Research Article

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Modeling benzene physicochemical properties using Zagreb upsilon indices

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Abstract: Quantitative structure–property relationship (QSPR) frameworks leverage topological indices to model the physicochemical attributes of molecular structures. In this study, we introduce the concept of upsilon degree and define the Zagreb upsilon indices based on this concept. Our findings demonstrate that the second Zagreb upsilon index exhibits the highest predictive accuracy for the π–electron energy of benzenes, surpassing existing degree-based topological indices with correlation coefficients exceeding 0.93. This accuracy was measured using statistical correlation analysis, and a direct comparison with the Randić and geometric-arithmetic indices further supports the superior performance of the second Zagreb upsilon index. Furthermore, structural sensitivity and abruptness analyses, which assess the stability and variation of an index across different molecular structures, indicate that Zagreb upsilon indices offer superior performance compared to alternative indices. These results suggest that Zagreb upsilon indices have significant potential as a new and effective tool for QSPR research.

Keywords: QSPR studies, benzenes, topological indices, Upsilon degree, Zagreb upsilon indices

1 Introduction

Topological indices are essential tools for obtaining real-valued metrics that are inherently connected to molecular structures, enabling a comprehensive analysis of their structural characteristics. The numerical metrics derived from topological indices can be employed to develop mathematical frameworks that incorporate parameters collected from empirical research in the physical and chemical sciences.

The current work on chemical graph theory includes thousands of distinct topological indices. The adoption of a new index requires evidence of its relative excellence compared to existing indices across three critical dimensions:

The proposed index must exhibit a correlation coefficient greater than 0.99 with at least one physical or chemical attribute of the molecules in question.

The correlation coefficients between the newly added index and the values of existing indices must surpass 0.9.

An analysis of the structural characteristics, particularly regarding smoothness and degeneracy, of the new index must produce results that are demonstrably superior to those obtained from existing indices.

When we examined the relevant literature, we noticed that none of the degree-based indices calculate the exponent of the degree based on a parameter obtained from the degree. To fill this gap, we defined the upsilon degree and the Zagreb upsilon indices accordingly. Also, a new index is defined in the chemical graph theory literature; the correlation values of this index are first calculated in either octanes or benzenes [1–7]. In this study, the values in similar ones are first examined, and in subsequent studies, the correlation results for octanes will be examined.

This academic discourse presents the concept of the upsilon degree of a vertex, representing a novel contribution to the field of graph theory. We introduce the Zagreb upsilon indices for the first time based on this underlying concept. We conduct a comprehensive study of the newly established indices based on the specified criteria, focusing on factors such as boiling point (BP), pi-electron energy (Pi-ele), molecular weight (MW), polarization (PO), molecular volume (MV), and relative formula mass of benzene derivatives. This article aims to deliver a comprehensive understanding of the subject, systematically organized as follows: The introduction part defines essential terms and clarifies the most often used indices in the literature, including the upsilon degrees and Zagreb upsilon indices used in this study. The following section outlines the Zagreb upsilon indices relevant to benzene molecules. We conducted analyses of the correlations between several properties – specifically BP, Pi-ele, MW,

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PO, MV, and relative formula mass of benzene – and the values related to the Zagreb upsilon indices in this section. These values were methodically contrasted with all relevant values documented in the current academic literature. We observed the second largest correlation linked to the third Zagreb upsilon index. Thus, we developed mathematical models for benzene's BP, Pi-ele, MW, PO, MV, and relative formula mass with the Zagreb upsilon indices. The fourth part delineates the correlation coefficients connecting benzene's Zagreb upsilon indices with other topological indices. The fifth segment includes a variety of structural evaluations. These inquiries collectively demonstrate that the Zagreb upsilon indices are unique tools particularly well-suited for quantitative structure-activity relationship studies.

In Figure 1, images symbolizing the chemical structure of the benzenoid hydrocarbons (BHs) whose properties we examined are given.

MAPLE software was used for the validation of calculations. Additional statistical analyses, including regression equations and fundamental parameters, were performed using ORIGIN software.

2 Basic definitions

The discourse on topological indices began in 1947, when Harold Wiener formulated the boiling temperatures of

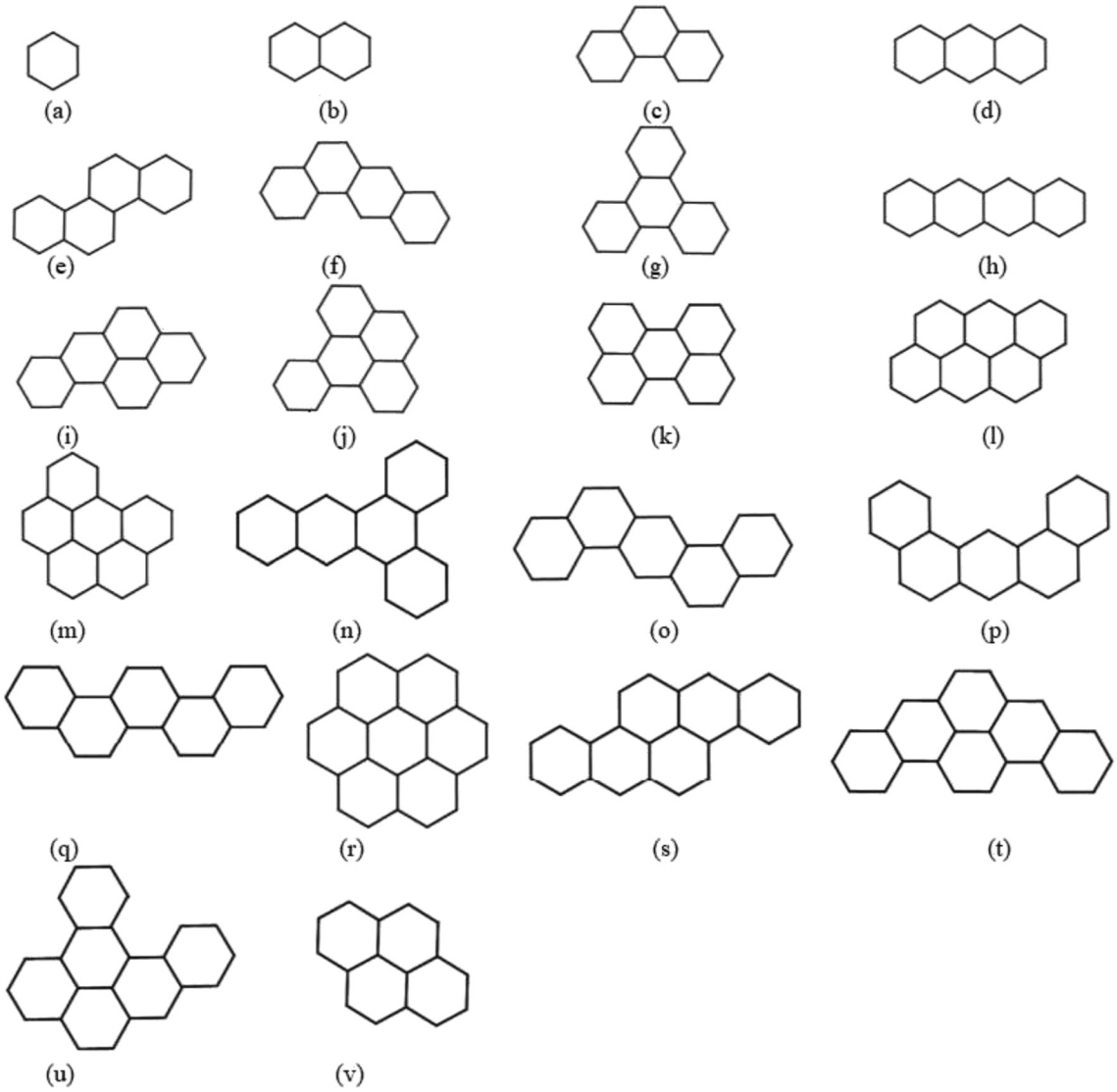

Figure 1: (a) Benzene, (b) naphthalene, (c) phenanthrene, (d) anthracene, (e) chrysene, (f) benzo[*a*]anthracene, (g) triphenylene, (h) tetracene, (i) benzo[*a*]pyrene, (j) benzo[*e*]pyrene, (k) perylene, (l) anthanthrene, (m) benzo[*ghi*]perylene, (n) dibenz[*a,c*]anthracene, (o) dibenz[*a,h*]anthracene, (p) dibenz[*a,j*]anthracene, (q) picene, (r) coronene, (s) dibenzo[*a,h*]pyrene, (t) dibenzo[*a,i*]pyrene, (u) dibenzo[*a,l*]pyrene, and (v) pyrene [8].

Table 1: Indices and their definitions

Name of index	Symbol	Formula	Reference
The first Zagreb	M_1	$M_1 = \sum_{v \in V(G)} \deg v^2$	[9]
The second Zagreb	M_2	$M_2 = \sum_{uv \in E(G)} \deg u \deg v$	[9]
Randić	R	$R = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u \deg v}}$	[10]
Reciprocal Randić	RR	$\mathrm{RR} = \sum_{uv \in E(G)} \sqrt{\deg u \deg v}$	[11]
Sum-connectivity	SCI	$\mathrm{SCI} = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u + \deg v}}$	[12]
Symmetric division deg	SDD	$\mathrm{SDD} = \sum_{uv \in E(G)} \left(\frac{\deg u}{\deg v} + \frac{\deg v}{\deg u} \right)$	[13]
Harmonic	H	$H = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u + \deg v}}$	[14]
Inverse sum index	ISI	$\mathrm{ISI} = \sum_{uv \in E(G)} \frac{\deg u \deg v}{\deg u + \deg v}$	[13]
Atom-bond connectivity	ABC	$\mathrm{ABC} = \sum_{uv \in E(G)} \sqrt{\frac{\deg u + \deg v - 2}{\deg u \deg v}}$	[15]
Augmented Zagreb index	AZI	$\mathrm{AZI} = \sum_{uv \in E(G)} \left(\frac{\deg u \deg v}{\deg u + \deg v - 2} \right)^3$	[16]
The first hyper-Zagreb	HM_1	$\mathrm{HM}_1 = \sum_{uv \in E(G)} (\deg u + \deg v)^2$	[17]
The second hyper-Zagreb	HM_2	$\mathrm{HM}_2 = \sum_{uv \in E(G)} (\deg u \deg v)^2$	[18]
Geometric-arithmetic	GA	$GA = \sum_{uv \in E(G)} \frac{2\sqrt{\deg u \deg v}}{\deg u + \deg v}$	[19]
The fourth geometric-arithmetic	GA_4	$\mathrm{GA}_4 = \sum_{uv \in E(G)} \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v}$	[20]
Arithmetic-geometric index	AG	$\mathrm{AG} = \sum_{uv \in E(G)} \frac{\deg u + \deg v}{2\sqrt{\deg u \deg v}}$	[21]
Sombor	SO	$\mathrm{SO} = \sum_{uv \in E(G)} \sqrt{\deg u^2 + \deg v^2}$	[22]
Modified Sombor	SO^m	$\mathrm{SO}^m = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u^2 + \deg v^2}}$	[23]
Nirmala	N	$N = \sum_{uv \in E(G)} \sqrt{\deg u + \deg v}$	[24]
The first inverse Nirmala	IN_1	$\mathrm{IN}_1 = \sum_{uv \in E(G)} \sqrt{\frac{1}{\deg u} + \frac{1}{\deg v}}$	[25]
The second inverse Nirmala	IN_2	$\mathrm{IN}_2 = \sum_{uv \in E(G)} \frac{1}{\sqrt{\frac{1}{\deg u} + \frac{1}{\deg v}}}$	[25]

alkanes using his proposed index [26]. The Wiener index quantifies distances between vertices in a graph. Contrary to common belief, the Zagreb index is not the first degree-based index. The Platt index, developed in 1947 [27], is acknowledged as the inaugural degree-based index. The Hosoya index subsequently appeared in the literature as the third topological index in 1971. For a compelling exposition of the Hosoya index, consult source 29. Subsequent to this evolution, the Randić and Zagreb indices were defined [9,10].

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 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 [28]. We will be able to compare these results with the Zagreb upsilon indices we define in this article in the fifth section of this study.

The upsilon degree was introduced to address a gap in the literature specifically, the absence of a degree-based parameter that could act as an exponent in topological indices. While many existing indices use the degree of a vertex directly or in a linear form, our approach introduces a nonlinear, multiplicative structure based on the degrees of neighboring vertices.

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

$$U(v) = \deg v^{1/M(v)}. \tag{1}$$

Here, $M(v)$ is the multiplication of the degrees of all vertices neighboring v.

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

$$UZ_1(G) = \sum_{v \in V(G)} U(v)^2. \tag{2}$$

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

$$UZ_2(G) = \sum_{uv \in E(G)} U(u)U(v). \tag{3}$$

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

$$UZ_3(G) = \sum_{uv \in E(G)} (U(u) + U(v)). \tag{4}$$

These definitions enable the proposed indices to not only reflect the degree of each vertex but also to capture the complexity of their local structural environments. This multiplicative design increases the sensitivity of the indices for distinguishing between molecular structures in quantitative structure–property relationship (QSPR) modeling.

The upsilon degree is defined based on the product of the degrees of neighboring vertices. This formulation allows Zagreb upsilon indices to capture structural differences more effectively than conventional indices.

For instance, consider two molecular structures with similar vertex degrees but different neighborhood compositions. Traditional indices may yield nearly identical values for these structures, whereas upsilon degree-based indices can differentiate them due to the exponential effect of degree multiplication. This property provides a critical advantage in QSPR modeling, where identifying molecular structural differences is essential.

Furthermore, the multiplicative formulation of the upsilon degree, defined as the product of the degrees of the neighboring vertices of a given vertex v, is not arbitrary but is rooted in its ability to amplify local structural variations in a molecular graph. Mathematically, the product

$$\prod_{u \in N(v)} \mathrm{d}(u),$$

captures the interaction intensity among the neighbors of v, and its use as an exponent in the Zagreb upsilon indices leads to nonlinear growth with respect to local connectivity. This is particularly valuable in QSPR applications where subtle structural differences can lead to significant changes in molecular properties. Unlike additive formulations, which may smooth out such distinctions, the multiplicative form magnifies them, making the index more sensitive to topological changes. Moreover, this formulation aligns with principles found in entropy-based descriptors and multiplicative connectivity indices, where exponential growth or suppression accurately reflects structural complexity and branching. Thus, the multiplicative form is not only novel but also mathematically justified in enhancing the discriminatory power of the proposed indices. This reasoning is consistent with prior studies that emphasize the sensitivity and nonlinearity advantages of multiplicative degree-based indices in molecular topology [15,29].

3 Zagreb upsilon indices for benzenes

This section demonstrates correlations greater than 0.95 between the Zagreb upsilon indices and the physico-chemical properties of benzenes, including BP, Pi-ele, MW, PO, MV, and relative formula mass (MR). Therefore, we present the mathematical models that define the chemical characteristics of benzene based on the Zagreb upsilon indices. Refer to studies [8,25,29–36] for the current findings. Benzene concentrations are derived from these research studies.

Table 2: Zagreb upsilon indices of benzenes

Benzenes	The first Zagreb upsilon index	The second Zagreb upsilon index	The third Zagreb upsilon index
Benzene	8,485	8,485	14,270
Naphthalene	13,098	14,289	25,069
Phenanthrene	17,878	20,194	35,936
Anthracene	17,833	20,225	35,965
Chrysene	22,657	26,099	46,804
Benzo[*a*]anthracene	22,613	26,131	46,832
Triphenylene	22,823	26,189	46,872
Tetracene	22,568	26,161	46,860
Benzo[*a*]pyrene	24,722	29,318	53,032
Benzo[*e*]pyrene	24,690	29,202	52,927
Perylene	24,827	29,341	53,053
Anthanthrene	26,940	32,689	59,394
Benzo[*ghi*]perylene	26,830	32,510	59,233
Dibenz[*a*,*c*]anthracene	27,558	32,126	57,767
Dibenz[*a*,*h*]anthracene	27,392	32,035	57,700
Dibenz[*a*,*j*]anthracene	27,392	32,036	57,700
Picene	27,437	32,005	57,671
Coronene	28,833	35,677	65,413
Dibenzo[*a*,*h*]pyrene	29,562	35,286	63,949
Dibenzo[*a*,*i*]pyrene	29,562	35,286	63,949
Dibenzo[*a*,*l*]pyrene	29,692	35,355	64,003
Pyrene	20,238	23,866	42,595

The correlation between Zagreb upsilon indices and the physicochemical properties of benzenes was analyzed. The second Zagreb upsilon index exhibited the strongest correlation ($r > 0.99$) with π-electron energy, outperforming traditional degree-based indices.

Table 2 provides the computed values of the Zagreb upsilon indices for benzenes.

Table 3 shows some physical–chemical properties of benzenes.

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

As evidenced in Table 4, the correlation coefficients between the three newly established indices and the characteristics of benzenes exceed 0.95. Consequently, it can be concluded that the initial criterion necessary for the formulation of a new index, as delineated in the present article, has been satisfied.

We present the results obtained from the before studies conducted in the literature on BHs used in this study in the tables below.

In 1998, Nikolić et al. calculated correlation results for the Pi-ele levels and BPs of benzenoid hydrocarbons [37]. These results can be seen in Table 5.

When compared with Table 4, it is seen that the Zagreb upsilon indices defined in this study give better results than Randić and edge-connectivity indices estimating pi-electron levels.

Table 4: The correlation coefficients between properties of benzenes and the Zagreb upsilon indices

	The first Zagreb upsilon index	The second Zagreb upsilon index	The third Zagreb upsilon index
BP	0.98664	0.98147	0.97915
Pi-ele	0.99772	0.9998	0.99973
MW	0.99951	0.99906	0.99832
PO	0.99548	0.99952	0.99992
MV	0.97479	0.95777	0.95289
MR	0.99544	0.99952	0.99992

In 2020, Hayat et al. calculated correlation coefficients between the pi electron levels of BHs for 17 different indices known in the literature [31]. We present their results in Table 6.

Again, when Tables 4 and 6 are examined together, it will be seen that the second Zagreb upsilon index gives the largest coefficient.

Despite the high correlation between all Zagreb upsilon indices and the physicochemical properties of benzenes, only the graphs of the indices with the highest correlation coefficients are given in order not to bore the reader and to increase the readability of the article.

The minimum root mean square error (RMSE) increases the accuracy of a regression model. RMSE is calculated with the following formula:

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*]anthracene	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 5: The correlation coefficients between π-electron energies and BPs of BHs and the vertex-connectivity and edge-connectivity indices

	The vertex-connectivity index (Randić)	The edge-connectivity index
BP	0.9954	0.9954
Pi-ele	0.9986	0.9993

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(a_i - b_i)^2}{n}},$$

where a_i is the observed value and b_i is the predicted value. In all the graphs below, R^2 and RMSE values are given for a healthy interpretation [38].

Figure 2 shows a linear regression model of benzene BP**s** using the first Zagreb upsilon index (UZ_1).

The linear regression model of pi-electron energy levels of benzenes via the second Zagreb upsilon index (UZ_2) is shown in Figure 3.

The linear regression model of MW of benzenes via the first Zagreb upsilon index (UZ_1) is shown in Figure 4.

The linear regression model of PO of benzenes via the third Zagreb upsilon index (UZ_3) is shown in Figure 5.

The linear regression model of MV of benzenes via the first Zagreb upsilon index (UZ_1) is shown in Figure 6.

The linear regression model of **MR** of benzenes via the third Zagreb upsilon index (UZ_3) is shown in Figure 7.

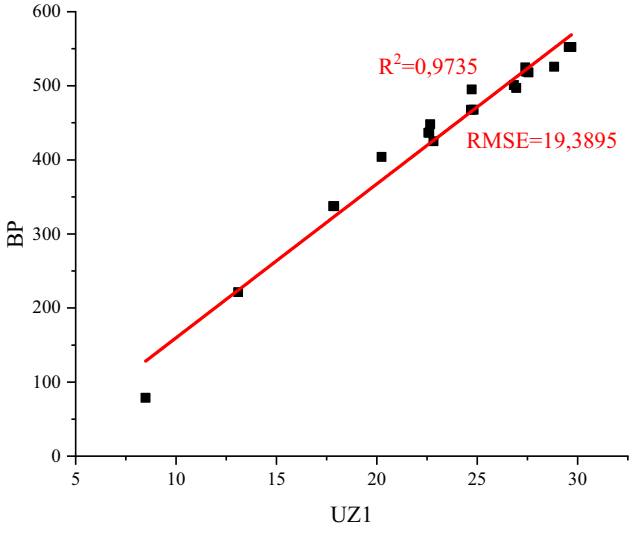

Figure 2: The linear fitting modeling of BPs of benzenes via the first Zagreb upsilon index (UZ_1).

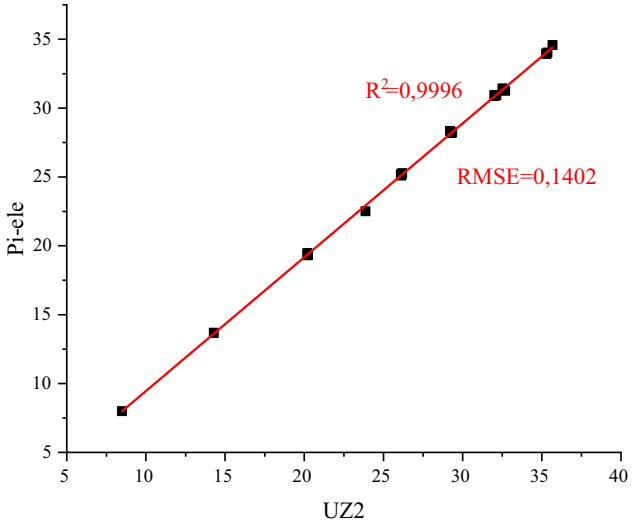

Figure 3: The linear fitting modeling of Pi-ele levels of benzenes via the second Zagreb upsilon index (UZ_2).

4 Relations with other indices

This section presents correlation coefficients between the Zagrep upsilon indices of benzene and established degree-based topological indices, including Randić (R), atom-bond connectivity (ABC), augmented Zagreb (AZI), geometric-arithmetic (GA), and the first and second Zagreb indices (M_1, M_2), as well as the Sombor (SO) index. The values derived from sources [30] and [33] are shown in Table 7.

Table 6: The correlation coefficients between π-electron energies of 17 topological indices

Index	Correlation	Index	Correlation
Wiener	0.9437	ABC_5 (atom-bond con.)	0.9656
Szeged	0.8907	GA_4 (geometric-arithmetic)	0.9991
Padmakar–Ivan	0.9684	Schultz	0.9418
Revised Szeged	0.8907	Degree-distance	0.9400
Eccentric connectivity	0.9292	Gutman	0.9334
Total eccentricity	0.9146	Additive weighted Harary	0.9763
ABC_2 (atom-bond con.)	0.9837	multiplicative weighted Harary	0.9628
GA_2 (geometric-arithmetic)	0.9874	Hyper-Wiener	0.8428

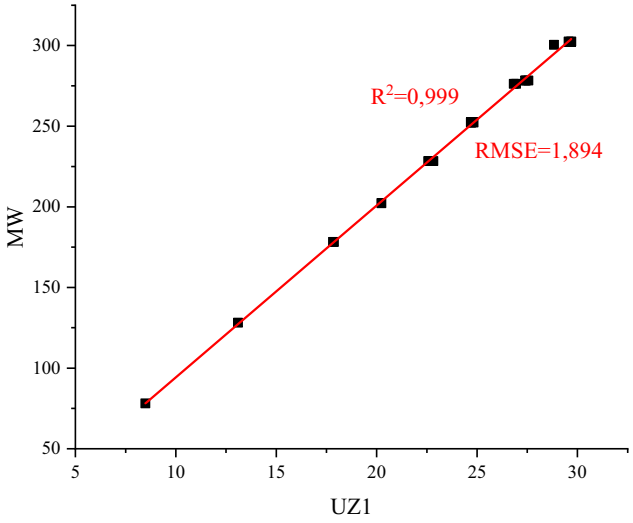

Figure 4: The linear fitting modeling of MW of benzenes via the first Zagreb upsilon index (UZ_1).

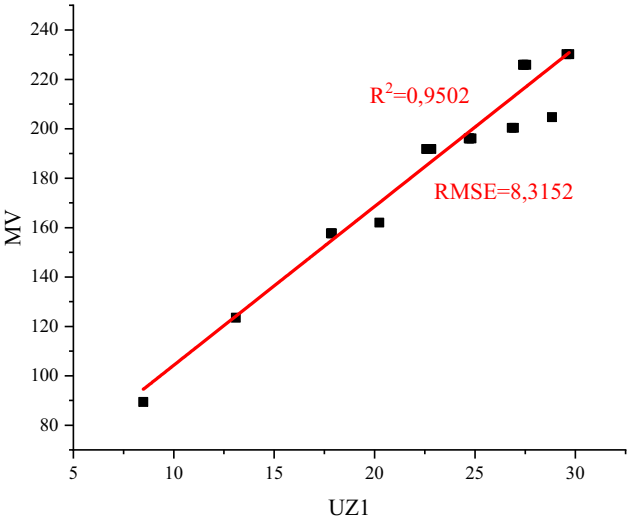

Figure 6: The linear fitting modeling of MV of benzenes via the first Zagreb upsilon index (UZ_1).

Table 8 shows the correlations between the R, R, ABC, AZI, GA, the first and second Zagreb (M_1, M_2), Sombor (SO) topological indices, and the newly defined Zagreb upsilon indices.

As can be seen from Table 8, the correlation coefficients between the first Zagreb upsilon indices and the R, ABC, AZI, GA, the first and second Zagreb (M_1, M_2), Sombor (SO) topological indices are greater than 0.93.

The correlation coefficients between the second Zagreb upsilon indices and the R, ABC, AZI, GA, the first and second Zagreb (M_1, M_2), Sombor (SO) topological indices are greater than 0.99.

The correlation coefficients between the third Zagreb upsilon indices and the R, ABC, AZI, GA, the first and second Zagreb (M_1, M_2), Sombor (SO) topological indices are greater than 0.98.

To further validate the effectiveness of Zagreb upsilon indices, their correlations with existing indices such as ABC and GA indices were analyzed. The second Zagreb upsilon index consistently demonstrated the highest correlation values.

These indicate a very strong relationship.

5 Smoothness analysis

This section examines the smoothness characteristics of specific Zagreb upsilon topological indices and does a

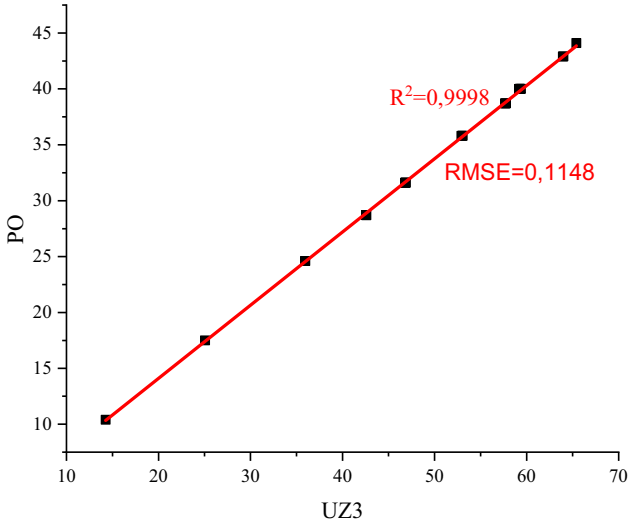

Figure 5: The linear fitting modeling of PO of benzenes via the third Zagreb upsilon index (UZ_3).

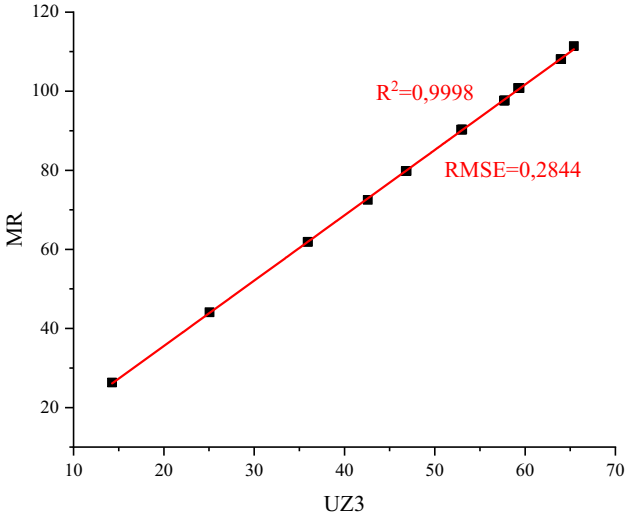

Figure 7: The linear fitting modeling of MR of benzenes via the third Zagreb upsilon index (UZ_3).

Table 7: Well-known degree-based topological indices of benzenes

Benzenes	R	ABC	AZI	GA	M_1	M_2	SO
Benzene	3,000	42,426	48	6	24	24	169,706
Naphthalene	4,966	77,377	913,906	109,192	50	57	356,354
Phenanthrene	6,950	111,924	1,381,719	158,788	76	91	541,602
Anthracene	6,933	112,328	1,347,813	158,384	76	90	543,003
Chrysene	8,933	14,647	1,849,531	208,384	102	125	72,785
Benzo[*a*]anthracene	8,916	146,875	1,815,625	20,798	102	124	728,251
Triphenylene	8,950	146,066	1,883,438	208,788	102	126	72,545
Tetracene	8,899	147,279	1,781,719	207,576	102	123	729,651
Benzo[*a*]pyrene	9,916	16,647	219,125	238,384	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	238,384	120	152	85,413
Anthanthrene	10,899	187,279	2,465,156	267,576	138	177	984,209
Benzo[*ghi*]perylene	10,916	186,875	2,499,063	26,798	138	178	982,809
Dibenz[*a*,*c*]anthracene	10,916	181,017	2,317,344	25,798	128	159	912,098
Dibenz[*a*,*h*]anthracene	10,899	181,421	2,283,438	257,576	128	158	913,499
Dibenz[*a*,*j*]anthracene	10,899	181,421	2,283,438	257,576	128	158	913,499
Picene	10,915	181,017	2,317,344	25,798	128	159	912,098
Coronene	11,899	207,279	2,806,875	297,576	156	204	1,111,489
Dibenzo[*a*,*h*]pyrene	11,582	201,421	2,625,156	287,576	146	185	1,040,778
Dibenzo[*a*,*i*]pyrene	11,566	201,421	2,625,156	287,576	146	185	1,040,778
Dibenzo[*a*,*l*]pyrene	11,491	201,017	2,659,063	28,798	146	186	1,039,378
Pyrene	11,915	132,328	1,689,531	188,384	94	117	670,282

Table 8: The correlation coefficients between the well-known topological indices and the Zagreb upsilon indices

İndices	R	ABC	AZI	GA	M_1	M_2	SO
The first Zagreb upsilon index	0.93029	0.93678	0.93543	0.93029	0.93678	0.93543	0.93029
The second Zagreb upsilon index	0.99578	0.99962	0.99994	0.99578	0.99962	0.99994	0.99578
The third Zagreb upsilon index	0.9866	0.99463	0.99617	0.9866	0.99463	0.99617	0.9866

comparative analysis with existing results related to several prominent topological indices. Furtula et al. [29] introduced two unique graph structural metrics: structural sensitivity (SS) and abruptness (Abr) to evaluate the smoothness of a molecular descriptor. Recent scholarly articles have examined the SS of eigenvalue-based topological indices and the continuity of graph energy in chemical graphs, as detailed in publications [34–36], respectively. Refer Furtula et al. [29] for the algorithm developed to calculate the SS and Abr of a topological index related to a specified class of linked networks. Kumar and Das performed a smoothness analysis of the 15°-based topological indices listed in Table 1 for all tree graphs containing 4–10 vertices, employing the algorithm developed to calculate the SS and Abr of a topological index.

Additionally, smoothness analysis was conducted using SS and Abr metrics. A high SS value indicates an index's sensitivity to molecular structural variations, while a low Abr value suggests stability. Our findings reveal that Zagreb

Table 9: SS and Abr analysis results of Zagreb upsilon indices on tree graphs

Zagreb upsilon 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
UZ_1	0.7506	0.7506	0.4911	0.7597	0.3059	0.6055	0.2207	0.4648	0.146	0.3233	0.1066	0.3365
UZ_2	0.6640	0.6640	0.4649	0.6671	0.2992	0.547	0.2192	0.4266	0.1559	0.3248	0.1219	0.3501
UZ_3	0.4647	0.4647	0.3326	0.4662	0.2040	0.3759	0.1531	0.2892	0.1063	0.215	0.0806	0.2249

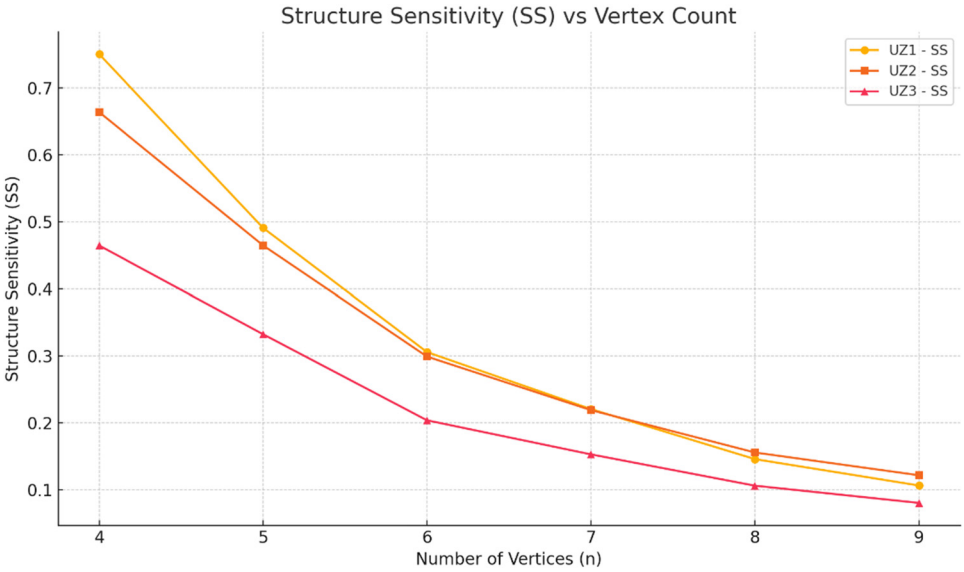

Figure 8: SS of UZ_1, UZ_2, and UZ_3 across different vertex counts.

Upsilon indices exhibit higher SS values than conventional indices, making them particularly suitable for QSPR applications.

The results of the SS and Abr analysis for Zagreb upsilon indices, utilizing the same algorithm, have been calculated for tree graphs with four to nine vertices and are presented in Table 9.

The exact computation of SS and Abr follows the algorithm proposed by Furtula et al. [29], which systematically evaluates the variation of a topological index over structurally distinct but size-equivalent graphs.

For a topological index to be effective, it is necessary to optimize the SS value while simultaneously reducing the Abr value. In the context of nine-vertex tree graphs, it has been shown that the SS value of the Zagreb Upsilon indices exceeds the values of the first Zagreb, Randić, ABC, and GA indices for $n = 9$ vertex trees. Additionally, in line with this observation, it has been noted that the Abr value of the Zagreb upsilon indices is greater than the values of all other indices.

To improve the interpretability of the smoothness analysis, we visualized the behavior of SS and Abr values

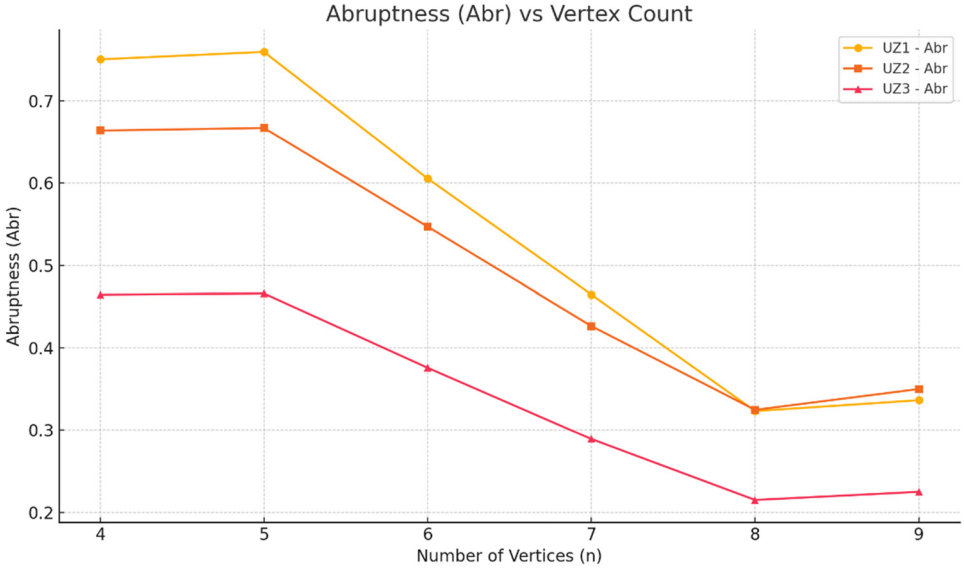

Figure 9: Abr of UZ_1, UZ_2, and UZ_3 across different vertex counts.

across different graph sizes (from four to nine vertices). The line plots in Figures 8 and 9 illustrate the trends of these metrics for each of the three proposed Zagreb upsilon indices. Figure 8 displays a consistent decrease in SS values as the number of vertices increases, indicating that the indices become less sensitive to minor structural changes in larger graphs. Among the three, the first Zagreb upsilon index (UZ_1) exhibits the highest SS values, affirming its high sensitivity to structural variations in small trees.Figure 9 shows the corresponding trends in Abr values. A downward trend is visible until $n = 8$, after which a slight increase is observed. This suggests a balance between SS and stability, where Zagreb upsilon indices maintain moderate abruptness across growing tree sizes. UZ_3 consistently shows the lowest Abr values, highlighting its smooth behavior.

These visualizations support the conclusion that Zagreb upsilon indices strike a desirable trade-off between sensitivity and stability, which is crucial for QSPR applicability.

6 Conclusion

This study introduces the Zagreb upsilon indices, derived from the novel concept of upsilon degree, as a promising addition to chemical graph theory. The results indicate that these indices provide highly accurate correlations with key physicochemical properties of benzenes, including BP, π-electron energy, MW, PO, MV, and relative formula mass. The second Zagreb upsilon index, in particular, outperforms well-established topological indices in predicting π-electron energy levels. Additionally, SS and Abr analyses confirm the robustness and reliability of these indices. Given these findings, Zagreb upsilon indices hold significant potential for enhancing QSPR studies and advancing predictive modeling in computational chemistry. Their application can extend to drug design, environmental chemistry, and materials science, where accurate molecular property predictions are crucial for developing new compounds and optimizing existing ones.

Future research will extend this analysis to a broader range of chemical compounds and incorporate additional validation metrics such as MAE and cross-validation. Furthermore, comparisons with eigenvalue-based indices will be explored to expand the scope of the study.

Additionally, future investigations will incorporate nonlinear modeling approaches and machine learning-based validation techniques to complement the current linear analysis. Methods such as support vector machines (SVM) and random forest regression will be applied to examine the robustness and generalizability of Zagreb upsilon indices in modeling complex physicochemical properties. These methods are particularly effective in identifying nonlinear relationships and interactions that may not be captured by traditional regression, offering a more nuanced perspective for QSPR applications.

To further enhance the statistical reliability of our models, future studies will incorporate additional error metrics such as mean absolute error (MAE) alongside RMSE. MAE provides a more interpretable and less variance-sensitive measure of prediction accuracy, which can complement RMSE in evaluating model performance. Additionally, *k*-fold cross-validation techniques will be employed to ensure that the developed models are not overfitted and generalize well to unseen data. These statistical tools will help validate the robustness and predictive power of the Zagreb upsilon indices in diverse QSPR scenarios.

To assess the generalizability of the proposed Zagreb upsilon indices, future research will focus on expanding the validation process to include diverse datasets beyond BHs. This will involve applying the indices to a broader spectrum of organic molecules, including heterocyclic compounds, polycyclic systems, and aliphatic hydrocarbons. Such an extension is crucial to demonstrate the adaptability and robustness of the indices in capturing structural-property relationships across varied molecular topologies. Comprehensive validation across chemically diverse datasets will further support the indices' applicability in real-world QSPR and cheminformatics contexts.

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Ethical approval: The conducted research is not related to either human or animal use.

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