Research Article

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Mostar index of graphs associated to groups

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Abstract: A bond-additive connectivity index, named as the Mostar index, is used to measure the amount of peripheral edges of a simple connected graph, where a peripheral edge in a graph is an edge whose one end vertex has more number of vertices closer as compared to the other end vertex. In this study, we count the contribution of peripheral edges in commuting, non-commuting, and non-conjugate graphs associated to the dihedral and semi-dihedral groups. In fact, we compute the Mostar index of these graphs.

Keywords: distance, Mostar index, group, commuting graph, non-commuting graph, non-conjugate graph

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1 Introduction

A connectivity index is a form of molecular attribute whose computation depends upon a chemical graph of a chemical substance in the subject of mathematical chemistry. A large variety of numerical values, also known as topological indices, have been suggested and explored in attempt to distil and collect, or summarie, the content contained in graph connectivity patterns (Todeschini and Conosonni, 2002). Topological indices are numerical quantities that describe the topology of a graph and are generally graph invariant (Qiu and Akl, 1995). For instance, the Wiener index is based on the topological proximity of vertices in a graph, and was defined by Wiener in 1947 to estimate the boiling properties of various alkane isomers. Since then, more than 3,000 topological indices of graphs have been recorded in chemical databases. Another type of topological index aims to measure the nonbalancedness among the bonds of a chemical graph on the base of peripherality of bonds (edges), which is named as the Mostar index (Akhter et al., 2021; Došlić et al., 2018). The Mostar index recently discovered as a bond-additive connectivity index determines the quantity of peripherality of certain edges as well as the graph as a whole (Akhter et al., 2021; Došlić et al., 2018). It is a distinct geometric index which counts the contribution $|\eta_\lambda - \eta_\mu|$ of every edge $e = \lambda\mu$ in a connected graph, where η_λ is the quantity of vertices that are closer to the vertex λ than the vertex μ, and η_μ is defined in the same way (Ali and Doslic, 2021). Accordingly, this index indicates the degree of specific edges and the degree of peripherality of the graph as a whole. This index attracted many graph theorists to measure the peripherality of various (chemical) graphs. Tepeh addressed the first conjecture about the Mostar index of bicyclic graphs (Tepeh, 2019), which was proposed by Došlić et al. (2018). Further, remarkable work on the Mostar index of carbon nanostructures, trees, and hexagonal chains has been supplied by Arockiaraj et al. (2019), Hayat and Zhou (2019), and Huang et al. (2020).

A classical study of graphs associated with groups attracted many researchers to explore the various theoretical and topological properties of graph. A large number of interesting work have been published by supplying the articles by Abdollahi et al. (2006), Ali et al. (2016), Alolayan et al. (2019), Bhuniya and Bera (2016), Bunday (2006), Cameron and Ghosh (2011), Chakrabarty et al. (2009), and Rahman (2017). Some of the graphs associated to group are defined as follows: Let a group Γ and the center of group Γ be $\zeta(\Gamma) = \{\lambda \in \Gamma: \lambda\mu = \mu\lambda \forall \mu \in \Gamma\}$. Γ_G denotes the commuting graph of Γ with the vertex set Γ and two distinct vertices λ and $\mu \in \Gamma$ from an edge in Γ_G if and only if $\lambda\mu = \mu\lambda$ in Γ (Ali et al., 2016; Bunday, 2006). The non-commuting graph of Γ is denoted by G_Γ with the vertex set $\Gamma - \zeta(\Gamma)$ and two distinct vertices λ and

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$\mu \in \Gamma$ from an edge in G_Γ if and only if $\lambda\mu \neq \mu\lambda$ in Γ (Abdollahi et al., 2006; Moghaddamfar et al., 2005; Wei et al., 2020). If $\lambda = g\mu g^{-1}$ or $\mu = g^{-1}\lambda g$ for $g \in \Gamma$, then λ and μ are said to be conjugate of each other. This relation between elements of Γ is an equivalence relation and is called the conjugacy relation. Due to this equivalence relation, Γ is partitioned into disjoint classes each of which is called a conjugacy class. Mathematically, the conjugacy class of $\lambda \in \Gamma$ is $\mathrm{Cl}(\lambda) = \{g\lambda g^{-1}: g \in \Gamma\}$. $G(\Gamma)$ denotes a non-conjugate graph with the vertex set Γ and two different vertices λ and $\mu \in \Gamma$ from an edge in $G(\Gamma)$ if and only if λ and μ belong to different conjugacy classes (Alolayan et al., 2019).

Graphs associated with the dihedral group have been considered by Abbas et al. (2021), Salman et al. (2022), and Wei et al. (2020) to study their topological properties such as the Wiener related indices, Harary index, Randić indices, geometric arithmetic indices, atom bond connectivity indices, harmonic index, Hosoya index, and polynomials. This study is aimed to investigate the Mostar index of graphs (commuting, non-commuting, and non-conjugate graphs) associated with the dihedral and semi-dihedral groups.

2 Preliminaries

This section provides partitions of groups under consideration, some basic terminologies of a graph, and the mechanism to compute the Mostar index.

The generating form $D_n = \langle a, b | a^n = b^2 = e, ab = ba^{-1}\rangle$ represents the dihedral group of order $2n$, which is the collection of symmetries of regular n-polygon. The center of D_n is:

$$\zeta(D_n) = \begin{cases} \{e\}, & \text{if } n \text{ is odd} \\ \{e, a^{\frac{n}{2}}\}, & \text{if } n \text{ is even} \end{cases}$$

Let us partition D_n as follows:

$\Omega_1 = \{e, a, a^2, \ldots, a^{n-1}\}$, $\Omega_2 = \{b, ab, a^2b, \ldots, a^{n-1}b\}$, and $\Omega_3 = \Omega_1 - \zeta(D_n)$, then $|\Omega_1| = |\Omega_2| = n$. Further for even n, let $\Omega_2 = \bigcup_{i=0}^{\frac{n}{2}-1}\Omega_2^i$ with $\Omega_2^i = \left\{a^i b, a^{i+\frac{n}{2}}\right\}$ be the subsets according to the commuting elements from Ω_2, and conjugacy classes of D_n are:

$$\mathrm{Cl}(D_n) = \begin{cases} \{e\}, & \text{for any } n \\ \left\{a^{\frac{n}{2}}\right\}, & \text{when } n \text{ is even} \\ \{a^i b : 0 \le i \le n-1\}, & \text{when } n \text{ is odd} \\ \{a^i, a^{n-i}\}; 1 \le i \le \frac{n-1}{2}, & \text{when } n \text{ is odd} \\ \left\{a^{2i} b : 0 \le i < \frac{n}{2}\right\}, & \text{when } n \text{ is even} \\ \left\{a^{2i+1} b : 0 \le i < \frac{n}{2}\right\}, & \text{when } n \text{ is even} \\ \{a^i, a^{n-i}\}; 1 \le i < \frac{n}{2}, & \text{when } n \text{ is even} \end{cases} \tag{1}$$

The generating form $\mathrm{SD}_{8n} = \langle a, b | a^{4n} = b^2 = e, ba = a^{2n-1}b\rangle$ represents the semi-dihedral group of order $8n$ with:

$$ba^i = \begin{cases} a^{4n-i}b, & \text{if } n \text{ is even} \\ a^{2n-i}b, & \text{if } n \text{ is odd} \end{cases}$$

and

$$\zeta(\mathrm{SD}_{8n}) = \begin{cases} \{e, a^{2n}\}, & \text{if } n \text{ is even} \\ \{e, a^n, a^{2n}, a^{3n}\}, & \text{if } n \text{ is odd} \end{cases}$$

Let us partition SD_{8n} as follows:

$\Omega_1 = \{e, a, a^2, \ldots, a^{4n-1}\}$, $\Omega_2 = \{b, ab, a^2b, \ldots, a^{4n-1}b\}$, and $\Omega_3 = \Omega_1 - \zeta(D_n)$, then $|\Omega_1| = |\Omega_2| = 4n$. For odd $n \ge 3$, let $\Omega_2 = \bigcup_{i=0}^{n-1}\Omega_2^i$ with $\Omega_2^i = \{a^i b, a^{i+n}b, a^{i+2n}b, a^{i+3n}b\}$ be the subsets according to the commuting elements from Ω_2, and conjugacy classes of SD_{8n} are:

$$\mathrm{Cl}(\mathrm{SD}_{8n}) = \begin{cases} \{e\} \\ \{a^{in}\}; 1 \le i \le 3 \\ \Phi_2^j = \{a^{4i+j}b : 0 \le i \le n-1\}; 0 \le j \le 3 \\ \Phi_3^i = \{a^i, a^{2n-i}\};\ \text{for odd } i, 1 \le i \\ \quad \le n-1 \text{ and } 2n+1 \le i \le 3n-2 \\ \Phi_3^i = \{a^i, a^{4n-i}\};\ \text{for even } i, 2 \le i \\ \quad \le 2n-2 \end{cases} \tag{2}$$

where $\bigcup_{j=0}^{3}\Phi_2^j = \Omega_2$ and $\bigcup_{\text{odd } i=1}^{n-1}\Phi_3^i \bigcup_{\text{odd } i=2n+1}^{3n-2}\Phi_3^i \bigcup_{\text{even } i=2}^{2n-2}\Phi_3^i = \Omega_3$.

For even $n \ge 2$, let $\Omega_2 = \bigcup_{i=0}^{2n-1}\Omega_2^i$ with $\Omega_2^i = \{a^i b, a^{i+2n}b\}$ be the subsets according to the commuting elements from Ω_2, and conjugacy classes of SD_{8n} are:

$$\mathrm{Cl}(\mathrm{SD}_{8n}) = \begin{cases} \{e\} \\ \{a^{2n}\} \\ \Phi_2^2 = \{a^i b: \text{ for even } i, 0 \le i \le 4n-2\} \\ \Phi_2^1 = \{a^i b: \text{ for odd } i, 1 \le i \le 4n-1\} \\ \Phi_3^i = \{a^i, a^{2n-i}\}; \text{ for odd } i, 1 \le i \\ \quad \le n-1 \text{ and } 2n+1 \le i \le 3n-1 \\ \Phi_3^i = \{a^i, a^{4n-i}\}; \text{ for even } i, 2 \le i \\ \quad \le 2n-2 \end{cases} \quad (3)$$

where $\bigcup_{j=1}^{2}\Phi_2^j = \Omega_2$ and $\bigcup_{\text{odd } i=1}^{n-1}\Phi_3^i \bigcup_{\text{odd } i=2n+1}^{3n-1}\Phi_3^i \bigcup_{\text{even } i=2}^{2n-2}\Phi_3^i = \Omega_3$.

Let a connected and simple graph G have vertex and edge sets symbolized by $V(G)$ and $E(G)$, respectively. We denote the number of edges(size) of a graph G by $S(G)$. The notation $K + H$ denotes the sum of two graphs K and H with $V(K) \cup V(H)$ as the vertex set and $E(K) \cup E(H) \cup \{\lambda \sim \mu: \lambda \in V(K) \wedge \mu \in V(H)\}$ as the edge set. The number of edges in a shortest path between two distinct vertices λ and μ is defined as the distance across λ and μ, indicated by $d(\lambda, \mu)$. The eccentricity of a vertex μ is the number

$$\mathrm{ecc}(\lambda) = \max_{\mu \in V(G)} d(\lambda, \mu)$$

For an edge $e = \lambda\mu$, peripheral neighborhoods of e according to its end vertices λ and μ are defined, Arockiaraj et al. (2020), as follows:

$$N_\lambda(e|\Gamma_G) = \{x \in V(\Gamma_G) : d(\lambda, x) < d(\mu, x)\},$$
$$N_\mu(e|\Gamma_G) = \{x \in V(\Gamma_G) : d(\mu, x) < d(\lambda, x)\}$$

Then, $\eta_\lambda(e|G) = |N_\lambda(e|\Gamma_G)|$ and $\eta_\mu(e|G) = |N_\mu(e|\Gamma_G)|$ are the peripheral degrees of e. Akhter et al. in 2021 and Došlić et al. in 2018 provided the following formula to compute the Mostar index of a graph G

$$\mathrm{Mo}(G) = \sum_{e=\lambda\mu \in E(G)} |\eta_\lambda(e|G) - \eta_\mu(e|G)|$$

The number of vertices adjacent to a vertex λ in G is called the degree of λ and it is denoted by $d(\lambda)$. A vertex of degree 1 is known as a leaf in G. Whenever we need to find the size, $S(G)$ of a graph G, we will use the formula $\sum_{\lambda \in V(G)} d(\lambda) = 2S(G)$ provided by the well-known handshake lemma (Rahman, 2017).

Proposition 1. *If λ is a leaf in G, then for an edge $e = \lambda\mu$, $N_\lambda(e|G) = \{\lambda\}$ and $N_\mu(e|G) = V(G) - \{\lambda\}$.*

Proof. Since λ is a leaf in G, so $d(\lambda, x) \le d(\mu, x)$ if and only if $x = \lambda$, and $d(\lambda, x) > d(\mu, x)$ for all $x \in V(G) - \{\lambda\}$. Therefore, the result is as follows.

For a non-negative integer k, the set $N_k(\lambda) = \{\mu \in V(G) | d(\lambda, \mu) = k\}$ is known as the k-distance neighborhood of λ in G, where $0 \le k \le \mathrm{ecc}(\lambda)$. □

Proposition 2. *Let $e = \lambda\mu$ be any edge in G, if $x \in N_k(\lambda) \cap N_k(\mu)$, then $x \notin N_\lambda(e|G) \cup N_\mu(e|G)$.*

Proof. As $d(\lambda, x) = k = d(\mu, x)$, so the result followed from the definitions of $N_\lambda(e|G)$ and $N_\mu(e|G)$. □

Remark 1. For any edge $e = \lambda\mu$ in G, let us define a set:

$$N_{k'}(\lambda) = \{x \in V(G) | d(\lambda, x) = k < d(\mu, x)\}, \text{ for } 0 \le k \le \mathrm{ecc}(\lambda).$$

Then, $N_{k'}(\lambda) = N_k(\lambda) - (\cup_{t \le k} N_t(\mu))$. Accordingly, $N_\lambda(e|G) = \bigcup_{k=0}^{\mathrm{ecc}(\lambda)} N_{k'}(\lambda)$.

A neighbor of λ is a vertex adjacent to it in a graph G. The open neighborhood, $N(\lambda)$, of λ in G is the set of all the neighbors of λ. The closed neighborhood of λ is $N[\lambda] = N(\lambda) \cup \{\lambda\}$. Two vertices λ and μ are false twins in G whenever $N(\lambda) = N(\mu)$, and are true twins whenever $N[\lambda] = N[\mu]$.

Proposition 3. *If λ and μ are true twins and $e = \lambda\mu \in E(G)$, then $N_\lambda(e|G) = \{\lambda\}$ and $N_\mu(e|G) = \{\mu\}$.*

Proof. Since $N[\lambda] = N[\mu]$, so $d(\lambda, x) = d(\mu, x))$ for each $x \in V(G) - \{\lambda, \mu\}$ and

$$d(\lambda, \lambda) = 0 \ne 1 = d(\mu, \lambda), d(\lambda, \mu) = 1 \ne 0 = d(\mu, \mu)$$

Thus, for each $x \in V(G) - \{\lambda, \mu\}$, $x \in N_k(\lambda) \cap N_k(\mu)$ for all $k \ne 0$. Hence, by Proposition 2, $x \notin N_\lambda(e|G) \cup N_\mu(e|G)$ for each $x \in V(G) - \{\lambda, \mu\}$. In fact, only $\lambda \in N_\lambda(e|G)$ and only $\mu \in N_\mu(e|G)$. □

3 Commuting graphs

The Mostar index of commuting graphs on the dihedral and semi-dihedral groups is computed in this section.

Theorem 1. *For $n \ge 3$, let Γ be a dihedral group D_n. Then,*

$$\mathrm{Mo}(\Gamma_G) = \begin{cases} 3n(n-1), & \text{when } n \text{ is odd} \\ 6n(n-2), & \text{when } n \text{ is even} \end{cases}$$

Proof. In a study by Ali et al. (2016), the following graph theoretical definition of the commuting graph on D_n was provided:

$$\Gamma_G = \begin{cases} K_1 + (K_{|\Omega_3|} \cup N_{|\Omega_2|}), & \text{if } n \text{ is odd} \\ K_2 + \left(K_{|\Omega_3|} \cup \frac{n}{2}K_2\right), & \text{if } n \text{ is even} \end{cases}$$

Then,

$$V(\Gamma_G) = \begin{cases} \zeta(\Gamma) \cup \Omega_3 \cup \Omega_2, & \text{if } n \text{ is odd} \\ \zeta(\Gamma) \cup \Omega_3 \bigcup_{i=0}^{n-1} \Omega_2, & \text{if } n \text{ is even} \end{cases}$$

Now, we discuss the following two cases. □

Case 1 (*n* is odd):

Let $E(\Gamma_G) = \bigcup_{i=1}^{3} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G) | e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \Omega_3$.
- Type T_2: $e = \lambda\mu \in E_2(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \zeta(\Gamma)$.
- Type T_3: $e = \lambda\mu \in E_3(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_2$.

Let *e* is of type T_1: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_3 = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_1 be the number of type T_1 edges. Since Ω_3 induces a complete graph K_{n-1}, so $t_1 = S(K_{n-1}) = \binom{n-1}{2}$.

Let *e* is of type T_2: Since $\mathrm{ecc}(\lambda) = 2$ and $\mathrm{ecc}(\mu) = 1$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_1$, $N_2(\lambda) = \Omega_2 N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_3 \cup \Omega_2$. Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = N_{2'}(\lambda) = \varnothing, N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2$$

and hence $\eta_\lambda(e|\Gamma_G) = 1$ and $\eta_\mu(e|\Gamma_G) = n + 1$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_3| \times |\zeta(\Gamma)| = n - 1$.

Let *e* is of type T_3: Note that μ is a leaf in Γ_G, so Proposition 1 yields that $\eta_\mu(e|\Gamma_G) = 1$ and $\eta_\lambda(e|\Gamma_G) = 2n - 1$. Let t_3 be the number of type T_3 edges, then $t_3 = |\zeta(\Gamma)| \times |\Omega_2| = n$. Now, the Mostar index of Γ_G is:

$$\begin{aligned} \mathrm{Mo}(\Gamma_G) &= \sum_{i=1}^{3} \sum_{\lambda\mu \in E_i(\Gamma_G)} |\eta_\lambda(e|\Gamma_G) - \eta_\mu(e|\Gamma_G)| \\ &= t_1|1-1| + t_2|n+1-1| + t_3|2n-1-1| \\ &= 3n(n-1) \end{aligned}$$

Case 2 (*n* is even):

Let $E(\Gamma_G) = \bigcup_{i=1}^{5} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G) | e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \Omega_3$.
- Type T_2: $e = \lambda\mu \in E_2(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \zeta(\Gamma)$.
- Type T_3: $e = \lambda\mu \in E_3(\Gamma_G)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_2^i$.
- Type T_4: $e = \lambda\mu \in E_4(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \zeta(\Gamma)$.
- Type T_5: $e = \lambda\mu \in E_5(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_2^i$.

Let *e* is of type T_1: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_3 = N[\mu]$. Thus λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_1 be the number of type T_1 edges. Since Ω_3 induces a complete graph K_{n-2}, so $t_1 = S(K_{n-2}) = \binom{n-2}{2}$.

Let *e* is of type T_2: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_3 \cup \Omega_2 = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_2 be the number of type T_2 edges. Since $\zeta(\Gamma)$ induces a complete graph K_2, so $t_2 = S(K_2) = 1$.

Let *e* is of type T_3: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_2^i = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_3 be the number of type T_3 edges. Since each Ω_2^i induces the complete graph K_2 and $0 \le i \le \frac{n}{2} - 1$, so $t_3 = \frac{n}{2} \times S(K_2) = \frac{n}{2}$.

Let *e* is of type T_4: Since $\mathrm{ecc}(\lambda) = 2$ and $\mathrm{ecc}(\mu) = 1$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = (\Omega_3 - \{\lambda\}) \cup \zeta(\Gamma), N_2(\lambda) = \Omega_2,$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = \Omega_3 \cup \zeta(\Gamma) - \{\mu\} \cup \Omega_2$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = N_{2'}(\lambda) = \varnothing, N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2$$

and hence $\eta_\lambda(e|\Gamma_G) = 1$ and $\eta_\mu(e|\Gamma_G) = n + 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\Omega_3| \times |\zeta(\Gamma)| = 2(n-2)$.

Let *e* is of type T_5: As $\mathrm{ecc}(\lambda) = 2$ and $\mathrm{ecc}(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = \Omega_3 \cup \zeta(\Gamma) - \{\lambda\} \cup \Omega_2$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = \Omega_2^i - \{\mu\} \cup \zeta(\Gamma), N_2(\mu) = \Omega_3 \cup \Omega_2 - \Omega_2^i$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i),$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|\Gamma_G) = 2n - 3$ and $\eta_\mu(e|\Gamma_G) = 1$. Let t_5 be the number of type T_5 edges, then $t_5 = |\Omega_2| \times |\zeta(\Gamma)| = 2n$.

Now, the Mostar index of Γ_G is:

$$\begin{aligned} \mathrm{Mo}(\Gamma_G) &= \sum_{i=1}^{5} \sum_{\lambda\mu \in E_i(\Gamma_G)} |\eta_\lambda(e|\Gamma_G) - \eta_\mu(e|\Gamma_G)| \\ &= t_1|1-1| + t_2|1-1| + t_3|1-1| + t_4|n+1-1| \\ &\quad + t_5|2n-3-1| \\ &= 6n(n-2) \end{aligned}$$

Theorem 2. *For $n \ge 2$, let Γ be a semi-dihedral group. Then,*

$$\mathrm{Mo}(\Gamma_G) = \begin{cases} 192n(n-1), & \textit{when } n \textit{ is odd} \\ 48n(2n-1), & \textit{when } n \textit{ is even} \end{cases}$$

Proof. Mathematically, the commuting graph on SD_{8n} is defined by Kumar et al. (2020) as follows:

$$\Gamma_G = \begin{cases} K_4 + (K_{|\Omega_3|} \cup nK_4), & \text{if } n \text{ is odd} \\ K_2 + (K_{|\Omega_3|} \cup 2nK_2), & \text{if } n \text{ is even} \end{cases}$$

$$V(\Gamma_G) = \begin{cases} \zeta(\Gamma) \cup \Omega_3 \bigcup_{i=0}^{n-1} \Omega_2^i, & \text{if } n \text{ is odd} \\ \zeta(\Gamma) \cup \Omega_3 \bigcup_{i=0}^{2n-1} \Omega_2^i, & \text{if } n \text{ is even} \end{cases}$$

Now, we discuss the following two cases. □

Case 1 (*n* is odd):

Let $E(\Gamma_G) = \bigcup_{i=1}^{5} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G) | e \text{ is of type } T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \Omega_3$.
- Type T_2: $e = \lambda\mu \in E_2(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \zeta(\Gamma)$.
- Type T_3: $e = \lambda\mu \in E_3(\Gamma_G)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_2^i$.
- Type T_4: $e = \lambda\mu \in E_4(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \zeta(\Gamma)$.
- Type T_5: $e = \lambda\mu \in E_5(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_2^i$.

Let *e* is of type T_1: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_3 = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_1 be the number of type T_1 edges. Since Ω_3 induces a complete graph K_{4n-4}, so $t_1 = S(K_{4n-4}) = \binom{4n-4}{2}$.

Let *e* is of type T_2: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_3 \cup \Omega_2 = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_2 be the number of type T_2 edges. Since $\zeta(\Gamma)$ induces a complete graph K_4, so $t_2 = S(K_4) = \binom{4}{2}$.

Let *e* is of type T_3: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_2^i = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_3 be the number of type T_3 edges. Since each Ω_2^i induces the complete graph K_4 and $0 \le i \le n-1$, so $t_3 = n \times S(K_4) = 6n$.

Let *e* is of type T_4: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 1$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = \Omega_3 - \{\lambda\} \cup \zeta(\Gamma), N_2(\lambda) = \Omega_2$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = \Omega_3 \cup \zeta(\Gamma) - \{\mu\} \cup \Omega_2$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = N_{2'}(\lambda) = \emptyset$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2$$

and hence $\eta_\lambda(e|\Gamma_G) = 1$ and $\eta_\mu(e|\Gamma_G) = 4n + 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\Omega_3| \times |\zeta(\Gamma)| = 4(4n-4)$.

Let *e* is of type T_5: Since $ecc(\lambda) = 1$ and $ecc(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup \zeta(\Gamma) - \{\lambda\} \cup \Omega_2$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_2^i - \{\mu\} \cup \zeta(\Gamma)$, and $N_2(\mu) = \Omega_3 \cup \Omega_2 - \Omega_2^i$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \{\Omega_3 \cup \Omega_2 - \Omega_2^i\}$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = N_{2'}(\mu) = \emptyset$$

and hence $\eta_\lambda(e|\Gamma_G) = 8n - 7$ and $\eta_\mu(e|\Gamma_G) = 1$. Let t_5 be the number of type T_5 edges, then $t_5 = |\Omega_2| \times |\zeta(\Gamma)| = 16n$.

Now, the Mostar index of Γ_G is:

$$\begin{aligned} Mo(\Gamma_G) &= \sum_{i=1}^{5} \sum_{\lambda\mu \in E_i(\Gamma_G)} |\eta_\lambda(e|\Gamma_G) - \eta_\mu(e|\Gamma_G)| \\ &= t_1|1-1| + t_2|1-1| + t_3|1-1| + t_4|4n+1-1| \\ &\quad + t_5|8n-7-1| \\ &= 192n(n-1) \end{aligned}$$

Case 2 (*n* is even):

Let $E(\Gamma_G) = \bigcup_{i=1}^{5} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G) | e \text{ is of type } T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \Omega_3$.
- Type T_2: $e = \lambda\mu \in E_2(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \zeta(\Gamma)$.
- Type T_3: $e = \lambda\mu \in E_3(\Gamma_G)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_2^i$.
- Type T_4: $e = \lambda\mu \in E_4(\Gamma_G)$ such that $\lambda \in \Omega_3$ and $\mu \in \zeta(\Gamma)$.
- Type T_5: $e = \lambda\mu \in E_5(\Gamma_G)$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_2^i$.

Let *e* is of type T_1: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_3 = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_1 the number of type T_1 edges. Since Ω_3 induces a complete graph K_{4n-2}, so $t_1 = S(K_{4n-2}) = \binom{4n-2}{2}$.

Let *e* is of type T_2: Note that $N[\lambda] = V(\Gamma_G) = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_2 be the number of type T_2 edges. Since $\zeta(\Gamma)$ induces a complete graph K_2, so $t_2 = S(K_2) = 1$.

Let *e* is of type T_3: Note that $N[\lambda] = \zeta(\Gamma) \cup \Omega_2^i = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|\Gamma_G) = 1 = \eta_\mu(e|\Gamma_G)$. Let t_3 be the number of type T_3 edges. Since each Ω_2^i induces the complete graph $K_{2|}$ and $0 \le i \le 2n-1$, so $t_3 = 2n \times S(K_2) = 2n$.

Let *e* is of type T_4: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 1$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = (\Omega_3 - \{\lambda\}) \cup \zeta(\Gamma)$, $N_2(\lambda) = \Omega_2$, $N_0(\mu) = \{\mu\}$, and $N_1(\mu) = V(\Gamma_G) - \{\mu\}$. Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = N_{2'}(\lambda) = \emptyset$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2$$

and hence $n_\lambda(e|\Gamma_G) = 1$ and $n_\mu(e|\Gamma_G) = 4n + 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\Omega_3| \times |\zeta(\Gamma)| = 2(4n - 2)$.

Let *e* is of type T_5: Since $\mathrm{ecc}(\lambda) = 1$ and $\mathrm{ecc}(\mu) = 2$. So $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\zeta(\Gamma) - \{\lambda\} \cup \Omega_2$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = (\Omega_2^i - \{\mu\}) \cup \zeta(\Gamma)$, and $N_2(\mu) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \{\Omega_3 \cup \Omega_2 - \Omega_2^i\}$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $n_\lambda(e|\Gamma_G) = 8n - 3$ and $n_\mu(e|\Gamma_G) = 1$. Let t_5 be the number of type T_5 edges, then $t_5 = |\Omega_2| \times |\zeta(\Gamma)| = 8n$.

Now, the Mostar index of Γ_G is:

$$\begin{aligned} \mathrm{Mo}(\Gamma_G) &= \sum_{i=1}^{5} \sum_{\lambda\mu \in E_i(\Gamma_G)} |\eta_\lambda(e|\Gamma_G) - \eta_\mu(e|\Gamma_G)| \\ &= t_1|1-1| + t_2|1-1| + t_3|1-1| + t_4|4n+1-1| \\ &\quad + t_5|8n-3-1| \\ &= 48n(2n-1) \end{aligned}$$

4 Non-commuting graphs

In this section, by measuring the amount of peripherality of each edge, we investigate the Mostar index of non-commuting graphs associated with D_n and SD_{8n}.

Theorem 3. *For $n \geq 3$, let Γ be a dihedral group. Then,*

$$\mathrm{Mo}(G_\Gamma) = \begin{cases} n(n-1)(n-2), & \text{when } n \text{ is odd} \\ n(n-2)(n-4), & \text{when } n \text{ is even} \end{cases}$$

Proof. The non-commuting graph on $\Gamma = D_n$ is mathematically defined by Wei et al. (2020) as follows:

$$G_\Gamma = \begin{cases} K_{|\Omega_2|} + N_{|\Omega_3|}, & \text{if } n \text{ is odd} \\ K_{\underbrace{2,2,\ldots,2}_{\frac{n}{2}-\text{times}},|\Omega_3|}, & \text{if } n \text{ is even} \end{cases}$$

Then,

$$V(G_\Gamma) = \begin{cases} \Omega_2 \cup \Omega_3, & \text{if } n \text{ is odd} \\ \bigcup_{i=0}^{\frac{n}{2}-1} \Omega_2^i \cup \Omega_3, & \text{if } n \text{ is even} \end{cases}$$

Next we discuss the following two cases.

Case 1 (*n* is odd):

Let $E(\Gamma_G) = \bigcup_{i=1}^{2} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G)|e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G_\Gamma)$ such that $\lambda \in \Omega_2$ and $\mu \in \Omega_2$.
- Type T_2: $e = \lambda\mu \in E_2(G_\Gamma)$ such that $\lambda \in \Omega_2$ and $\mu \in \Omega_3$.

Let *e* is of type T_1: Note that $N[\lambda] = V(G_\Gamma) = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|G_\Gamma) = 1 = \eta_\mu(e|G_\Gamma)$. Let t_1 be the number of type T_1 edges. Since Ω_2 induces a complete graph K_n, so $t_1 = S(K_n) = \binom{n}{2}$.

Let *e* is of type T_2: Since $\mathrm{ecc}(\lambda) = 1$ and $\mathrm{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \{\lambda\}$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_2$, and $N_2(\mu) = \Omega_3 - \{\mu\}$. Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3 - \{\mu\}$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = n - 1$ and $\eta_\mu(e|G_\Gamma) = 1$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = n(n-1)$.

Now, the Mostar index of G_Γ is:

$$\begin{aligned} \mathrm{Mo}(G_\Gamma) &= \sum_{i=1}^{2} \sum_{\lambda\mu \in E_i(G_\Gamma)} |\eta_\lambda(e|G_\Gamma) - \eta_\mu(e|G_\Gamma)| \\ &= t_1|n-1-1| + t_2|1-1| \\ &= n(n-1)(n-2) \end{aligned}$$

Case 2 (*n* is even):

Let $E(\Gamma_G) = \bigcup_{i=1}^{2} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G)|e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G_\Gamma)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_2^j$ for $i \neq j$.
- Type T_2: $e = \lambda\mu \in E_2(G_\Gamma)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_3$.

Let *e* is of type T_1: Since $\mathrm{ecc}(\lambda) = 2$ and $\mathrm{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$, and $N_2(\lambda) = \Omega_2^i - \{\lambda\}$,

$$N_0(\mu) = \{\mu\}, N_1(\mu) = \Omega_3 \cup (\Omega_2 - \Omega_2^j) N_2(\mu) = \Omega_2^j - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_2^j - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = 2$ and $\eta_\mu(e|G_\Gamma) = 2$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_2 with parts Ω_2^i induces a complete multipartite graph, so for any $\lambda \in \Omega_2^i$, $d(\lambda) = 2\left(\frac{n}{2} - 1\right) = n - 2$ in the subgraph of G_Γ induced by the set $\bigcup_{i=0}^{\frac{n}{2}-1} \Omega_2^i$. Since $|\Omega_2^i| = 2$ and there are $\frac{n}{2}$ such sets, so by the formula of handshake lemma, $t_1 = \frac{n(n-2)}{2}$.

Let *e* is of type T_2: Since $\mathrm{ecc}(\lambda) = 2$ and $\mathrm{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$, $N_2(\lambda) = \Omega_2^i - \{\lambda\}$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_2$, and $N_2(\mu) = \Omega_3 - \{\mu\}$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3 - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = n - 2$ and $\eta_\mu(e|G_\Gamma) = 2$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = n(n-2)$.

Now, the Mostar index of G_Γ is:

$$\begin{aligned}\text{Mo}(G_\Gamma) &= \sum_{i=1}^{2} \sum_{\lambda\mu \in E_i(G_\Gamma)} |\eta_\lambda(e|G_\Gamma) - \eta_\mu(e|G_\Gamma)| \\ &= t_1|2-2| + t_2|n-2-2| \\ &= n(n-2)(n-4)\end{aligned}$$

Theorem 4. *For $n \geq 2$, let Γ be a semi-dihedral group. Then,*

$$\text{Mo}(G_\Gamma) = \begin{cases} 64n(n-1)(n-2), & \text{when } n \text{ is odd} \\ 32n(n-1)(2n-1), & \text{when } n \text{ is even} \end{cases}$$

Proof. Mathematically, the non-commuting graph on $\Gamma = SD_{8n}$ can be expressed as follows:

$$G_\Gamma = \begin{cases} nN_4 + N_{4n-4}, & \text{if } n \text{ is odd} \\ 2nN_2 + N_{4n-2}, & \text{if } n \text{ is even} \end{cases}$$

$$V(G_\Gamma) = \begin{cases} \bigcup_{i=0}^{n-1} \Omega_2^i \cup \Omega_3, & \text{if } n \text{ is odd} \\ \bigcup_{i=0}^{2n-1} \Omega_2^i \cup \Omega_3, & \text{if } n \text{ is even} \end{cases}$$

Next we discuss the following two cases. □

Case 1 (*n* is odd):

Let $E(\Gamma_G) = \bigcup_{i=1}^{2} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G)|e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G_\Gamma)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_2^j$ for $i \neq j$.
- Type T_2: $e = \lambda\mu \in E_2(G_\Gamma)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_3$.

Let *e* is of type T_1: Since $\text{ecc}(\lambda) = 2$ and $\text{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$, $N_2(\lambda) = \Omega_2^i - \{\lambda\}$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_3 \cup (\Omega_2 - \Omega_2^j)$, and $N_2(\mu) = \Omega_2^j - \{\mu\}$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_2^j - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = 4$ and $\eta_\mu(e|G_\Gamma) = 4$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_2 with parts Ω_2^i induces a complete multipartite graph, so for any $\lambda \in \Omega_2^i$, $d(\lambda) = 4(n-1) = 4n-4$ in the subgraph of G_Γ induced by the set $\bigcup_{i=0}^{n-1}\Omega_2^i$. Since $|\Omega_2^i| = 4$ and there are n such sets, so by the formula of handshake lemma, $t_1 = 2n(4n-4)$.

Let *e* is of type T_2: Since $\text{ecc}(\lambda) = 2$ and $\text{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$, $N_2(\lambda) = \Omega_2^i - \{\lambda\}$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_2$, $N_2(\mu) = \Omega_3 - \{\mu\}$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3 - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = 4n - 4$ and $\eta_\mu(e|G_\Gamma) = 4$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = 4n(4n-4)$.

Now, the Mostar index of G_Γ is:

$$\begin{aligned}\text{Mo}(G_\Gamma) &= \sum_{i=1}^{2} \sum_{\lambda\mu \in E_i(G_\Gamma)} |\eta_\lambda(e|G_\Gamma) - \eta_\mu(e|G_\Gamma)| \\ &= t_1|4-4| + t_2|4n-4-4| \\ &= 64n(n-1)(n-2)\end{aligned}$$

Case 2 (*n* is even):

Let $E(\Gamma_G) = \bigcup_{i=1}^{2} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G)|e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G_\Gamma)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_2^j$ for $i \neq j$.
- Type T_2: $e = \lambda\mu \in E_2(G_\Gamma)$ such that $\lambda \in \Omega_2^i$ and $\mu \in \Omega_3$.

Let *e* is of type T_1: Since $\text{ecc}(\lambda) = 2$ and $\text{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$, $N_2(\lambda) = \Omega_2^i - \{\lambda\}$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_3 \cup (\Omega_2 - \Omega_2^j)$, and $N_2(\mu) = \Omega_2^j - \{\mu\}$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_2^j - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = 2$ and $\eta_\mu(e|G_\Gamma) = 2$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_2 with parts Ω_2^i induces a complete multipartite graph, so for any $\lambda \in \Omega_2^i$, $d(\lambda) = 2(2n-1) = 4n-2$ in the subgraph of G_Γ induced by the set $\bigcup_{i=0}^{2n-1}\Omega_2^i$. Since $|\Omega_2^i| = 2$ and there are $2n$ such sets, so by the formula of handshake lemma, $t_1 = 2n(4n-2)$.

Let *e* is of type T_2: Since $\text{ecc}(\lambda) = 2$ and $\text{ecc}(\mu) = 2$, so $N_0(\lambda) = \{\lambda\}$, $N_1(\lambda) = \Omega_3 \cup (\Omega_2 - \Omega_2^i)$, $N_2(\lambda) = \Omega_2^i - \{\lambda\}$, $N_0(\mu) = \{\mu\}$, $N_1(\mu) = \Omega_2$, and $N_2(\mu) = \Omega_3 - \{\mu\}$.

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3 - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $n_\lambda(e|G_\Gamma) = 4n - 2$ and $n_\mu(e|G_\Gamma) = 2$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = 4n(4n-2)$.

Now, the Mostar index of G_Γ is:

$$\begin{aligned} Mo(G_\Gamma) &= \sum_{i=1}^{2} \sum_{\lambda\mu \in E_i(G_\Gamma)} |\eta_\lambda(e|G_\Gamma) - \eta_\mu(e|G_\Gamma)| \\ &= t_1|2-2| + t_2|4n-2-2| \\ &= 32n(2n-1)(n-1) \end{aligned}$$

5 Non-conjugate graphs

In this section, non-conjugate graphs associated with D_n and SD_{8n} are considered in the context of Mostar index.

Theorem 5. *For $n \geq 3$, let Γ be a dihedral group. Then,*

$$Mo(G(\Gamma)) = \begin{cases} (n-1)(n^2-n+1), & \text{when } n \text{ is odd} \\ \left(\frac{n-2}{2}\right)(n^2-2n+4), & \text{when } n \text{ is even} \end{cases}$$

Proof. From conjugacy classes, written in Eq. 1, the number of conjugacy classes of order 1, 2, and n is 1, $\frac{n-1}{2}$, and 1, respectively, whenever n is odd, and the number of conjugacy classes of order 1, 2, and $\frac{n}{2}$ is 2, $\frac{n-2}{2}$, and 2, respectively, whenever n is even. Thus, the non-conjugate graph $G(\Gamma)$ on $\Gamma = D_n$ can be described as follows:

$$G(\Gamma) = \begin{cases} K_{1,\underbrace{2,2,\ldots,2}_{\frac{n-1}{2}-\text{times}},n}, & \text{if } n \text{ is odd} \\ K_{1,1,\underbrace{2,2,\ldots,2}_{\frac{n-2}{2}-\text{times}},\frac{n}{2},\frac{n}{2}}, & \text{if } n \text{ is even} \end{cases}$$

Here $K_{1,\underbrace{2,2,\ldots,2}_{\frac{n-1}{2}-\text{times}},n}$, is a complete $\frac{n+3}{2}$-partite graph having $\frac{n-1}{2}$ parts $\Omega_3^i = \{a^i, a^{n-i}\}$ for $1 \leq i \leq \frac{n-1}{2}$ with $\bigcup_{i=1}^{\frac{n-1}{2}} \Omega_3^i = \Omega_3$; one part is $\zeta(\Gamma)$; and one part is Ω_2. Similarly, $K_{1,1,\underbrace{2,2,\ldots,2}_{\frac{n-2}{2}-\text{times}},\frac{n}{2},\frac{n}{2}}$, is a complete $\frac{n+6}{2}$-partite graph having $\frac{n-2}{2}$ parts $\Omega_3^i = \{a^i, a^{n-i}\}$ for $1 \leq i < \frac{n}{2}$ with $\bigcup_{i=1}^{\frac{n-2}{2}} \Omega_3^i = \Omega_3$; two parts $\{e\}$, $\{a^{\frac{n}{2}}\}$; and two parts $\Omega_2^j = \left\{a^{2i+j}b : \forall 0 \leq i < \frac{n}{2}\right\}$ for $i = 0,1$ with $\Omega_2^0 \cup \Omega_2^1 = \Omega_2$. □

Now, we discuss the following two cases.

Case 1 (*n* is odd):

Let $E(\Gamma_G) = \bigcup_{i=1}^{4} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G) | e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G(\Gamma))$ such that $\lambda \in \Omega_3^i$ and $\mu \in \Omega_3^j$ for $i \neq j$.
- Type T_2: $e = \lambda\mu \in E_2(G(\Gamma))$ such that $\lambda \in \Omega_3^i$ and $\mu \in \Omega_2$.
- Type T_3: $e = \lambda\mu \in E_3(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_3^i$.
- Type T_4: $e = \lambda\mu \in E_4(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_2$.

Let *e* is of type T_1: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\},\ N_1(\lambda) = V(G(\Gamma)) - \Omega_3^i,\ N_2(\lambda) = \Omega_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\},\ N_1(\mu) = V(G(\Gamma)) - \Omega_3^j,\ N_2(\mu) = \Omega_3^j - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\},\ N_{1'}(\lambda) = \Omega_3^j - \{\mu\},\ N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\},\ N_{1'}(\mu) = \Omega_3^i - \{\lambda\},\ N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = 2$ and $\eta_\mu(e|G_\Gamma) = 2$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_3 with parts Ω_3^i induces a complete multipartite graph, so for any $\lambda \in \Omega_3^i$, $d(\lambda) = 2\left(\frac{(n-1)}{2} - 1\right) \underset{n-1}{=} n - 3$ in the subgraph of G_Γ induced by the set $\bigcup_{i=1}^{\frac{n-1}{2}} \Omega_3^i$. Since $|\Omega_3^i| = 2$ and there are $\frac{n-1}{2}$ such sets, therefore by the formula of handshake lemma, $t_1 = \frac{(n-1)(n-3)}{2}$.

Let *e* is of type T_2: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\},\ N_1(\lambda) = V(G(\Gamma)) - \Omega_3^i,\ N_2(\lambda) = \Omega_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\},\ N_1(\mu) = \zeta(\Gamma) \cup \Omega_3,\ N_2(\mu) = \Omega_2 - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\},\ N_{1'}(\lambda) = \Omega_2 - \{\mu\},\ N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\},\ N_{1'}(\mu) = \Omega_3^i - \{\lambda\},\ N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = n$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = n(n-1)$.

Let *e* is of type T_3: Since $ecc(\lambda) = 1$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\},\ N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\},\ N_1(\mu) = V(G(\Gamma)) - \Omega_3^i,\ N_2(\mu) = \Omega_3^i - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\},\ N_{1'}(\lambda) = \Omega_3^i - \{\mu\},$$
$$N_{0'}(\mu) = \{\mu\},\ N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = n$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\zeta(\Gamma)| \times |\Omega_2| = n$.

Now, the Mostar index of $G(\Gamma)$ is:

$$\begin{aligned}Mo(G(\Gamma)) &= \sum_{i=1}^{4}\sum_{\lambda\mu\in E_i(G(\Gamma))}|\eta_\lambda(e|G(\Gamma)) - \eta_\mu(e|G(\Gamma))|\\ &= t_1|2-2| + t_2|n-2| + t_3|2-1| + t_4|n-1|\\ &= (n-1)(n^2-n+1)\end{aligned}$$

Case 2 (*n* is even):

Let $E(\Gamma_G) = \bigcup_{i=1}^{6} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G)|e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G(\Gamma))$ such that $\lambda \in \Omega_3^i$ and $\mu \in \Omega_3^k$ for $i \neq k$.
- Type T_2: $e = \lambda\mu \in E_2(G(\Gamma))$ such that $\lambda \in \Omega_3^i$ and $\mu \in \Omega_2^j$.
- Type T_3: $e = \lambda\mu \in E_3(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_3^i$.
- Type T_4: $e = \lambda\mu \in E_4(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Omega_2^j$.
- Type T_5: $e = \lambda\mu \in E_5(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \zeta(\Gamma)$.
- Type T_6: $e = \lambda\mu \in E_6(G(\Gamma))$ such that $\lambda \in \Omega_2^j$ and $\mu \in \Omega_2^k$ for $j = 0,1$, $k = 0,1$, and $j \neq k$.

Let *e* is of type T_1: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Omega_3^i, N_2(\lambda) = \Omega_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Omega_3^k, N_2(\mu) = \Omega_3^k - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3^k - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_3^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_3 with parts Ω_3^i induces a complete multipartite graph, so for any $\lambda \in \Omega_3^i$, $d(\lambda) = 2\left(\frac{(n-2)}{2}\frac{-}{n-2}1\right) = n-4$ in the subgraph of G_Γ induced by the set $\bigcup_{i=1}^{\frac{n-2}{2}} \Omega_3^i$. Since $|\Omega_3^i| = 2$ and there are $\frac{n-2}{2}$ such sets, so by the formula of handshake lemma, $t_1 = \frac{(n-2)(n-4)}{2}$.

Let *e* is of type T_2: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Omega_3^i, N_2(\lambda) = \Omega_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Omega_2^j, N_2(\mu) = \Omega_2^j - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_2^j - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_3^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = \frac{n}{2}$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = n(n-2)$.

Let *e* is of type T_3: Since $ecc(\lambda) = 1$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Omega_3^i, N_2(\mu) = \Omega_3^i - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_3^i - \{\mu\}, N_{0'}(\mu) = \{\mu\}$$
$$N_{1'}(\mu) = \varnothing, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_3 be the number of type T_3 edges, then $t_3 = |\zeta(\Gamma)| \times |\Omega_3| = 2(n-2)$.

Let *e* is of type T_4: Since $ecc(\lambda) = 1$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Omega_2^j, N_2(\mu) = \Omega_2^j - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_2^i - \{\mu\}, N_{0'}(\mu) = \{\mu\}$$
$$N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = \frac{n}{2}$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\zeta(\Gamma)| \times |\Omega_2| = 2n$.

Let *e* is of type T_5: Note that $N[\lambda] = V(G(\Gamma)) = N[\mu]$. Thus, λ and μ are true twins, so Proposition 3 yields that $\eta_\lambda(e|G_\Gamma) = 1 = \eta_\mu(e|G_\Gamma)$. Let t_5 be the number of type T_5 edges. Since $\zeta(\Gamma)$ induces a complete graph K_2, so $t_1 = S(K_2) = 1$.

Let *e* is of type T_6: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Omega_2^j, N_2(\lambda) = \Omega_2^j - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Omega_2^k, N_2(\mu) = \Omega_2^k - \{\mu\}$$

Accordingly, Remark 1 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Omega_2^k - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Omega_2^j - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = \frac{n}{2}$ and $\eta_\mu(e|G(\Gamma)) = \frac{n}{2}$. Let t_6 be the number of type T_6 edges, then $t_6 = |\Omega_2^j| \times |\Omega_2^k| = \frac{n^2}{4}$.

Now, the Mostar index of $G(\Gamma)$ is:

$$\begin{aligned}Mo(G(\Gamma)) &= \sum_{i=1}^{6}\sum_{\lambda\mu\in E_i(G(\Gamma))}|\eta_\lambda(e|G(\Gamma)) - \eta_\mu(e|G(\Gamma))|\\ &= t_1|2-2| + t_2\left|\frac{n}{2}-2\right| + t_3|2-1|\\ &\quad + t_4\left|\frac{n}{2}-1\right| + t_5|1-1| + t_6\left|\frac{n}{2}-\frac{n}{2}\right|\\ &= \left(\frac{n-2}{2}\right)(n^2-2n+4)\end{aligned}$$

Theorem 6. *For $n \geq 2$, let Γ be a semi-dihedral group. Then:*

$$Mo(G(\Gamma)) = \begin{cases}4(2n-1)(4n^2-2n+1), & \text{when } n \text{ is even}\\ 16(n-1)(n^2-2n+4), & \text{when } n \text{ is odd}\end{cases}$$

Proof. From conjugacy classes, written in Eqs. 2 and 3, the number of conjugacy classes of order 1, 2 and, n is 4, $2n-2$, and 4, respectively, whenever n is odd, and the number of conjugacy classes of order 1, 2, and $2n$ is 2, $2n-1$, and 2, respectively, whenever n is even. Thus, the non-conjugate graph on $\Gamma = SD_{8n}$ can be expressed as follows:

$$G(\Gamma) = \begin{cases} K_{1,1,1,1,\underbrace{2,2,\ldots,2}_{2n-2\text{ times}},n,n,n,n}, & \text{if } n \text{ is odd} \\ K_{1,1,\underbrace{2,2,\ldots,2}_{2n-1\text{ times}},2n,2n}, & \text{if } n \text{ is even} \end{cases}$$

Here $K_{1,1,1,1,\underbrace{2,2,\ldots,2}_{2n-2-\text{times}},n,n,n,n}$, is a complete$(2n+6)$-partite graph having $n-1$ parts Φ_3^i for odd i; $n-1$ parts Φ_3^i for even i; four parts from $\zeta(\Gamma)$; and four parts Φ_2^j. Similarly, $K_{1,1,\underbrace{2,2,\ldots,2}_{2n-1-\text{times}},2n,2n}$, is a complete $(2n+3)$-partite graph having n parts Φ_3^i for odd i;

$n-1$ parts Φ_3^i for even i; two parts from $\zeta(\Gamma)$, and two parts Φ_2^1 and Φ_2^2.

Now, we discuss the following two cases. □

Case 1 (n is odd):

Let $E(\Gamma_G) = \bigcup_{i=1}^{6} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G) | e \text{ is of type } T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G(\Gamma))$ such that $\lambda \in \Phi_3^i$ and $\mu \in \Phi_3^k$ for $i \neq k$.
- Type T_2: $e = \lambda\mu \in E_2(G(\Gamma))$ such that $\lambda \in \Phi_3^i$ and $\mu \in \Phi_2^j$.
- Type T_3: $e = \lambda\mu \in E_3(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Phi_3^i$.
- Type T_4: $e = \lambda\mu \in E_4(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Phi_2^j$.
- Type T_5: $e = \lambda\mu \in E_5(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \zeta(\Gamma)$.
- Type T_6: $e = \lambda\mu \in E_6(G(\Gamma))$ such that $\lambda \in \Phi_2^j$ and $\mu \in \Phi_2^k$ for $j \neq k$.

Let e is of type T_1: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_3^k - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Phi_3^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_3 with parts Φ_3^i induces a complete multipartite graph, so for any $\lambda \in \Phi_3^i$, $d(\lambda) = 2(2n-2-1) = 4n-6$ in the subgraph of $G(\Gamma)$ induced by the set $\bigcup_{\text{odd } i=1}^{n-1}\Phi_3^i \bigcup_{\text{odd } i=2n+1}^{3n-2}\Phi_3^i \bigcup_{\text{even } i=2}^{2n-2}\Phi_3^i$. Since $|\Phi_3^i| = 2$ and there are $2n-2$ such sets, so by the formula of handshake lemma, $t_1 = (2n-2)(4n-6)$.

Let e is of type T_2: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Phi_3^i, N_2(\lambda) = \Phi_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_2^j, N_2(\mu) = \Phi_2^j - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_2^j - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Phi_3^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = n$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = 4n(n-4)$.

Let e is of type T_3: Since $ecc(\lambda) = 1$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_3^i, N_2(\mu) = \Phi_3^i - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_3^i - \{\mu\}, N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_3 be the number of type T_3 edges, then $t_3 = |\zeta(\Gamma)| \times |\Omega_3| = 4(4n-4)$.

Let e is of type T_4: Since $ecc(\lambda) = 1$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_2^j, N_2(\mu) = \Phi_2^j - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_2^j - \{\mu\}, N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = n$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\zeta(\Gamma)| \times |\Omega_2| = 16n$.

Let e is of type T_5: Note that $N[\lambda] = V(G(\Gamma)) = N[\mu]$. Thus, λ and μ are true twins, so Proposition 4 yields that $\eta_\lambda(e|G_\Gamma) = 1 = \eta_\mu(e|G_\Gamma)$. Let t_5 be the number of type T_5 edges. Since $\zeta(\Gamma)$ induces a complete graph $K_{|\zeta(\Gamma)|}$, so $t_1 = S(K_4) = 4_2$.

Let e is of type T_6: Since $ecc(\lambda) = 2$ and $ecc(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Phi_2^j, N_2(\lambda) = \Phi_2^j - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_2^k, N_2(\mu) = \Phi_2^k - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_2^k - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Phi_2^j - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = n$ and $\eta_\mu(e|G(\Gamma)) = n$. Let t_6 be the number of edges of type T_6. Since the partition of Ω_2 with parts Φ_2^j induces a complete multipartite graph, so for any $\lambda \in \Phi_2^j$, $d(\lambda) = 3n$ in the subgraph of $G(\Gamma)$ induced by the set $\bigcup_{j=0}^{3}\Phi_2^j$. Since $|\Phi_2^j| = n$ and there are 4 such sets, so by the formula of handshake lemma, $t_6 = 6n^2$.

Now, the Mostar index of $G(\Gamma)$ is:

$$\begin{aligned}\text{Mo}(G(\Gamma)) &= \sum_{i=1}^{6}\sum_{\lambda\mu\in E_i(G(\Gamma))}|\eta_\lambda(e|G(\Gamma)) - \eta_\mu(e|G(\Gamma))|\\ &= t_1|2-2| + t_2|n-2| + n(T-3)|2-1|\\ &\quad + n(T-4)|n-1| + t_5|1-1| + t_6|n-n|\\ &= 16(n-1)(n^2-n+1)\end{aligned}$$

Case 2 (*n* is even):

Let $E(\Gamma_G) = \bigcup_{i=1}^{6} E_i(\Gamma_G)$ with $E_i(\Gamma_G) = \{e \in E(\Gamma_G)|e$ is of type $T_i\}$.

- Type T_1: $e = \lambda\mu \in E_1(G(\Gamma))$ such that $\lambda \in \Phi_3^i$ and $\mu \in \Phi_3^k$ for $i \neq k$.
- Type T_2: $e = \lambda\mu \in E_2(G(\Gamma))$ such that $\lambda \in \Phi_3^i$ and $\mu \in \Phi_2^j$.
- Type T_3: $e = \lambda\mu \in E_3(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Phi_3^i$.
- Type T_4; $e = \lambda\mu \in E_4(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \Phi_2^j$.
- Type T_5: $e = \lambda\mu \in E_5(G(\Gamma))$ such that $\lambda \in \zeta(\Gamma)$ and $\mu \in \zeta(\Gamma)$.
- Type T_6: $e = \lambda\mu \in E_6(G(\Gamma))$ such that $\lambda \in \Phi_2^j$ and $\mu \in \Phi_2^k$ for $j \neq k$.

Let *e* is of type T_1: Since ecc$(\lambda) = 2$ and ecc$(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Phi_3^i, N_2(\lambda) = \Phi_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_3^k, N_2(\mu) = \Phi_3^k - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_3^k - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Phi_3^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_1 be the number of edges of type T_1. Since the partition of Ω_3 with parts Φ_3^i induces a complete multipartite graph, so for any $\lambda \in \Phi_3^i$, $d(\lambda) = 2(2n-1-1) = 4n-4$ in the subgraph of $G(\Gamma)$ induced by the set $\bigcup_{\text{odd } i=1}^{n-1}\Phi_3^i \bigcup_{\text{odd } i=2n+1}^{3n-1}\Phi_3^i \bigcup_{\text{even } i=2}^{2n-2}\Phi_3^i$. Since $|\Phi_3^i| = 2$ and there are $2n-1$ such sets, so by the formula of handshake lemma, $t_1 = (2n-2)(4n-2)$.

Let *e* is of type T_2: Since ecc$(\lambda) = 2$ and ecc$(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Phi_3^i, N_2(\lambda) = \Phi_3^i - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_2^j, N_2(\mu) = \Phi_2^j - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_2^j - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Phi_3^i - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2n$ and $\eta_\mu(e|G(\Gamma)) = 2$. Let t_2 be the number of type T_2 edges, then $t_2 = |\Omega_2| \times |\Omega_3| = 4n(n-2)$.

Let *e* is of type T_3: Since ecc$(\lambda) = 1$ and ecc$(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_3^i, N_2(\mu) = \Phi_3^i - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_3^i - \{\mu\}$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \varnothing, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_3 be the number of type T_3 edges, then $t_3 = |\zeta(\Gamma)| \times |\Omega_3| = 4(2n-1)$.

Let *e* is of type T_4: Since ecc$(\lambda) = 1$ and ecc$(\mu) = 2$, so

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_2^j, N_2(\mu) = \Phi_2^j - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_2^j - \{\mu\}$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \varnothing, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G_\Gamma) = 2n$ and $\eta_\mu(e|G(\Gamma)) = 1$. Let t_4 be the number of type T_4 edges, then $t_4 = |\zeta(\Gamma)| \times |\Omega_2| = 8n$.

Let *e* is of type T_5: Note that $N[\lambda] = V(G(\Gamma)) = N[\mu]$. Thus, λ and μ are true twins, so Proposition 4 yields that $\eta_\lambda(e|G_\Gamma) = 1 = \eta_\mu(e|G_\Gamma)$. Let t_5 be the number of type T_5 edges. Since $\zeta(\Gamma)$ induces a complete graph K_2, so $t_1 = S(K_2) = 1$.

Let *e* is of type T_6: Since ecc$(\lambda) = 2$ and ecc$(\mu) = 2$, so:

$$N_0(\lambda) = \{\lambda\}, N_1(\lambda) = V(G(\Gamma)) - \Phi_2^j, N_2(\lambda) = \Phi_2^j - \{\lambda\}$$
$$N_0(\mu) = \{\mu\}, N_1(\mu) = V(G(\Gamma)) - \Phi_2^k, N_2(\mu) = \Phi_2^k - \{\mu\}$$

Accordingly, Remark 3 implies that:

$$N_{0'}(\lambda) = \{\lambda\}, N_{1'}(\lambda) = \Phi_2^k - \{\mu\}, N_{2'}(\lambda) = \varnothing$$
$$N_{0'}(\mu) = \{\mu\}, N_{1'}(\mu) = \Phi_2^j - \{\lambda\}, N_{2'}(\mu) = \varnothing$$

and hence $\eta_\lambda(e|G(\Gamma)) = 2n$ and $\eta_\mu(e|G(\Gamma)) = 2n$. Let t_6 be the number of type T_6 edges, then $t_6 = |\Phi_2^j| \times |\Phi_2^k| = 4n^2$.

Now, the Mostar index of $G(\Gamma)$ is:

$$\begin{aligned}\text{Mo}(G(\Gamma)) &= \sum_{i=1}^{6}\sum_{\lambda\mu\in E_i(G(\Gamma))}|\eta_\lambda(e|G(\Gamma)) - \eta_\mu(e|G(\Gamma))|\\ &= t_1|2-2| + t_2|2n-2| + t_3|2-1| + t_4|2n-1|\\ &\quad + t_5|1-1| + t_6|2n-2n|\\ &= 4(2n-1)(4n^2-2n+1)\end{aligned}$$

6 Conclusion

A classical field of study associating graphs with algebraic structures is extended by exploring graph distance neighborhood-based property (which is also known as a bond-additive property) of commuting, non-commuting, and non-conjugate graphs associated with the group of symmetries of regular polygon and its semi version. In fact, we determined the Mostar index of these graphs. Basic theme of this work was to propose a different technique which is quite easy and interesting as compares with any of the other direct methods to measure the peripherality of edges. It is based upon the distance structure of a graph captured through observing distance degree neighborhoods. Researchers working on the peripherality measurement of edges of various graphs, especially graphs having twins, can get a remarkable help by understanding the proposed technique.

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