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Modelling Physico-Chemical Properties of Benzenes Via Zagreb Tau Indices

Kerem Yamaç[1*]

[1]Van Yuzuncu Yil University, Faculty of Education, Department of Mathematics, 65080 Van, Türkiye.
* kyamac@yyu.edu.tr
*Orcid No: 0000-0001-5018-0618

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Abstract

Quantitative structure-property relationship (QSPR) studies use topological indices to explain the chemical and physical properties of molecular entities. In this study, we primarily determined the tau degree of a vertex along with the Zagreb tau indices for connected graphs, which represents a significant advancement in the field of (chemical) graph theory. It has been shown that there are correlations exceeding 0.95 between Zagreb tau indices and the physicochemical properties of benzenes, including boiling point, pi-electron energy, molecular weight, polarization, molecular volume, and relative formula mass. The findings show that the correlation coefficients between Zagreb tau indices and the degree-based topological indices of benzenes exceed 0.92. Additionally, structural sensitivity and abrupt change analyses were conducted on these new indices, and they were compared with other topological indices. The results and analyses confirm that the Zagreb tau indices are applicable in QSPR research efforts.

Keywords: QSPR studies, Benzenes, Topological indices, Tau degree, Zagreb tau indices.

1. Introduction

Topological indices are mathematical descriptors that transform the structure of a molecule into real-valued numbers, thereby enabling the exploration of structural characteristics and quantitative modeling of physicochemical properties [1]. Since the seminal work of Wiener in 1947 [1], thousands of distinct topological indices have been proposed, including Platt [2], Zagreb [4], Randić [5], hyper-Zagreb [12,13], and Sombor indices [17,18], which have been extensively applied in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) analyses [21–25]. Despite their success, existing indices often exhibit limitations in capturing subtle aspects of local connectivity, neighbor-degree distributions, and abrupt structural variations, especially in polycyclic aromatic hydrocarbons. As a result, new descriptors are needed to better correlate structural features with molecular properties and improve predictive performance in QSPR/QSAR models [3,24].

In this study, we introduce a novel degree-related concept called the tau degree of a vertex and, based on this, define the Zagreb tau indices for the first time. These indices aim to overcome some of the shortcomings of classical indices by simultaneously accounting for the sum and product of the degrees of neighboring vertices. Specifically, we hypothesize that the Zagreb tau indices will (i) exhibit stronger correlations with key physicochemical properties of benzenes compared to classical indices, (ii) maintain high consistency with other degree-based indices, and (iii) provide more stable structural sensitivity (smoothness) and abruptness characteristics [26–28]. To test this hypothesis, we calculated three Zagreb tau indices for a set of benzenoid hydrocarbons and modeled their boiling point, π-electron energy, molecular weight, polarization, molecular volume, and relative formula mass. We also compared these new indices to widely used topological descriptors and performed a smoothness analysis to evaluate their structural sensitivity.

The remainder of this article is organized as follows. Section 2 provides the basic definitions of the tau degree and Zagreb tau indices along with a brief overview of commonly used degree-based topological indices. Section 3 presents the calculated Zagreb tau indices for benzenes and their correlations with physicochemical properties, including linear regression models. Section 4 analyzes the relationship between the Zagreb tau indices and well-known degree-based indices, while Section 5 discusses the smoothness and abruptness properties of the new descriptors. Finally, the Conclusion summarizes

the novelty, significance, and potential applications of the Zagreb tau indices in QSPR and QSAR studies.

2. Basic Definitions

The story of topological indices began in 1947, when Harold Wiener modelled the boiling points of alkanes using the index he defined [1]. The Wiener index is defined based on the concept of distance between vertices in a graph. Contrary to popular belief, the Zagreb index is not the first degree-based index. The Platt index, which was also defined in 1947 [2], was the first degree-based index. The Hosoya index took its place in the literature as the third topological index in 1971. For the interesting story of the Hosoya index, see reference [29]. And after that Randić and Zagreb indices were defined [4,5].

Let G be a graph, and v be a vertex of this graph. This vertex's degree, $deg\ v$, is the number of edges adjacent to it. We denote the set of vertices of a graph as $V(G)$, and the set of edges as $E(G)$. Table 1 below gives the definitions of degree-based topological indices found in the literature and used in this study. We selected the indices in Table 1 due to the smoothness analysis results provided by Kumar and Das in 2024 [3]. We will be able to compare these results with the Zagreb tau indices we define in this article in the fifth section of this study.

Table 1. Indices and their definitions.

Name of Index	Symbol	Formula	Reference
The first Zagreb	M_1	$M_1 = \sum_{v\in V(G)} \deg v^2$	[4]
The second Zagreb	M_2	$M_2 = \sum_{uv\in E(G)} \deg u \deg v$	[4]
Randić	R	$R = \sum_{uv\in E(G)} \frac{1}{\sqrt{\deg u \deg v}}$	[5]
Reciprocal Randić	RR	$RR = \sum_{uv\in E(G)} \sqrt{\deg u \deg v}$	[6]
Sum-connectivity	SCI	$SCI = \sum_{uv\in E(G)} \frac{1}{\sqrt{\deg u + \deg v}}$	[7]
Symmetric division deg	SDD	$SDD = \sum_{uv\in E(G)} (\frac{\deg u}{\deg v} + \frac{\deg v}{\deg u})$	[8]
Harmonic	H	$H = \sum_{uv\in E(G)} \frac{1}{\sqrt{\deg u + \deg v}}$	[9]
Inverse sum indeg	ISI	$ISI = \sum_{uv\in E(G)} \frac{\deg u \deg v}{\deg u + \deg v}$	[8]
Atom-bond connectivity	ABC	$ABC = \sum_{uv\in E(G)} \sqrt{\frac{\deg u + \deg v - 2}{\deg u \deg v}}$	[10]
Augmented Zagreb index	AZI	$AZI = \sum_{uv\in E(G)} (\frac{\deg u \deg v}{\deg u + \deg v - 2})^3$	[11]
The first hyper-Zagreb	HM_1	$HM_1 = \sum_{uv\in E(G)} (\deg u + \deg v)^2$	[12]
The second hyper-Zagreb	HM_2	$HM_2 = \sum_{uv\in E(G)} (\deg u \deg v)^2$	[13]
Geometric-arithmetic	GA	$GA = \sum_{uv\in E(G)} \frac{2\sqrt{\deg u \deg v}}{\deg u + \deg v}$	[14]
The fourth geometric-arithmetic	GA_4	$GA_4 = \sum_{uv\in E(G)} \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v}$	[15]

Arithmetic-geometric index	AG	$AG = \sum_{uv\in E(G)} \frac{\deg u + \deg v}{2\sqrt{\deg u \deg v}}$	[16]
Sombor	SO	$SO = \sum_{uv\in E(G)} \sqrt{\deg u^2 + \deg v^2}$	[17]
Modified Sombor	SO^m	$SO^m = \sum_{uv\in E(G)} \frac{1}{\sqrt{\deg u^2 + \deg v^2}}$	[18]
Nirmala	N	$N = \sum_{uv\in E(G)} \sqrt{\deg u + \deg v}$	[19]
The first inverse Nirmala	IN_1	$IN_1 = \sum_{uv\in E(G)} \sqrt{\frac{1}{\deg u} + \frac{1}{\deg v}}$	[20]
The second inverse Nirmala	IN_2	$IN_2 = \sum_{uv\in E(G)} \frac{1}{\sqrt{\frac{1}{\deg u} + \frac{1}{\deg v}}}$	[20]

At this juncture, we are prepared to articulate the definition of the tau degree associated with a vertex, as well as the delineation of three distinct Zagreb tau indices, which constitute the foundational framework of this investigation.

Definition 2.1 Let G be an n-vertex connected graph, and let v be a vertex of G. The tau degree of the vertex v is defined as,

$$\tau(v) = \frac{1}{\sqrt[n]{S_v * M_v}} \quad (1)$$

Here, S_v is the sum of the degrees of all vertices neighboring v, and M_v is the product of the degrees of all vertices neighboring v.

Definition 2.2 The first Zagreb tau index of an n-vertex connected graph G is defined as;

$$M_1\mathrm{T}(G) = \sum_{v\in V(G)} \tau(v)^2 \quad (2)$$

Definition 2.3 The second Zagreb tau index of an n-vertex connected graph G is defined as;

$$M_2\mathrm{T}(G) = \sum_{uv\in E(G)} \tau(u)\tau(v) \quad (3)$$

Definition 2.4 The third Zagreb tau index of an n-vertex connected graph G is defined as;

$$M_3\mathrm{T}(G) = \sum_{uv\in E(G)} \big(\tau(u) + \tau(v)\big) \quad (4)$$

3. Zagreb Tau Indices for Benzenes

In this section, we demonstrate that there are correlations higher than 0.95 between the Zagreb tau indices and the physico-chemical properties of benzenes such as boiling point (BP), pi electron energy (Pi-ele), molecular weight (MW), polarization (PO), molecular volume (MV) and relative formula mass (MR). Therefore, we present the mathematical models of benzene chemical properties based on the Zagreb tau indices. For the studies so far, see [20-29]. Benzene values are taken from these studies.

3.1. Data and Computational Details

The physicochemical properties of benzenoid hydrocarbons (boiling point, π-electron energy, molecular weight, polarization, molecular volume, and relative formula mass) used in this study were taken directly from the published literature [20–29]. The Zagreb tau indices were calculated using our own implementations based on the formal definitions given in Section 2. All correlation and regression analyses were performed in Python 3.12 (NumPy, pandas, and SciPy libraries) and cross-checked in Microsoft Excel 365. Standard errors and 95% confidence intervals of the regression parameters were computed to assess the statistical reliability of the models. This combined approach ensured transparency and reproducibility of the reported results.

Table 2 shows the calculated values of Zagreb tau indices in benzenes.

Table 2. Zagreb tau indices of benzenes.

Benzenes	The first Zagreb Tau index	The second Zagreb Tau index	The third Zagreb Tau index
Benzene	2.381	2.381	7.559
Naphthalene	5.148	5.546	15.609
Phenanthrene	8.428	9.434	24.554
Anthracene	8.408	9.460	24.590
Chrysene	11.947	13.694	33.899

Benzo[a] anthracene	11.932	13.718	33.931
Triphenylene	11.975	13.686	33.879
Tetracene	11.916	13.742	33.964
Benzo[a]pyrene	13.578	16.033	39.214
Benzo[e]pyrene	13.550	15.970	39.131
Perylene	13.598	16.017	39.189
Anthanthrene	15.301	18.506	44.687
Benzo[ghi] perylene	15.270	18.442	44.608
Dibenz[a,c] nthracene	15.615	18.181	43.462
Dibenz[a,h]anthracene	15.593	18.191	43.482
Dibenz[a,j]anthracene	15.593	18.191	43.831
Picene	15.605	18.168	43.454
Coronene	16.982	20.942	50.113
Dibenzo[a,h] pyrene	17.308	20.633	48.906
Dibenzo[a,i] pyrene	17.308	20.633	48.906
Dibenzo[a,l] pyrene	17.327	20.621	48.887
Pyrene	10.099	11.805	29.950

Table 3 shows some physical-chemical properties of benzenes.

Table 3. Some physical-chemical properties of benzenes.

Benzenes	BP	Pi-ele	MW	PO	MV	MR
Benzene	78.800	8.000	78.110	10.400	89.400	26.300
Naphthalene	221.500	13.683	128.170	17.500	123.500	44.100
Phenanthrene	337.400	19.448	178.230	24.600	157.700	61.900
Anthracene	337.400	19.314	178.230	24.600	157.700	61.900
Chrysene	448.000	25.192	228.300	31.600	191.800	79.800
Benzo[a] anthracene	436.700	25.101	228.300	31.600	191.800	79.800
Triphenylene	425.000	25.275	228.300	31.600	191.800	79.800
Tetracene	436.700	25.188	228.300	31.600	191.800	79.800
Benzo[a]pyrene	495.000	28.222	252.300	35.800	196.100	90.300
Benzo[e]pyrene	467.500	28.336	252.300	35.800	196.100	90.300
Perylene	467.500	28.245	252.300	35.800	196.100	90.300
Anthanthrene	497.100	31.253	276.300	40.000	200.400	100.800
Benzo[ghi] perylene	501.000	31.425	276.300	40.000	200.400	100.800
Dibenz[a,c] nthracene	518.000	30.942	278.300	38.700	225.900	97.600
Dibenz[a,h]anthracene	524.700	30.881	278.300	38.700	225.900	97.600
Dibenz[a,j]anthracene	524.700	30.880	278.300	38.700	225.900	97.600
Picene	519.000	30.943	278.300	38.700	225.900	97.600
Coronene	525.600	34.572	300.400	44.100	204.700	111.400
Dibenzo[a,h] pyrene	552.300	33.928	302.400	42.900	230.200	108.100
Dibenzo[a,i] pyrene	552.300	33.954	302.400	42.900	230.200	108.100
Dibenzo[a,l] pyrene	552.300	34.031	302.400	42.900	230.200	108.100
Pyrene	404.000	22.506	202.250	28.700	162.000	72.500

Table 4 shows the correlation coefficients between the properties of benzenes and the Zagreb tau indices.

Table 4. The correlation coefficients between properties of benzenes and the Zagreb tau indices.

	The first Zagreb Tau index	**The second Zagreb Tau index**	**The third Zagreb Tau index**
BP	0.97833	0.97095	0.9747
Pi-ele	0.99803	0.99832	0.99934
MW	0.99888	0.99711	0.99787
PO	0.9964	0.99826	0.99951
MV	0.96847	0.95338	0.95228
MR	0.99637	0.99824	0.99951

As can be seen from Table 4, the correlation coefficients between the three new indices and the properties of benzenes are greater than 0,95. Therefore, it is seen that the first condition required to define a new index presented in this article is met.

Now we give the linear regression graphs of the physico-chemical properties with the help of the index giving the highest correlation.

Linear regression model of boiling points of benzenes via the first Zagreb tau index is showed in Figure 1.

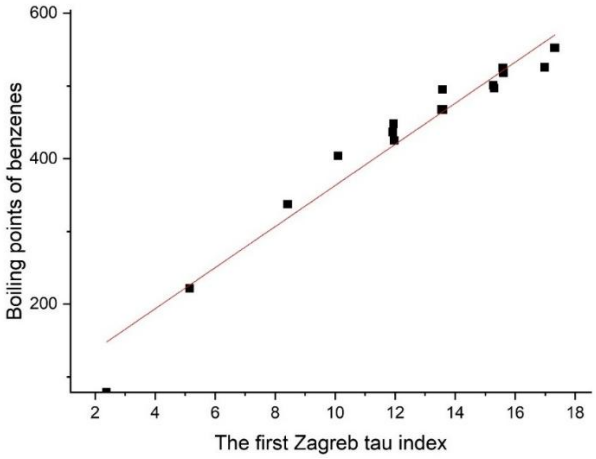

Figure 1. The linear fitting modelling of boiling points of benzenes via the first Zagreb tau index

The technical details of the graph given in Figure 1 are given below in Table 5.

Table 5. Details of linear regression model of boiling points of benzenes via the first Zagreb tau index.

Equation	Linear regression model of boiling points of benzenes via the first Zagreb tau index
Intercept	80.51723 ± 18.09627
Slope	28.26323 ± 1.3374
Pearson's R	0.97833
R-Square (COD)	0.95714
Adj. R-Square	0.95499

Linear regression model of **pi-electron energy levels** of benzenes via the second Zagreb tau index is showed in Figure 2.

Figure 2. The linear fitting modelling of pi electron energy levels of benzenes via the second Zagreb tau index

The technical details of the graph given in Figure 2 are given below in Table 6.

Table 6. Details of linear regression model of pi electron energy levels of benzenes via the second Zagreb tau index.

Equation	Linear regression model of pi electron energy levels of benzenes via the first Zagreb tau index
Intercept	6.01066 ± 0.2842
Slope	1.37453 ± 0.01782
Pearson's R	0.99832
R-Square (COD)	0.99665
Adj. R-Square	0.99648

Linear regression model of **molecular weight** of benzenes via the first Zagreb tau index is showed in Figure 3.

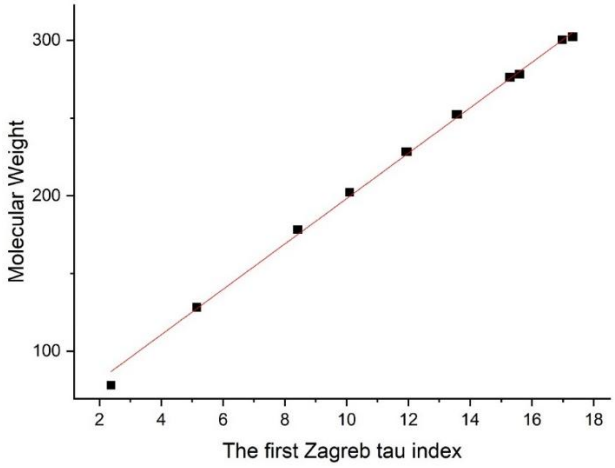

Figure 3. The linear fitting modelling of molecular weight of benzenes via the first Zagreb tau index

The technical details of the graph given in Figure 3 are given below in Table 7.

Table 7. Details of linear regression model of molecular weight of benzenes via the first Zagreb tau index.

Equation	Linear regression model of molecular weight of benzenes via the first Zagreb tau index
Intercept	52.18749 ± 2.0927
Slope	14.60484 ± 0.15466
Pearson's R	0.99888
R-Square (COD)	0.99776
Adj. R-Square	0.99765

Linear regression model of **polarization** of benzenes via the second Zagreb tau index is showed in Figure 4.

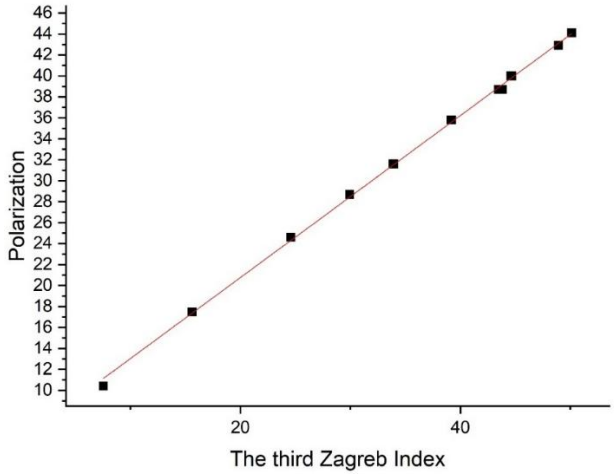

Figure 4. The linear fitting modelling of polarization of benzenes via the first Zagreb tau index

The technical details of the graph given in Figure 4 are given below in Table 8.

Table 8. Details of linear regression model of polarization of benzenes via the third Zagreb tau index.

Equation	Linear regression model of polarization of benzenes via the third Zagreb tau index
Intercept	5.30677 ± 0.20926
Slope	0.7728 ± 0.00541
Pearson's R	0.99951
R-Square (COD)	0.99902
Adj. R-Square	0.99897

Linear regression model of **molecular volume** of benzenes via the first Zagreb tau index is showed in Figure 5.

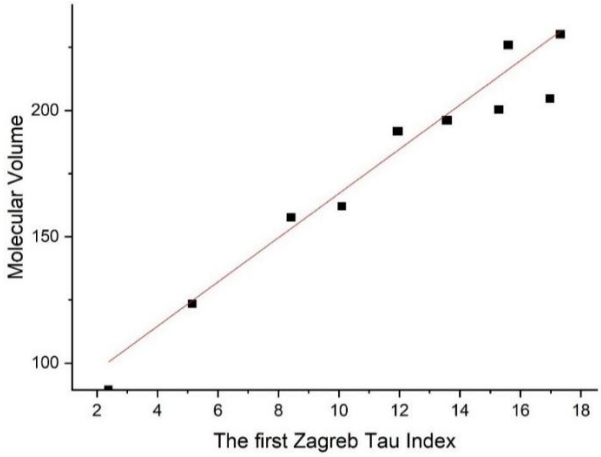

Figure 5. The linear fitting modelling of molecular volume of benzenes via the first Zagreb tau index

The relatively lower correlation observed for molecular volume compared to other properties may stem from the fact that molecular volume reflects three-dimensional packing and steric effects, which are less directly encoded by the neighbor-degree patterns captured by the Zagreb tau indices.

The technical details of the graph given in Figure 5 are given below in Table 9.

Table 9. Details of linear regression model of molecular volume of benzenes via the first Zagreb tau index.

Equation	Linear regression model of molecular volume of benzenes via the first Zagreb tau index
Intercept	79.53736 ± 6.81869
Slope	8.76101 ± 0.50393
Pearson's R	0.96847
R-Square (COD)	0.93794
Adj. R-Square	0.93483

Linear regression model of **MR** of benzenes via the third Zagreb tau index is showed in Figure 6.

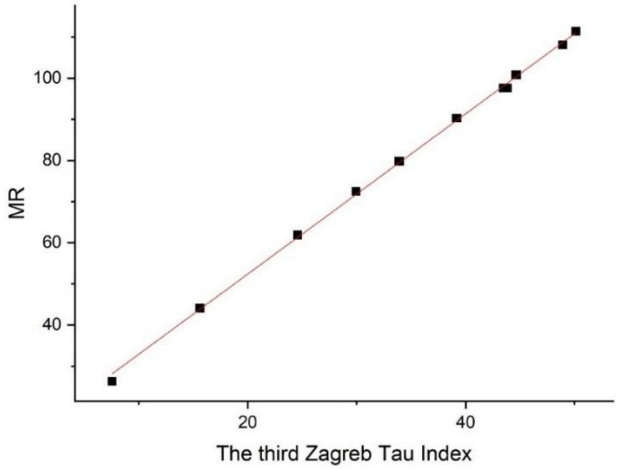

Figure 6. The linear fitting modelling of MR of benzenes via the third Zagreb tau index

The technical details of the graph given in Figure 6 are given below in Table 10.

Table 10. Details of linear regression model of MR of benzenes via the third Zagreb tau index.

Equation	Linear regression model of MR of benzenes via the third Zagreb tau index
Intercept	13.41676 ± 0.52785
Slope	1.94818 ± 0.01366
Pearson's R	0.99951
R-Square (COD)	0.99902
Adj. R-Square	0.99897

4. Relations With Other Indices

The fourth section provided correlation coefficients between the Zagrep tau indices of benzene and well-known degree based topological indices such as; Randić (R), Atom-Bond Connectivity (ABC), Augmented Zagreb (AZI), Geometric-Arithmetic (GA), the first and second Zagreb (M_1, M_2), Sombor (S) topological indices. The values taken from the references [21] and [25].

Table 11. Well-known degree based topological indices of benzenes.

Benzenes	*R*	*ABC*	*AZI*	*GA*	M_1	M_2	*SO*
Benzene	3.000	4.2426	48	6	24	24	16.9706
Naphthalene	4.966	7.7377	91.3906	10.9192	50	57	35.6354
Phenanthrene	6.950	11.1924	138.1719	15.8788	76	91	54.1602

Anthracene	6.933	11.2328	134.7813	15.8384	76	90	54.3003
Chrysene	8.933	14.647	184.9531	20.8384	102	125	72.785
Benzo[a] anthracene	8.916	14.6875	181.5625	20.798	102	124	72.8251
Triphenylene	8.950	14.6066	188.3438	20.8788	102	126	72.545
Tetracene	8.899	14.7279	178.1719	20.7576	102	123	72.9651
Benzo[a]pyrene	9.916	16.647	219.125	23.8384	120	152	85.413
Benzo[e]pyrene	9.933	16.647	219.125	23.798	120	151	85.553
Perylene	9.933	16.647	219.125	23.8384	120	152	85.413
Anthanthrene	10.899	18.7279	246.5156	26.7576	138	177	98.4209
Benzo[ghi] perylene	10.916	18.6875	249.9063	26.798	138	178	98.2809
Dibenz[a,c] Anthracene	10.916	18.1017	231.7344	25.798	128	159	91.2098
Dibenz[a,h]anthracene	10.899	18.1421	228.3438	25.7576	128	158	91.3499
Dibenz[a,j]anthracene	10.899	18.1421	228.3438	25.7576	128	158	91.3499
Picene	10.915	18.1017	231.7344	25.798	128	159	91.2098
Coronene	11.899	20.7279	280.6875	29.7576	156	204	111.1489
Dibenzo[a,h] pyrene	11.582	20.1421	262.5156	28.7576	146	185	104.0778
Dibenzo[a,i] pyrene	11.566	20.1421	262.5156	28.7576	146	185	104.0778
Dibenzo[a,l] pyrene	11.491	20.1017	265.9063	28.798	146	186	103.9378
Pyrene	11.915	13.2328	168.9531	18.8384	94	117	67.0282

Table 12 shows the correlations between the Randić (R), the Randić (R), Atom-Bond Connectivity (ABC), Augmented Zagreb (AZI), Geometric-Arithmetic (GA), the first and second Zagreb (M_1, M_2), Sombor (S) topological indices and the newly defined Zagreb tau indices.

Table 12. The correlation coefficients between the well-known topological indices and the Zagreb tau indices.

Indices	*R*	*ABC*	*AZI*	*GA*	M_1	M_2	*SO*
The first Zagreb Tau index	0.92417	0.9257	0.93027	0.92417	0.9257	0.93027	0.92417
The second Zagreb Tau index	0.99657	0.99822	0.99949	0.99657	0.99822	0.99949	0.99657
The third Zagreb Tau index	0.98926	0.99454	0.99601	0.98926	0.99454	0.99601	0.98926

As can be seen from Table 12, the correlation coefficients between the firstZagreb tau indices, and the Randić (R), Atom-Bond Connectivity (ABC), Augmented Zagreb (AZI), Geometric-Arithmetic (GA), the first and second Zagreb (M1, M2), Sombor (S) topological indices are greater than 0,92.

The correlation coefficients between the third Zagreb tau indices, and the Randić (R), Atom-Bond Connectivity (ABC), Augmented Zagreb (AZI), Geometric-Arithmetic (GA), the first and second Zagreb (M1, M2), Sombor (S) topological indices are greater than 0,98. These indicate a very strong relationship.

5. Smoothness Analysis

In this section, we investigate the smoothness properties of particular Zagreb tau topological indices and conduct a comparative evaluation against the esTablelished findings pertaining to various noTable topological indices. Two innovative graph structural metrics, namely structure sensitivity (denoted as SS) and abruptness (symbolized as Abr), were introduced in reference [26] to assess the smoothness of a molecular descriptor. Recent academic literature has scrutinized the structure sensitivity (SS) of eigenvalue-based topological indices and the smoothness of graph energy within chemical graphs, as discussed in publications [27] and [28], respectively. Refer to reference 26 for the algorithm formulated to compute the SS and Abr of a topological index associated with a designated class of connected graphs. Kumar and Das conducted a smoothness analysis of the fifteen degree-based topological indices presented in Table 1 for all tree graphs comprising between four and ten vertices, utilizing the algorithm devised to compute the SS and Abr of a topological index.

Employing the same algorithm, the results of the structure sensitivity (SS) and abruptness (Abr) analysis for Zagreb tau indices have been computed for tree graphs ranging from four to nine vertices and are delineated in Table 13.

These smoothness and abruptness results indicate that the Zagreb tau indices exhibit favorable structural sensitivity and can therefore be applied reliably to chemical graphs for QSPR/QSAR modeling, offering a balanced combination of sensitivity to local structural changes and overall stability.

Table 13. Structure sensitivity (SS) and abruptness (Abr) analysis results of Zagreb tau indices on tree graphs.

Zagreb Tau Indices	n=4		n=5		n=6		n=7		n=8		n=9	
	SS	Abr	SS	Abr	SS	Abr	SS	Abr	SS	Abr	SS	Abr
$M_1\Psi$	0.1422	0.1422	0.1312	0.1366	0.0745	0.1034	0.0583	0.0912	0.0440	0.0713	0.0400	0.0804
$M_2\Psi$	0.0030	0.0030	0.0493	0.061	0.062	0.1069	0.0446	0.0851	0.0424	0.0782	0.0352	0.0754
$M_3\Psi$	0.0103	0.0103	0.0284	0.0326	0.0341	0.0564	0.0224	0.0421	0.0210	0.0385	0.0174	0.0373

For a topological index to exhibit efficacy, it is imperative that the SS value be optimized while simultaneously reducing the Abr value. In the context of nine-vertex tree graphs, a comparative analysis of the outcomes presented in Table 8 alongside the findings in Table 1 of the third reference and Table 3 of the twenty-sixth reference reveals that the SS value of the Zagreb Tau indices surpasses that of the first inverse Nirmala index. Furthermore, in alignment with this observation, it is noted that the Abr value of the Zagreb Tau indices also exceeds that of the first inverse Nirmala index. Consequently, the proximity of the Abr values to the minimum threshold can be regarded as a favorable aspect for the Zagreb Tau indices. Nevertheless, the closeness of the SS values to the minimum threshold may be construed as a disadvantage for the Zagreb Tau indices.

6. Conclusion

In this study, we proposed the tau degree of a vertex and introduced, for the first time, three Zagreb tau indices as novel degree-based topological descriptors. Using a comprehensive dataset of benzenoid hydrocarbons, we demonstrated that the Zagreb tau indices exhibit very strong correlations (Pearson's R > 0.95) with key physicochemical properties such as boiling point, π-electron energy, molecular weight, polarization, molecular volume, and relative formula mass [20–25]. We also showed that these indices maintain high consistency (R > 0.92) with other established degree-based topological indices, confirming their robustness and compatibility with existing descriptors. Furthermore, the structural sensitivity (SS) and abruptness (Abr) analyses revealed favorable smoothness properties of the Zagreb tau indices compared to several classical indices [26–28].

Beyond reporting correlations, we provided a chemical interpretation of the observed trends. In particular, the strong association between the Zagreb tau indices and π-electron energy or polarization reflects their ability to capture the delocalized electron environment in benzenoid systems, while the slightly lower correlation for molecular volume indicates structural aspects that are less directly encoded by neighbor-degree patterns. These insights highlight the conceptual advantage of the tau-based formulation over traditional indices.

Overall, the findings suggest that the Zagreb tau indices constitute a promising addition to the toolkit of chemical graph theory and QSPR/QSAR modeling. By integrating sum–product information of neighboring degrees, they offer improved sensitivity to subtle structural variations and enhanced predictive performance for physicochemical properties. Future research may extend these indices to other classes of molecular graphs, explore nonlinear and machine-learning-based regression models, and evaluate their applicability in the prediction of biological activities or nanomaterial properties [3,24]. Thus, the present study not only introduces a new family of indices but also provides a foundation for their broader use in chemical informatics and theoretical chemistry.

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Author's Contributions

Kerem Yamaç: Conceived and designed the study, performed the experiments and data analysis, interpreted the results, and wrote the manuscript.

Ethics

There are no ethical issues after the publication of this manuscript.

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