Some Results on Topological Indices of Graphs Associated to Groups and Rings

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7th Biennial International Group Theory Conference

7-11 August 2023

Presentation Outline

INTRODUCTION

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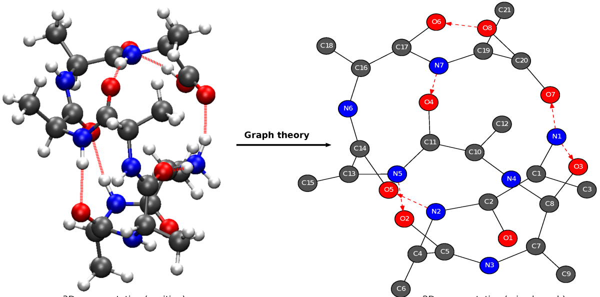


3D representation (position) 2D representation (mixed graph)

- Topological indices provide numerical descriptors that capture important structural features of molecules.
- They serve as powerful tools for the analysis and prediction of various physicochemical properties and biological activities.

- The significance of topological indices lies in their ability to transform complex molecular structures into numerical representations, enabling the development of computational models and the efficient exploration of chemical space for various applications in drug discovery, materials science, and reaction chemistry [1].
- Various types of topological indices have been developed based on either chemistry or mathematical perspectives.

[1]I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry, Springer Science and Business Media*, 2012.

TOPOLOGICAL INDICES

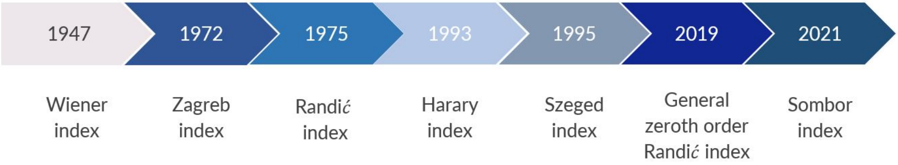


Figure 1: Different Types of Topological Indices

DEFINITIONS OF TOPOLOGICAL INDICES

Wiener Index

- The first type of topological index has been discovered by Wiener [2] in 1947, in which the concept of Wiener number considering the path in a graph is introduced.
- The Wiener number of some paraffins are determined and their boiling points are also predicted.
- Then, Hosoya [3] reformulated the formula of Wiener number, known as Wiener index of a graph, $W(\Gamma)$, and its formula is given in the following.

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

where $d(i,j)$ is the distance between vertices i and j, and m is the total number of vertices in a graph Γ.

[2] K. Wiener, *Structural determination of paraffin boiling points, Journal of the American Chemical Society*, **69(1)** (1947), 17-20.
[3] H. Hosoya, *Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bulletin of the Chemical Society of Japan*, **44(9)** (1971), 2332–2339.

Example of Wiener Index

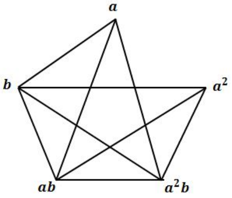


Figure 2: The non-commuting graph D_6

$$
\begin{aligned}
W(\Gamma) &= \frac{1}{2}\sum_{i=a}^{a^2b}\sum_{j=a}^{a^2b} d(i,j) \\
&= \frac{1}{2}\Big[d(a,a^2)+d(a,b)+d(a,ab)+d(a,a^2b)+d(a^2,b)+ \\
&\quad d(a^2,ab)+d(a^2,a^2b)+d(b,ab)+d(ab,a^2b)+d(b,a^2b)\Big] \\
&= 2+9(1) \\
&= 11.
\end{aligned}
$$

Wiener Index of the Non-commuting Graph

Proposition 1.1 [4]

Let G be a finite group and Γ_G^{NC} be the non-commuting graph. Then, the Wiener index of the non-commuting graph of G is given as

$$W(\Gamma_G^{\mathrm{NC}}) = \frac{1}{2}\left[\left(|G| - |Z(G)|\right)\left(|G| - 2|Z(G)| - 2\right) + |G|\left(k(G) - |Z(G)|\right)\right].$$

[4]A. Azad and M. Eliasi, *Distance in the non-commuting graph of groups. Ars Comb.* **99** (2011), 279-287.

Zagreb Index

In 1972, Gutman and Trinajstić [5] introduced the degree-based topological index, Zagreb index, which is divided into two types; first Zagreb index, M_1, and second Zagreb index, M_2, defined as follows.

$$M_1(\Gamma) = \sum_{v \in v(\Gamma)} (\deg(v))^2$$

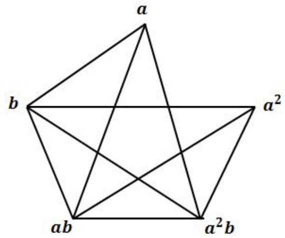
and

$$M_2(\Gamma) = \sum_{\{u,v\} \in E(\Gamma)} \deg(u)\deg(v).$$

[5] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, Chemical Physics Letters*, **17(4)** (1972), 535-538.

Example of First Zagreb Index

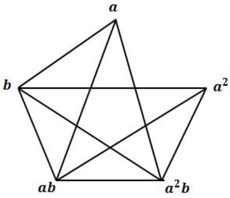
Based on Figure 2,



$$
\begin{aligned}
M_1(\Gamma) &= \sum_{v \in v(\Gamma)} (\deg(v))^2 \\
&= deg(a)^2 + deg(a^2)^2 + deg(b)^2 + deg(ab)^2 + deg(a^b)^2 \\
&= 3 + 3 + 4 + 4 + 4 \\
&= 18.
\end{aligned}
$$

Example of Second Zagreb Index

Based on Figure 2,



$$
\begin{aligned}
M_2(\Gamma) &= \sum_{\{u,v\}\in E(\Gamma)} \deg(u)\deg(v) \\
&= deg(a)deg(b) + deg(a)deg(ab) + deg(a)deg(a^2b) + deg(a^2)deg(b) + \\
&\quad deg(a^2)deg(ab) + deg(a^2)deg(a^2b) + deg(b)deg(ab) + deg(ab)deg(a^2b) \\
&\quad + deg(b)deg(a^2b) \\
&= 3(4) + 3(4) + 3(4) + 3(4) + 3(4) + 3(4) + 4(4) + 4(4) + 4(4) \\
&= 120.
\end{aligned}
$$

Zagreb Index of the Non-commuting Graph

Proposition 1.2 [6]

Let G be a finite group and Γ_G^{NC} be the non-commuting graph of G. Then, the first Zagreb index of the non-commuting graph of G,

$$M_1(\Gamma_G^{\mathrm{NC}}) = |G|^2(|G| + |Z(G)| - 2k(G)) - \sum_{x \in G - Z(G)} |C_G(x)|^2.$$

Proposition 1.3 [6]

Let G be a finite group and Γ_G^{NC} be the non-commuting graph. Then, the second Zagreb index of the non-commuting graph of G,

$$M_2(\Gamma_G^{\mathrm{NC}}) = -|G|^2|E(\Gamma_G^{\mathrm{NC}})| + |G|M_1(\Gamma_G^{\mathrm{NC}}) + \sum_{x,y \in E(\Gamma_G^{\mathrm{NC}})} |C_G(x)||C_G(y)|.$$

[6] M. Mizargar and A. Ashrafi, *Some distance-based topological indices of a non-commuting graph. Hacettepe Journal of Mathematics ans Staristics.* **41(4)** (2012), 515-526.

DEFINITIONS OF TOPOLOGICAL INDICES

Szeged Index

Let Γ be a simple connected graph with vertex set $V(\Gamma) = \{1, 2, \ldots, n\}$. The Szeged index, $Sz(\Gamma)$ is given as 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,

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

and

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

which means that $n_1(e|\Gamma)$ counts the Γ's vertices are closer to one edge's terminal x than the other while $n_2(e|\Gamma)$ is vice versa [7].

[7] P.V. Khadikar, N.V. Deshpande, V. Narayan, P. Kale, P. Prabhakar, A. Dobrynin, I. Gutman, and G. Domotor, *The Szeged index and an analogy with the Wiener index*, *Journal of Chemical Information and Computer Sciences*, **35(3)** (1995), 547-550.

Example of Szeged Index

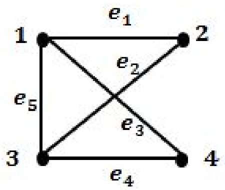


Figure 3: A simple connected graph

Note that $N_1(e_i|\Gamma)$ is the vertices of Γ lying closer to one endpoint x of the edge e_i than to its other endpoint y while $N_2(e_i|\Gamma)$ is vice versa. First, $N_1(e_i|\Gamma)$ and $N_2(e_i|\Gamma)$ are calculated for all i.
For $e_1 = \{1, 2\}$,

$$\begin{aligned} N_1(e_1|\Gamma) &= \{x \in V(\Gamma) : d(x,1) < d(x,2)\}, \quad n_1(e_1|\Gamma) = 2, \\ &= \{1, 4\}, \\ N_2(e_1|\Gamma) &= \{y \in V(\Gamma) : d(y,1) > d(y,2)\}, \quad n_2(e_1|\Gamma) = 1. \\ &= \{2\}, \end{aligned}$$

Example of Szeged Index (CONT.)

For $e_2 = \{2, 3\}$,

$$\begin{aligned} N_1(e_2|\Gamma) &= \{x \in V(\Gamma) : d(x,2) < d(x,3)\}, \quad n_1(e_2|\Gamma) = 1, \\ &= \{2\}, \\ N_2(e_2|\Gamma) &= \{y \in V(\Gamma) : d(y,2) > d(y,3)\}, \quad n_2(e_2|\Gamma) = 2. \\ &= \{3, 4\}, \end{aligned}$$

For $e_3 = \{1, 4\}$,

$$\begin{aligned} N_1(e_3|\Gamma) &= \{x \in V(\Gamma) : d(x,1) < d(x,4)\}, \quad n_1(e_3|\Gamma) = 2, \\ &= \{1, 2\}, \\ N_2(e_3|\Gamma) &= \{y \in V(\Gamma) : d(y,1) > d(y,4)\}, \quad n_2(e_3|\Gamma) = 1. \\ &= \{4\}, \end{aligned}$$

Example of Szeged Index (CONT.)

For $e_4 = \{3,4\}$,

$$\begin{aligned} N_1(e_4|\Gamma) &= \{x \in V(\Gamma) : d(x,3) < d(x,4)\}, \quad n_1(e_4|\Gamma) = 2, \\ &= \{2,3\}, \\ N_2(e_4|\Gamma) &= \{y \in V(\Gamma) : d(y,3) > d(y,4)\}, \quad n_2(e_4|\Gamma) = 1. \\ &= \{4\}, \end{aligned}$$

For $e_5 = \{1,3\}$,

$$\begin{aligned} N_1(e_5|\Gamma) &= \{x \in V(\Gamma) : d(x,1) < d(x,3)\}, \quad n_1(e_5|\Gamma) = 1, \\ &= \{1\}, \\ N_2(e_5|\Gamma) &= \{y \in V(\Gamma) : d(y,1) > d(y,3)\}, \quad n_2(e_5|\Gamma) = 1. \\ &= \{3\}, \end{aligned}$$

Example of Szeged Index (CONT.)

Hence,

$$
\begin{aligned}
Sz(\Gamma) &= \sum_{i=1}^{5} n_1(e_i|\Gamma)n_2(e_i|\Gamma) \\
&= n_1(e_1|\Gamma)n_2(e_1|\Gamma) + n_1(e_2|\Gamma)n_2(e_2|\Gamma) + n_1(e_3|\Gamma)n_2(e_3|\Gamma) + \\
&\quad n_1(e_4|\Gamma)n_2(e_4|\Gamma) + n_1(e_5|\Gamma)n_2(e_5|\Gamma) \\
&= (2)(1) + (1)(2) + (2)(1) + (2)(1) + (1)(1) \\
&= 9.
\end{aligned}
$$

DEFINITIONS OF TOPOLOGICAL INDICES

Harary Index

Let Γ be a connected graph with vertex set $V = \{1, 2, \ldots, n\}$. Half the elements' sum in the reciprocal distance matrix, $D^r = D^r(\Gamma)$, is what is known as the Harary index, written as

$$H = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} D^r(i, j),$$

where

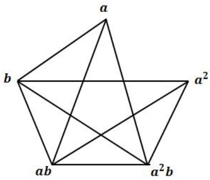
$$D^r(i, j) = \begin{cases} \frac{1}{d(i,j)} & \text{if} \quad i \neq j, \\ 0 & \text{if} \quad i = j, \end{cases}$$

and $d(i, j)$ is the shortest distance between vertex i and j [8].

[8] D. Plavšić, S. Nikolić, N. Trinajstić, and Z. Mihalić, *On the Harary index for the characterization of chemical graphs, Journal of Mathematical Chemistry*, **12** (1993), 235-250.

Example of Harary Index

Based on Figure 2,



$$
\begin{aligned}
H &= \frac{1}{2}\sum_{i=a}^{a^2b}\sum_{j=a}^{a^2b} D^r(i,j) \\
&= \frac{1}{2}\big[D^r(a,a) + D^r(a,a^2) + D^r(a,b) + D^r(a,ab) + D^r(a,a^2b) + \\
&\quad D^r(a^2,a) + D^r(a^2,a^2) + D^r(a^2,b) + D^r(a^2,ab) + D^r(a^2,a^2b) + \\
&\quad D^r(b,a) + D^r(b,a^2) + D^r(b,b) + D^r(b,ab) + D^r(b,a^2b) + \\
&\quad D^r(ab,a) + D^r(ab,a^2) + D^r(ab,b) + D^r(ab,ab) + D^r(ab,a^2b) + \\
&\quad D^r(a^2b,a) + D^r(a^2b,a^2) + D^r(a^2b,b) + D^r(a^2b,ab) + D^r(a^2b,a^2b)\big]
\end{aligned}
$$

Example of Harary Index (CONT.)

$$
\begin{aligned}
H &= \frac{1}{2}\sum_{i=a}^{a^2b}\sum_{j=a}^{a^2b} D^r(i,j) \\
&= \frac{1}{2}\Big[0+\frac{1}{2}+1+1+1+\frac{1}{2}+0+1+1+1+ \\
&\quad 1+1+0+1+1+1+1+1+0+1+1+1+1+1+0] \\
&= 9.5
\end{aligned}
$$

Randić Index

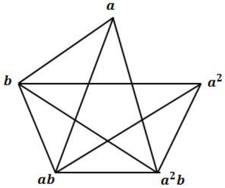
- The Randić index is a graph-theoretical descriptor that quantifies the complexity or branching structure of a molecular graph.
- It was introduced by Milan Randić [9] in 1975 and has found applications in various fields of chemistry.
- It is defined as the sum of the reciprocal square roots of the product of the degrees of connected pairs of vertices, written as

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

[9] M. Randić , *Characterization of molecular branching. Journal of the American Chemical Society*, **97(23)** (1975), 6609-6615.

Example of Randić Index

Based on Figure 2,



$$
\begin{aligned}
R(\Gamma) &= \sum_{u,v \in E(\Gamma)} \frac{1}{\sqrt{deg(u)deg(v)}} \\
&= \frac{1}{\sqrt{(3)(4)}} + \frac{1}{\sqrt{(3)(4)}} + \frac{1}{\sqrt{(3)(4)}} + \frac{1}{\sqrt{(3)(4)}} + \frac{1}{\sqrt{(3)(4)}} \\
&\quad \frac{1}{\sqrt{(3)(4)}} + \frac{1}{\sqrt{(4)(4)}} + \frac{1}{\sqrt{(4)(4)}} + \frac{1}{\sqrt{(4)(4)}} \\
&= 2.48
\end{aligned}
$$

DEFINITIONS OF TOPOLOGICAL INDICES

General Zeroth Order Randić Index

The Randić index is modified and introduced a concept of general zeroth order Randić index, which is defined as

$$^{0}R_{\alpha} = \sum_{u \in V(\Gamma)} (deg(u))^{\alpha},$$

where α can be any non-zero real number [10].

Sombor Index

Recently, in 2021, a new topological index, Sombor index has been established by Gutman [11]. The Sombor index of a graph, $SO(\Gamma)$, is defined as follows.

$$SO(\Gamma) = \sum_{u,v \in E(\Gamma)} \sqrt{\deg(u)^2 + \deg(v)^2}.$$

[10] H. Ahmed, A.A. Bhatti, and A. Ali, *Zeroth-order general Randić index of cactus graphs. AKCE International Journal of Graphs and Combinatorics*, **16(2)** (2019), 182-189.
[11] I. Gutman, *Geometric approach to degree-Based topological indices: Sombor indices. MATCH Commun. Math. Comput. Chem.*, **86** (2021), 11–16.

Example of Sombor Index

Based on Figure 2,

$$
\begin{aligned}
SO(\Gamma) &= \sum_{u,v\in E(\Gamma)} \sqrt{\deg(u)^2+\deg(v)^2} \\
&= \sqrt{deg(a)^2+deg(b)^2}+\sqrt{deg(a)^2+deg(ab)^2}+\sqrt{deg(a)^2+deg(a^2b)^2}+ \\
&\quad \sqrt{deg(a^2)^2+deg(b)^2}+\sqrt{deg(a^2)^2+deg(ab)^2}+ \\
&\quad \sqrt{deg(a^2)^2+deg(a^2b)^2}+\sqrt{deg(b)^2+deg(ab)^2}+ \\
&\quad \sqrt{deg(b)^2+deg(a^2b)^2}+\sqrt{deg(ab)^2+deg(a^2b)^2} \\
&= \sqrt{3^2+4^2}+\sqrt{3^2+4^2}+\sqrt{3^2+4^2}+\sqrt{3^2+4^2}+\sqrt{3^2+4^2} \\
&\quad \sqrt{3^2+4^2}+\sqrt{4^2+4^2}+\sqrt{4^2+4^2}+\sqrt{4^2+4^2} \\
&= 46.97
\end{aligned}
$$

GRAPHS ASSOCIATED TO GROUPS

Definition 2.1 [12] The Non-commuting Graph

Let G be a finite group. The non-commuting graph of G, denoted by Γ_G, is the graph of vertex set $G - Z(G)$ and two distinct vertices x and y are joined by an edge whenever $xy \neq yx$.

Example :

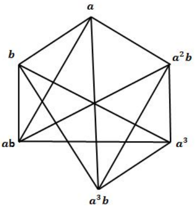


Figure 4: The non-commuting graph of D_8

[12] A. Abdollahi, S. Akbari, H. Maimani, *Non-commuting graph of a group. Journal of Algebra.* **298** (2006), 468-492.

Propisition 2.1 [13]

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

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

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

THE NON-COMMUTING GRAPH ASSOCIATED TO SOME FINITE GROUPS

Propisition 2.2 [13]

Let G be the generalised quaternion group, $Q_{4n} = \langle a, b | a^n = b^2, a^{2n} = b^4 = 1, bab = a^{-1} \rangle$ of order $4n$ where $n \geq 2, n \in \mathbb{N}$ and let Γ_G be the non-commuting graph of G. Then,

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

Propisition 2.3 [13]

Let G be the quasidihedral group, $QD_{2^n} = \langle a, b | a^{2^{n-1}} = b^2 = 1, bab = a^{2^{n-2}-1} \rangle$ of order 2^n where $n \geq 4, n \in \mathbb{N}$ and let Γ_G be the non-commuting graph of G. Then,

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

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

Definition 2.2 [14] The Coprime Graph

Coprime graph of a group G is a graph that consists the elements in G as the set of vertices where two distinct vertices are adjacent if and only if the order of both vertices are coprime.

Example:

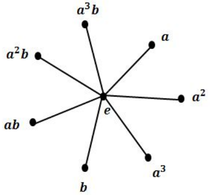


Figure 5: The coprime graph of D_8

[14] X.L. Ma, H.Q. Wei, and L.Y. Yang, *The coprime graph of a group. International Journal of Group Theory,* **3(3)** (2014), 13-23.

THE COPRIME GRAPH ASSOCIATED TO DIHEDRAL GROUPS

In 2014, Ma *et al.* [14] generalized the coprime graph for certain order of dihedral groups, as stated in the following propositions.

Proposition 2.4 [14]

Let G be the dihedral groups of order $2n$ and the coprime graph of G is denoted as Γ_G^{CO}. Then, Γ_G^{CO} is isomorphic to a multipartite graph $K_{1,n-1,n}$ if n is an odd prime.

Proposition 2.5 [14]

Let G be the dihedral groups of order $2n$ and the coprime graph of G is denoted as Γ_G^{CO}. Then, Γ_G^{CO} is isomorphic to a star graph, $K_{1,2^{k+1}-1}$ if $n = 2^k$ for some positive integer k.

[14] X.L. Ma, H.Q. Wei, and L.Y. Yang, *The coprime graph of a group.* *International Journal of Group Theory,* **3(3)** (2014), 13-23.

GRAPHS ASSOCIATED TO RINGS

Zero Divisor Graph [15]

Let R be a commutative ring with identity, $Z(R)$ its set of zero divisors. The zero divisor graph of R is $\Gamma(R) = Z(R) - 0$, with distinct vertices a and b adjacent if and only if $ab = 0$ or $ba = 0$.

Example :

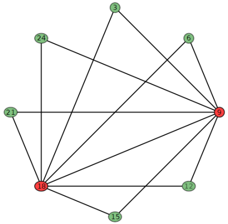


Figure 6: The zero divisor graph for $\mathbb{Z}_{27}$, $\Gamma\left(\mathbb{Z}_{27}\right)$

[15] D.F. Anderson and P.S. Livingston, *The zero-divisor graph of a commutative ring.* *Journal of Algebra,* **217(2)** (1999), 434–447.

TOPOLOGICAL INDICES OF GRAPHS ASSOCIATED TO GROUPS

The Wiener Index of the Non-commuting Graph for Some Finite Groups

Theorem 1 [16]

Let G be the dihedral groups, D_{2n} of order $2n$ where $n \geq 3$, Γ_G is the non-commuting graph of G and $W(\Gamma_G^{NC})$ is the Wiener index of Γ_G. Then,

$$W(\Gamma_G^{NC}) = \frac{1}{2}(5n^2 - 9n + 4).$$

[16] N.I. Alimon, *Topological Indices of a Class of Graphs of Some Finite Groups and Applications to Molecular Structures*, Ph.D Thesis. Universiti Teknologi Malaysia (2021).

Proof

For n is odd and $n \geq 3$,

$$\begin{aligned}
W(\Gamma_G^{\mathrm{NC}}) &= \frac{1}{2}\left[\left(|G| - |Z(G)|\right)\left(|G| - 2|Z(G)| - 2\right) + |G|\left(k(G) - |Z(G)|\right)\right] \\
&= \frac{1}{2}\left[(2n-1)\left(2n - 2(1) - 2\right) + (2n)\left(\frac{n+3}{2} - 1\right)\right] \\
&= \frac{1}{2}\left[(2n-1)(2n-4) + n(n+1)\right] \\
&= \frac{1}{2}\left[4n^2 - 8n - 2n + 4 + n^2 + n\right] \\
&= \frac{1}{2}(5n^2 - 9n + 4).
\end{aligned}$$

Proof (Cont.)

For n is even and $n \geq 4$,

$$\begin{aligned} W(\Gamma_G^{\mathrm{NC}}) &= \frac{1}{2}\left[(|G| - |Z(G)|)\,(|G| - 2|Z(G)| - 2) + |G|\,(k(G) - |Z(G)|)\right] \\ &= \frac{1}{2}\left[(2n-2)\,(2n - 2(2) - 2) + (2n)\left(\frac{n+6}{2} - 2\right)\right] \\ &= \frac{1}{2}\left[(2n-2)(2n-6) + n(n+2)\right] \\ &= \frac{1}{2}\left[4n^2 - 12n - 4n + 12 + n^2 + 2n\right] \\ &= \frac{1}{2}\left[5n^2 - 14n + 12\right]. \end{aligned}$$

■

The Wiener Index of the Non-commuting Graph for Some Finite Groups

Theorem 2 [17]

Let G be the generalised quaternion group, Q_{4n} of order $4n$ where $n \geq 2$, Γ_G is the non-commuting graph of G and $W(\Gamma_G^{NC})$ is the Wiener index of Γ_G. Then,

$$W(\Gamma_G^{NC}) = 2n(5n - 7) + 6.$$

Theorem 3 [16]

Let G be the quasidihedral group, QD_{2^n} of order 2^n where $n \geq 4$, Γ_G is the non-commuting graph of G and $W(\Gamma_G^{NC})$ is the Wiener index of Γ_G. Then,

$$W(\Gamma_G^{NC}) = 2^{2n-1} + 2^{2n-3} - 7(2^{n-1}) + 6.$$

[16] N.I. Alimon, *Topological Indices of a Class of Graphs of Some Finite Groups and Applications to Molecular Structures,* Ph.D Thesis. Universiti Teknologi Malaysia (2021).

[17] N.H. Sarmin, N.I. Alimon, and A. Erfanian, *Topological indices of the non-commuting graph for generalised quaternion group. Bulletin of the Malaysian Mathematical Sciences Society*, **43(5)** (2020), 3361-3367.

The Wiener Index of the Coprime Graph for Some Finite Groups

The cases are only limited to n is an odd prime and $n = 2^k, k \in \mathbb{Z}$ since the coprime graph associated to the dihedral groups of the other cases of n cannot be generalized.

Theorem 4 [18]

Let G be the dihedral group, D_{2n} of order $2n$ where n is an odd prime. Then, the Wiener index of the coprime graph of G, Γ_G^{CO} is stated as follows :

$$W(\Gamma_G^{\mathrm{CO}}) = (n-1)(3n-1) + n.$$

Proof

- The coprime graph of D_{2n}, when n is an odd prime, is $K_{1,n-1,n}$.
- Then, the total number of vertices in $K_{1,n-1,n}$ is $1 + n - 1 + n = 2n$ vertices. Its coprime graph has three independent sets which are $1, n-1$ and n elements, respectively.

[18] N.I. Alimon, N.H. Sarmin, and A. Erfanian, *The Szeged and Wiener indices for coprime graph of dihedral groups. In AIP Conference Proceedings*, **2266(1)** (2020), 060006.

Proof (Cont.)

- The coprime graph of dihedral groups has n^2+n-1 edges where the number of edges for a complete graph, K_{2n} minus the number of edges for K_{n-1} and K_n, as shown in the following.

$$\begin{aligned}|E(K_{1,n-1,n})| &= \frac{2n(2n-1)}{2} - \frac{n(n-1)}{2} - \frac{(n-1)(n-2)}{2} \\ &= n^2+n-1.\end{aligned}$$

Thus, there are n^2+n-1 edges which have a distance of 1, while $\frac{(n-1)(n-2)}{2}$ and $\frac{n(n-1)}{2}$ edges have a distance of 2.
By using the definition of the Wiener index,

$$\begin{aligned}W(\Gamma_G^{CO}) &= \frac{1}{2}\sum_{i=1}^{2n}\sum_{j=1}^{2n} d(i,j) \\ &= 1\times\left[n^2+n-1\right] + 2\times\left[\frac{n(n-1)}{2}\right] + 2\times\left[\frac{(n-1)(n-2)}{2}\right] \\ &= (n-1)(3n-1)+n.\end{aligned}$$

The Wiener Index of the Coprime Graph for Some Finite Groups

Theorem 5 [18]

Let G be the dihedral group, D_{2n} of order $2n$ where $n = 2^k, k \in \mathbb{Z}^+$. Then, the Wiener index of the coprime graph for G,

$$W(\Gamma_G^{\mathrm{CO}}) = (2n-1)^2.$$

Theorem 6 [16]

Let G be the generalized quaternion group, Q_{4n} of order $4n$ where $n = 2^{k-1}, k \geq 2$ Then, the Wiener index of the coprime graph for G, Γ_G^{CO} is stated as follows :

$$W(\Gamma_G^{\mathrm{CO}}) = (4n-1)^2.$$

[16] N.I. Alimon, *Topological Indices of a Class of Graphs of Some Finite Groups and Applications to Molecular Structures,* Ph.D Thesis. Universiti Teknologi Malaysia (2021).
[18] N.I. Alimon, N.H. Sarmin, and A. Erfanian, *The Szeged and Wiener indices for coprime graph of dihedral groups. In AIP Conference Proceedings*, **2266(1)** (2020), 060006.

The Wiener Index of the Coprime Graph for Some Finite Groups

Theorem 7 [16]

Let G be the quasidihedral group, Q_{2^n} of order 2^n where $n \geq 4$. Then, the Wiener index of the coprime graph for G, Γ_G^{CO} is stated as follows :

$$W(\Gamma_G^{\mathrm{CO}}) = (2^n - 1)^2.$$

[16] N.I. Alimon, *Topological Indices of a Class of Graphs of Some Finite Groups and Applications to Molecular Structures,* Ph.D Thesis. Universiti Teknologi Malaysia (2021).

The Zagreb Index of the Non-commuting Graph for Some Finite Groups

Theorem 8[19]

Let G be a dihedral group, D_{2n} of order $2n$ where $n \geq 3$. Then,

$$M_1(\Gamma_G^{NC}) = \begin{cases} n(5n-4)(n-1) & \text{if} \quad n \text{ is odd,} \\ n(5n-8)(n-2) & \text{if} \quad n \text{ is even,} \end{cases}$$

[19] N.I. Alimon, N.H., Sarmin, and A. Erfanian, *Topological indices of non-commuting graph of dihedral groups. Malaysian Journal of Fundamental and Applied Sciences*, (2018), 473-476.

Proof

For n is odd,

$$\begin{aligned} M_1(\Gamma_G^{\mathrm{NC}}) &= |G|^2\left(|G| + |Z(G)| - 2k(G)\right) - \sum_{x \in G - Z(G)} |C_G(x)|^2 \\ &= 4n^2\left[2n + 1 - 2\left(\frac{n+3}{2}\right)\right] - 2^2 n + n^2(n-1) \\ &= n\left(5n-4\right)\left(n-1\right). \end{aligned}$$

For n is even,

$$\begin{aligned} M_1(\Gamma_G^{\mathrm{NC}}) &= |G|^2\left(|G| + |Z(G)| - 2k(G)\right) - \sum_{x \in G - Z(G)} |C_G(x)|^2 \\ &= 4n^2\left[2n + 1 - 2\left(\frac{n+6}{2}\right)\right] - 4^2 n + n^2(n-2) \\ &= n\left(5n-8\right)\left(n-2\right). \end{aligned}$$

■

The Zagreb Index of the Non-commuting Graph for Some Finite Groups

Theorem 9 [19]

Let G be a dihedral group, D_{2n} of order $2n$ where $n \geq 3$. Then,

$$M_2(\Gamma_G^{NC}) = \begin{cases} 2n(n-1)^2(2n-1) & \text{if} \quad n \text{ is odd}, \\ 4n(n-2)^2(n-1) & \text{if} \quad n \text{ is even}. \end{cases}$$

Theorem 10 [17]

Let G be the generalised quaternion group, Q_{4n} of order $4n$ where $n \geq 2$. Then,

$$M_1(\Gamma_G^{NC}) = 8n(5n^2 - 9n + 4),$$

and

$$M_2(\Gamma_G^{NC}) = 32n(2n^3 - 5n^2 + 4n - 1).$$

[19] N.I. Alimon, N.H., Sarmin, and A. Erfanian, *Topological indices of non-commuting graph of dihedral groups. Malaysian Journal of Fundamental and Applied Sciences*, (2018), 473-476.
[17] N.H. Sarmin, N.I. Alimon, and A. Erfanian, *Topological indices of the non-commuting graph for generalised quaternion group. Bulletin of the Malaysian Mathematical Sciences Society*, **43(5)** (2020), 3361-3367.

The Zagreb Index of the Non-commuting Graph for Some Finite Groups

Theorem 11 [16]

Let G be the quasidihedral group, QD_{2^n} of order 2^n where $n \geq 4$. Then,

$$M_1(\Gamma_G^{\mathrm{NC}}) = \left[5(2^{3n-3}) - 9(2^{2n-1}) + 8(2^n)\right],$$

and

$$M_2(\Gamma_G^{\mathrm{NC}}) = \left[2^{4n-2} - 5(2^{3n-1}) + 8(3^n) - 8(2^n)\right].$$

[16] N.I. Alimon, *Topological Indices of a Class of Graphs of Some Finite Groups and Applications to Molecular Structures*, Ph.D Thesis. Universiti Teknologi Malaysia (2021).

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

Theorem 12 [20]

Let G be the dihedral groups, D_{2n}, where $n \geq 3$. Then, the Szeged index of the non-commuting graph of G,

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

Proof

By Proposition 2.1, the non-commuting graph of D_{2n} is

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

[20] N.I. Alimon, N.H., Sarmin, and A. Erfanian, *On the Szeged index and its non-commuting graph, Jurnal Teknologi*, **85(3)** (2023), 105-110.

Proof (Cont.)

For n is odd and $n \geq 3$:

- There are $n(n-1)$ edges have $n_1(e|\Gamma) = 1$ since there is only one element of vertices which is closer to a vertex a^i of the edge than the other vertex of the edge, $a^j b$, where $i = \{1, 2, \ldots, n-1\}$ and $j = \{0, 1, \ldots, n-1\}$.
- Then, $n_2(e|\Gamma) = n-1$ since $n-1$ elements of vertices which are closer to $a^k b$ than to $a^l b$, where $k, l = \{0, 1, \ldots, n-1\}$. Meanwhile, the rest of the edges have $n_1(e|\Gamma) = n_2(e|\Gamma) = 1$.

Thus, by definition of the Szeged index,

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

Proof (Cont.)

For n is even and $n \geq 3$:

- There are $2n(n-2)$ edges have $n_1(e|\Gamma) = 2$ since there are two elements of vertices which are closer to a vertex of edge, a^i than the other vertex of edge, $a^j b$, where a^i is non-central elements and $j = \{0, 1, \ldots, n-1\}$.

Then, $n_2(e|\Gamma) = n-2$ since there is $n-2$ elements of vertices which re closer to $a^k b$ than to $a^l b$, where $k, l = \{0, 1, \ldots, n-1\}$. Meanwhile, the rest of the edges have $n_1(e|\Gamma) = n_2(e|\Gamma) = 2$. Thus, by the definition of Szeged index:

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

■

The Szeged Index of the Non-commuting Graph for Q_{4n} and QD_{2^n}

Theorem 13 [20]

Let G be the generalized quaternion groups, Q_{4n} where $n \geq 2$. Then, the Szeged index of the non-commuting graph of G,

$$Sz(\Gamma_G^{\mathrm{NC}}) = 8n(2n-1)(n-1).$$

Theorem 14 [20]

Let G be the quasidihedral groups of order 2^n where $n \geq 4$. Then, the Szeged index of the non-commuting graph of G,

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

[20] N.I. Alimon, N.H., Sarmin, and A. Erfanian, *On the Szeged index and its non-commuting graph*, *Jurnal Teknologi*, **85(3)** (2023), 105-110.

The Szeged Index of the Coprime Graph for D_{2n}

Theorem 15 [18]

Let G be the dihedral groups, D_{2n} where $n \geq 3$. If n is an odd prime, then the Szeged index of the coprime graph of G,

$$Sz(\Gamma_G^{\mathrm{CO}}) = n^4 - 2n^3 + 3n^2 - 2n + 1.$$

Theorem 16 [18]

Let G be a dihedral group, D_{2n} and Γ_G^{CO} is coprime graph of G. Then, if $n = 2^k$, where $k \in \mathbb{Z}^+$, the Szeged index of coprime graph for D_{2n} is as follows :

$$Sz(\Gamma_G^{CO}) = 4n^2 - 4n + 1.$$

[18] N.I. Alimon, N.H. Sarmin, and A. Erfanian, *The Szeged and Wiener indices for coprime graph of dihedral groups. In AIP Conference Proceedings*, **2266(1)** (2020), 060006.

The Szeged Index of the Coprime Graph for Q_{4n} and QD_{2^n}

Theorem 17 [16]

Let G be the generalized quaternion groups of order $4n$ where $n \geq 2$. If $n = 2^{k-1}, k \geq 2$, then the Szeged index of the coprime graph of G,

$$Sz(\Gamma_G^{\mathrm{CO}}) = (4n-1)^2.$$

Theorem 18 [16]

Let G be the quasidihedral groups of order 2^n where $n \geq 4$. Then, the Szeged index of the coprime graph of G,

$$Sz(\Gamma_G^{\mathrm{CO}}) = (2^n-1)^2.$$

[16] N.I. Alimon, *Topological Indices of a Class of Graphs of Some Finite Groups and Applications to Molecular Structures,* Ph.D Thesis. Universiti Teknologi Malaysia (2021).

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

Theorem 19 [21]

Let G be a dihedral group, D_{2n} and Γ_G^{NC} is a non-commuting graph of G. Then,

$$H(\Gamma_G^{NC}) = \begin{cases} \frac{1}{4}\left[(n-2)(7n-3)+n\right] & \text{if} \quad n \text{ is even,} \\ \frac{1}{4}\left[(n-1)(7n-2)\right] & \text{if} \quad n \text{ is odd.} \end{cases}$$

[21] N.I. Alimon, N.H. Sarmin, and A. Erfanian, *The Harary index of the non-commuting graph for dihedral groups. Southeast Asian Bull. Math*, **44(6)** (2020), 763-768.

Proof

The Harary index of the non-commuting graph for dihedral group where n is odd is the same as half of the total of all entries in its distance matrix, D^r. The entries of D^r in this case is either 1 if two vertices are connected or $\frac{1}{2}$ if two vertices are not connected to each other. Hence,
for n is even and $n \geq 4$,

$$
\begin{aligned}
H &= |E(\Gamma_G)| + \left(\frac{1}{2} \times \frac{n}{2}\right) + \left(\frac{(n-2)(n-3)}{2} \times \frac{1}{2}\right) \\
&= \frac{3}{2}n(n-2) + \frac{n}{4} + \frac{(n-2)(n-3)}{4} \\
&= \frac{1}{4}\left[6n(n-2) + n + (n-2)(n-3)\right] \\
&= \frac{1}{4}\left[(n-2)(7n-3) + n\right],
\end{aligned}
$$

Proof (Cont.)

for n is odd and $n \geq 3$,

$$\begin{aligned} H(\Gamma_G) &= |E(\Gamma_G)| + \frac{1}{2}\left[\frac{(n-1)(n-2)}{2}\right] \\ &= \frac{3n}{2}(n-1) + \frac{1}{4}(n-1)(n-2) \\ &= \frac{1}{2}(n-1)\left(3n + \frac{1}{2}(n-2)\right) \\ &= \frac{1}{2}(n-1)\left(\frac{7}{2}n - 1\right) \\ &= \frac{1}{4}(n-1)(7n-2). \end{aligned}$$

Therefore,

$$H(\Gamma_G) = \begin{cases} \frac{1}{4}[(n-2)(7n-3)+n], & \text{if} \quad n \text{ is even}, \\ \frac{1}{4}(n-1)(7n-2), & \text{if} \quad n \text{ is odd}. \end{cases} \qquad \blacksquare$$

The Harary Index of the Non-commuting Graph for Q_{4n} and QD_{2^n}

Theorem 20 [21]

Let G be the generalized quaternion groups of order $4n$, where $n \geq 2$. Then, the Harary index of the non-commuting graph of G,

$$H(\Gamma_G^{\mathrm{NC}}) = 7n^2 - 8n + \frac{3}{2}.$$

Theorem 21 [21]

Let G be the quasidihedral groups of order 2^n, where $n \geq 4$. Then, the Harary index of the non-commuting graph of G,

$$H(\Gamma_G^{\mathrm{NC}}) = 7(2^{2n-4}) - 2^{n+1} + \frac{3}{2}.$$

[21] N.I. Alimon, N.H. Sarmin, and A. Erfanian, *The Harary index of the non-commuting graph for dihedral groups. Southeast Asian Bull. Math*, **44(6)** (2020), 763-768.

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

Theorem 22 [22]

Let G be a dihedral group, D_{2n} and Γ_G^{NC} is a non-commuting graph of G. Then,

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

[22] S.R.D. Roslly, N.F.A.Z. Ab Halem, N.S.S. Zailani, and N.I. Alimon, *Generalization of Randić index of the non-commuting graph for a family of finite groups. Malaysian Journal of Fundamental and Applied Sciences*, In Review.

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

Theorem 23 [22]

Let G be the generalised quaternion group, Q_{4n} and Γ_G^{NC} is a non-commuting graph of G. Then,

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

Theorem 24 [22]

Let G be the quasidihedral group, QD_{2^n} and Γ_G^{NC} is a non-commuting graph of G. Then,

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

[22] S.R.D. Roslly, N.F.A.Z. Ab Halem, N.S.S. Zailani, and N.I. Alimon, *Generalization of Randić index of the non-commuting graph for a family of finite groups. Malaysian Journal of Fundamental and Applied Sciences*, In Review.

The Sombor Index of the Non-commuting Graph for Some Finite Groups

Theorem 25 [23]

Let Γ_G be the non-commuting graph of G where G is the dihedral groups of order $2n$, $n \geq 3$. Then, the Sombor index of Γ_G,

$$SO(\Gamma_G) = \begin{cases} (n-1)[\sqrt{2}(n-1) + \sqrt{4(n-1)^2 + n^2}] & \text{if} \quad n \text{ is odd,} \\ (n-2)[\sqrt{2}(n-2) + \sqrt{4(n-2)^2 + n^2}] & \text{if} \quad n \text{ is even.} \end{cases}$$

Theorem 26 [23]

Let Γ_G be the non-commuting graph of G where G is the generalized quaternion groups of order $4n$, $n \geq 2$. Then, the Sombor index of Γ_G,

$$SO(\Gamma_G) = n(n-1)[\sqrt{2}(n-1) + \sqrt{4(n-1)^2 + n^2}].$$

[23] S.M.S. Khasraw, N.H. Sarmin, N.I. Alimon and N. Najmuddin, *The Sombor index and Sombor polynomial of the power graph associated to some finite groups, ASIA International Multidisciplinary Conference 2023 Proceedings*. Submitted.

The Sombor Index of the Non-commuting Graph for Some Finite Groups

Theorem 27 [23]

Let Γ_G be the non-commuting graph of G where G is the quasidihedral groups of order 2^n, $n \geq 4$. Then, the Sombor index of Γ_G,

$$SO(\Gamma_G) = \sqrt{2}(2^n - 4)\left(2^{2n-3} - 2^{n+1}\right) + \left(2^{2n-2} - 2\right)\sqrt{(2^n - 4)^2 + 2^{2n-2}}.$$

[23] S.M.S. Khasraw, N.H. Sarmin, N.I. Alimon and N. Najmuddin, *The Sombor index and Sombor polynomial of the power graph associated to some finite groups, ASIA International Multidisciplinary Conference 2023 Proceedings*. Submitted.

TOPOLOGICAL INDICES OF GRAPHS ASSOCIATED TO RINGS

Theorem 28 [24]

The first Zagreb index of the zero divisor graph for the ring $\mathbb{Z}_{p^k}$ is $2(p^{k-1} - p^k)\left(k - 1 + \lceil \frac{k-1}{2} \rceil\right) + (p^k + 1)(p^{k-1} - 1) + 3\left(p^{\lceil \frac{k-1}{2} \rceil} - 1\right)$ where $k \geq 3$ for $p = 2$ and $k \geq 2$ for odd prime p.

Theorem 29 [25]

The general zeroth-order Randić index of the zero divisor graph for the ring $\mathbb{Z}_{p^k q}$ when $\alpha = 1$,

$$R_1^0 = k(p^k - p^{k-1})(2q - 1) - p^k - p + 2 - \left(\frac{p^k - p^{\lceil \frac{k+3}{2} \rceil}}{p^{\lceil \frac{k+1}{2} \rceil}}\right).$$

[24] G. Semil @ Ismail, N.H. Sarmin, N.I. Alimon, and F. Maulana, *The first Zagreb index of zero divisor graph for the ring of integers modulo power of primes, Jurnal Teknologi.* In Review.
[25] G. Semil @ Ismail, N.H. Sarmin, N.I. Alimon, and F. Maulana, *The general zeroth-order Randić index of a graph for the commutative ring $\mathbb{Z}_{p^k q}$.* Submitted.

THE TOPOLOGICAL INDICES OF THE POINT GROUPS OF ORDER EIGHT FOR A MOLECULAR STRUCTURE

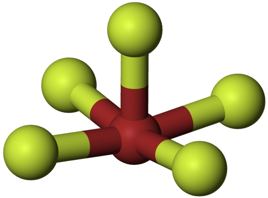


Figure 7: Bromine Pentafluoride, BrF_5

- The BrF_5 has rotation axis of order four and four vertical planes.
- Its point group is C_{4v} with elements $E, C_4, C_4^2, C_4^3, \sigma_{v_1}, \sigma_{v_2}, \sigma_{d_1}, \sigma_{d_2}$.
- Let ϕ be the mapping from D_8 to C_{4v}. It is found that ϕ satisfies the homomorphism property.
- Therefore, $D_8 \cong C_{4v}$.

THE TOPOLOGICAL INDICES OF THE POINT GROUPS OF ORDER EIGHT FOR A MOLECULAR STRUCTURE

Since $D_8 \cong C_4$, then Wiener index of the non-commuting graph of D_8 is used to calculate the Wiener index of the non-commuting graph of C_{4v}. Based on Theorem 1 where $n = 4$,

$$\begin{aligned} W(\Gamma_G^{\mathrm{NC}}) &= \frac{1}{2}\left(5n^2 - 14n + 12\right) \\ &= 18. \end{aligned}$$

CONCLUSION

- Some topological indices, which are the Wiener index, the Zagreb index, the Szeged index, the Harary index and the Randić index of some graphs associated to some finite groups are found.
- Based on the results, the higher the order of the groups, the higher the value of topological indices. This is due to the increasing of the number of vertices and edges.
- The general formulas of the topological indices can be used to help chemists and biologists to predict the chemical and physical properties of the molecules by developing a mathematical model.

RECOMMENDATIONS

- Other types of topological indices of some graphs associated to groups can be computed.
- Similar to other types of topological indices of some graphs associated to rings can also be computed.
- The topological indices for graphs representing chemical structures in drugs are a valuable approach to determine both the physicochemical properties and biological activities of these molecules can be constructed.

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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.

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