molecule [2]. For instance, pharmaceutical QSAR is studied using the topological index in order to quantitatively compute their molecular features [3]. The majority of topological indices are determined by the degree of a vertex or the distance between two vertices.

This paper focuses on the Szeged index of the non-commuting graph for the quasidihedral groups, the dihedral groups, and the generalized quaternion groups, which are denoted as QD_{2^n}, D_{2n} and Q_{4n}, respectively. In [3], the presentation of the quasidihedral group, QD_{2^n} that has order 2^n is given in the following:

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

where $n \geq 4$.

Meanwhile, Humphreys [4] also stated the presentation of the non-abelian dihedral group that has order $2n$ is given in the following :

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

where $n \geq 3$.

The presentation of the generaized quarternion group of order $4n$ as follows.

$$Q_{4n} = \left\langle a,b \middle| a^n = b^2, a^{2n} = 1, bab = a^{-1} \right\rangle,$$

where $n \geq 2$ [5].

Next, the non-commuting graph of G, denoted as Γ_G, is a graph with non-central vertex set where two distinct vertices are adjacent whenever they do not commute [5]. If all vertices of the graph are adjacent to each other, then it is called the complete graph, which is denoted as K_n, where n is the vertex number of the graph.

Many types of topological indices have been introduced for the past decades and it started with the Wiener index of a graph, which is denoted as $W(\Gamma)$, introduced by Wiener [6] in 1947. The Wiener index takes into account the distance of two vertices. Then, the Zagreb index has been developed by Gutman and Trinajstić [7] in 1972 and the researches are still continuing up until today. In 2019, Yurtas *et al.* [8] determined that any positive even number, excluding 4 and 8, may be the first Zagreb index of a connected graph. Any positive integer is possible to be the second Zagreb index of connected graph other than 2, 3, 5, 6, 7, 10, 11, 13 and 17. Besides that, Xu *et al.* [9] studied on the distinction of the Zagreb indices of graphs and discovered a formula and its applications. Meanwhile, in 1993, Plavšić *et al.* [10] invented the Harary index. Xu and Das [11] determined the upper and lower bounds for the graphs' Harary index which involves the clique and chromatic numbers.

Particularly, this paper focuses on finding the Szeged index of graph, which is denoted as $Sz(\Gamma)$, has been introduced by Gutman and Dobrynin in [12]. The basic idea of developing the Szeged index came from the Wiener index since the Wiener index does not apply to graph containing cycles. If the graph is a tree which is not containing cycles, then the value of the Szeged and Wiener indices are the same. The research on the relation of the Wiener and Szeged indices on monocyclic molecules is done by Gutman *et al.* [13] in 1997. In 2011, Nadjafi-Arani *et al.* [14] also discovered a connection between a graph's Wiener and Szeged indices, and proved that $Sz(\Gamma) = W(\Gamma)$. Later, in 2017, Bonamy *et al.*[15] then proved this conjecture for the 2−connected non-complete n vertices graph and found that $Sz(\Gamma) - W(\Gamma) \geq 2n-6$. Additionally, for n −vertex unicyclic graphs with a certain diameter, Wang *et al.* [16] identified their minimum edge-Szeged index in 2018. Pattabiraman and Kandan have introduced the weighted Szeged index of a splice graph and link graph [17]. Meanwhile, in 2022, Liu [18] discovered the smallest revised Szeged index among all conjugated unicyclic graphs.

In this paper, there are four sections. The introduction is stated in the first section, followed by preliminaries that lay out some fundamental terms and notions related to the theory of groups and graphs. The third section explains on the relationship of the molecule in chemistry with group theory. The fourth section includes the main results and the conclusion is stated in the last section.

2.0 PRELIMINARIES

This section contains some fundamental ideas and prior findings in group and graph theories which are needed to develop the general form of the topological indices.

Mahmoud *et al*. [19] generalized the types of the non-commuting graph for the quasidihedral groups, the dihedral groups, and the generalized quaternion groups are as complete multipartite graphs. The complete p-partite graph, $K_{n_1,n_2,\ldots,n_p}$ has vertices partitioned into p subsets of $n_1, n_2, \ldots, n_p$ elements each, and vertices are only considered to be contiguous if they belong to separate subsets of the partition [20].

Based on the given graph, some properties of the graph are considered in computing its topological index. In calculating the index, two information are needed from the graph which are the vertex degree and the shortest path between the two vertices. In a chemical compound, the atoms represent the vertices of the graph while the bond between atoms represent the edge of the graph. The number of edges at a vertex in a graph is known as its vertex degree, while the distance between two vertices is the shortest path from a vertex to another vertex of the graph [21].

The following propositions are from previous results that are used in generalizing the topological index of the non-commuting graph for the quasidihedral groups, the dihedral groups, and the generalized quaternion groups. The number of conjugacy classes of dihedral groups and its center are stated as follows:

Proposition 1. [22] Let G be a dihedral group, D_{2n}. Then, the total conjugacy classes number of G, which denoted as $k(G)$ is

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

Proposition 2. [22] Let G be a dihedral group, D_{2n} and $Z(G)$ is the center of G. Then,

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

The center of generalized quaternion group and quasidihedral group are stated in the following propositions.

Proposition 3. [23] Let G be a generalized quaternion group, Q_{4n}. Then, the center of G is $Z(G)=\{1,a^n\}$, where $n\geq 2, n\in Z$.

Proposition 4. [24] Let G be a quasidihedral group, QD_{2^n}. Then, the center of G is $Z(G)=\left\{1,a^{2^{n-2}}\right\}$, where $n\geq 4, n\in Z$.

Furthermore, the total edges numbers in the non-commuting graph has been determined by Abdollahi *et al.* [22] as presented in the following proposition.

Proposition 5. [25] Let G be a finite group and the non-commuting graph of G is denoted as Γ_G. Then,

$$\left|E(\Gamma_G)\right|=\frac{|G|^2-k(G)|G|}{2}.$$

Mahmoud *et al.* [19] have found the non-commuting graph of the quasidihedral groups, the dihedral groups, and the generalized quaternion groups which are presented in the following three propositions.

Proposition 6. [19] Let G be the quasidihedral groups of order 2^n where $n\geq 4, n\in Z$. Then, the non-commuting graph of G is

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

Proposition 7. [19] Let G be the dihedral group of order $2n$ where $n\geq 3, n\in Z$ and let Γ_G be the non-commuting graph of G. Then,

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

Proposition 8. [19] Let G be the generalized quaternion groups, Q_{4n}. Then, the non-commuting graph of G is

$$\Gamma_G = K_{\underbrace{2,2,\cdots,2}_{n\text{ times}},2n-2},$$

where $n\geq 2, n\in Z$.

The computation of the Szeged index involves the distance between all vertices in the graph, where the graph considered is a connected graph only. Let such graph be Γ, then the Szeged index, $Sz(\Gamma)$ is given in the following:

$$Sz(\Gamma)=\sum_{e\in E(\Gamma)} n_1(e|\Gamma)n_2(e|\Gamma),$$

where the summation embraces all edges of Γ,

$$n_1(e|\Gamma)=\left|\left\{v|v\in V(\Gamma), d(v,x|\Gamma)<d(v,y|\Gamma)\right\}\right|$$

and

$$n_2(e|\Gamma)=\left|\left\{v|v\in V(\Gamma), d(v,x|\Gamma)>d(v,y|\Gamma)\right\}\right|$$

which means, $n_1(e|\Gamma)$ counts the vertices of Γ that are closer to one endpoint x of the edge than to its other endpoint y, whereas $n_2(e|\Gamma)$ does the opposite [12].

3.0 RESULTS AND DISCUSSION

The Szeged index of the non-commuting graph for the quasidihedral groups, dihedral groups, and generalised quaternion groups is established in this section as the primary results. The general formula of the Szeged index for QD_{2^n}, D_{2n} and Q_{4n}, are stated in the following three theorems.

Theorem 1. Let G be the quasidihedral group and the non-commuting graph of G is denoted as Γ_G. Then, the Szeged index of the non-commuting graph for QD_{2^n} is

$$Sz(\Gamma_G)=2^n\left[2^{2n-2}-3\left(2^{n-1}\right)+2\right],$$

where $n\geq 4$.

Proof From Proposition 8, $2^{n-1}\left(2^{n-1}-2\right)$ edges have $n_1\left(e|\Gamma\right)=2$ since there are only two elements of vertices which are closer to a vertex of edge, namely x, than the other vertex of edge, namely y. Then, $n_2\left(e|\Gamma\right)=2^{n-1}-2$ since there are $2n-2$ elements of vertices which are closer to y than to x. Meanwhile, the rest of the edges have $n_1\left(e|\Gamma\right)=n_2\left(e|\Gamma\right)=2$. Thus, according to the Szeged index definition,

$$\begin{aligned}Sz\left(\Gamma_G\right)&=\left(2^{n-1}\right)\left(2^{n-1}-2\right)\left[2\left(2^{n-1}-2\right)\right]+\\&\quad\left[\left|E\left(\Gamma_G\right)\right|-\left(2^{n-1}\right)\left(2^{n-1}-2\right)\right]\left[2\times 2\right]\\&=\left(2^{n-1}\right)\left(2^{n-1}-2\right)\left[2\left(2^{n-1}-2\right)\right]+\\&\quad\left[\frac{2^{2n}-2^n\left(2^{n-2}+3\right)}{2}-2^{n-1}\left(2^{n-1}-2\right)\right]\left[4\right]\\&=2^n\left(2^{n-1}-2\right)^2+2^{2n+1}-2^{2n-1}-3\left(2^{n+1}\right)-2^{2n}\\&\quad+2\left(2^{n+1}\right)\\&=2^n\left[\left(2^{n-1}-2\right)^2+2^{n+1}-2^{n-1}-2-2^n\right]\\&=2^n\left[\frac{2^{2n}}{4}+2-\frac{2^n}{2}-2^n\right]\\&=2^n\left[2^{2n-2}-3\left(2^{n-1}\right)+2\right],\end{aligned}$$

where $n\geq 4$. □

Theorem 2. Let G be the dihedral group and the non-commuting graph of G is denoted as Γ_G. Then, the Szeged index of the non-commuting graph for D_{2n} is

$$Sz(\Gamma_G)=\begin{cases}n\left(n-1\right)\left(n-\frac{1}{2}\right), & \text{if } n \text{ is odd,}\\ 2n\left(n-2\right)\left(n-1\right), & \text{if } n \text{ is even,}\end{cases}$$

where $n\geq 3$.

Proof Case 1: n is odd and $n\geq 3$:
Let Γ be the non-commuting graph of D_{2n}. Based on Proposition 6, $n\left(n-1\right)$ edges have $n_1\left(e|\Gamma\right)=1$ since there is only one element of vertices which is closer to a vertex x of the edge than the other vertex of the edge, namely y. Then, $n_2\left(e|\Gamma\right)=n-1$ since $n-1$ elements of vertices which are closer to y than to x. Meanwhile, the rest of the edges have $n_1\left(e|\Gamma\right)=n_2\left(e|\Gamma\right)=1$. Thus, by the Szeged index definition,

$$\begin{aligned}Sz\left(\Gamma_G\right)&=n(n-1)\left[1\times\left(n-1\right)\right]+\left[\left|E\left(\Gamma_G\right)\right|-n\left(n-1\right)\right]\left[1\times 1\right]\\&=n(n-1)(n-1)+\left[\frac{|G|^2-k(G)|G|}{2}-n\left(n-1\right)\right]\\&=n(n-1)(n-1)+\left[2n^2-n\left(\frac{n+3}{2}\right)-n\left(n-1\right)\right]\\&=n\left(n-1\right)^2+\frac{n^2}{2}-\frac{n}{2}\\&=n\left(n-1\right)\left(n-\frac{1}{2}\right).\end{aligned}$$

Case 2: n is even and $n\geq 3$:
Let Γ be the non-commuting graph of D_{2n}. Based on Proposition 6, $2n\left(n-2\right)$ edges have $n_1\left(e|\Gamma\right)=2$ since there are two elements of vertices which are closer to a vertex x of the edge than the other vertex of the edge, namely y. Then, $n_2\left(e|\Gamma\right)=n-2$ since $n-2$ elements of vertices which are closer to y than to x. Meanwhile, the rest of the edges have $n_1\left(e|\Gamma\right)=n_2\left(e|\Gamma\right)=2$. Thus, by the definition of Szeged index,

$$\begin{aligned}Sz\left(\Gamma_G\right)&=n(n-2)\left[2\times\left(n-2\right)\right]+\left[\left|E\left(\Gamma_G\right)\right|-n\left(n-2\right)\right]\left[2\times 2\right]\\&=2n(n-2)(n-2)+\left[\frac{|G|^2-k(G)|G|}{2}-n\left(n-2\right)\right]\left[4\right]\\&=2n(n-2)^2+\left[\frac{4n^2-\left(n+6\right)\left(n\right)}{2}-n\left(n-2\right)\right]\left[4\right]\\&=2n(n-2)^2+2\left[4n^2-n\left(n+6\right)-2n\left(n-2\right)\right]\\&=2n\left(n-2\right)^2+2n\left(n-2\right)\\&=2n\left(n-2\right)\left(n-1\right).\end{aligned}$$

Therefore,

$$Sz(\Gamma_G)=\begin{cases}n(n-1)\left(n-\frac{1}{2}\right), & \text{if } n \text{ is odd,}\\ 2n(n-2)(n-1), & \text{if } n \text{ is even.}\end{cases}$$

Theorem 3. Let G be the generalized quaternion group and the non-commuting graph of G is denoted as Γ_G. Then, the Szeged index of the non-commuting graph for Q_{4n} is

$$Sz\left(\Gamma_G\right)=8n\left(n-1\right)\left(2n-1\right),$$

where $n\geq 2$.

Proof From Proposition 7, there are $4n\left(n-1\right)$ edges that have $n_1\left(e|\Gamma\right)=2$ since there are two elements of vertices which are closer to a vertex of edge, namely x than the other vertex of edge, namely y. Then, $n_2(e|\Gamma) = 2n-2$ since $2n-2$ elements of vertices which are closer to y than to x. Meanwhile, the rest of the edges have $n_1(e|\Gamma) = n_2(e|\Gamma) = 2$. Thus, by the Szeged index definition,

$$Sz(\Gamma_G) = 4n(n-1)\left[2\times(2n-2)\right] + \left[\left|E(\Gamma_G)\right| - 4n(n-1)\right]\left[2\times 2\right]$$

$$= 8n(n-1)(2n-2) + \left[\frac{|G|^2 - k(G)|G|}{2} - 4n(n-1)\right][4]$$

$$= 16n(n-1)^2 + \left[\frac{(4n)^2 - (n+3)(4n)}{2} - 4n(n-1)\right][4]$$

$$= 16n(n-1)^2 + 2n(n-1)(4)$$

$$= 8n(n-1)(2n-1).$$

Next, the main theorem will be used to compute the Szeged index of the ammonia molecule via its point group and isomorphism with a particular group in group theory.

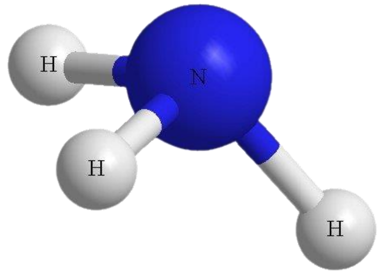


Figure 1 Ammonia molecule

In group theory, there are a few operations involved to develop a group. Particularly, dihedral group is created from the operation of rotation and reflection. In this section, the relationship between the ammonia molecule, NH_3 and the dihedral group of order six, D_6 is shown. In consequence, the Szeged index of NH_3 can be determined from the main result.

The dihedral group of order six can be represented as a triangle with three vertices. The elements of D_6 are denoted as $\rho_0, \rho_1, \rho_2, \mu_1, \mu_2$,and μ_3 which can be written by $D_6 = \{\rho_0, \rho_1, \rho_2, \mu_1, \mu_2, \mu_3\}$.

Meanwhile, the ammonia molecule has four atoms which are a nitrogen(N) atom and three hydrogen(H) atoms, as shown in Figure 1. The molecule can be classified into symmetry group based on symmetry element and symmetry operation. Symmetry operation is an action such that the molecule is transformed into a state indistinguishable from the starting state [26].

The symmetry elements are the identity (E), inversion center (i), symmetry plane (σ), rotation (C_n), and improper axis (S_n). These combinations of elements are called the point group [27]. In other word, point groups can be defined when there is at least a point in a molecule that remains unchanged and not affected by any symmetry operation from the group [28]. Molecule of ammonia is a non-linear molecule which has elements of $E, C_3, C_3^2, \sigma_{v(xy)}, \sigma_{v'(yz)}$ and $\sigma_{v''(xz)}$ where the x, y, z axis is at nitrogen atom. Hence, it has a point group, C_{3v} where its Cayley table is presented in Figure 2.

$\cdot$	E	C_3	C_3^2	$\sigma_{v(xy)}$	$\sigma_{v'(yz)}$	$\sigma_{v''(xz)}$
E	E	C_3	C_3^2	$\sigma_{v(xy)}$	$\sigma_{v'(yz)}$	$\sigma_{v''(xz)}$
C_3	C_3	C_3^2	E	$\sigma_{v'(yz)}$	$\sigma_{v''(xz)}$	$\sigma_{v(xy)}$
C_3^2	C_3^2	E	C_3	$\sigma_{v''(xz)}$	$\sigma_{v(xy)}$	$\sigma_{v'(yz)}$
$\sigma_{v(xy)}$	$\sigma_{v(xy)}$	$\sigma_{v''(xz)}$	$\sigma_{v'(yz)}$	E	C_3^2	C_3
$\sigma_{v'(yz)}$	$\sigma_{v'(yz)}$	$\sigma_{v(xy)}$	$\sigma_{v''(xz)}$	C_3	E	C_3^2
$\sigma_{v''(xz)}$	$\sigma_{v''(xz)}$	$\sigma_{v'(yz)}$	$\sigma_{v(xy)}$	C_2	C_3	E

Figure 2 Cayley table of C_{3v}

Next, the isomorphism of D_6 and $C_{3v} = \{E, C_3, C_3^2, \sigma_{v(xy)}, \sigma_{v'(yz)}, \sigma_{v''(yz)}\}$ is shown in the following. First, the elements from each set are mapped to those of the same order. Let ϕ be the mapping from D_6 to C_{3v}, then let $\phi(\rho_0) = E, \phi(\rho_1) = C_3, \phi(\rho_2) = C_3^2, \phi(\mu_1) = \sigma_{v(xy)}, \phi(\mu_2) = \sigma_{v'(yz)}$, and $\phi(\mu_3) = \sigma_{v''(xz)}$. Thus, ϕ is one-to-one and onto. Next, ϕ can be shown to be homomorphism i.e. $\phi(gh) = \phi(g)\phi(h)$ for all $g, h \in D_6$. Thus, ϕ is an isomorphism and D_6 is isomorphic to C_{3v}, $D_6 \cong C_{3v}$ and the main theorem can be used to determine the Szeged index of the molecular structure.

Since $D_6 \cong C_{3v}$, then the Szeged index of the non-commuting graph for the ammonia molecule can be calculated from the general formula of the Szeged index of the non-commuting graph for dihedral group of order six, D_6. From Theorem 1, the Szeged index is $n(n-1)(n-0.5)$ when n is odd. Hence, $Sz(\Gamma_{NH_3}) = 3(2)(2.5) = 15.$

4.0 CONCLUSION

In this article, the general formula of the Szeged index of the non-commuting graph associated to the quasidihedral, the dihedral, and the generalized quaternion groups in terms of n are determined. These formulas can help the scientists especially chemists to compute the physicochemical properties in a faster way. An example is presented to illustrate the application and calculation of any topological index for molecular structure of chemical compound. In future, other types of topological indices for various type of graphs associated to the semidirect product of two groups can be investigated.

Conflicts of Interest

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

Acknowledgement

This work was funded by Ministry of Higher Education Malaysia (MoHE) under Fundamental Research Grant Scheme (FRGS/1/2020/STG06/UTM/01/2) and Universiti Teknologi Malaysia Fundamental Research Grant (UTMFR) Vote Number 20H70.

References

[1] Gutman, I. and Polansky, O. E. 1986. *Mathematical Concepts in Organic Chemistry*. Springer-Verlag Berlin Heidelberg.

[2] Basak, S. C., Niemi, G. J., and Veith, G. D. 1991. Predicting Properties of Molecules using Graph Invariants. *Journal of Mathematical Chemistry*. 1: 243-272. Doi: https://doi.org/10.1007/bf01200826.

[3] Ali, P., Kirmani, S. A. K., Al Rugaie, O., and Azam, F. 2020. Degree-based Topological Indices and Polynomials of Hyaluronic Acid-curcumin Conjugates. *Saudi Pharmaceutical Journal*. 28(9): 1093-1100. https://doi.org/10.1016/j.jsps.2020.07.010.

[4] Humphreys, J. F., Humphreys, M. J., and Liu, Q. 1996. A Course in Group Theory. Vol. 6. Oxford University Press on Demand. Doi: https://doi.org/10.2307/2005904.

[5] Raza, Z. and Faizi, S. 2013. Non-commuting Graph of Finitely Presented Group. Sci. Int. (Lahore). 25 (4): 883-885.

[6] Wiener, H. 1947. Structural Determination of Paraffin Boiling Points. *Journal of the American Chemical Society*. 69(1): 17-20. Doi: https://doi.org/10.1021/ja01193a005.

[7] Gutman, I. and Trinajstić, N. 1972. Graph Theory and Molecular Orbitals. Total φ-electron Energy of Alternant Hydrocarbons. *Chemical Physics Letters*. 17(4): 535-538. Doi: https://doi.org/10.1016/0009-2614(72)85099-1.

[8] Gutman, I., Togan, M., Yurttas, A., Cevik, A. S. and Cangul, I. N. 2018. Inverse Problem for Sigma Index. *MATCH Commun. Math. Comput. Chem*. 79(2): 491-508.

[9] Xu, K., Gao, F., Das, K. C. and Trinajstić, N. 2019. A Formula with its Applications on the Difference of Zagreb Indices of Graphs. *Journal of Mathematical Chemistry*. 57(6): 1618-1626. Doi: https://doi.org/10.1007/s10910-019-01025-0.

[10] Plavšić, D., Nikolić, S., Trinajstić, N., and Mihalić, Z. 1993. On the Harary Index for the Characterization of Chemical Graphs. *Journal of Mathematical Chemistry*. 12(1): 235-250. Doi: https://doi.org/10.1007/BF01164638.

[11] Xu, K. and Das, K. C. 2011. On Harary Index of Graphs. *Discrete Applied Mathematics*. 159(15): 1631-1640. Doi: https://doi.org/10.1016/j.dam.2011.06.003.

[12] Gutman, I. and Dobrynin, A. A. 1998. The Szeged Index–A Success Story. Graph Theory Notes NY. 34: 37-44.

[13] Gutman, I., Popovic, L., Khadikar, P., Karmarkar, S., Joshi, S. and Mandloi, M. 1997. Relations between Wiener and Szeged Indices of Monocyclic Molecules. *MATCH Commun. Math. Comput. Chem*. 35: 91-103.

[14] Nadjafi-Arani, M. J., Khodashenas, H. and Ashrafi, A. 2011. On the Differences between Szeged and Wiener Indices of Graphs. *Discrete Mathematics*. 20: 2233-2237. Doi: https://doi.org/10.1016/j.disc.2011.06.019.

[15] Bonamy, M., Knor, M., Lužar, B., Pinlou, A. and Śkrekovski, R. 2017. On the Difference between the Szeged and the Wiener Index. *Applied Mathematics and Computation*. 312: 202-213. Doi: https://doi.org/10.1016/j.amc.2017.05.047.

[16] Wang, G., Li, S., Qi, D. and Zhang, H. 2018. On the Edge-Szeged Index of Unicyclic Graphs with Given Diameter. *Applied Mathematics and Computation*. 336: 94-106.

[17] Pattabiraman, K., & Kandan, P. 2018. Weighted Szeged Index of Graphs. *Bulletin Of International Mathematical Virtual Institute*. 8(1): 11-19. https://doi.ord/ 10.7251/BIMVI1801011P.

[18] Liu, H. 2022. On Revised Szeged Index of a Class of Unicyclic Graphs. *Discrete Mathematics, Algorithms and Applications*. 14(02): 2150115. https://doi.org/10.1142/S1793830921501159.

[19] Mahmoud, R. 2018. Energy and Laplacian Energy of Graphs Related to a Family of Finite Groups. Ph.D. Thesis. Universiti Teknologi Malaysia.

[20] Rosen, K. H. and Krithivasan, K. 2012. *Discrete Mathematics and Its Applications: With Combinatorics and Graph Theory*. Tata McGraw-Hill Education.

[21] Bondy, J. A and Murty, J. A. 1976. *Graph Theory with Applications*. Vol.210 290. Macmillan London.

[22] Samaila, D., Abba, B. I. and Pur, M. P. 2013. On the Conjugacy Classes, Centers and Representation of the Groups S_n and D_n. *International Journal of Pure and Applied Sciences and Technology*. 15 (1): 87-89.

[23] Roman, S. 2011. *Fundamentals of Group Theory: An Advanced Approach*. Springer Science & Business Media.

[24] Dummit, D. S. and Foote, R. M. 2004. *Abstract Algebra*. Vol. 3. Wiley Hoboken.

[25] Abdollahi, A., Akbari, S. and Maimani, H. 2006. Non-commuting Graph of a Group. *Journal of Algebra*. 298(2): 468-492. Doi: https://doi.org/10.1016/j.jalgebra.2006.02.015.

[26] Thakkar, A. J. 2017. *Quantum Chemistry*. Morgan & Claypool Publisher.

[27] Zeldin, M. 1966. An Introduction to Molecular Symmetry and Symmetry Point Groups. *Journal of Chemical Education*. 43(1): 17. Doi: https://doi.org/10.1021/ed043p17.

[28] Aruldhas, G. 2007. *Molecular Structure and Spectroscopy*. PHI Learning Pvt. Ltd.