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Eccentric Connectivity Index of the Power Graph for Dihedral Groups: A Case of Bromine Pentafluoride

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Abstract
Eccentric connectivity index is one of the topological indices, which is a numerical value derived from the graph representation of a molecule, where atoms are vertices and bonds are edges, used to characterize its topology. By efficiently encoding molecular information, topological indices enable quick and effective correlation with various molecular properties, facilitating advanced predictive modelling. Since 1947, numerous topological indices have been introduced, and the development of new indices continues actively to this day. The eccentric connectivity index of a molecular graph is defined as the sum of the products of the vertex degrees and their eccentricities, where the eccentricity of a vertex is the greatest distance from that vertex to any other vertex in the graph. Meanwhile, a power graph is a graph where two different vertices are connected by an edge if and only if one is the power of the other. The graph's vertex set consists of all the elements in a group. In this paper, the eccentric connectivity index of the power graph for dihedral groups is determined. Next, the eccentric connectivity index of a molecular structure, namely the Bromine Pentafluoride, is computed using point groups and isomorphism. It is found that the eccentric connectivity index of the power graph for the group increases when the power graph becomes more complex, where the number of vertices and edges increases.
Keywords: Eccentric connectivity index; power graph; molecular structure; group theory; graph theory.

Introduction
Topological index (TI) is a number that expresses the measurable properties of the molecules. The information provided in the molecular graph must be translated into numerical features in order to establish a connection between molecular topology and any actual molecular property [1]. Since 1947, various types of topological indices have been developed, starting with the Wiener index which has been introduced by Harold Wiener [2], followed by Hosoya index [3], Zagreb index [4], Randiċ index [5], Harary index [6], eccentric connectivity index [7] and many more. The research in this field are not limited to the computation of the topological index of certain graphs in general, but a significant amount of applications have been explored such as Quantitative Structure-Activity Relationship (QSAR) studies, Quantitative Structure-Property Relationships (QSPR) studies, and the usage of TI in the development drugs to cure many diseases. Some recent research can be found in [8-12].

In addition, the TI of graphs associated with groups is receiving much attention, nowadays. The study of the graphs of groups is important for understanding their algebraic and symmetrical properties, in which the properties are very useful in studying the properties of molecular graphs in chemistry. In 2018, Sarmin et al. [13] found the Wiener and Zagreb indices of the non-commuting graph associated with the generalised quaternion groups. Next, the Wiener and Zagreb indices of the conjugacy class graph of the dihedral groups are determined in 2019 [14]. Since there is a lack of research connecting the topological indices and the power graph, hence this study focuses on computing the topological index of the power graph associated with dihedral groups. The group presentation of the dihedral group is given in the following,

$$D_{2\alpha} = \langle a, b | a^{\alpha} = b^2 = 1, bab = a^{-1} \rangle,$$

where $\alpha \geq 3$.

This paper consists of three sections. Section 1 is the Introduction section, followed by Section 2, namely the Preliminaries where some definitions and previous results are stated. In Section 3, the main result, which is the eccentric connectivity index of a power graph for dihedral groups is presented. Then, based on the new theorem, the eccentric connectivity index of Bromine Pentafluoride is computed, by using the isomorphism of its point group and the dihedral group of order eight.

Preliminaries

This section presents some basic concepts, definitions, and previous results that will be used to prove the main theorems.

Definition 1 [15] Degree of a vertex

Degree of a vertex, i is the number of edges attached to vertex i and it is denoted as $\deg(i)$.

Definition 2 [15] Distance between two vertices

The distance between two vertices, which are i and j, is the shortest path from vertex i to vertex j, denoted as $d(i, j)$.

Definition 3 [16] Eccentric connectivity index

The eccentric connectivity index (ECI) is defined as the sum of the product of eccentricity and degree of each vertex in a graph with n total vertices, is written as

$$ECI = \sum_{i=1}^{n} E(i)\deg(i),$$

where $\deg(i)$ is the degree of vertex i and the eccentricity of a vertex i, $E(i)$ is a maximum distance between vertex i with the other vertices in a graph.

Example 1 Given a simple graph as in the following figure.

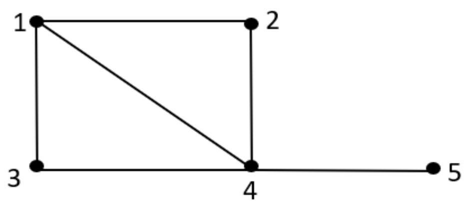

Figure 1 Simple graph

Based on Figure 1, $\deg(1) = 3, \deg(2) = 2, \deg(3) = 2, \deg(4) = 4$ and $\deg(5) = 1$. Then, the distance between two vertices in the graph are stated in Table 1.

Table 1 The distances between two vertices in a graph

Vertex	**1**	**2**	**3**	**4**	**5**	
1	0	1	1	1	2	$E(1) = 2$
2	1	0	2	1	2	$E(2) = 2$
3	1	2	0	1	2	$E(3) = 2$
4	1	1	1	0	1	$E(4) = 1$
5	2	2	2	1	0	$E(5) = 2$

Hence, $ECI = \sum_{i=1}^{5} E(i)\deg(i)$

$$= E(1)\deg(1) + E(2)\deg(2) + E(3)\deg(3) + E(4)\deg(4) + E(5)\deg(5)$$
$$= 2(3) + 2(2) + 2(2) + 1(4) + 2(1)$$
$$= 20.$$

Definition 4 [17] Power graph
A power graph is an undirected graph where two distinct vertices i and j are adjacent if and only if $i^r = j$ or $j^r = i$, where $r \in \mathbb{Z}^+$.

In 2018, Chattopadhyay and Panigrahi [18] studied the connectivity and planarity of power graphs of finite cyclic, dihedral and dicyclic groups. They determined the general forms of the power graph for dihedral and generalised quaternion groups. The degree of each vertex in the power graph for dihedral group is found, as stated in Proposition 2.

Proposition 1 [18] Let $K(H) = \langle a \rangle$ be a cyclic subgroup of the $D_{2\alpha}$, where $\alpha \geq 3$. Suppose that $K(H)$ is a complete graph. Then, the power graph of $D_{2\alpha}$ can be illustrated as in Figure 2.

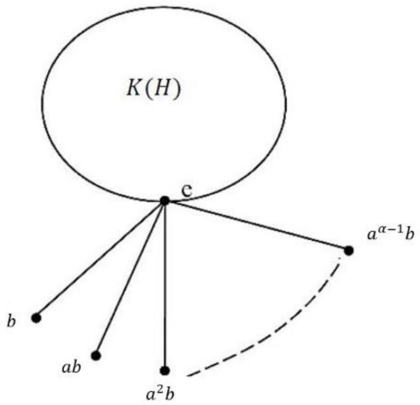

Figure 2 [18] A power graph of $D_{2\alpha}$

Proposition 2 [19] The vertex degree in the power graph for $D_{2\alpha}$, where $\alpha \geq 3$, is

1. $\deg(e) = 2\alpha - 1,$
2. $\deg(a^i) = \alpha - 1, \;\; 1 \leq i \leq \alpha - 1,$
3. $\deg(a^i b) = 1, \;\; 0 \leq i \leq \alpha - 1.$

Next, bromine pentafluoride, BrF_5 is an interhalogen compound and a strong fluorination agent, as shown in Figure 3. In the last part of the paper, the computation of its eccentric connectivity index is shown.

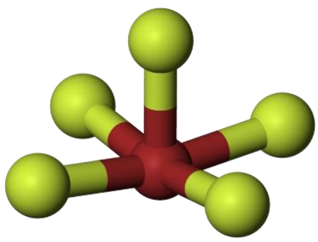

Figure 3 A bromine pentafluoride

Results and Discussion

In this section, the general formula of the eccentric connectivity index of the power graph for dihedral groups is presented as the main theorem. Then, based on the result, the eccentric connectivity index of the bromine pentafluoride, BrF_5, is calculated. The isomorphism of the point group of BrF_5 and the dihedral groups is also determined.

Theorem 1 Let Γ be the power graph for the dihedral groups, $D_{2\alpha}$. Then, its eccentric connectivity index, $ECI = 2\alpha^2 + 1$, where $\alpha \geq 3$.

Proof Based on Proposition 1, $K(H)$ is a complete graph, but the element of a^i is not adjacent to vertices $a^j b$, where $1 \leq i \leq \alpha - 1$ and $0 \leq j \leq \alpha - 1$. Then, $E(a^i) = 2$. Meanwhile, the vertex e is the only vertex that is adjacent to all other vertices. The vertex $a^j b$, where $0 \leq j \leq n - 1$, is adjacent only to vertex e. Then, $E(a^i b) = 2$. Hence, there are $|K(H)|$ that has the same eccentricity and degrees of a^i, $|e|$ that has the same eccentricity and degree of e and $|a^j b|$ that has the same eccentricity and degrees of $a^j b$. By Definition 3 and Proposition 2,

$$
\begin{aligned}
ECI &= \sum_{i=1}^{\alpha} E(i)\deg(i) \\
&= |K(H)|E(a^i)\deg(a^i) + |e|E(e)\deg(e) + |a^j b|E(a^j b)\deg(a^j b) \\
&= (\alpha - 1)(2)(\alpha - 1) + (1)(1)(2\alpha - 1) + \alpha(2)(1) \\
&= 2\alpha^2 + 1.
\end{aligned}
$$

In [20], the point group of bromine pentafluoride, BrF_5, is given as $C_{4v} = \{E, C_4, C_4^2, C_4^3, \sigma_{v_1}, \sigma_{v_2}, \sigma_{d_1}, \sigma_{d_2}\}$, where C_4 is the 90-degree rotation, σ_{v_1} and σ_{v_2} are the planes of symmetry that are standing vertically perpendicular to XZ –plane (horizontal plane) in between the molecules, and σ_{d_1} and σ_{d_2} are the vertical diagonal planes on the molecules. The commutative elements can be seen in the following Cayley table (Figure 4). The operation used depends on the element at the right of $*$. For instance, if $C_4 * C_4^2$, it means the 180-degree rotation is applied to C_4 element and it is C_4^3 element. Meanwhile, if $\sigma_{v_1} * \sigma_{d_1}$, it means the operation σ_{d_1} is applied to σ_{v_1}.

$*$	E	C_4	C_4^2	C_4^3	σ_{v_1}	σ_{v_2}	σ_{d_1}	σ_{d_2}
E	E	C_4	C_4^2	C_4^3	σ_{v_1}	σ_{v_2}	σ_{d_1}	σ_{d_2}
C_4	C_4	C_4^2	C_4^3	E	σ_{d_1}	σ_{d_2}	σ_{v_2}	σ_{v_1}
C_4^2	C_4^2	C_4^3	E	C_4	σ_{v_2}	σ_{v_1}	σ_{d_2}	σ_{d_1}
C_4^3	C_4^3	E	C_4	C_4^2	σ_{d_2}	σ_{d_1}	σ_{v_1}	σ_{v_2}
σ_{v_1}	σ_{v_1}	σ_{d_2}	σ_{v_2}	σ_{d_1}	E	C_4^2	C_4^3	C_4
σ_{v_2}	σ_{v_2}	σ_{d_1}	σ_{v_1}	σ_{d_2}	C_4^2	E	C_4	C_4^3
σ_{d_1}	σ_{d_1}	σ_{v_1}	σ_{d_2}	σ_{v_2}	C_4	C_4^3	E	C_4^2
σ_{d_2}	σ_{d_2}	σ_{v_2}	σ_{d_1}	σ_{v_1}	C_4^3	C_4	C_4^2	E

Figure 4 Cayley table of C_{4v}

Based on the Cayley table of C_{4v}, its isomorphism with D_8 can be determined. First, the elements from each set are mapped to those of the same order. The order of an element, a, is the least positive integer α such that $a^\alpha = e$. Hence, based on the Cayley table of D_8 and C_{4v}, the order of each element is listed in the following.

D_8	C_{4v}
$\|\rho_0\| = 1$	$\|E\| = 1$
$\|\rho_{90}\| = 4$	$\|C_4\| = 4$
$\|\rho_{180}\| = 2$	$\|C_4^2\| = 2$
$\|\rho_{270}\| = 4$	$\|C_4^3\| = 4$
$\|v\| = 2$	$\|\sigma_{v_1}\| = 2$
$\|h\| = 2$	$\|\sigma_{v_2}\| = 2$
$\|d_1\| = 2$	$\|\sigma_{d_1}\| = 2$
$\|d_2\| = 2$	$\|\sigma_{d_2}\| = 2$

Let ϕ be the mapping from D_8 to C_{4v}. Based on the order of the elements in D_8 and C_{4v}, ϕ is one-to-one and onto. Next, ϕ can be shown to be a homomorphism, that is $\phi(gh) = \phi(g)\phi(h)$ for all $g, h \in D_8$, as shown in the following.

Let $g = \rho_{90}$ and h be the elements in D_8. The homomorphism can be shown below.

$$\begin{aligned}
&\phi(\rho_{90} \cdot \rho_{180}) = \phi(\rho_{270}) = C_4^3, && \phi(\rho_{90})\phi(\rho_{180}) = C_4 \cdot C_4^2 = C_4^3,\\
&\phi(\rho_{90} \cdot \rho_{270}) = \phi(\rho_0) = E, && \phi(\rho_{90})\phi(\rho_{270}) = C_4 \cdot C_4^3 = E,\\
&\phi(\rho_{90} \cdot \rho_v) = \phi(\rho_{d_1}) = \sigma_{d_1}, && \phi(\rho_{90})\phi(\rho_v) = C_4 \cdot \sigma_{v_1} = \sigma_{d_1},\\
&\phi(\rho_{90} \cdot \rho_h) = \phi(\rho_{d_2}) = \sigma_{d_2}, && \phi(\rho_{90})\phi(\rho_h) = C_4 \cdot \sigma_{v_2} = \sigma_{d_2},\\
&\phi(\rho_{90} \cdot \rho_{d_1}) = \phi(\rho_h) = \sigma_{v_2}, && \phi(\rho_{90})\phi(\rho_{d_1}) = C_4 \cdot \sigma_{d_1} = \sigma_{v_2},\\
&\phi(\rho_{90} \cdot \rho_{d_2}) = \phi(\rho_v) = \sigma_{v_1}, && \phi(\rho_{90})\phi(\rho_{d_2}) = C_4 \cdot \sigma_{d_2} = \sigma_{v_1}.
\end{aligned}$$

Same goes to all others g and h in D_8. Thus, ϕ is an isomorphism and $D_8 \cong C_{4v}$. Therefore, the eccentric connectivity index of the power graph for bromine pentafluoride can computed by using Theorem 1.

Theorem 2 The eccentric connectivity index of the power graph for BrF_5 is 33.

Proof By using Theorem 1 and $\alpha = 4$, since BrF_5 is isomorphic to D_8, $ECI = 2\alpha^2 + 1 = 2(4)^2 + 1 = 33$.

Conclusion

In conclusion, the eccentric connectivity index of a power graph for dihedral groups in terms of α is determined. The properties of the power graph such as the degree of each vertex and the eccentricity of the vertex are first found based on the power graph obtained. Then, the eccentric connectivity index of the power graph of bromine pentafluoride is computed by using the main result and the isomorphism between the point group of BrF_5 with the dihedral group of order eight. In addition, the main result is useful in predicting any physical and biological properties of the molecules in chemistry by establishing a new mathematical model. This can improve the computational efficiency while also reducing the energy and cost.

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