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Degree-based topological indices and m-polynomial of benzimidazole molecular graph

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Abstract

Chemical graph theory plays an important role in understanding thestructural and physicochemical behaviour of graph-based descriptors. In this work, the hydrogen-suppressed molecular graph of benzimidazole is investigated using degree-based topological indices and the M-polynomial approach. The molecular structure of benzimidazole is represented as a graph, and the corresponding edge partitions are determined based on the degrees of end vertices. Using these edge partitions, several important degree-based topological indices, namely the First Zagreb index, Second Zagreb index, Randi´c index, Atom-Bond Connectivity index, Geometric-Arithmetic index, Harmonic index, Sum Connectivity index, Hyper Zagreb index, Forgotten index, and Symmetric Division Degree index, are computed systematically. Further, the M-polynomial of the benzimidazole molecular graph is derived and employed to obtain selected topological descriptors. In addition, a simple statistical analysis is performed between selected topological indices and physicochemical properties of benzimidazole using Pearson correlation and linear regression techniques. The correlation coefficient was found to be $r \approx -0.207$, indicating a weak negative relationship, while the coefficient of determination was obtained as $R^2 \approx 0.0428$, showing limited predictive capability for the considered dataset. The obtained results provide structural insight into the benzimidazole molecular graph and establish a mathematical basis for future studies involving benzimidazole derivatives and QSPR/QSAR modeling.

Keywords: Benzimidazole; Adjacency Matrix; Vertex degrees; Edge partitions

1. Introduction

Chemical graph theory is an important interdisciplinary area that combines graph theory, chemistry, and mathematical modeling to study molecular structures through graphical representations. In chemical graph theory, atoms are represented as vertices and chemical bonds are represented as edges, thereby transforming molecular structures into mathematical graphs for systematic investigation [1, 13, 15, 16]. This graphical representation enables researchers to investigate structural properties of chemical compounds without depending entirely on experimental procedures. Over the years, graph-theoretic techniques have gained considerable attention in chemistry, pharmaceutical sciences, computational biology, and material science because of their ability to model complex molecular systems efficiently [9, 14]. The application of graph theory in chemistry has become particularly important in understanding molecular connectivity, branching behaviour, and physicochemical properties.

Topological indices are numerical descriptors derived from molecular graphs that characterize the structural nature of chemical compounds. These graph invariants have found widespread applications in Quantitative Structure Property Relationship (QSPR) and Quantitative Structure Activity Relationship (QSAR) studies for predicting molecular properties and biological activities [12, 14]. Topological indices are generally classified into degree-based, distance-based, and neighborhood-based descriptors depending on the structural information used in their formulation. Among

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these, degree-based topological indices are particularly significant due to their computational simplicity and strong applicability in molecular characterization [13, 9]. Such indices are frequently employed to estimate physicochemical properties including boiling point, melting point, toxicity, molecular stability, and biological effectiveness.

The earliest and most widely studied degree-based topological descriptors include the Zagreb indices introduced by Gutman and Trinajsti´c [2]. The First Zagreb index and Second Zagreb index have been successfully used to describe molecular branching and structural complexity in chemical compounds. Another highly influential descriptor is the Randi´c index, introduced by Randi´c [3], which is widely recognized for measuring molecular branching and has extensive applications in chemical property prediction. Several modifications and extensions of classical descriptors have subsequently emerged to provide deeper insights into molecular structures and their chemical significance.

In addition to classical descriptors, modern degree-based topological indices such as the Atom-Bond Connectivity (ABC) index and Geometric-Arithmetic (GA) index have gained substantial importance in mathematical chemistry. The ABC index introduced by Estrada et al. [5] has shown strong applicability in modeling physicochemical properties and stability of molecular compounds. Similarly, the Geometric-Arithmetic index proposed by Vuki˘cevi´c and Furtula [7] has attracted considerable attention due to its predictive capabilities in chemical graph theory. Other descriptors such as the Harmonic index, Sum Connectivity index, Forgotten index, Hyper Zagreb index, and Symmetric Division Degree index have also contributed significantly to the structural characterization of chemical compounds [4, 6, 8,19].

In recent years, the M-polynomial has emerged as an effective algebraic tool for deriving degree-based topological indices in a unified framework. The concept of the M-polynomial provides an efficient representation of edge partitions based on vertex degrees and significantly reduces the complexity involved in computing multiple graph invariants [10, 11]. Once the edge partition of a molecular graph is determined, various topological indices can be obtained systematically through differential and integral operators applied to the polynomial representation. Due to its efficiency and compactness, the M-polynomial method has become increasingly popular in studies involving nanotubes, dendrimers, chemical networks, and pharmaceutical compounds [11, 10].

Benzimidazole is an important heterocyclic aromatic compound formed by the fusion of benzene and imidazole rings. It possesses significant pharmaceutical relevance because of its diverse biological and medicinal properties. Benzimidazole derivatives are commonly used in the development of antibacterial, antifungal, antiviral, anti-inflammatory, antiparasitic, and anticancer drugs [18, 17]. Several clinically important drugs contain benzimidazole moieties, making it an attractive subject for graph-theoretic and pharmaceutical investigations. Owing to its fused ring system and unique connectivity, benzimidazole provides an interesting framework for analysing molecular descriptors and graph invariants.

The hydrogen-suppressed molecular graph of benzimidazole enables researchers to study its structural behaviour using graph-theoretic tools and topological descriptors. Through degree-based edge partitioning, it becomes possible to compute multiple indices that characterize molecular complexity and connectivity [13, 9]. Such graph-based analysis not only contributes to the mathematical characterization of molecular compounds but also assists in understanding their potential physicochemical significance. Furthermore, preliminary statistical investigations involving molecular descriptors may provide useful insights regarding the relationship between graph invariants and physicochemical properties [12, 14].

Motivated by the growing importance of chemical graph theory and the medicinal significance of benzimidazole, the present work investigates the benzimidazole molecular graph using degree-based topological descriptors and the M-polynomial framework. The corresponding molecular graph is constructed, and the edge partitions are determined based on vertex degrees. Using these edge partitions, several important topological indices including the First Zagreb index, Second Zagreb index, Randi´c index, Atom-Bond Connectivity index, Geometric-Arithmetic index, Harmonic index, Sum Connectivity index, Hyper Zagreb index, Forgotten index, and Symmetric Division Degree index are computed systematically. In addition, a simple statistical investigation involving Pearson correlation and linear regression is carried out between selected topological indices and physicochemical properties of benzimidazole to examine possible structural relationships.

2. Molecular Graph of Benzimidazole

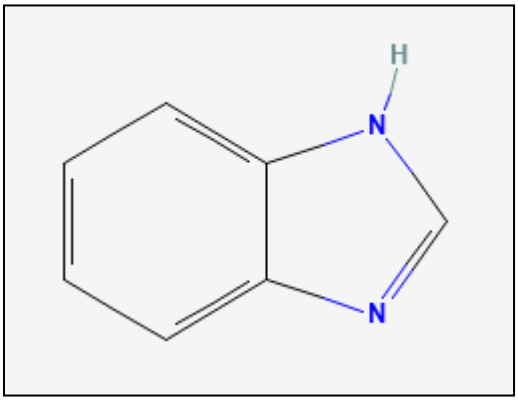

Figure 1 Molecular Graph of Benzimidazole

2.1. Adjacency Matrix

$$A(G) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

2.2. Vertex Degrees

$$d(v_1) = 2, \quad d(v_2) = 2, \quad d(v_3) = 2, \quad d(v_4) = 3, \quad d(v_5) = 2,$$

$$d(v_6) = 3, \quad d(v_7) = 2, d(v_8) = 2, \quad d(v_9) = 2.$$

Table 1 Physicochemical Properties of Benzimidazole

Property Name	Property Value
Molecular Weight	118.14
XLogP3	1.3
Exact Mass	118.053098200
Monoisotopic Mass	118.053098200
Topological Polar Surface Area	28.7
Heavy Atom Count	9
Complexity	103

Edge Partitions

Let $E_1(G) = E_{(2,2)}$ and $E_2(G) = E_{(2,3)}$ where $|E_1(G)| = 4, |E_2(G)| = 6$.

2.3. Definitions

Definition 1 First Zagreb Index

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

Definition 2 Second Zagreb Index

$$M_2(G) = \sum_{uv \in E(G)} [d(u)d(v)]$$

Definition 3 Randi´c Index

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{[d(u)d(v)]}}$$

Definition 4 Atom-Bond Connectivity Index

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

Definition 5 Geometric-Arithmetic Index

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

Definition 6 Harmonic Index

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$$

Definition 7 Sum Connectivity Index

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}$$

Definition 8 Hyper Zagreb Index

$$\mathrm{HM}(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2$$

Definition 9 Forgotten Index

$$\mathrm{F}(G) = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2]$$

Definition 10 Symmetric Division Degree Index

$$\mathrm{SDD}(G) = \sum_{uv \in E(G)} \left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right)$$

3. Results

Theorem 11 For the Benzimidazole Molecular Graph, the topological indices are calculated and are given by

Topological Index	Value
$M_1(G)$	46
$M_2(G)$	52
$R(G)$	4.449
$ABC(G)$	7.071
$GA(G)$	9.879
$H(G)$	4.4
$\chi(G)$	4.683
$HM(G)$	214
$F(G)$	110
$SDD(G)$	21

Proof

(i) First Zagreb Index

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

$$= \sum_{uv \in E_1(G)} [d(u) + d(v)] + \sum_{uv \in E_2(G)} [d(u) + d(v)]$$

$$= 4\big(d(u) + d(v)\big) + 6\big(d(u) + d(v)\big)$$

$$= 4(2 + 2) + 6(2 + 3)$$

$$= 4(4) + 6(5)$$

$$= 16 + 30$$

$$= 46$$

(ii) Second Zagreb Index

$$M_2(G) = \sum_{uv \in E(G)} [d(u)d(v)]$$

$$= \sum_{uv \in E_1(G)} [d(u)d(v)] + \sum_{uv \in E_2(G)} [d(u)d(v)]$$

$$= 4\big(d(u)d(v)\big) + 6\big(d(u)d(v)\big)$$

$$= 4(2 \times 2) + 6(2 \times 3)$$

$$= 4(4) + 6(6)$$

$= 16 + 36$

$= 52$

(iii) Randi´c Index

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{[d(u)d(v)]}}$$

$$= \sum_{uv \in E_1(G)} \frac{1}{\sqrt{[d(u)d(v)]}} + \sum_{uv \in E_2(G)} \frac{1}{\sqrt{[d(u)d(v)]}}$$

$$= 4\left(\frac{1}{\sqrt{[d(u)d(v)]}}\right) + 6\left(\frac{1}{\sqrt{[d(u)d(v)]}}\right)$$

$$= 4\left(\frac{1}{\sqrt{2 \times 2}}\right) + 6\left(\frac{1}{\sqrt{[2 \times 3]}}\right)$$

$$= 4\left(\frac{1}{\sqrt{4}}\right) + 6\left(\frac{1}{\sqrt{6}}\right)$$

$$= 4\left(\frac{1}{2}\right) + \frac{6}{\sqrt{6}}$$

$$= 2 + \sqrt{6}$$

$$\approx 2 + 2.449$$

$$\approx 4.449$$

(iv) Atom-Bond Connectivity Index

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

$$= \sum_{uv \in E_1(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}} + \sum_{uv \in E_2(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}$$

$$= 4\left(\sqrt{\frac{2 + 2 - 2}{2 \times 2}}\right) + 6\left(\sqrt{\frac{2 + 3 - 2}{2 \times 3}}\right)$$

$$= 4\left(\sqrt{\frac{1}{2}}\right) + 6\left(\sqrt{\frac{1}{2}}\right)$$

$$= \left(\frac{4}{\sqrt{2}}\right) + \left(\frac{6}{\sqrt{2}}\right)$$

$$= \frac{10}{\sqrt{2}}$$

$$= 5\sqrt{2}$$

≈ 7.071

(v) Geometric-Arithmetic Index

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$$

$$= \sum_{uv \in E_1(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)} + \sum_{uv \in E_2(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$$

$$= 4\left(\frac{2\sqrt{2\times 2}}{2+2}\right) + 6\left(\frac{2\sqrt{2\times 3}}{2+3}\right)$$

$$= 4\left(\frac{4}{4}\right) + 6\left(\frac{2\sqrt{6}}{5}\right)$$

$$= 4(1) + \frac{12\sqrt{6}}{5}$$

$$= 4 + \frac{12\sqrt{6}}{5}$$

≈ 9.879

(vi) Harmonic Index

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$$

$$= \sum_{uv \in E_1(G)} \frac{2}{d(u)+d(v)} + \sum_{uv \in E_2(G)} \frac{2}{d(u)+d(v)}$$

$$= 4\left(\frac{2}{2+2}\right) + 6\left(\frac{2}{2+3}\right)$$

$$= 4\left(\frac{2}{4}\right) + 6\left(\frac{2}{5}\right)$$

$$= 2 + \frac{12}{5}$$

$$= \frac{22}{5}$$

$= 4.4$

(vii) Sum Connectivity Index

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$$

$$= \sum_{uv \in E_1(G)} \frac{1}{\sqrt{d(u)+d(v)}} + \sum_{uv \in E_2(G)} \frac{1}{\sqrt{d(u)+d(v)}}$$

$$= 4\left(\frac{1}{\sqrt{2+2}}\right) + 6\left(\frac{1}{\sqrt{2+3}}\right)$$

$$= 4\left(\frac{1}{2}\right) + 6\left(\frac{1}{\sqrt{5}}\right)$$

$$= 2 + \frac{6}{\sqrt{5}}$$

$$\approx 4.683$$

(viii) Hyper Zagreb Index

$$\mathrm{HM}(G) = \sum_{uv \in E(G)} [d(u)+d(v)]^2$$

$$= \sum_{uv \in E_1(G)} [d(u)+d(v)]^2 + \sum_{uv \in E_2(G)} [d(u)+d(v)]^2$$

$$= 4([2+2]^2) + 6([2+3]^2)$$

$$= 4(16) + 6(25)$$

$$= 64 + 150$$

$$= 214$$

(ix) Forgotten Index

$$\mathrm{F}(G) = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2]$$

$$= \sum_{uv \in E_1(G)} [d(u)^2 + d(v)^2] + \sum_{uv \in E_2(G)} [d(u)^2 + d(v)^2]$$

$$= 4([2^2+2^2]) + 6([2^2+3^2])$$

$$= 4(4+4) + 6(4+9)$$

$$= 4(8) + 6(13)$$

$$= 32 + 78$$

$$= 110$$

(x) Symmetric Division Degree Index

$$\mathrm{SDD}(G) = \sum_{uv \in E(G)} \left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right)$$

$$= \sum_{uv \in E_1(G)} \left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right) + \sum_{uv \in E_2(G)} \left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right)$$

$$= 4\left(\left(\frac{2}{2} + \frac{2}{2}\right)\right) + 6\left(\left[\frac{2}{3} + \frac{3}{2}\right]\right)$$

$$= 4(2) + 6\left(\frac{13}{6}\right)$$

$$= 8 + 13$$

$$= 21$$

3.1. Pearson Correlation and Linear Regression Analysis

Let $x = \{46, 52, 4.449, 7.071, 9.879, 4.4, 4.683\}$ and $y = \{118.14, 1.3, 118.0530982, 118.0530982, 28.7, 9, 103\}$.

3.2. Pearson Correlation Coefficient

The Pearson correlation coefficient is given by $r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}$

Substituting the values,

$r = -0.20688$

$$\approx -0.207$$

Thus, the Pearson correlation coefficient between x and y is, $r \approx -0.207$. This indicates a weak negative correlation.

3.3. Linear Regression Equation

The linear regression model is given by $y = ax + b$ where $a = \frac{n\sum xy - (\sum x)(\sum y)}{[n\sum x^2 - (\sum x)^2]}$ and $b = \bar{y} - a\bar{x}$. After Computation $a = -0.539572$ and $b = 80.795930$

Hence, the regression equation is $y = -0.539572x + 80.795930$ (1)

or approximately, $y = -0.540x + 80.796$.

3.4. Coefficient of Determination

The coefficient of determination is

$R^2 = r^2$

$R^2 = (-0.20688)^2$ (2)

$= 0.042799$ (3)

≈ 0.0428 (4)

Therefore, $R^2 \approx 0.0428$.

This means that approximately 4.28% of the variation in y is explained by x.

4. Conclusion

In this work, the hydrogen-suppressed molecular graph of benzimidazole was investigated using degree-based topological descriptors. The molecular graph was constructed, and the corresponding edge partitions were obtained. Using the edge partition technique and M-polynomial approach, several important topological indices including the First Zagreb index, Second Zagreb index, Randi´c index, Atom-Bond Connectivity index, Geometric-Arithmetic index, Harmonic index, Sum Connectivity index, Hyper Zagreb index, Forgotten index, and

Symmetric Division Degree index were computed. Further, a correlation and regression analysis was carried out between selected topological indices and physicochemical properties of benzimidazole. The Pearson correlation

coefficient was found to be $r \approx -0.207$, indicating a weak negative correlation between the considered variables. The obtained linear regression model is given by $y = -0.540x + 80.796$, with coefficient of determination

$R^2 \approx 0.0428$.

The low value of R^2indicates that only 4.28% of the variation in the physicochemical properties is explained by the selected topological descriptors, suggesting weak predictive capability for the present dataset. Nevertheless, the computed topological indices provide useful structural characterization of the benzimidazole molecular graph and may serve as a basis for future studies involving larger datasets of benzimidazole derivatives for improved QSPR/QSAR modeling.

Compliance with ethical standards

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Disclosure of conflict of interest

We declare that there is no conflict of interest regarding the publication of this manuscript.

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