Cumhuriyet Sci. J., 46(2) (2025) 360-368
DOI: https://doi.org/10.17776/csj.1617573

Cumhuriyet Science Journal

| csj.cumhuriyet.edu.tr | Founded: 2002 ISSN: 2587-2680 e-ISSN: 2587-246X Publisher: Sivas Cumhuriyet University

Modeling The Physicochemical Characteristics of Benzene Compounds Through the Application of Zagreb Omicron Indices

İdris Çiftçi [1,a,*]

[1] *Department of Mathematics, Faculty of Education, Van Yüzüncü Yıl University, Van, Türkiye*

**Corresponding author*

Research Article

History
Received: 10/01/2025
Accepted: 26/05/2025

ABSTRACT

Quantitative structure–property relationship (QSPR) studies commonly utilize topological indices to describe the chemical and physical characteristics of molecular structures. This study primarily focuses on the omicron degree of vertices and the corresponding Zagreb omicron indices for connected graphs, representing a notable contribution to the field of chemical graph theory. It has been demonstrated that the Zagreb omicron indices exhibit correlations greater than 0.995 with various physicochemical properties of benzene derivatives, including π-electron energy, molecular weight, polarization, and relative formula mass. The findings reveal that the first Zagreb omicron index correlates with degree-based topological indices of benzene derivatives with coefficients exceeding 0.96. Additionally, structural sensitivity and abruptness analyses of the proposed indices were conducted and compared with those of other established topological indices. The overall results provide compelling evidence that Zagreb omicron indices serve as valuable tools in QSPR research applications.

Keywords: QSPR studies, Benzenes, Topological indices, Omicron degree, Zagreb omicron indices.

[a] *idrisciftci@yyu.edu.tr* *https://orcid.org/0000-0002-2698-0807*

Introduction

Topological indices are essential tools used to derive real-valued descriptors closely linked to molecular structures, allowing for comprehensive analysis of their structural characteristics. These descriptors can be used to develop mathematical models that incorporate parameters obtained from experimental studies in chemistry and physics.

Recent research in chemical graph theory has introduced thousands of different topological indices. To propose a new index, it is essential to demonstrate its superiority over existing indices based on three key criteria:

I. The new index should show a correlation coefficient greater than 0.99 with at least one physicochemical property of the studied molecules.
II. It should have correlation coefficients above 0.9 with known topological indices.
III. The index should demonstrate clear superiority in structural characteristics, such as smoothness and degeneracy, compared to existing indices [1].

This study introduces the concept of the omicron degree of a vertex, representing a new contribution to graph theory. We present the Zagreb omicron indices for the inaugural time, predicated upon this foundational concept. A thorough investigation of the newly formulated indices is conducted based on the designated criteria, concentrating on parameters such as boiling point, pi electron energy, molecular weight, polarization, molecular volume, and relative formula mass of benzene derivatives. The structure of this paper is as follows: The introductory section defines pivotal terms and elucidates the most frequently employed indices within the literature, including the omicron degrees and Zagreb omicron indices pertinent to this study. The subsequent section delineates the Zagreb omicron indices pertinent to benzene molecules. In this segment, we executed analyses of the correlations among several properties—specifically boiling point, pi electron energy, molecular weight, polarization, molecular volume, and relative formula mass of benzene—and the values associated with the Zagreb omicron indices. These values were systematically juxtaposed with all relevant data documented in the extant academic literature. We identified the second highest correlation associated with the third Zagreb omicron index. Consequently, we formulated mathematical models for benzene's boiling point, pi electron energy, molecular weight, polarization, molecular volume, and relative formula mass in conjunction with the Zagreb omicron indices. The fourth section elucidates the correlation coefficients that link benzene's Zagreb omicron indices with other topological indices. The fifth segment encompasses a diverse array of structural evaluations. These investigations collectively substantiate that the Zagreb omicron indices represent distinctive instruments particularly adept for quantitative structure-activity relationship (QSAR) analyses.

Basic Definitions

The study of topological indices began in 1947, when Harold Wiener introduced an index to estimate the boiling points of alkanes [2]. The Wiener index is based on the sum of distances between all pairs of vertices in a graph. Contrary to common belief, the Zagreb index was not the first degree-based topological index. The first degree-based index is the Platt index, proposed in 1947 [3]. The third topological index, known as the Hosoya index, appeared in the literature in 1971. For a detailed discussion on the Hosoya index, refer to reference [4]. Subsequently, the Randić and Zagreb indices were introduced [5,6].

Let G be a graph and v a vertex in G. The degree of v, denoted as $deg\ v$, is the number of edges incident to it. We denote the set of vertices of a graph as $V(G)$, and the set of edges as $E(G)$. Table 1 provides definitions of the degree-based topological indices referenced in the literature and applied in this study. We selected the indices in Table 1 due to the smoothness analysis results in [1]. These indices will later be compared with the Zagreb omicron indices defined in this study, particularly in Section 5.

Table 1. Indices and their definitions

Name of Index	Symbol	Formula	Reference
The first Zagreb	M_1	$M_1 = \sum_{v \in V(G)} \deg v^2$	[6]
The second Zagreb	M_2	$M_2 = \sum_{uv \in E(G)} \deg u \deg v$	[6]
Randić	R	$R = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u \deg v}}$	[1]
Reciprocal Randić	RR	$RR = \sum_{uv \in E(G)} \sqrt{\deg u \deg v}$	[7]
Sum-connectivity	SCI	$SCI = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u + \deg v}}$	[8]
Symmetric division deg	SDD	$SDD = \sum_{uv \in E(G)} (\frac{\deg u}{\deg v} + \frac{\deg v}{\deg u})$	[9]
Inverse sum indeg	ISI	$ISI = \sum_{uv \in E(G)} \frac{\deg u \deg v}{\deg u + \deg v}$	[9]
Harmonic	H	$H = \sum_{uv \in E(G)} \frac{1}{\sqrt{\deg u + \deg v}}$	[10]
Atom-bond connectivity	ABC	$ABC = \sum_{uv \in E(G)} \sqrt{\frac{\deg u + \deg v - 2}{\deg u \deg v}}$	[11]
Augmented Zagreb index	AZI	$AZI = \sum_{uv \in E(G)} (\frac{\deg u \deg v}{\deg u + \deg v - 2})^3$	[12]
The first hyper-Zagreb	HM_1	$HM_1 = \sum_{uv \in E(G)} (\deg u + \deg v)^2$	[13]
The second hyper-Zagreb	HM_2	$HM_2 = \sum_{uv \in E(G)} (\deg u \deg v)^2$	[14]
Geometric-arithmetic	GA	$GA = \sum_{uv \in E(G)} \frac{2\sqrt{\deg u \deg v}}{\deg u + \deg v}$	[15]
The fourth geometric-arithmetic	GA_4	$GA_4 = \sum_{uv \in E(G)} \frac{2\sqrt{\varepsilon_u \varepsilon_v}}{\varepsilon_u + \varepsilon_v}$	[16]
Arithmetic-geometric index	AG	$AG = \sum_{uv \in E(G)} \frac{\deg u + \deg v}{2\sqrt{\deg u \deg v}}$	[17]
Sombor	SO	$SO = \sum_{uv \in E(G)} \sqrt{\deg u^2 + \deg v^2}$	[18]

Modified Sombor	SO^m	$SO^m = \sum_{uv\in E(G)} \frac{1}{\sqrt{\deg u^2 + \deg v^2}}$	[19]
Nirmala	N	$N = \sum_{uv\in E(G)} \sqrt{\deg u + \deg v}$	[20]
The first inverse Nirmala	IN_1	$IN_1 = \sum_{uv\in E(G)} \sqrt{\frac{1}{\deg u} + \frac{1}{\deg v}}$	[21]
The second inverse Nirmala	IN_2	$IN_2 = \sum_{uv\in E(G)} \frac{1}{\sqrt{\frac{1}{\deg u} + \frac{1}{\deg v}}}$	[21]

The indices presented in Table 1 were selected based on their high structural smoothness scores and frequent application in recent QSPR studies, particularly those analyzed in [1]. While alternative indices such as F-index or Y-index are also effective, they were not included due to their limited coverage in recent smoothness-focused comparisons.

We are now ready to offer the formal definition of the omicron degree related to a vertex, together with the specification of three unique Zagreb omicron indices, which represent the essential basis of this research.

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

$$o(v) = \deg v^{1/deg(v)} \quad (1)$$

Here, M_v is the multiplication of the degrees of all vertices neighbouring *v*.

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

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

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

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

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

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

Zagreb Omicron Indices For Benzenes

This section presents correlations greater than 0.95 between the Zagreb omicron indices and the physicochemical properties of benzene derivatives, including boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarization (PO), molecular volume (MV), and relative formula mass (MR). Consequently, we introduce mathematical models that describe the chemical properties of benzene derivatives based on Zagreb omicron indices. The latest related findings can be found in studies [4], [21–29]. The concentrations of benzene derivatives used in this study were obtained from the current dataset.

Table 2. Zagreb omicron indices of benzenes.

Benzenes	The first Zagreb Omicron index	The second Zagreb Omicron index	The third Zagreb Omicron index
Benzene	12,000	12,000	16,970
Naphthalene	20,160	22,238	31,280
Phenanthrene	28,320	32,478	45,590
Anthracene	28,320	32,477	45,590
Chrysene	36,481	42,717	59,901
Benzo[a] anthracene	36,481	42,716	59,901
Triphenylene	36,481	42,719	59,901
Tetracene	36,481	42,715	59,901
Benzo[a]pyrene	40,641	48,957	68,554
Benzo[e]pyrene	40,641	48,958	68,554
Perylene	40,641	49,786	68,554
Anthanthrene	44,801	55,196	77,207

Benzo[ghi] perylene	44,801	55,197	77,207
Dibenz[a,c] nthracene	44,641	52,957	74,211
Dibenz[a,h]anthracene	44,641	52,956	74,211
Dibenz[a,j]anthracene	44,641	52,956	74,211
Picene	44,641	52,957	74,211
Coronene	48,961	61,436	85,860
Dibenzo[a,h] pyrene	48,801	59,196	82,864
Dibenzo[a,i] pyrene	48,801	59,196	82,864
Dibenzo[a,l] pyrene	48,801	59,197	82,864
Pyrene	32,481	38,717	54,244

Table 3 presents selected physicochemical properties of benzene derivatives.

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 summarizes the correlation coefficients between the physicochemical properties of benzene derivatives and the Zagreb omicron indices.

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

	The first Zagreb Omicron index	The second Zagreb Omicron index	The third Zagreb Omicron index
BP	0,9835	0,9755	0,9761
Pi-ele	0,9998	0,9990	0,9993
MW	0,9998	0,9967	0,9971
PO	0,9988	0,9998	1,0000
MV	0,9639	0,9458	0,9472
MR	0,9988	0,9998	1,0000

As shown in Table 4, the correlation coefficients between the three newly defined indices and the physicochemical characteristics of benzene derivatives exceed 0.9458. The third Zagreb omicron index shows a perfect correlation (r = 1.000) with both PO and MR. This result is the best found in the literature so far. These results satisfy the first criterion proposed in this study for validating a newly defined index. Now we provide the linear regression graphs of the physico-chemical properties using the index that provides the greatest correlation.

Figure 1 shows a linear regression model of benzene boiling points using the first Zagreb omicron index.

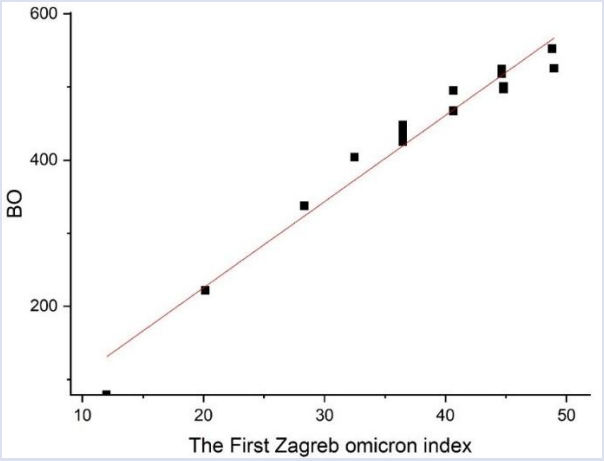

Figure 1. The linear fitting modelling of boiling points of benzenes via the first Zagreb omicron index

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 omicron index

Equation	Linear regression model of boiling points of benzenes via the first Zagreb omicron index
Intercept	-10,75115 ± 19,39041
Slope	11,79726 ± 0,48604
Pearson's R	0,98345
R-Square (COD)	0,96717
Adj. R-Square	0,96553

Linear regression model of pi-electron energy levels of benzenes via the first Zagreb omicron index is shown in Figure 2.

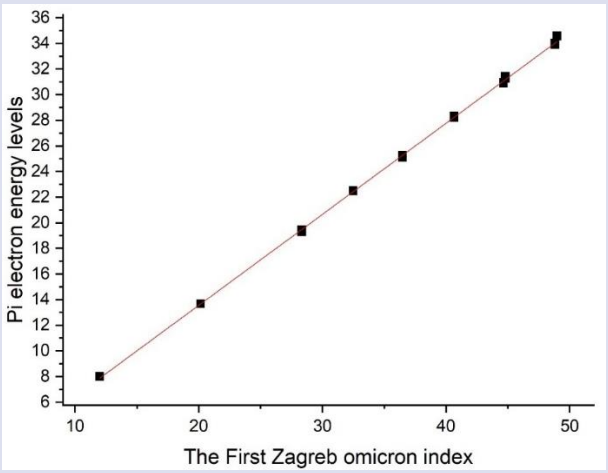

Figure 2. The linear fitting modelling of pi electron energy levels of benzenes via the first Zagreb omicron index

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 third Zagreb omicron index

Equation	Linear regression model of pi electron energy levels of benzenes via the first Zagreb omicron index
Intercept	-0,65859 ± 0,13755
Slope	0,71049 ± 0,00345
Pearson's R	0,99976
R-Square (COD)	0,99953
Adj. R-Square	0,99951

Linear regression model of molecular weight of benzenes via the first Zagreb omicron index is shown in Figure 3.

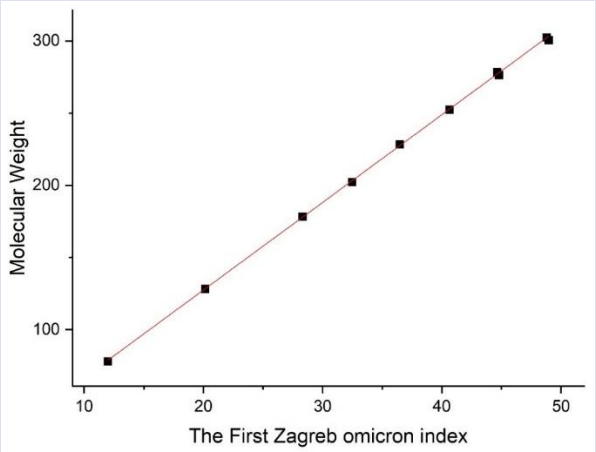

Figure 3. The linear fitting modelling of molecular weight of benzenes via the first Zagreb omicron index

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 omicron index

Equation	Linear regression model of molecular weight of benzenes via the first Zagreb omicron index
Intercept	6,03113 ± 1,01243
Slope	6,0702 ± 0,02538
Pearson's R	0,99983
R-Square (COD)	0,99965
Adj. R-Square	0,99963

Linear regression model of polarization of benzenes via the third Zagreb omicron index is shown in Figure 4.

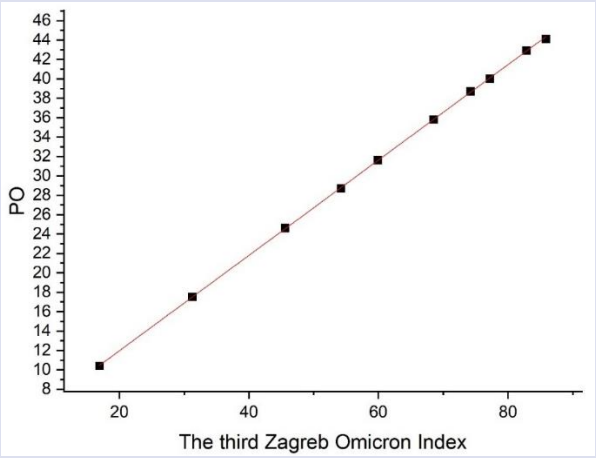

Figure 4. The linear fitting modelling of polarization of benzenes via the third Zagreb omicron index

The technical details of the graph given in Fig 4 are given below in Tab 8.

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

Equation	Linear regression model of polarization of benzenes via the third Zagreb omicron index
Intercept	2,13198 ± 0,06761
Slope	0,49156 ± 0,00101
Pearson's R	0,99996
R-Square (COD)	0,99992
Adj. R-Square	0,99991

Linear regression model of molecular volume of benzenes via the first Zagreb omicron index is shown in Figure 5.

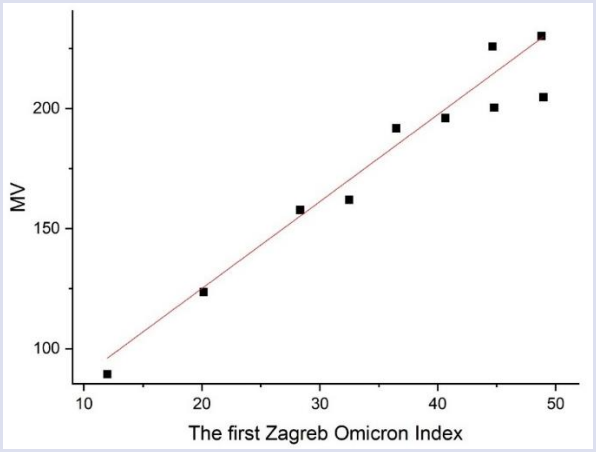

Figure 5. The linear fitting modelling of molecular volume of benzenes via the first Zagreb omicron index

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 omicron index

Equation	Linear regression model of molecular volume of benzenes via the first Zagreb omicron index
Intercept	52,6429 ± 8,91779
Slope	3,62086 ± 0,22353
Pearson's R	0,97479
R-Square (COD)	0,95022
Adj. R-Square	0,94773

Linear regression model of MR of benzenes via the third Zagreb omicron index is shown in Figure 6.

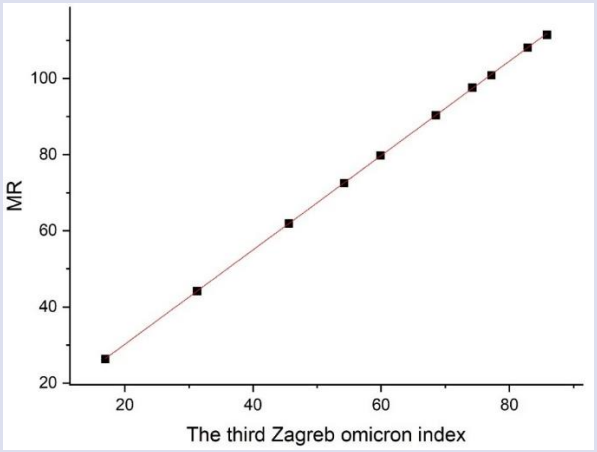

Figure 6. The linear fitting modelling of MR of benzenes via the third Zagreb omicron index

The technical details of the graph given in Fig 6 are given below in Tab 10.

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

Equation	Linear regression model of MR of benzenes via the third Zagreb omicron index
Intercept	5,41268 ± 0,15478
Slope	1,2392 ± 0,00231
Pearson's R	0,99997
R-Square (COD)	0,99993
Adj. R-Square	0,99993

Relations With Other Indices

Section 4 presents correlation coefficients between the Zagreb omicron indices and established degree-based topological indices—Randić (R), atom–bond connectivity (ABC), augmented Zagreb index (AZI), geometric–arithmetic index (GA), the first and second Zagreb indices (M_1, M_2), and the Sombor index (SO). The values derived from sources [22] and [26].

Table 11 shows the values of classical degree-based indices calculated for the same set of benzene derivatives. These data serve as the basis for correlation analysis with the newly proposed Zagreb omicron indices.

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 summarizes the correlation coefficients between the classical indices—Randić (R), ABC, AZI, GA, M_1, M_2, SO—and the newly defined Zagreb omicron indices.

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

İndices	*R*	*ABC*	*AZI*	*GA*	M_1	M_2	*SO*
The first Zagreb Omicron index	0,96274	0,96119	0,96033	0,96274	0,96119	0,96033	0,96274
The second Zagreb Omicron index	0,86228	0,86371	0,86214	0,86228	0,86371	0,86214	0,86228
The third Zagreb Omicron index	0,85	0,85311	0,85132	0,85	0,85311	0,85132	0,85

As shown in Table 12, the first Zagreb omicron index correlates with other classical indices with coefficients exceeding 0.96119, indicating a very strong relationship.

To further justify the relevance of the new indices, we also examine correlations between established indices and physicochemical properties. Table 13 displays the correlation coefficients between classical indices (R, ABC, AZI, GA, M_1, M_2, SO) and the physicochemical properties of benzene derivatives. The results show that some established indices, such as M_1 and M_2, yield correlation coefficients near unity, underscoring the need to demonstrate the structural and mathematical advantages of the Zagreb omicron indices.

Table 13. Pearson Correlation Coefficients Between Classical Degree-Based Topological Indices and Physicochemical Properties of Benzene Derivatives

Property	R	ABC	AZI	GA	M1	M2	SO
BP	0,9408	0,5111	0,6324	0,3456	0,9672	0,9555	0,5286
Pi-ele	0,932	0,565	0,661	0,33	0,996	0,991	0,587
MW	0,9299	0,5664	0,6631	0,3277	0,9922	0,9848	0,5861
PO	0,933	0,565	0,658	0,336	0,998	0,994	0,591
MV	0,8802	0,5522	0,6548	0,2822	0,9302	0,9112	0,547
MR	0,9336	0,564	0,6581	0,3365	0,9983	0,9943	0,5902

Legend: This table presents the correlation coefficients between several well-known degree-based topological indices (R, ABC, AZI, GA, M1, M2, SO) and key physicochemical properties of benzene derivatives, including boiling point (BP), pi-electron energy (Pi-ele), molecular weight (MW), polarization (PO), molecular volume (MV), and molar refractivity (MR). These results provide a comparative context for evaluating the predictive strength of the newly introduced Zagreb omicron indices.

Smoothness Analysis

This section investigates the smoothness characteristics of the Zagreb omicron indices and compares them with previously established results for various well-known topological indices. Reference [27] introduced two graph-based structural metrics—structure sensitivity (SS) and abruptness (Abr)—used to evaluate the smoothness of molecular descriptors. Recent studies have examined the structural sensitivity of eigenvalue-based topological indices and the continuity of graph energy in chemical structures, as reported in references [28] and [29], respectively. Reference [27] provides the algorithm used to compute SS and Abr values for topological indices applied to specific classes of connected graphs. Kumar and Das applied this algorithm to evaluate the smoothness of fifteen degree-based topological indices (listed in Table 1) on all tree graphs with 4 to 10 vertices.

Using the same algorithm, SS and Abr values of the Zagreb omicron indices were calculated for tree graphs with 4 to 9 vertices, and the results are presented in Table 13.

Table 14. Structure sensitivity (SS) and abruptness (Abr) analysis results of Zagreb omicron indices on tree graphs

Zagreb Omicron 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_1O	0.1672	0.1672	0,1453	0,1491	0,1000	0,1231	0,068	0,108	0,0590	0,0919	0,0513	0,0966
M_2O	0.1098	0.1098	0,0949	0,0999	0,0652	0,0822	0,0561	0,1009	0,0394	0,0620	0,0339	0,0661
M_3O	0.0441	0.0441	0,0411	0,0438	0,0293	0,0373	0,0286	0,0508	0,0181	0,0288	0,0805	0,2247

An effective topological index should exhibit a low Abr value and a relatively high SS value, indicating stable structural behavior. For tree graphs with 9 vertices, comparison of Table 13 with Table 1 in reference [5] and Table 3 in reference [27] reveals that the SS value of the Zagreb omicron indices exceeds those of the first Zagreb, Randić, ABC, and GA indices. However, it is also observed that the Abr values of the Zagreb omicron indices are higher than those of all other indices.

Conclusion

This study introduced the concept of the omicron degree within the framework of chemical graph theory. Based on this new degree concept, three Zagreb omicron indices were defined. Their applicability was evaluated in QSAR studies modeling key physicochemical properties of benzene derivatives, including boiling point, π-electron energy, molecular weight, polarization, molecular volume, and relative formula mass. The results showed that Zagreb omicron indices correlated strongly ($r > 0.995$) with properties such as π-electron energy, molecular weight, polarization, and molar refractivity. Additionally, structural sensitivity and abruptness analyses were carried out and compared with those of established topological indices. Overall, the findings demonstrate that the Zagreb omicron indices are highly suitable for use in QSPR research.

Although this study focused on degree-based indices, future research could investigate the inclusion of distance-based indices—such as the Wiener, Harary, and Balaban indices—to determine whether stronger correlations with physicochemical properties can be obtained.

Conflicts of interest

There are no conflicts of interest in this work.

References

[1] Kumar V., Das S., On Structure Sensitivity and Chemical Applicability of Some Novel Degree-Based Topological Indices, *MATCH Commun. Math. Comput. Chem.,* 92 (2024) 165–203.

[2] Wiener H., Structural determination of paraffin boiling points, *J. Am. Chem. Soc.,* 69 (1947) 17–20.

[3] Platt J. R., Influence of neighbour bonds on additive bond properties in paraffins, *J. Chem. Phys.,* 15 (1947) 419-420.

[4] Hosoya H., The most private features of the topological index, *MATI.,* (1) (2019) 25-33.

[5] Gutman I., Trinajstić N., Graph theory and molecular orbitals, Total π electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17 (1972) 535–538.

[6] Randić M., Characterization of molecular branching, *J. Am. Chem. Soc.,* 97 (1975) 6609–6615.

[7] Gutman I., Furtula B., Elphick C., Three new/old vertex-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.*, 72 (2014) 617–632.

[8] Zhou B., Trinajstić N., On a novel connectivity index*, J. Math. Chem*., 46 (2009) 1252–1270.

[9] Vukičević D., Gašperov M., Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta.,* 83 (2010) 243–260.

[10] Favaron O., Mahéo M., Saclé J. F., Some eigenvalue properties in graphs (conjectures of graffiti-II), *Discrete Math.*, 111 (1993) 197–220.

[11] Estrada E., Torres L., Rodriguez L., Gutman I., An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem.,* 37A (1998) 849–855.

[12] Furtula B., Graovac A., Vukičević D., Augmented Zagreb index, *J. Math. Chem.,* 48 (2010) 370–380.

[13] Shirdel G., Rezapour H., Sayadi A., The hyper-Zagreb index of graph operations, *Iran. J. Math. Chem.,* 4 (2013) 213–220.

[14] Alameri A., Second hyper-Zagreb index of titania nanotubes and their applications, *IEEE Access.,* 9 (2021) 9567–9571.

[15] Vukičević D., Furtula B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.,* 46 (2009) 1369–1376.

[16] Ediz S., Computing GA4 index of an infinite class of nano star dendrimers, *Optoelectronics and Advanced Materials Rapid Communications.,* 4 (12) (2010) 2198-2199.

[17] Shegehalli V., Kanabur R., Arithmetic-Geometric indices of path graph, *J. Comput. Math. Sci.,* 16 (2015) 19–24.

[18] Gutman I., Geometric approach to degree-based topological indices:Sombor indices, *MATCH Commun. Math. Comput. Chem.,* 86 (2021) 11–16.

[19] Kulli V., Gutman I., Computation of Sombor indices of certain networks, *SSRG Int. J. Appl. Chem.,* 8 (2021) 1–5.

[20] Kulli V., Nirmala index, *Int. J. Math. Trends Technol.,* 67 (2021) 8–12.

[21] Kulli V., Lokesha V., Nirupadi K., Computation of inverse Nirmala indices of certain nanostructures, *Int. J. Math. Comb.,* 2 (2021) 33–40.

[22] Nikolić S., Trinajstić N., Comparison between the Vertex- and Edge-Connectivity Indices for Benzenoid Hydrocarbons, *J. Chem. Inf. Comput. Sci.,* 38 (1998) 42-46.

[23] Hayat S., Khan S., Khan A., Imran M., Distance-based topological descriptors for measuring the π-electronic energy of benzenoid hydrocarbons with applications to carbon nanotubes, *Math. Meth. Appl. Sci.,* (2020) 1–20.

[24] Hayat S., Khani S., Khan A., Imran M., A Computer-Based Method to Determine Predictive Potential of Distance-Spectral Descriptors for Measuring the π-Electronic Energy of Benzenoid Hydrocarbons with Applications, *IEEE Access.,* 9 (2021) 19238-19253.

[25] Shanmukha M. C., Usha A., Kulli V. R., Shilpa K. C., Chemical applicability and curvilinear regression models of vertex-degree-based topological index: Elliptic Sombor index, *Int J Quantum Chem.,* (2024) 124: e27376.

[26] Malik M. Y. H., Binyamin M. A., Hayat S., Correlation ability of degree-based topological indices for physicochemical properties of polycyclic aromatic hydrocarbons with applications, *Polycyclic Aromatic Compounds.,* 42 (2022) 6267-6281.

[27] Furtula B., Gutman I., Dehmer M., On structure-sensitivity of degree-based topological indices, *Appl. Math. Comput.,* 219 (2013) 8973–8978.

[28] Redˇzepovi´c I., Furtula B., Comparative study on structural sensitivity of eigenvalue-based molecular descriptors*, J. Math. Chem.,* 59 (2021) 476–487.

[29] Zemljič K., Žigert Pleteršek P., Smoothness of graph energy in chemical graphs, *Mathematics.,* 11 (2023) #552.