International Journal of Applied Mathematics

Volume 38 No. 4 2025, 513–521
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)
doi: http://dx.doi.org/10.12732/ijam.v38i4.5

THE TOTAL ECCENTRICITY INDEX OF SOME BENZENOID SYSTEMS

Shahistha Hanif [1], **K. Arathi Bhat** [1,*]

[1] Department of Mathematics

Manipal Institute of Technology

Manipal Academy of Higher Education

Manipal-576104, Karnataka, INDIA

e-mail: shahistha.hanif@manipal.edu

e-mail: arathi.bhat@manipal.edu (* corresponding author)

Abstract

This article offers an extensive examination of the significance, calculation methodologies, and applications of one of the eccentricity-based topological indices in molecular chemistry. New closed formulae are developed for the total eccentricity index of linear and triangular systems of benzenoids. Further, the correlation of the total eccentricity index of benzenoids with some of its physical properties is studied with the help of regression analysis. It is found that the index exhibits a strong correlation with molecular weight and *Log P*, where *P* is the partition coefficient.

Math. Subject Classification: 05C30, 05C90, 05C92

Key Words and Phrases: topological indices, regression analysis, eccentricity, diameter, radius, degree

Received: March 22, 2025

1. **Introduction**

In graph theory, a topological index is a numerical value that characterizes the topology (structure) of a graph. It is often used to describe the molecular structure of chemical compounds, where atoms are represented as vertices and bonds as edges in a molecular graph. Topological indices help in understanding the physical, chemical, and biological properties of molecules without conducting experimental studies. They are widely applied in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies, [1].

$G(V, X)$ represents a graph with the vertex set V and the edge set X. Throughout the article, we consider only simple, connected, and undirected graphs. In a graph G, two vertices u, v are adjacent (denoted by $u \sim v$) if and only if there is an edge e between them, which is represented as $e = uv$. The degree of a vertex u, denoted by d_u is the number of vertices adjacent to it. The distance D_{uv} between two vertices u and v is the length of the shortest path between them. The eccentricity of a vertex u is given by $e_u = max\{D_{uv} : v \in V\}$. The maximum and the minimum eccentricities in a graph G, respectively are the diameter $dia(G)$ and the radius $rad(G)$.

The journey of topological indices started when the chemist Harold Wiener introduced the Wiener index in 1947 [2]. In recent decades, numerous topological indices have been introduced based on degree, distance, and eccentricity. Furthermore, the existing topological indices are continuously being redefined and modified in an effort to achieve better approximations and strengthen correlations. One of the well-known eccentricity-based topological indices defined by Farooq et.al. [3] in 2015 is the total eccentricity index

$$T(G) = \sum_{v \in V} e_v.$$

The normalized version of the total eccentricity index gives the average eccentricity of the graph. That is, the average eccentricity of a graph $G(V, X)$, denoted by $avec(G)$ is

$$avec(G) = \frac{T(G)}{|V|}.$$

The total eccentricity index is found useful in analyzing the physico-chemical, pharmacological, and toxicological properties of the oxide network [4]. The total eccentricity index is also studied by the name of eccentricity sum or total eccentricity ([5], [6]). The eccentricity-based

indices for copper oxide are computed in [7]. Gao et al. calculated the eccentric version some of the well-known degree-based indices of linear polycene parallelogram benzenoids in [8].

2. **Motivation and methodology**

The eccentricity-based topological indices often leads to sharper correlations than the classical degree-based indices, leading to novel discoveries and insights in QSPR/QAPR studies. This turns out to be the strongest driving force to take up this study for a class of aromatic hydrocarbons.

To compute our results, we use the method of combinatorial computing, graph theoretical tools like vertex and edge partitioning, and analytic techniques. Moreover, we use MATLAB for mathematical calculations and verifications. A statistical technique called regression analysis is used to capture the correlation between the dataset containing the physicochemical properties and the indices.

3. **Total eccentricity index of some benzenoid systems**

Benzenoids are a class of organic compounds that consist of fused benzene rings (hexagons) arranged in a specific geometric pattern. They are a subset of polycyclic aromatic hydrocarbons and are characterized by their conjugated $\pi-$electron systems, which provide them with aromatic stability. Benzenoids are used in the production of dyes, pigments, and plastics also as intermediates in pharmaceuticals and agrochemicals. A linear system of benzenoids contains benzene rings arranged linearly in a row (refer to Fig. 1). Let L_p represent the benzenoid, containing p hexagons, arranged in linear order. For example, naphthalene is represented by L_2 and anthracene is represented by L_3.

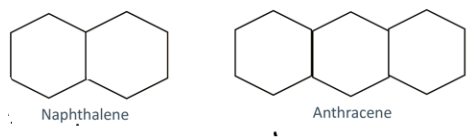

FIGURE 1. L_2 and L_3

THEOREM 3.1. *Let $G(V, X) = L_p$. Then,*

$$T(G) = 6p^2 + 8p + 2,$$
$$avec(G) = \frac{3p^2 + 4p + 1}{2p + 1}.$$

P r o o f. It is clear that $|V| = 4p + 2$ and $|X| = 5p + 1$. The vertex eccentricities in G are given as in Figure 2.

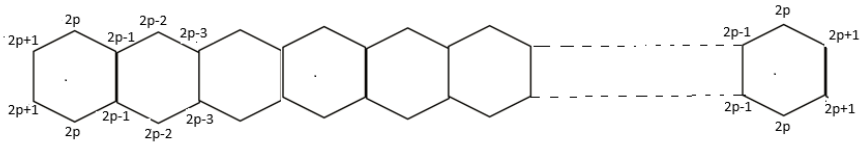

FIGURE 2. Eccentricity of vertices in L_p

The two vertices with degree 2 in the extreme ends of the hexagons have the largest eccentricity and it goes on decreasing by one as shown. The diameter being $2p + 1$ and the vertices belonging to hexagon in the median position have the least eccentricity $p + 1$. When p is odd, the two vertices of degree two belonging to hexagon in $\left(\frac{p+1}{2}\right)^{th}$ position has the least eccentricity of $p + 1$. But when p is even, the vertices of degree 3 shared by two hexagons in the positions $\frac{p}{2}$ and $\left(\frac{p}{2} + 1\right)$ have the least eccentricity. The graph L_p has 4 vertices of eccentricity k, for each $k = p+2, p+3, \ldots, 2p+1$. Further, there are 2 vertices of eccentricity $p+1$ in the median position. On enumerating and adding the eccentricities of all the vertices in G, one can get the expression for $T(G)$ and $avec(G)$. □

Another system of benzenoids most commonly available is the triangular system. The benzene rings are arranged in triangular patterns, sharing one or more edges (refer to Fig. 3). A triangular benzene T_p has p hexagons in the base graph (the lowest row L_p, containing the maximum number of hexagons).

THEOREM 3.2. *Let $G(V, X) = T_p$. Then*

$$T(G) = \frac{4p^3 + 13p^2 + 17p + 2}{2}$$
$$avec(G) = \frac{4p^3 + 13p^2 + 17p + 2}{2(p^2 + 4p + 1)}.$$

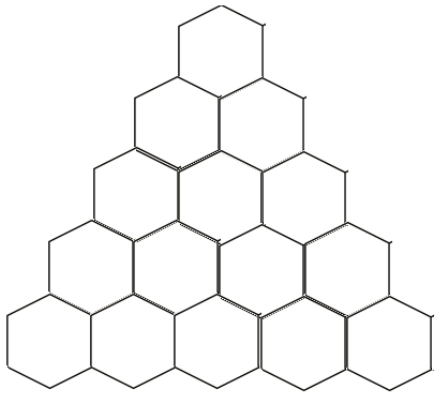

FIGURE 3. A triangular system of benzenoid T_5

P r o o f. Observe that $|V| = p^2+4p+1$ and all vertices are of degree 2 or 3. From Fig. 3, one can note that there are $(3p+3)$ vertices of degree 2, which lie in the exterior of the graph (belonging to exactly one hexagon). Remaining all the other vertices are of degree 3, out of them some lie in the exterior (shared by two hexagons) of the graph, and some lie in the interior (shared by three hexagons). We now use the technique of vertex partition based on their eccentricities as below. Let $V = V_1 \cup V_2 \cup V_3 \cup V_4$, where:

V_i	$\lvert V_i \rvert$
$V_1 = \{v \in V : d_v = 2 \text{ and } e_v = 2p+1\}$	$3p+3$
$V_2 = \{v \in V : d_v = 3 \text{ and } e_v = 2p\}$	$3p-3$
$V_3 = \{v \in V : d_v = 3 \text{ and } e_v = 2p-1\}$	$\frac{p(p-1)}{2}$
$V_4 = \{v \in V : d_v = 3 \text{ and } e_v = 2p-2\}$	$\frac{(p-1)(p-2)}{2}$

The set V_1 contains all the vertices of degree 2. The set V_2 contains all the exterior vertices of degree 3. The remaining vertices of degree 3 are contained in V_3 and V_4. On enumerating and adding the eccentricities of all the vertices in G, one can get the expression for the total eccentricity index and the average eccentricity index. □

4. **Correlation analysis**

Benzenoids are primarily used as components in fuels (particularly gasoline) as solvents, and as building blocks for the synthesis of a wide

range of chemicals including plastics, detergents, dyes, and pharmaceuticals, [10]. Monocyclic aromatic hydrocarbons also represent very important petrochemical and other intermediate, [11]. For example, toluene is used as a starting material for the synthesis of benzoic acid and benzaldehyde (used as food preservatives and flavoring and fragrance agents in food and cosmetics).

Correlation analysis is a statistical method that is used to discover if there is a relationship between two variables/datasets, and how strong that relationship may be. To quantify the strength of the relationship between two variables shown to have a linear relationship on the scatter plot, the coefficient of determination, denoted by R^2 is computed. The coefficient of determination, R^2 is a measure that provides information about the goodness of fit of a model. The range is 0 to 1, indicating 0% to 100% of the variation in the relationship.

The physical properties include molecular weight m(g/mol), boiling point BP(^0C), melting point MP(^0C), Complexity (C), and $LogP$ (where P is the partition coefficient) (refer to Table 1 for the data set). The empirical data (source: PubChem database) containing the properties of various compounds used for the analysis is given in Table 1.

4.1. **Discussion.** When exploring the relationship between two numerical variables, the first and essential step is to graphically depict the relationship on a scatter plot. For each of the parameter, a linear regression model is derived and the coefficient of determination R^2 associated with both the total eccentricity index and average eccentricity index are given.

Though we have considered several properties, not all of them yield a good correlation with all the indices. For example, the melting point does not correlate with both the indices considered here. The description of the correlation and the strength is interpreted in Table 2.

5. Conclusion

From Table 2, the properties like melting point, boiling point, complexity do not correlate with two of the eccentricity-based indices we have considered. But the total eccentricity index shows a strong correlation with the molar mass and *Log P*. The scatter plots of the two parameters are given in Figures 4 and 5.

It is noteworthy that this study concerns the prediction of physical properties like boiling point, molecular weight and *Log P* on the basis

Compound G	$T(G)$	$ave(G)$	m	C	BP	MP	$logP$
Benzene	18	3	78.11	15.5	80.1	5.53	2.13
Naphthalene	42	4.2	128.17	80.6	217.9	78.2	3.34
Phenantherene	80	5.7142	178.23	335	338	101	4.68
Chrysene	130	7.2222	228.29	264	448	448	5.73
Tetraphene	130	7.222	228.29	294	438	158	5.8
Triphenylene	130	7.2222	228.29	217	438	198	5.14
Tetrahelicene	130	7.2222	228.29	266	436	68	4.46
Naphathcene	130	7.2222	228.29	304	440	357	5.91
Pyrene	86	5.0588	202.25	236	404	150	4.88
Perylene	122	6.1	252.31	217	467	276	6.3
Benzo[a]pyrene	122	6.1	253.30	372	495	179	6.13
Benzo[e]pyrene	122	6.1	252.31	372	492.2	177	6.44
Anthracene	80	5.7142	178.23	154	341.3	216	4.56
Picene	192	8.7272	278.33	361	693	366	7.14
Coronene	150	6.25	300.35	376	525	437	6.05
Heptacene	352	11.733	378.45		677.2		
Triangulene	139	6.3181	276.33		410	171	
Benzopyrene	135	6.75	252.31	372	496	178	
Phenalene	60	4.6152	166.22	216	70	159	

TABLE 1. Index values and physicochemical properties of benzenoid systems (source: PubChem database)

Parameter	R^2 with $T(G)$	R^2 with $avec(G)$
Molar mass	**0.8375**	0.733
Complexity	0.6219	0.4725
Boiling point	0.3619	0.3219
Melting point	0.4366	0.3566
$LogP$	**0.8291**	0.6737

TABLE 2. The coefficient of determination obtained by linear regression model between the topological indices and the physicochemical properties.

of some eccentricity based topological indices. This inference is expected to contribute significantly to the Quantitative Structure-Property Relationship analysis.

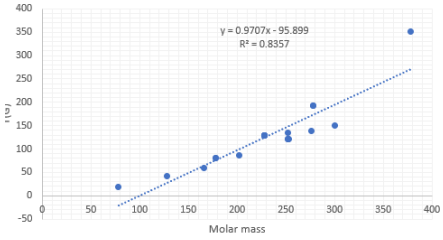

FIGURE 4. Molar mass vs total eccentricity index with $R^2 = 0.8375$

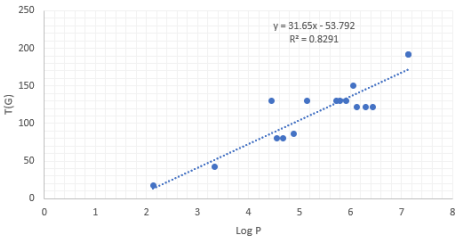

FIGURE 5. *Log P* vs total eccentricity index with $R^2 = 0.8291$

References

[1] N. Trinajstic, *Chemical Graph Theory*, CRC Press (2018).

[2] H. Wiener, Structural determination of paraffin boiling points, *Journal of the American Chemical Society*, **69**, No 1 (1947), 17-20.

[3] R. Farooq, M. Ali Malik, On some eccentricity based topological indices of nanostar dendrimers, *Optoelectronics and Advanced Materials-Rapid Communications*, **9**, No 5-6 (2015), 842-849.

[4] M. Imran, M. Kamran Siddiqui, A. A. E. Abunamous, D. Adi, S. Hafsa Rafique, A. Qudair Baig, Eccentricity based topological indices of an oxide network, *Mathematics*, **6**, No 7 (2018).

[5] K. Fathalikhani, H. Faramarzi, H. Yousefi-Azari, Total eccentricity of some graph operations, *Electronic Notes in Discrete Mathematics*, **45** (2014), 125-131.

[6] H. Smith, L. Szekely, H. Wang, Eccentricity sums in trees, *Discrete Applied Mathematics*, **207** (2016), 120-131.

[7] M. Imran, A. Q. Baig, M. Razwan Azhar, M. Reza Farahani, X. Zhang, Eccentricity based geometric-arithmetic and atom-bond connectivity indices of copper oxide CuO[372], *International Journal of Pure and Applied Mathematics*, **17**, No 3 (2018), 481–502.

[8] W. Gao, M. Reza Farahani, M. Kamran Jamil, The eccentricity version of atom-bond connectivity index of linear polycene parallelogram benzenoid ABC5(P(n,n)), *Acta Chim. Slov.*, **63** (2016), 376–379.

[9] E. Estrada, E. Uriarte, Recent advances on the role of topological indices in drug discovery research, *Current Medicinal Chemistry*, **8**, No 13 (2001), 1573-1588.

[10] H. Pan, X. Zhou, S. Xie, Z. Du, G. Li, C. Zhang, Y. Luo, X. Zhang, Selective production of monocyclic aromatic hydrocarbon from agricultural waste wheat straw for aviation fuel using Ni/ZSM-5 catalyst, *Biomass and Bioenergy*, **165** (2022), 106592.

[11] G. Busca, Production of gasolines and monocyclic aromatic hydrocarbons: from fossil raw materials to green processes, *Energies*, *14*, No 13 (2021), 4061.