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Hosoya properties of the commuting graph associated with the group of symmetries

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Abstract: A vast amount of information about distance based graph invariants is contained in the Hosoya polynomial. Such an information is helpful to determine well-known distance based molecular descriptors. The Hosoya index or Z-index of a graph G is the total number of its matching. The Hosoya index is a prominent example of topological indices, which are of great interest in combinatorial chemistry, and later on it applies to address several chemical properties in molecular structures. In this article, we investigate Hosoya properties (Hosoya polynomial, reciprocal Hosoya polynomial and Hosoya index) of the commuting graph associated with an algebraic structure developed by the symmetries of regular molecular graphs (constructed by atoms with regular atomic-bonding).

Keywords: geodesic, Hosoya polynomial, reciprocal Hosoya polynomial, Hosoya index, molecular structure, network

AMS Subject Classification Numbers: 15A27; 05C07; 05C12; 05C92

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1 Introduction

A numeral quantity which captures the symmetry of a molecular structure is known as a topological index. In fact, a topological index is a numerical characterization of a chemical graph and it provides a mathematical function of the structure in quantitative structure-activity relationship (QSAR)/quantitative structure-property relationship (QSPR) studies. It correlates certain physico-chemical properties such as boiling point, stability and strain energy of chemical compounds of a molecular structure (graph). Several properties of chemical compounds in a molecular structure can be determined with the assistance of mathematical languages rendered by various types of topological indices. Harold Wiener, introduced the concept of first (distance based) topological index while working on the boiling point of Paraffin and named this index as path number (Wiener, 1947). Next off, it was renamed as the Wiener index, and that was the time theory of topological indices began.

We consider simple and connected graph (chemical structure) G with vertex set $V(G)$ and edge set $E(G)$. We denote the two adjacent vertices u and v in G as $u \sim v$ and non-adjacent vertices as $u \not\sim v$. Starting from a vertex u and ending at a vertex v in G , a shortest alternating sequences of vertices and edges without repetition of any vertex is known as a $u-v$ geodesic. The number of edges in a $u-v$ geodesic is denoted by $d(u, v)$, and is called the distance between u and v in G . The sum of two graphs G_1 and G_2 , denoted by $G_1 + G_2$, is a graph with vertex set $V(G_1) \cup V(G_2)$ and an edge set $E(G_1) \cup E(G_2) \cup \{u \sim v : u \in V(G_1) \wedge v \in V(G_2)\}$. The maximum distance of a vertex v among all of its distances with all the vertices of G is called the eccentricity of v , denoted by $\text{ecc}(v)$. The number $\text{diam}(G) = \max_{v \in V(G)} \text{ecc}(v)$ is the diameter of G .

1.1 Hosoya properties

Many chemist used the concept of counting polynomial, introduced by Polya (1936), in order to obtain the molecular

orbitals of unsaturated hydrocarbons. In this regard, the spectra of the characteristic polynomial of graphs were studied extensively. In 1988, Hosoya used this concept to find the polynomials of many chemical structures (Hosoya, 1986b), known as Hosoya polynomials and seeks a lot of attention afterwards. In 1996, the Hosoya polynomial was renamed as Wiener polynomial by Sagan *et al.* (1996), but now a days, majority of researchers used the term Hosoya polynomial. The Hosoya polynomial provides a pile of information about distance based graph invariants. The relationship between the Hosoya polynomial and the hyper Wiener index was observed by Cash (2002). Several other applications of extended Wiener indices were studied by Estrada *et al.* (1998).

Consider a connected graph G of n vertices. Hosoya defined the polynomial of G with variable x in the following way:

$$H(G, x) = \sum_{k \geq 0} d(G, k) x^k.$$

The coefficient $d(G, k)$ denotes the number of unordered pairs (u, v) of vertices such that $d(u, v) = k$, where $k \leq \text{diam}(G)$. The reciprocal status Hosoya polynomial of G was introduced by Ramane and Talwar (2019), and is defined as follows:

$$H_{rs}(G, x) = \sum_{u \sim v \in E(G)} x^{rs(u) + rs(v)},$$

where:

$$rs(v) = \sum_{u \in V(G), v \neq u} \frac{1}{d(v, u)}$$

is called the reciprocal status (transmission) of a vertex v .

The Hosoya index or Z-index of a graph G is the total number of its matchings (independent edge subsets, the empty set is also consider one matching in G). The Hosoya index is the prominent example of topological indices which is of great interest in combinatorial chemistry. The Z-index was introduced by Hosoya (1971, 1986a) and it turned out to be applicable to molecular chemistry, such as boiling point, entropy or heat of vaporization are well studied. Several researcher studied extremal problems with respect to the Hosoya index for various graph structures. With respect to Hosoya and Merrifield-Simmons indices, extremal properties of various graph, trees and unicyclic graph have been studies in the articles of Deng and Chen (2008), Wagner (2007), and Yu and Tian (2006). The minimal Hosoya index for cyclic systems was computed by Hou (2002). In 2008, Deng investigated the largest Hosoya index for every simple connected garph having n vertices and $n+1$ edges (Deng, 2008).

1.2 Group of symmetries and commuting graph

Group of symmetries finds its notable use in the theory of molecular vibrations and electron structures. Due to their noteworthy employment in chemical structures, in the context of topological indices, we consider the group of symmetries of a regular molecular polygon (also called a regular molecular n -gon constructed on $n \geq 2$ atoms with their regular atomic-bonding). A regular molecular n -gon is a molecular structure whose corners are atoms and sides are atom-bonds of same length, and each internal angle between atom-bonds is of the measurement $\pi - \frac{2k\pi}{n}$ radian. The group of symmetries of a regular molecular n -gon consists of $2n$ elements, which are n rotations about its center through an angle of $\frac{2k\pi}{n}$ radian, where $k = 0, 1, \dots, n-1$, either all clockwise or all anti-clockwise) and n reflections (for even n , the reflections through a line joining the mid-points of the opposite atom-bonds or through a line joining two opposite atoms; and for odd n , the reflections through those lines which join an atom with the mid-point of the opposite atom-bond). Symbolically, the group of symmetries is denoted by D_n and is called the dihedral group (a group theoretic name) of order $2n$ (Majeed, 2013). If we denote a rotation by ' a ' and a reflection by ' b ', then $2n$ elements of D_n are $a, a^2, \dots, a^{n-1}, a^n = e$ and $b, ab, a^2b, \dots, a^{n-1}b$ (here e is the identical shape molecular n -gone). In generating form, D_n can be represented as follows:

$$D_n = \langle a, b \mid a^n = b^2 = e, ab = ba^{-1} \rangle.$$

The center of D_n is:

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

Let $\Omega_1 = \{e, a, a^2, \dots, a^{n-1}\}$, $\Omega_2 = \{b, ab, a^2b, \dots, a^{n-1}b\}$ and $\Omega_3 = \Omega_1 - \zeta(D_n)$. Then $|\Omega_1| = n = |\Omega_2|$ and

$$|\Omega_3| = \begin{cases} n-1 & , \text{ when } n \text{ is odd} , \\ n-2 & , \text{ when } n \text{ is even} . \end{cases}$$

In the case of even value of $n \geq 4$, we partitioned Ω_2 into $\frac{n}{2}$ two element subsets $\Omega_2^i = \{a^i b, a^{\frac{n}{2}+i} b\}$, $0 \leq i \leq \frac{n}{2} - 1$, so that $\Omega_2 = \bigcup_{i=0}^{\frac{n}{2}-1} \Omega_2^i$.

The commuting graph of a non-abelian group Γ is denoted by $\Gamma_G = C(\Gamma, \Omega)$ with vertex set $\Omega \subseteq \Gamma$. For two

unlike elements $x, y \in \Omega, x \sim y$ in Γ_G if and only if $xy = yx$ in Γ . The notion of commuting graphs on non-central elements of a group has been studied by many researchers – see for instance Ali et al. (2016) and Bunday (2006), and the references therein. The commuting graph on D_n is defined by Ali et al. (2016) in the following result.

Proposition 1

For all $n \geq 3$, let $\Gamma_G = \mathcal{C}(D_n, D_n)$ be a commuting graph on $\Gamma = D_n$, then:

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

Here K_1 is the trivial graph, K_p is a complete graph on p vertices, N_t is a null graph on t vertices, $\frac{n}{2} K_2$ is the union of $\frac{n}{2}$ copies of K_2 .

2 Hosoya polynomials

In this section, we find Hosoya polynomial and reciprocal status Hosoya polynomial of Γ_G .

2.1 Hosoya polynomial

Our first two results of this section provide the coefficients for the Hosoya polynomial of the commuting graph on D_n .

Proposition 2

Consider the commuting graph Γ_G associated with the group $\Gamma = D_n$ for odd values of $n \geq 3$. Then:

$$d(\Gamma_G, k) = \begin{cases} 2n & , \text{ for } k=0, \\ \frac{n(n+1)}{2} & , \text{ for } k=1, \\ \frac{3n(n-1)}{2} & , \text{ for } k=2. \end{cases}$$

Proof. Note that $\text{diam}(\Gamma_G) = 2$. So, we have to find $d(\Gamma_G, 0)$, $d(\Gamma_G, 1)$ and $d(\Gamma_G, 2)$. Consider the set V_p of all the pairs of vertices (same and distinct) of Γ_G , then:

$$|V_p| = \binom{|\Gamma_G|}{2} + |\Gamma_G| = n(2n+1).$$

Let $S(\Gamma_G, k) = \{(l, m); l, m \in V(\Gamma_G) | d(l, m) = k\}$ and $d(\Gamma_G, k) = |S(\Gamma_G, k)|$. Then:

$$V_p = S(\Gamma_G, 0) \cup S(\Gamma_G, 1) \cup S(\Gamma_G, 2). \quad (1)$$

Since, $d(l, l) = 0$ for all $l \in V(\Gamma_G)$, so $S(\Gamma_G, 0) = \{(l, l); l \in V(\Gamma_G)\} = V(\Gamma_G)$. Thus, $d(\Gamma_G, 0) = 2n$. By Proposition 1, $\Gamma_G = K_1 + (K_{|\Omega_3|} \cup N_{|\Omega_2|})$ with $V(K_1) = \zeta(\Gamma)$, $V(K_{|\Omega_3|}) = \Omega_3$ and $V(N_{|\Omega_2|}) = \Omega_2$. Therefore:

$$\begin{aligned} S(\Gamma_G, 1) &= \{(l, m); l \in \zeta(\Gamma), m \in \Omega_3\} \\ &\cup \{(l, m); l \in \zeta(\Gamma), m \in \Omega_2\} \\ &\cup \{(l, m); l, m \in \Omega_3 \text{ and } l \neq m\}. \end{aligned}$$

Accordingly,

$$d(\Gamma_G, 1) = n - 1 + n + \binom{n-1}{2} = \frac{n(n+1)}{2}.$$

By Eq. 1, we have $|V_p| = d(\Gamma_G, 0) + d(\Gamma_G, 1) + d(\Gamma_G, 2)$. Therefore:

$$\begin{aligned} d(\Gamma_G, 2) &= |V_p| - d(\Gamma_G, 0) - d(\Gamma_G, 1) = n(2n+1) \\ &- 2n - \frac{n(n+1)}{2} = \frac{3n(n-1)}{2}. \end{aligned}$$

Proposition 3

Consider the commuting graph Γ_G associated with the group $\Gamma = D_n$ for even values of $n \geq 4$. Then:

$$d(\Gamma_G, k) = \begin{cases} 2n & , \text{ for } k=0, \\ \frac{n(n+4)}{2} & , \text{ for } k=1, \\ \frac{3n(n-2)}{2} & , \text{ for } k=2. \end{cases}$$

Proof. As $\text{diam}(\Gamma_G) = 2$, so we have to find the coefficients $d(\Gamma_G, 0)$, $d(\Gamma_G, 1)$ and $d(\Gamma_G, 2)$. If V_p denotes the set of all the pairs of vertices (same and distinct) of Γ_G , then $|V_p| = n(2n+1)$, by Proposition 2. Let $S(\Gamma_G, k) = \{(l, m); l, m \in V(\Gamma_G) | d(l, m) = k\}$, then $d(\Gamma_G, k) = |S(\Gamma_G, k)|$ and

$$V_p = S(\Gamma_G, 0) \cup S(\Gamma_G, 1) \cup S(\Gamma_G, 2). \quad (2)$$

Since, $d(l, l) = 0 \quad \forall \quad l \in V(\Gamma_G)$, so $S(\Gamma_G, 0) = \{(l, l); l \in V(\Gamma_G)\} = V(\Gamma_G)$. Thus, $d(\Gamma_G, 0) = 2n$. By Proposition 1, $\Gamma_G = K_2 + (K_{|\Omega_3|} \cup \frac{n}{2} K_2)$ with $V(K_2) = \zeta(\Gamma)$, $V(K_{|\Omega_3|}) = \Omega_3$ and $V(\frac{n}{2} K_2) = \bigcup_{i=0}^{\frac{n-1}{2}} \Omega_2^i = \Omega_2$. Thus:

$$\begin{aligned} S(\Gamma_G, 1) &= \{(l, m); l \in \zeta(\Gamma), m \in \Omega_3 \\ &\cup \{(l, m); l \in \zeta(\Gamma), m \in \Omega_2\} \\ &\cup \{(l, m); (l, m) \in \zeta(\Gamma) \text{ and } l \neq m\} \\ &\cup \{(l, m); (l, m) \in \Omega_3 \text{ and } l \neq m\} \\ &\cup \bigcup_{i=0}^{\frac{n-1}{2}} \{(l, m); (l, m) \in \Omega_2^i \text{ and } l \neq m\}. \end{aligned}$$

Accordingly,

$$\begin{aligned} d(\Gamma_G, 1) &= 2(n-2) + 2(n) + 1 + \binom{n-2}{2} + \frac{n}{2}(1) \\ &= 2n - 4 + \frac{5n}{2} + 1 + \frac{(n-2)(n-3)}{2} = \frac{n(n+4)}{2}. \end{aligned}$$

From Eq. 2, we have $|V_p| = d(\Gamma_G, 0) + d(\Gamma_G, 1) + d(\Gamma_G, 2)$. Therefore

$$\begin{aligned} d(\Gamma_{G,2}) &= |V_p| - d(\Gamma_G, 0) - d(\Gamma_G, 1) \\ &= n(2n+1) - 2n - \frac{n(n+4)}{2} \\ &= \frac{3n(n-2)}{2}. \end{aligned}$$

The Hosoya polynomials of the commuting graph on D_n , for odd and even values of $n \geq 3$, is obtained in the following result.

Theorem 4

For $n \geq 3$, let Γ_G be the commuting graph on $\Gamma = D_n$, then:

$$H(\Gamma_G, x) = \begin{cases} \frac{n}{2} \{3(n-1)x^2 + (n+1)x + 4\} & , \text{ for odd } n, \\ \frac{n}{2} \{3(n-2)x^2 + (n+4)x + 4\} & , \text{ for even } n. \end{cases}$$

Proof. Using the coefficients $d(\Gamma_G, k)$, computed in Propositions 2 and 3, in the formula of the Hosoya polynomial, we have:

For odd n :

$$\begin{aligned} H(\Gamma_G, x) &= d(\Gamma_G, 0)x^0 + d(\Gamma_G, 1)x^1 + d(\Gamma_G, 2)x^2 \\ &= (2n)x^0 + \left(\frac{n(n+1)}{2}\right)x + \left(\frac{3n(n-1)}{2}\right)x^2 \\ &= \frac{n}{2} \{3(n-1)x^2 + (n+1)x + 4\}. \end{aligned}$$

For even n :

$$\begin{aligned} H(\Gamma_G, x) &= d(\Gamma_G, 0)x^0 + d(\Gamma_G, 1)x^1 + d(\Gamma_G, 2)x^2 \\ &= (2n)x^0 + \left(\frac{n(n+4)}{2}\right)x + \left(\frac{3n(n-2)}{2}\right)x^2 \\ &= \frac{n}{2} \{3(n-2)x^2 + (n+4)x + 4\}. \end{aligned}$$

2.2 Reciprocal status Hosoya polynomial

Firstly, we find the reciprocal status of each vertex of the commuting graph on D_n , for odd and even values of $n \geq 3$, in the following two results, respectively.

Proposition 5

If l is a vertex in the commuting graph on D_n for odd values of $n \geq 3$, then:

$$rs(l) = \begin{cases} 2n-1 & , \text{ whenever } l \in \zeta(D_n), \\ \frac{3n}{2}-1 & , \text{ whenever } l \in \Omega_3, \\ n & , \text{ whenever } l \in \Omega_2. \end{cases}$$

Proof. By Proposition 1, the commuting graph on D_n is $K_1 + (K_{|\Omega_3|} \cup N_{|\Omega_2|})$ with the vertex set $\zeta(D_n) \cup \Omega_3 \cup \Omega_2$. Accordingly, we have:

Whenever $l \in \zeta(D_n)$: $ecc(l) = 1$, and by the definition of reciprocal status, we get

$$rs(l) = \left(\frac{1}{1}\right)(n+n-1) = 2n-1.$$

Whenever $l \in \Omega_3$: $ecc(l) = 2$, and by the definition of reciprocal status, we get

$$rs(l) = \left(\frac{1}{1}\right)(n-1) + \left(\frac{1}{2}\right)n = \frac{3n}{2}-1.$$

Whenever $l \in \Omega_2$: $\text{ecc}(l)=2$, and by the definition of reciprocal status, we get

$$rs(l) = \left(\frac{1}{1}\right)1 + \left(\frac{1}{2}\right)(2n-2) = n.$$

Proposition 6

For even values of $n \geq 4$, if l is any vertex of the commuting graph on D_n , then:

$$rs(l) = \begin{cases} 2n-1 & , \text{ whenever } l \in \zeta(D_n), \\ \frac{3n}{2}-1 & , \text{ whenever } l \in \Omega_3, \\ n+1 & , \text{ whenever } l \in \Omega_2. \end{cases}$$

Proof. By Proposition 1, the commuting graph on D_n is $K_2 + (K_{|\Omega_2|} \cup \frac{n}{2} K_2)$ with the vertex set $\zeta(D_n) \cup \Omega_3 \cup \Omega_2$. Accordingly, we have:

Whenever $l \in \zeta(D_n)$: $\text{ecc}(l)=1$, and by the definition of reciprocal status, we get

$$rs(l) = \left(\frac{1}{1}\right)\left\{1 + n - 2 + \left(\frac{n}{2}\right)2\right\} = 2n-1.$$

Whenever $l \in \Omega_3$: $\text{ecc}(l)=2$, and by the definition of reciprocal status, we get

$$rs(l) = \left(\frac{1}{1}\right)(n-3+2) + \left(\frac{1}{2}\right)\left(\frac{n}{2}\right)2 = \frac{3n}{2}-1.$$

Whenever $l \in \Omega_2$: $\text{ecc}(l)=2$, and by the definition of reciprocal status, we get

$$rs(l) = \left(\frac{1}{1}\right)3 + \left(\frac{1}{2}\right)\left\{(n-2) + \left(\frac{2n}{2}-2\right)\right\} = n+1.$$

The next two results provide the reciprocal status Hosoya polynomial of the commuting graph on D_n .

Theorem 7

For odd $n \geq 3$, if Γ_G is the commuting graph on $\Gamma = D_n$. Then:

$$H_{rs}(\Gamma_G) = (n-1)x^{\frac{7n-2}{2}} + nx^{3n-1} + \binom{n-1}{2}x^{3n-2}.$$

Proof. Proposition 5 implies that there are three types ($a \sim b$, $a \sim c$, $b \sim b$) of edges in Γ_G according to the reciprocal statuses of their end vertices, where $a = 2n-1$, $b = \frac{3n}{2}-1$, $c = n$. Table 1 shows the edge partition accordingly.

By using the edge partition, given in the Table 1, in the formula of the reciprocal status Hosoya polynomial, we have:

$$\begin{aligned} H_{rs}(G) &= \sum_{E_{a-b}} x^{a+b} + \sum_{E_{a-c}} x^{a+c} + \sum_{E_{b-b}} x^{b+b} \\ &= (n-1)x^{2n-1+\frac{3n}{2}-1} + nx^{2n-1+n} + \binom{n-1}{2}x^{\frac{3n}{2}-1+\frac{3n}{2}-1} \\ &= (n-1)x^{\frac{7n-2}{2}} + nx^{3n-1} + \binom{n-1}{2}x^{3n-2}. \end{aligned}$$

Theorem 8

For even $n \geq 4$, if Γ_G is the commuting graph on $\Gamma = D_n$. Then:

$$H_{rs}(\Gamma_G) = \binom{n-2}{2}x^{3n-2} + (2n-4)x^{\frac{7n-2}{2}} + x^{4n-2} + 2nx^{3n} + \frac{n}{2}x^{2n+2}.$$

Proof. Proposition 6 implies that there are five types ($a \sim a$, $a \sim b$, $b \sim b$, $b \sim c$, $c \sim c$) of edges in Γ_G accordingly, the edge partition is given in the Table 2, according to the reciprocal statuses of their end vertices, where $a = \frac{3n}{2}-1$, $b = 2n-1$, $c = n+1$.

Table 1: Edge partition of Γ_G according to reciprocal statuses

Edges type	Partition of edge set	Number of edges
$a \sim b$	$E_{a-b} = \{uv \in E(\Gamma_G) \mid rs(u) = a, rs(v) = b\}$	$ E_{a-b} = n-1$
$a \sim c$	$E_{a-c} = \{uv \in E(\Gamma_G) \mid rs(u) = a, rs(v) = c\}$	$ E_{a-c} = n$
$b \sim b$	$E_{b-b} = \{uv \in E(\Gamma_G) \mid rs(u) = b, rs(v) = b\}$	$ E_{b-b} = \binom{n-1}{2}$

Table 2: Edge partition of Γ_G according to reciprocal statuses

Type of edges	Partition of edge set	Number of edges
$a \sim a$	$E_{a-a} = \{uv \in E(\Gamma_G) \mid rs(u) = a, rs(v) = a\}$	$ E_{a-a} = \binom{n-2}{2}$
$a \sim b$	$E_{a-b} = \{uv \in E(\Gamma_G) \mid rs(u) = a, rs(v) = b\}$	$ E_{a-b} = 2(n-2)$
$b \sim b$	$E_{b-b} = \{uv \in E(\Gamma_G) \mid rs(u) = b, rs(v) = b\}$	$ E_{b-b} = 1$
$b \sim c$	$E_{b-c} = \{uv \in E(\Gamma_G) \mid rs(u) = b, rs(v) = c\}$	$ E_{b-c} = 2n$
$c \sim c$	$E_{c-c} = \{uv \in E(\Gamma_G) \mid rs(u) = c, rs(v) = c\}$	$ E_{c-c} = \frac{n}{2}$

By using the edge partition of Γ_G , given in the Table 2, in the formula of the reciprocal Hosoya polynomial, we have:

$$\begin{aligned}
 H_{rs}(G) &= \sum_{E_{a-a}} x^{a+a} + \sum_{E_{a-b}} x^{a+b} + \sum_{E_{b-b}} x^{b+b} + \sum_{E_{b-c}} x^{b+c} + \sum_{E_{c-c}} x^{c+c} \\
 &= \binom{n-2}{2} x^{2\left(\frac{3n-1}{2}\right)} + 2(n-2)x^{\frac{3n}{2}-1+2n-1} + 1x^{2(2n-1)} \\
 &\quad + 2nx^{2n-1+n+1} + \left(\frac{n}{2}\right)x^{2(n+1)} \\
 &= \binom{n-2}{2} x^{3n-2} + (2n-4)x^{\frac{7n-2}{2}} + x^{4n-2} + 2nx^{3n} + \left(\frac{n}{2}\right)x^{2n+2}.
 \end{aligned}$$

3 Hosoya index

In this section, we investigate the Hosoya index of the commuting graph of the dihedral group. The largest possible value of the Hosoya index, on a graph with n vertices, is given by the complete graph K_n (Tichy and Wagner, 2005). Generally, the Hosoya index of a complete graph K_n , $n \geq 1$ is:

$$1 + \sum_{k=1}^{\lfloor \frac{n}{2} \rfloor} \frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2},$$

which can be viewed in accordance with the number of non-empty matchings given in Table 3, where m_k denotes the number of matchings of cardinality k , $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

For all odd values of $n \geq 3$, the Hosoya index is computed in the following result.

Theorem 9

Let Γ_G be a commuting graph on $\Gamma = D_n$, for odd $n \geq 3$. Then the Hosoya index of Γ_G is:

$$1 + \binom{n}{2} + n + \sum_{k=2}^{\lfloor \frac{n}{2} \rfloor} \left[\frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2} + \frac{n}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-1}{2} \right].$$

Proof. As $\Gamma_G = K_1 + (K_{|\Omega_3|} \cup N_{|\Omega_2|})$ with $V(\Gamma_G) = \zeta(D_n) \cup \Omega_3 \cup \Omega_2$, by Proposition 1, so there are three types of edges in Γ_G :

Type-1: $u \sim v$ for $u, v \in \Omega_3$;

Type-2: $u \sim v$ for $u \in \Omega_3$ and $v \in \zeta(D_n)$;

Type-3: $u \sim v$ for $u \in \Omega_2$ and $v \in \zeta(D_n)$.

As $\zeta(D_n) \cup \Omega_3 = \Omega_1$ induces a complete subgraph K_n on n vertices in Γ_G , so there are two types of matchings in Γ_G :

(M_1) Matchings of edges of Type-1 and Type-2;

(M_2) Matchings of edges of Type-1 and Type-3.

The number of matchings of each type can be found as follows:

(M_1) Since the edges of Type-1 and Type-2 are the edges of complete graph K_n induced by the vertices in $\zeta(D_n) \cup \Omega_3 = \Omega_1$, so the number of matchings in this type can be obtained by counting the matchings in K_n for all $n \geq 3$, which are given in Table 4, where m_k denotes the number of matchings of order k for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

(M_2) Each matching of this type can be obtained by adding one edge of Type-3 into each matching of the edges of Type-1. As each edge of Type-1 is an edge of a complete graph K_{n-1} induced by the vertices in Ω_3 , so each matching of the edges of Type-1 is actually the matching in a complete graph K_{n-1} . The numbers of such matchings are listed in Table 5, where m_k denotes the number of matchings of order k for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

Table 3: The number of non-empty matchings in a complete graph K_n

K_n	m_1	m_2	m_3	m_4	...	m_k
K_2	$\binom{2}{2}$					
K_3	$\binom{3}{2}$					
K_4	$\binom{4}{2}$	$\frac{1}{2}\binom{4}{2}\binom{2}{2}$				
K_5	$\binom{5}{2}$	$\frac{1}{2}\binom{5}{2}\binom{3}{2}$				
K_6	$\binom{6}{2}$	$\frac{1}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{3}\binom{6}{2}\binom{4}{2}\binom{2}{2}$			
K_7	$\binom{7}{2}$	$\frac{1}{2}\binom{7}{2}\binom{5}{2}$	$\frac{1}{3}\binom{7}{2}\binom{5}{2}\binom{3}{2}$			
K_8	$\binom{8}{2}$	$\frac{1}{2}\binom{8}{2}\binom{6}{2}$	$\frac{1}{3}\binom{8}{2}\binom{6}{2}\binom{4}{2}$	$\frac{1}{4}\binom{8}{2}\binom{6}{2}\binom{4}{2}\binom{2}{2}$		
K_9	$\binom{9}{2}$	$\frac{1}{2}\binom{9}{2}\binom{7}{2}$	$\frac{1}{3}\binom{9}{2}\binom{7}{2}\binom{5}{2}$	$\frac{1}{4}\binom{9}{2}\binom{7}{2}\binom{5}{2}\binom{3}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_n	$\binom{n}{2}$	$\frac{1}{2}\binom{n}{2}\binom{n-2}{2}$	$\frac{1}{3}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}$	$\frac{1}{4}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}\binom{n-6}{2}$	...	$\frac{1}{k}\prod_{i=0}^{k-1}\binom{n-2i}{2}$

Table 4: The number of non-empty matchings in a complete graph K_n for odd $n \geq 3$

K_n	m_1	m_2	m_3	m_4	...	m_k
K_3	$\binom{3}{2}$					
K_5	$\binom{5}{2}$	$\frac{1}{2}\binom{5}{2}\binom{3}{2}$				
K_7	$\binom{7}{2}$	$\frac{1}{2}\binom{7}{2}\binom{5}{2}$	$\frac{1}{3}\binom{7}{2}\binom{5}{2}\binom{3}{2}$			
K_9	$\binom{9}{2}$	$\frac{1}{2}\binom{9}{2}\binom{7}{2}$	$\frac{1}{3}\binom{9}{2}\binom{7}{2}\binom{5}{2}$	$\frac{1}{4}\binom{9}{2}\binom{7}{2}\binom{5}{2}\binom{3}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_n	$\binom{n}{2}$	$\frac{1}{2}\binom{n}{2}\binom{n-2}{2}$	$\frac{1}{3}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}$	$\frac{1}{4}\binom{n}{2}\binom{n-2}{2}\binom{n-4}{2}\binom{n-6}{2}$	...	$\frac{1}{k}\prod_{i=0}^{k-1}\binom{n-2i}{2}$

Now, since there are n edges of Type-3, so the required matchings can be obtained as follows:

Matchings of order 1: These are n such matchings corresponding to n edges of Type-3.

Matchings of order 2: Each of these matchings can be obtained by adding one edge of Type-3 into each matching of order 1 in K_{n-1} . There are n edges of Type-3 and $\binom{n-1}{2}$ matchings of order 1 in K_{n-1} , by Table 5. Therefore, by the rule of product, the number of matchings of order 2 is:

$$n \binom{n-1}{2}.$$

Matchings of order 3: Each of these matchings can be obtained by adding one edge of Type-3 into each matching of order 2 in K_{n-1} . There are n edges of Type-3 and $\frac{1}{2} \binom{n-1}{2} \binom{n-3}{2}$ matchings of order 2 in K_{n-1} , by Table 5. Therefore, by the rule of product, the number of matchings of order 3 is:

$$\frac{1}{2} n \binom{n-1}{2} \binom{n-3}{2}.$$

Matchings of order 4: Each of these matchings can be obtained by adding one edge of Type-3 into each matching of order 3 in K_{n-1} . There are n edges of Type-3 and

$$\frac{1}{3} \binom{n-1}{2} \binom{n-3}{2} \binom{n-5}{2}$$

matchings of order 3 in K_{n-1} , by Table 5. Therefore, by the rule of product, the number of matchings of order 4 is:

$$\frac{1}{3} n \binom{n-1}{2} \binom{n-3}{2} \binom{n-5}{2}.$$

Matchings of order k : Generally, each matching of order k can be obtained by adding one edge of Type-3 into each matching of order $k-1$ in K_{n-1} . There are n edges of Type-3 and

$$\frac{1}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-1}{2}.$$

matchings of order $k-1$ in K_{n-1} , by Table 5. Therefore, by the rule of product, the number of matchings of order k is:

$$\frac{n}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-1}{2}.$$

Now, by the rule of sum, the total number of matchings (matchings (M_1) + matchings (M_2)) in Γ_G of each order can be counted as follows:

The number of matching of order 1 is:

$$\binom{n}{2} + n.$$

The number of matching of order 2 is:

$$\frac{1}{2} \binom{n}{2} \binom{n-2}{2} + n \binom{n-1}{2}.$$

Table 5: The number of non-empty matchings in a complete graph K_{n-1} for odd $n \geq 3$

K_n	m_1	m_2	m_3	m_4	...	m_k
K_2	$\binom{2}{2}$					
K_4	$\binom{4}{2}$	$\frac{1}{2} \binom{4}{2} \binom{2}{2}$				
K_6	$\binom{6}{2}$	$\frac{1}{2} \binom{6}{2} \binom{4}{2}$	$\frac{1}{3} \binom{6}{2} \binom{4}{2} \binom{2}{2}$			
K_8	$\binom{8}{2}$	$\frac{1}{2} \binom{8}{2} \binom{6}{2}$	$\frac{1}{3} \binom{8}{2} \binom{6}{2} \binom{4}{2}$	$\frac{1}{4} \binom{8}{2} \binom{6}{2} \binom{4}{2} \binom{2}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_{n-1}	$\binom{n-1}{2}$	$\frac{1}{2} \binom{n-1}{2} \binom{n-3}{2}$	$\frac{1}{3} \binom{n-1}{2} \binom{n-3}{2} \binom{n-5}{2}$	$\frac{1}{4} \binom{n-1}{2} \binom{n-3}{2} \binom{n-5}{2} \binom{n-7}{2}$	...	$\frac{1}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-1}{2}$

The number of matching of order 3 is:

$$\frac{1}{3} \binom{n}{2} \binom{n-2}{2} \binom{n-4}{2} + \frac{1}{2} n \binom{n-1}{2} \binom{n-3}{2}.$$

The number of matching of order 4 is:

$$\frac{1}{4} \binom{n}{2} \binom{n-2}{2} \binom{n-4}{2} \binom{n-6}{2} + \frac{1}{3} n \binom{n-1}{2} \binom{n-3}{2} \binom{n-5}{2}.$$

Generally, the number of matching of order k is:

$$\frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2} + \frac{n}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-1}{2},$$

where $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

Hence, the Hosoya index of Γ_G is:

$$1 + \binom{n}{2} + n + \sum_{k=2}^{\lfloor \frac{n}{2} \rfloor} \left[\frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2} + \frac{n}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-1}{2} \right].$$

When $n=2$, then $\Gamma = D_2$ is an abelian group and so the commuting graph Γ_G is the complete graph K_4 . Hence, by Table 3, the Hosoya index of Γ_G is $1+m_1+m_2=10$. The following result provides the Hosoya index of the commuting graph of D_n for even values of $n > 3$.

Theorem 10

Let Γ_G be a commuting graph on $\Gamma = D_n$ for even $n > 3$. Then the Hosoya index of Γ_G is:

$$1 + \sum_{k=1}^{\frac{n}{2}} m_k^1 + \sum_{k=1}^2 m_k^2 + \sum_{k=1}^{\frac{n}{2}} m_k^3 + \sum_{k=2}^{\frac{n+1}{2}} m_k^4 + m_2^5 + \sum_{k=2}^{\frac{n}{2}} m_k^6 + \sum_{k=2}^n m_k^7,$$

where:

$$m_k^1 = \frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2},$$

$$m_1^2 = 2n, m_2^2 = n(n-1),$$

$$m_k^3 = \left\lfloor \frac{n}{2} \right\rfloor,$$

$$m_2^4 = 2n \binom{n-2}{2},$$

$$m_k^4 = n \left[\frac{2}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-2}{2} + \frac{n-1}{k-2} \prod_{i=0}^{k-3} \binom{n-2i-2}{2} \right]$$

for $3 \leq k \leq \frac{n}{2}$,

$$m_{\frac{n+1}{2}}^4 = \frac{n(n-1)}{k-2} \prod_{i=0}^{k-3} \binom{n-2i-2}{2},$$

$$m_2^5 = 2n(n-1),$$

$$m_2^6 = 2n \left(\frac{n}{2} - 1 \right),$$

$$m_k^6 = n \left[2 \binom{\frac{n}{2}-1}{k-1} + \binom{\frac{n}{2}-1}{k-2} + 2(n-2) \binom{\frac{n}{2}-2}{k-2} \right] \text{ for } 3 \leq k \leq \frac{n}{2},$$

$$m_k^7 = \sum_{j=1}^{k-1} \frac{1}{j} \prod_{i=0}^{j-1} \binom{n-2i}{2} \binom{\frac{n}{2}}{k-j} \text{ for } 2 \leq k \leq n.$$

Proof. By Proposition 1, $\Gamma_G = K_2 + (K_{|\Omega_3|} \cup \frac{n}{2} K_2)$ with $V(\Gamma_G) = \zeta(D_n) \cup \Omega_3 \cup \Omega_2$, where $\Omega_2 = \bigcup_{i=0}^{\frac{n}{2}-1} \Omega_2^i$. Thus, we have following types of edges in Γ_G .

Type-1: $x \sim y$ for $x, y \in \Omega_3$;

Type-2: $x \sim y$ for $x, y \in \zeta(D_n)$;

Type-3: $x \sim y$ for $x \in \Omega_3$ and $y \in \zeta(D_n)$;

Type-4: $x \sim y$ for $x \in \Omega_2$ and $y \in \zeta(D_n)$;

Type-5: $x \sim y$ for $x, y \in \Omega_2^i \subseteq \Omega_2$, where $0 \leq i \leq \frac{n}{2}-1$.

According to these types, following seven types of matchings between the edges of Γ_G exist:

- (m^1) Matchings between the edges of Type-1, Type-2 and Type-3;
- (m^2) Matchings between the edges of Type-4;
- (m^3) Matchings between the edges of Type-5;
- (m^4) Matchings between the edges of Type-1 and Type-4;
- (m^5) Matchings between the edges of Type-3 and Type-4;
- (m^6) Matchings between the edges of Type-4 and Type-5;
- (m^7) Matchings between the edges of Type-1, Type-2 Type-3 and the edges of Type-5.

The number of all these types of matchings is computed as follows:

- (m^1) Since $\zeta(D_n) \cup \Omega_3 = \Omega_1$ induces a complete graph k_n , so the edges of Type-1, Type-2 and Type-3 are the edges of k_n , and all the matchings between these edges are counted in Table 6, where m_k^1 denotes the number of matchings of order k , where $1 \leq k \leq \frac{n}{2}$.
- (m^2) Let m_k^2 denotes the number of matchings of order k , for $k=1, 2$.

For m_1^2 : The number of matchings of order 1 is equal to the number of edges of Type-4, which is $2n$. Hence $m_1^2 = 2n$.

For m_2^2 : Let $e = x \sim y$ be an edge of Type-4 with $x \in \Omega_2^i$ for fixed $0 \leq i \leq \frac{n}{2} - 1$ and $y \in \zeta(D_n)$. Then, together with the edge e , each edge of Type-4 having one end in $\Omega_2 - \{x\}$ and one end in $\zeta(D_n) - \{y\}$ form a matching of order 2. Therefore $m_2^2 = \frac{1}{2}(4(n-1) \times \frac{n}{2}) = n(n-1)$. There is no matching of order greater than two in this case.

- (m^3) There are $\frac{n}{2}$ edges of Type-5, and no two of them shares a common vertex. Therefore, there exists a matching of every order k such that $1 \leq k \leq \frac{n}{2}$. Let m_k^3 denotes the number of matchings of order k . Then:

$$m_k^3 = \binom{\frac{n}{2}}{k}.$$

- (m^4) Let m_k^4 denotes the number of matchings of order k , for $1 \leq k \leq \frac{n}{2} + 1$. Then $m_1^4 = 0$ in this case. In Γ , no edge of Type-1 shares a common vertex with any edge of Type-4. Therefore, in this case we can get a matching by combining any matching of the edges of Type-1 with each matching of the edges of Type-4. As there are m_j^1 matchings of order j , $1 \leq j \leq \frac{n-2}{2}$, between the edges of Type-1, which are the edges of a complete graph K_{n-2} , where each m_j^1 can be obtained from Table 6 and there are $m_1^2 = 2n$ and $m_2^2 = n(n-1)$ matching of order 1 and 2, respectively, between the edges of Type-4. Therefore, by the rule of product, we get:

$$m_2^4 = m_1^2 \times m_1^1 = 2nm_1^1,$$

for $3 \leq k \leq \frac{n}{2}$:

$$\begin{aligned} m_k^4 &= m_1^2 \times m_{k-1}^1 + m_2^2 \times m_{k-2}^1 \\ &= 2nm_{k-1}^1 + n(n-1)m_{k-2}^1 \end{aligned}$$

$$= n(2m_{k-1}^1 + (n-1)m_{k-2}^1),$$

and for $k = \frac{n}{2} + 1$:

$$m_k^4 = m_2^2 \times m_{k-2}^1 = n(n-1)m_{\frac{n}{2}-1}^1.$$

- (m^5) Let m_k^5 denotes the number of matchings of order k for $k=1, 2$. Then $m_1^5 = 0$ in this case. Here, we can use matchings of order 1 only between the edges of Type-4. For otherwise, we cannot use any edge of Type-3 because both types of edges commonly shared the vertices in $\zeta(D_n)$. Hence, we can get matchings of order 2 only in this case. Let $M = \{e = x \sim y\}$ be a matching of order 1 between the edges of Type-4 with $x \in \Omega_2^i$ for $0 \leq i \leq \frac{n}{2} - 1$ and $y \in \zeta(D_n)$. Then every edge of Type-3, not adjacent with y can contribute to form a matching of order 2. Since there are $n-2$ such edges of Type-3 each of which can be used in any of $2n$ matchings of order 1 between the edges of Type-4, so by the rule of product, we have:

$$m_2^5 = 2n(n-2).$$

- (m^6) Let m_k^6 denotes the number of matchings of order k for $1 \leq k \leq \frac{n}{2}$. Then $m_1^6 = 0$ in this case, because to find matchings, both the matchings of order 1 and 2 between the dges of Type-4 will be used, and any matching of order j , $1 \leq j \leq \frac{n}{2} - 1$ between the edges of Type-5 will be used. Accordingly, by counting these matchings with the rule of product, we get:

$$m_2^6 = 4 \times 1 \times \binom{\frac{n}{2}-1}{1} \times \frac{n}{2} = 2n \left(\frac{n}{2} - 1 \right),$$

and for $3 \leq k \leq \frac{n}{2}$,

$$m_k^6 = n \left[2 \binom{\frac{n}{2}-1}{k-1} + \binom{\frac{n}{2}-1}{k-2} + 2(n-2) \binom{\frac{n}{2}-2}{k-2} \right].$$

- (m^7) Since the edges of Type-1, Type-2 and Type-3 are the edges of a complete graph k_n induced by $\zeta(D_n) \cup \Omega_3 = \Omega_1$, so in this case we find the matchings between the edges of Type-5 and the edges of k_n . Let m_k^7 be the number of matchings of order k . Then $m_1^7 = 0$. Since no edge of Type-5 share a common vertex with any edge of k_n , so corresponds to each matching of the edges of Type-5, every matching of the edges of k_n can be used to find a matching in this case. As there are m_i^1 matchings

of order $1 \leq t \leq \frac{n}{2}$ between the edges of K_n , counted

in Table 6, and there are $m_j^3 = \binom{\frac{n}{2}}{j}$ matchings

of order $1 \leq j \leq \frac{n}{2}$ between the edges of Type-5. Thus, the maximum order of a matching in this case is $\frac{n}{2} + \frac{n}{2} = n$. Therefore, we can find m_k^7 for $2 \leq k \leq n$ as

follows:

$$m_2^7 = m_1^1 m_1^3,$$

$$m_3^7 = m_1^1 m_2^3 + m_2^1 m_1^3,$$

$$m_4^7 = m_1^1 m_3^3 + m_2^1 m_2^3 + m_3^1 m_1^3,$$

$$m_5^7 = m_1^1 m_4^3 + m_2^1 m_3^3 + m_3^1 m_2^3 + m_4^1 m_1^3,$$

and so on, generally, we have:

$$m_k^7 = \sum_{j=1}^{k-1} m_j^1 m_{k-j}^3.$$

Hence, by the rule of sum, the Hosoya index of Γ_G is:

$$1 + \sum_{i=1}^7 \text{the number of matchings}(m^i)$$

$$= 1 + \sum_{k=1}^{\frac{n}{2}} m_k^1 + \sum_{k=1}^2 m_k^2 + \sum_{k=1}^{\frac{n}{2}} m_k^3 + \sum_{k=2}^{\frac{n}{2}+1} m_k^4 + m_2^5 + \sum_{k=2}^{\frac{n}{2}} m_k^6 + \sum_{k=2}^n m_k^7,$$

with

$$m_k^1 = \frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2},$$

$$m_1^2 = 2n, m_2^2 = n(n-1),$$

$$m_k^3 = \binom{\frac{n}{2}}{k},$$

$$m_2^4 = 2n \binom{n-2}{2},$$

$$m_k^4 = n \left[\frac{2}{k-1} \prod_{i=0}^{k-2} \binom{n-2i-2}{2} + \frac{n-1}{k-2} \prod_{i=0}^{k-3} \binom{n-2i-2}{2} \right]$$

$$\text{for } 3 \leq k \leq \frac{n}{2},$$

$$m_{\frac{n}{2}+1}^4 = \frac{n(n-1)}{k-2} \prod_{i=0}^{k-3} \binom{n-2i-2}{2},$$

$$m_2^5 = 2n(n-1),$$

Table 6: The number of non-empty matchings in a complete graph K_n for even $n \geq 2$

K_n	m_1^1	m_2^1	m_3^1	m_4^1	...	m_k^1
K_2	$\binom{2}{2}$					
K_4	$\binom{4}{2}$	$\frac{1}{2} \binom{4}{2} \binom{2}{2}$				
K_6	$\binom{6}{2}$	$\frac{1}{2} \binom{6}{2} \binom{4}{2}$	$\frac{1}{3} \binom{6}{2} \binom{4}{2} \binom{2}{2}$			
K_8	$\binom{8}{2}$	$\frac{1}{2} \binom{8}{2} \binom{6}{2}$	$\frac{1}{3} \binom{8}{2} \binom{6}{2} \binom{4}{2}$	$\frac{1}{4} \binom{8}{2} \binom{6}{2} \binom{4}{2} \binom{2}{2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
K_{n-1}	$\binom{n}{2}$	$\frac{1}{2} \binom{n}{2} \binom{n-2}{2}$	$\frac{1}{3} \binom{n}{2} \binom{n-2}{2} \binom{n-4}{2}$	$\frac{1}{4} \binom{n}{2} \binom{n-2}{2} \binom{n-4}{2} \binom{n-6}{2}$	...	$\frac{1}{k} \prod_{i=0}^{k-1} \binom{n-2i}{2}$

$$m_2^6 = 2n \binom{\frac{n}{2}-1}{2},$$

$$m_k^6 = n \left[2 \binom{\frac{n}{2}-1}{k-1} + \binom{\frac{n}{2}-1}{k-2} + 2(n-2) \binom{\frac{n}{2}-2}{k-2} \right]$$

$$\text{for } 3 \leq k \leq \frac{n}{2},$$

$$m_k^7 = \sum_{j=1}^{k-1} \frac{1}{j} \prod_{i=0}^{j-1} \binom{n-2i}{2} \binom{\frac{n}{2}}{k-j} \text{ for } 2 \leq k \leq n.$$

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