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Jalappa, Vijendra. N, Boregowda H. S.

Department of Studies and Research in Mathematics,
Tumkur University,Tumkur-572103, Karnataka, India

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DEGREE-STATUS CONNECTIVITY INDICES: STRUCTURAL PROPERTIES AND QSPR APPLICATIONS TO BENZENOID HYDROCARBONS

Jalappa, Vijendra. N, Boregowda H. S.*

Department of Studies and Research in Mathematics,

Tumkur University,Tumkur-572103, Karnataka, India

Corresponding Auhtor: bgsamarasa@gmail.com

Abstract: *In this work, we introduce two new connectivity indices for a graph G, referred to as the first and second degree status connectivity indices. These indices are defined as follows:*
$PS_1(G) = \sum_{\{s,t\}\in E(G)} [\sigma(s) + \sigma(t)](d_s d_t)$ *and* $PS_2(G) = \sum_{\{s,t\}\in E(G)} [\sigma(s)\sigma(t)](d_s d_t)$ *where* $E(G)$ *denotes the edge set of the graph and* $d(s)$ *denotes degree of a vertex* s*. These indices have been evaluated for some standard class of graphs. Additionally, certain bounds were investigated. We further investigated the applicability of these indices in modeling the physicochemical properties of benzenoid hydrocarbons. Specifically, This study examines the predictive potential of the indices* $PS_1(G)$ *and* $PS_2(G)$ *through cubic regression modeling for benzenoid hydrocarbons. The results indicate that* $PS_1(G)$ *serves as a more effective predictive index compared to* $PS_2(G)$ *among the two newly introduced indices. Furthermore, a comparison between the actual and predicted physicochemical properties has been presented for both indices to provide clearer insights.*

Keywords: *Status, Status connectivity index, Zagreb index, Second status connectivity index.*

AMSC:*05C07; 05C09; 05C92*

1 Introduction

In Mathematical chemistry, molecular graphs are employed to represent molecular structures, with atoms modeled as vertices and covalent bonds as edges. These graph-theoretic models are fundamental in the investigation of QSPR and QSAR. Such studies heavily depend on numerical graph invariants, which reflect intrinsic molecular properties. One of the earliest and most influential topological indices is the Wiener index, introduced by Harold Wiener in 1947, initially used to examine the properties of paraffin compounds [7].

Let G be a connected graph comprising n vertices and m edges, with vertex and edge sets denoted by $V(G)$and $E(G)$, respectively. An edge linking two vertices s and t is written as st. The degree of a vertex s, noted as d_s, indicates the count of edges incident to it. A graph in which every vertex has same degree is called regular graph. For standard graph-theoretic concepts, we refer the reader to [9, 10].

Numerous topological descriptors have been extensively analyzed due to their relevance in chemical graph theory. For additional information, consult [1, 2, 3, 4, 5, 6].

Index	Definition
Eccentricity of vertex s, $\tilde{e}(s)$	$\tilde{e}(s) = \max_{t\in V(G)} d(s,t)$
Diameter of graph, $\text{diam}(G)$	$\text{diam}(G) = D = \max_{s\in V(G)} \tilde{e}(s)$
Status (transmission) of vertex s, $\sigma(s)$	$\sigma(s) = \sum_{t\in V(G)} d(s,t)$

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Wiener Index, [7] $W(G)$	$W(G)=\sum_{\{s,t\}\subseteq V(G)} d(s,t) = \frac{1}{2}\sum_{s\in V(G)} \sigma(s)$
First Zagreb Index, [11] $Z_1(G)$	$Z_1(G)=\sum_{st\in E(G)\in E(G)} (d_s+d_t)$
Second Zagreb Index, [11] $Z_2(G)$	$Z_2(G)=\sum_{st\in E(G)} d_s d_t$
Hyper-Zagreb Index, [13] $HM(G)$	$HM(G)=\sum_{st\in E(G)} (d_s+d_t)^2$
Second alpha-Gourava Index, [12] $G_2(G)$	$G_2(G)=\sum_{st\in E(G)} (d_s+d_t)d_s d_t$
First Eccentric Connectivity Index, [22, 23] $e_1(G)$	$e_1(G)=\sum_{st\in E(G)} (\tilde{e}(s)+\tilde{e}(t))$
Second Eccentric Connectivity Index, [22, 23] $e_2(G)$	$e_2(G)=\sum_{st\in E(G)} \tilde{e}(s)\tilde{e}(t)$
First Status Connectivity Index, [24] $S_1(G)$	$S_1(G)=\sum_{st\in E(G)} (\sigma(s)+\sigma(t))$
Second Status Connectivity Index, [24] $S_2(G)$	$S_2(G)=\sum_{st\in E(G)} \sigma(s)\sigma(t)$

These descriptors are foundational tools in the analysis of molecular structure and network properties [20, 21]. For further background, see [14, 15, 16, 17, 18, 19, 28]. These indices extend the concept of connectivity by leveraging transmission values, offering refined perspectives for graph-based molecular analysis.

The first and second degree status connectivity indices. For a given graph G, these are formulated as follows:

$$PS_1(G)=\sum_{st\in E(G)} [\sigma(s)+\sigma(t)]d_s d_t, \quad PS_2(G)=\sum_{st\in E(G)} \sigma(s)\sigma(t)\ d_s d_t.$$

2 Degree status connectivity indices of some families of graphs

Theorem 2.1 *Let* $G(\mathfrak{n},\mathfrak{m})$ *be a connected graph with* $diam(G)\leq 2$*, Then*

$$PS_1(G)=4(\mathfrak{n}-1)Z_2(G)-G_2(G)$$

and

$$PS_2(G)=4(\mathfrak{n}-1)^2 Z_2(G)-2(\mathfrak{n}-1)G_2(G)+HM_2(G)$$

Proof. 1 If $diam(G)\leq 2$, then d_s number of vertices are at distance 1 and $(\mathfrak{n}-1-d_s)$ vertices are at distance 2 from u. So, for each vertex u in G,

$$\sigma_s = 2\mathfrak{n}-2-d_s$$
$$PS_1(G)=\sum_{st\in E(G)} (\sigma_s+\sigma_t)(d_s d_t)$$
$$=\sum_{st\in E(G)} (4(\mathfrak{n}-1)-(d_s+d_t))(d_s d_t)$$
$$=4(\mathfrak{n}-1)Z_2(G)-G_2(G) \quad (1)$$

And

$$PS_2(G)=\sum_{st\in E(G)} (\sigma_s\cdot\sigma_t)(d_s d_t)$$
$$=\sum_{st\in E(G)} (2\mathfrak{n}-2-d_s)(2\mathfrak{n}-2-d_s)(d_s d_t)$$

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$$= 4(n-1)^2 Z_2(G) - 2(n-1)G_2(G) + HM_2(G) \tag{2}$$

Corollary 1 *Let $G(n,m)$ be r-regular connected graph with $diam(G) \leq 2$, Then*
$$PS_1(G) = 4(n-1)r^{2m} - 2mr^3$$
and
$$PS_2(G) = 4(n-1)^{2m}r^2 - 4(n-1)mr^3 + r^4$$

Corollary 2 *For n-vertex complete graph K_n, $PS_1(K_n) = n(n-1)^4$ and $PS_2(K_n) = \frac{n(n-1)^5}{2}$*

proposition 1 *For complete bipartite Graph $K_{n,m}$,*
$$PS_1(G) = (nm)^2[4(n+m-1) - (nm)(n+m)]$$
and
$$PS_2(G) = 4(n+m-1)^2(nm)^2 - 2(n+m-1)nm(n+m)(nm^2) + nm(n+m)^2$$

Corollary 3 *For a n-vertex star graph S_n, we have*
$$PS_1(S_n) = (n-1)^2(3n-8) \quad \text{and} \quad PS_2(S_n) = (n-2)^3(2n-5)$$

proposition 2 *For a cycle C_n on $n \geq 3$ vertices*
$$PS_1(C_n) = \begin{cases} 2n^3 & \text{ifniseven} \\ 2n(n^2-1) & \text{ifnisodd} \end{cases}$$
And
$$PS_1(C_n) = \begin{cases} \frac{n^5}{8} & \text{ifniseven} \\ \frac{n(n-1)^2(n+1)^2}{4} & \text{ifnisodd} \end{cases}$$

proposition 3 *For a friendship graph F_n, $n \geq 2$*
$$PS_1(F_n) = 16n[3n^2 + n - 1] \quad \text{and} \quad PS_2(F_n) = 16n(2-n)(2+n)$$

3 Bounds On degree Status Connectivity Index

Theorem 3.1 *For any graph G,*
$$2\sigma_{min}M_2(G) \leq PS_1(G) \leq 2\sigma_{max}M_2(G) \quad and \quad \sigma_{min}^2 M_2(G) \leq PS_2(G) \leq \sigma_{max}^2 M_2(G)$$

Proof. For any edge $uv \in E(G)$, we have, $\sigma_{min} \leq \sigma(u), \sigma(v) \leq \sigma_{max}$. Thus,
$$2\sigma_{min} \leq \sigma(u) + \sigma(v) \leq 2\sigma_{max}$$

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$2\sigma_{min} \sum_{uv\in E(G)} d_u d_v \le PS_1(G) \le 2\sigma_{max} \sum_{uv\in E(G)} d_u d_v$
$2\sigma_{min} M_2(G) \le PS_1(G) \le 2\sigma_{max} M_2(G)$
and
Similarly, $\sigma_{min}^2 \le \sigma(u) + \sigma(v) \le \sigma_{max}^2$
$\sigma_{min}^2 M_2(G) \le PS_2(G) \le \sigma_{max}^2 M_2(G)$

Corollary 4 *For any edge* $uv \in E(G)$, $\delta^2 \le d_u d_v \le \Delta^2$.

$$2m\sigma_{min}\delta^2 \le PS_1(G) \le 2m\sigma_{max}\Delta^2$$

$$m\sigma_{min}^2\delta^2 \le PS_2(G) \le m\sigma_{max}^2\Delta^2$$

Theorem 3.2 *Let* $G = (V, E)$ *be a connected graph on n vertices with diameter D. Then,*

$$PS_1(G) \le 2(n-1)DM_2(G) \quad and \quad PS_2(G) \le (n-1)^2 D^2 M_2(G)$$

Proof. For each $v \in V$ the ststus, $\sigma(v) = \sum_{u\in V} d(v,u) \le (n-1)D$. Since there are n-1 other vertices and each distance is atmost D. Hence,

$$\sigma_{max} = Max_v \sigma(v) \le (n-1)D. \quad (3)$$

Weknowthat, $\sigma(u) + \sigma(v) \le 2\sigma_{max}$; $\sigma(u)\sigma(v) \le \sigma_{max}^2$.

$PS_1(G) = \sum_{uv\in E(G)} (\sigma(u) + \sigma(v) d_u d_v) \le 2\sigma_{max} \sum_{uv\in E(G)} d_u d_v = 2\sigma_{max} M_2$
$PS_2(G) = \sum_{uv\in E(G)} (\sigma(u)\sigma(v) d_u d_v) \le \sigma_{max}^2 \sum_{uv\in E(G)} d_u d_v = \sigma_{max}^2 M_2$.

Combine with ?? to obtain,

$$PS_1(G) \le 2(n-1)DM_2(G) \quad and \quad PS_2(G) \le (n-1)^2 D^2 M_2(G)$$

Lemma 3.3 *[26, 27] Let* G *be any connected graph with* $D \le 2$. *Then [i]*

1. $1 \le \sigma_s \le (n-1)^2$
2. $1 \le \sigma_s \le (n-1)D$
3. $n - 1 \le \sigma_s \le \frac{(n-1)(n+2)}{2} - m$

Theorem 3.4 *For any connected graph G,*

$$2Z_2(G) \le PS_1(G) \le 2(n-1)^2 Z_2(G).$$

and

$$Z_2(G) \le PS_2(G) \le (n-1)^4 Z_2(G).$$

Proof. Using (i) of Lemma(3.3), we get,

$\sum_{st\in E(G)} (1+1) d_s d_t \le \sum_{st\in E(G)} (\sigma_s + \sigma_t) d_s d_t \le \sum_{st\in E(G)} ((n-1)^2 + (n-1)^2) d_s d_t$

$2Z_2(G) \le PS_1(G) \le 2(n-1)^2 Z_2(G)$.

And

$\sum_{st\in E(G)} (1 \cdot 1) d_s d_t \le \sum_{st\in E(G)} (\sigma_s \cdot \sigma_t) d_s d_t \le \sum_{st\in E(G)} ((n-1)^2 (n-1)^2) d_s d_t$

$Z_2(G) \le PS_2(G) \le (n-1)^4 Z_2(G)$.

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Corollary 5 *For any connected graph* G,

$$2Z_2(G) \leq PS_1(G) \leq 2(n-1)DZ_2(G).$$

and

$$Z_2(G) \leq PS_2(G) \leq (n-1)^2D^2Z_2(G).$$

Proof. Proof follows from the (ii) of the Lemma(3.3)

Corollary 6 *For any graph connected* G,

$$2(n-1)Z_2(G) \leq PS_1(G) \leq [(n+1)(n+2)-2m]Z_2(G).$$

and

$$(n-1)^2Z_2(G) \leq PS_2(G) \leq \frac{((n-1)(n+2)-2m)^2}{4}Z_2(G).$$

Proof. Proof follows from the (iii) of the Lemma(3.3)

Theorem 3.5 *For any connected graph* G,

$$\delta^2S_1(G) \leq PS_1(G) \leq \Delta^2S_1(G).$$

and

$$\delta^2S_2(G) \leq PS_2(G) \leq \Delta^2S_2(G).$$

Proof. Since $\delta \leq d_s \leq \Delta$

$$\delta^2 \sum_{st\in E(G)} (\sigma_s + \sigma_t) \leq PS_1(G) \leq \Delta^2 \sum_{st\in E(G)} (\sigma_s + \sigma_t)$$
$$\delta^2S_1(G) \leq PS_1(G) \leq \Delta^2S_1(G).$$

And

$$\delta^2 \sum_{st\in E(G)} (\sigma_s \cdot \sigma_t) \leq PS_1(G) \leq \Delta^2 \sum_{st\in E(G)} (\sigma_s \cdot \sigma_t)$$
$$\delta^2S_2(G) \leq PS_2(G) \leq \Delta^2S_2(G).$$

Corollary 7 *For any connected graph* G,

$$S_1(G) \leq PS_1(G) \leq (n-1)^2S_1(G).$$

and

$$S_2(G) \leq PS_2(G) \leq (n-1)^2S_2(G).$$

Proof. Proof follows from the (i) of the Lemma(3.3)

4 Regression models

4.1 Results and Discussion

The evaluation of regression models is performed as follows. The cubic regression model is expressed as:

$$y = a + b_1x + b_2x^2 + b_3x^3 \quad (4)$$

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The dependent variable is denoted by y, with a representing the regression constant, while b_i $(i = 1,2,3)$ are the regression coefficients associated with the independent variables x_i $(i = 1,2,3)$. The regression equation is obtained using sample data, where r denotes the correlation coefficient, SE is the standard error of the estimates, and F represents Fisher's statistic.

The root mean square error (RMSE) is a key metric for evaluating the performance of statistical models, as it quantifies the deviation between observed values and predicted values. The RMSE is defined as:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}$$

Specifically, n represents the number of data points, y_i is the actual value for the i^{th} observation, and $\hat{y}_i$ is the corresponding predicted value.

Benzenoid hydrocarbons are polycyclic, fully conjugated, and unsaturated hydrocarbons made up entirely of fused six-membered rings. The arrangement of π-electrons in a benzenoid hydrocarbon cannot be accurately depicted using a conventional structural formula that includes double bonds between specific carbon atom pairs.

Here we investigate the correlation between indices values with some physiochemical properties of benzenoid hydrocarbons. Experimental values of benzenoid hydrocarbons represented in Fig. 1 are taken from [25].

In this study, 5 pyhsicochemical properties (Table 1) of benzanoid hydrocarbons are considered such as Boiling point(BP), Entropy(S(Cal/mol.k)), Log P, Retension index(RI) and Enthalpy($\Delta(H_f)$) for which coefficient of correlation are calculated using the predicted values of Topological indices. Also we have shown a bar graph representaion, comparing Actual and Pridicted values of all the physicochemical properties with respect to the $PS_1(G)$ and $PS_2(G)$.

From the Table (4), it is obvious that of 2 degree based indices considered in the study, $PS_1(G)$ has high correlation with 5 (BP, S, Log P, RI, $\Delta(H)$) properties considered. The predicted values of the physichochemical properties for $PS_1(G)$ and $PS_2(G)$ are shown in tables(2) and (3), respectively. The comparison of the actual and predicted values of the two indices for the pyhsicochemical properties under consideration is shown in Figures (2, 3, 4, 5, 6).

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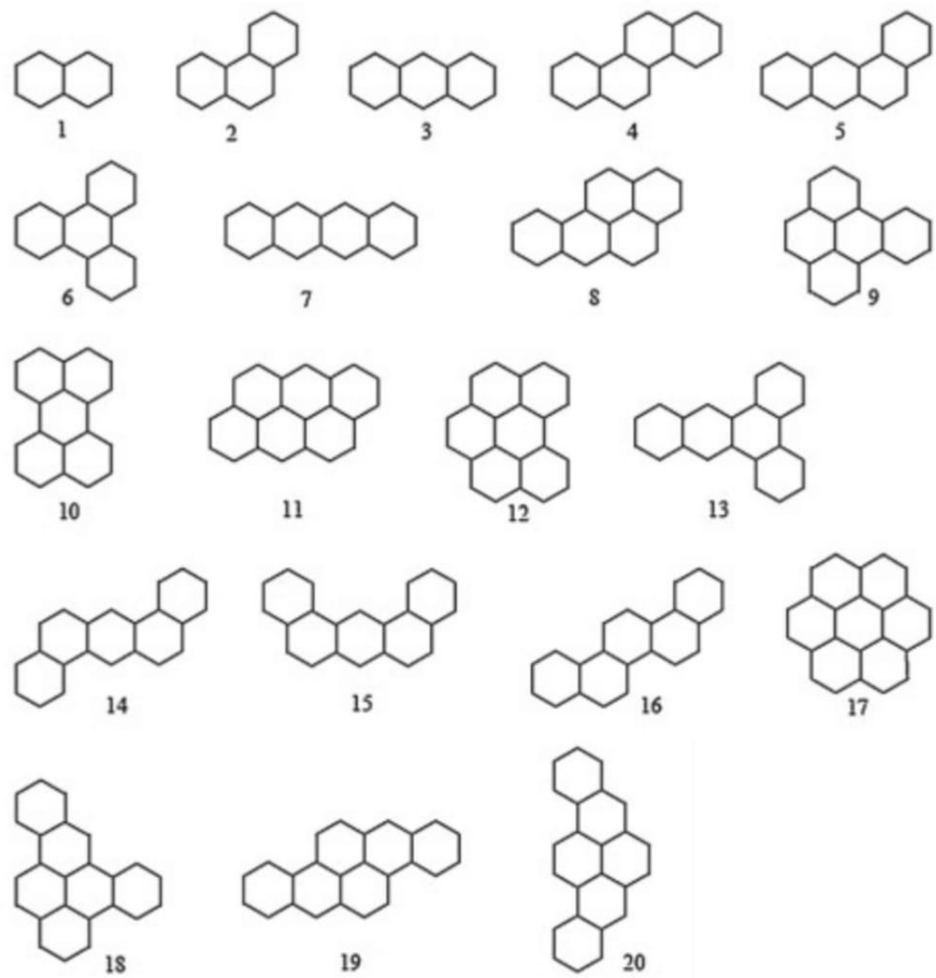

Figure 1: Molecular graph of benzenoid hydrocarbons under consideration

Benzenoid Hydrocarbons	**BP (˚C)**	$PS_1(G)$	$PS_2(G)$	**S (Cal/mol·K)**	**log P**	**RI**	$\Delta H_f(kJ/mol)$
Naphthalene	218	2354	24569	79.38	3.3	200	150.6
Phenanthrene	338	6582	121067	93.79	4.46	300	209.1
Anthracene	340.05	6772	129562	92.43	4.45	301.69	218.3
Chrysene	431	14170	410669	106.83	5.81	400	267.7
Tetraphene	425	14332	423008	108.22	5.76	398.5	276.9
Triphenylene	429	13212	353214	104.66	5.49	400	258.5
Naphthacene	440	14742	451227	105.47	5.76	408.3	286.1
Benzo[a]pyrene	496	19228	623836	111.85	6.13	453.44	279.9
Benzo[e]pyrene	493	18396	565240	110.46	6.44	450.73	289.1

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Perylene	497	18666	584432	109.10	6.25	456.22	279.9
Anthanthrene	547	25390	924893	114.10	7.04	503.89	310.5
Benzo[ghi]perylene	542	24180	812126	114.10	6.63	501.32	301.3
Dibenz[a,h]anthracene	536	26340	1125062	119.87	6.75	495.45	335.5
Dibenz[a,j]anthracene	531	25828	1078278	119.87	6.54	489.8	335.5
Picene	519	26206	1109023	119.87	7.11	500	326.3
Coronene	590	32052	1273848	116.36	7.64	549.67	322.7
Dibenzo[a,e]pyrene	592	30702	1299996	124.89	7.28	551.53	338.5
Dibenzo[a,h]pyrene	596	32972	1506532	123.50	7.28	559.9	347.7
Dibenzo[a,i]pyrene	594	31538	1379408	123.50	7.28	556.47	347.7
Dibenzo[a,l]pyrene	595	30256	1255352	131.69	7.71	553	351.2

Table 1: Experimental values of some physiochemical properties of benzenoid hydrocarbons.

S1	Pred. BP	Pred. LogP	Pred. RI	Pred. Enthalpy	Pred. Entropy
2354	227.09	3.33	202.72	156.55	80.73
6582	325.60	4.41	295.70	207.93	91.90
6772	329.37	4.45	299.27	209.91	92.34
14170	441.24	5.72	405.82	269.14	105.87
14332	443.07	5.74	407.57	270.11	106.10
13212	429.99	5.59	395.02	263.16	104.45
14742	447.60	5.80	411.93	272.52	106.67
19228	490.06	6.30	453.07	294.87	112.11
18396	482.99	6.22	446.18	291.19	111.20
18666	485.31	6.24	448.45	292.40	111.50
25390	537.48	6.85	499.67	318.41	117.93
24180	528.36	6.75	490.68	314.08	116.87
26340	544.79	6.93	506.88	321.82	118.75
25828	540.83	6.89	502.98	319.98	118.31
26206	543.75	6.92	505.85	321.34	118.64
32052	595.62	7.45	556.83	344.21	123.81
30702	582.09	7.32	543.59	338.42	122.56
32972	605.57	7.55	566.55	348.43	124.70
31538	590.33	7.40	551.66	341.95	123.33
30256	577.87	7.27	539.45	336.59	122.16

Table 2: Predicted Physical Properties for S1

S2	Pred. BP	Pred. LogP	Pred. RI	Pred. Enthalpy	Pred. Entropy
24569	248.66	3.58	222.16	169.91	83.61
121067	311.67	4.25	282.43	201.24	90.57
129562	316.69	4.31	287.24	203.75	91.13

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410669	442.36	5.72	407.31	267.30	105.54
423008	446.29	5.76	411.07	269.33	106.01
353214	422.48	5.48	388.32	257.11	103.19
451227	454.86	5.86	419.25	273.76	107.04
623836	496.00	6.36	458.60	295.36	112.15
565240	484.01	6.21	447.12	289.00	110.62
584432	488.14	6.26	451.07	291.18	111.14
924893	536.27	6.87	497.62	317.33	117.58
812126	524.28	6.72	485.86	310.70	115.91
1125062	555.01	7.08	516.47	327.46	120.07
1078278	550.52	7.03	511.91	325.10	119.50
1109023	553.45	7.06	514.88	326.64	119.87
1273848	571.83	7.22	533.65	335.94	122.01
1299996	575.40	7.25	537.30	337.68	122.39
1506532	613.84	7.52	576.44	355.83	126.21
1379408	587.80	7.34	549.96	343.63	123.67
1255352	569.44	7.20	531.21	334.76	121.75

Table 3: Predicted Physical Properties for S2

Property	R^2		RMSE		MAE	
	S1	S2	S1	S2	S1	S2
Boiling Point	0.9863	0.9638	11.6246	18.9163	10.4542	16.9001
Entropy	0.9324	0.9305	3.1595	3.2045	2.1223	2.2315
Log P	0.9744	0.9550	0.1807	0.2397	0.1399	0.1842
Refractive Index	0.9940	0.9769	7.4231	14.5284	6.5519	13.2694
Enthalpy	0.9596	0.9609	10.3306	10.1512	8.4534	8.3987

Table 4: Comparison of S1 and S2 cubic regression models for physicochemical properties

Table 4 presents the regression statistics of cubic models developed using the features $PS_1(G)$ and $PS_2(G)$ for predicting various physicochemical properties of benzenoid hydrocarbons, namely boiling point (BP), entropy, refractive index (RI), log P, and enthalpy. The quality of the models was evaluated using the coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), and statistical significance (F-test). The results show that both $PS_1(G)$ and $PS_2(G)$ features provide statistically significant models with $p < 0.0001$, confirming their strong predictive power. However, $PS_1(G)$ generally yields superior performance compared to $PS_2(G)$, as indicated by consistently higher R^2 values and lower RMSE and MAE values across most properties. For example, in predicting the Refractive Index, the cubic model with $PS_1(G)$ achieves an $R^2 = 0.0.9940$ with lower prediction errors (RMSE = 7.42, MAE = 6.55) compared to $PS_2(G)$ ($R^2 = 0.9769$, RMSE = 14.52, MAE = 13.26). Similarly, for the boiling point index, $PS_1(G)$ provides an excellent fit with $R^2 = 0.9863$.

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Overall, these findings highlight that the proposed product degree status connectivity indices, particularly $PS_1(G)$, are effective descriptors for modeling and correlating structural features of benzenoid hydrocarbons with their physical and chemical properties.

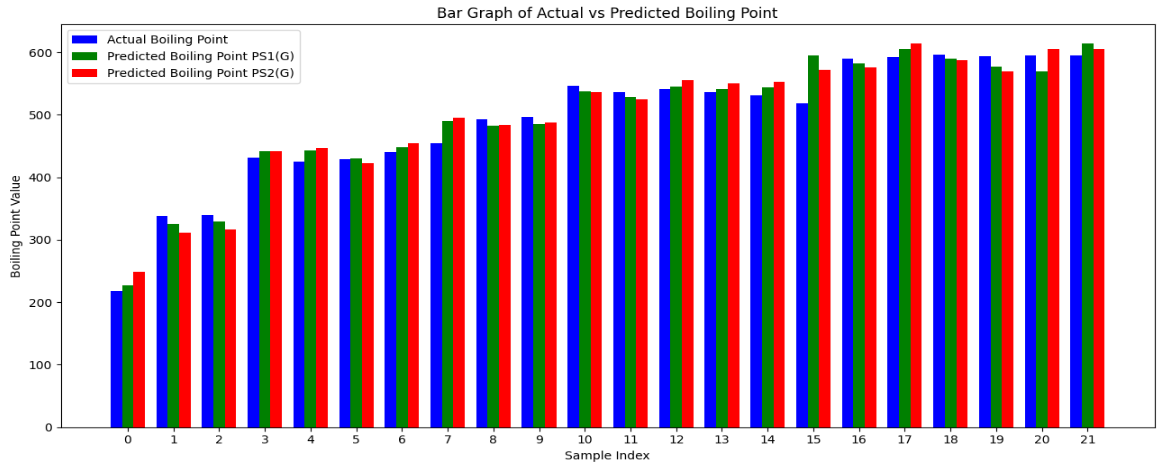

Figure 2: *Bar graph of Actual vs Predicted Boiling Point*

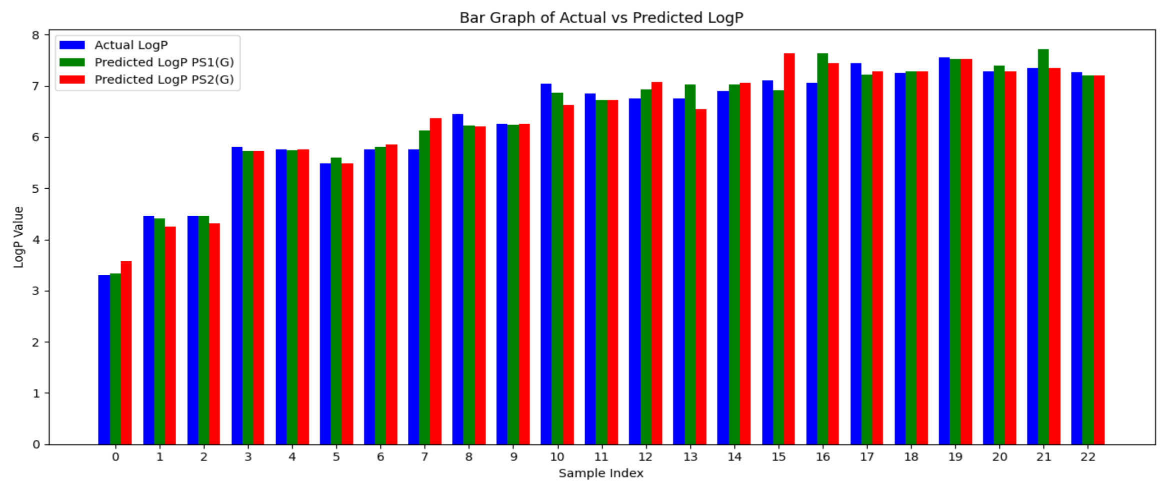

Figure 3: *Bar graph of Actual vs Predicted LogP*

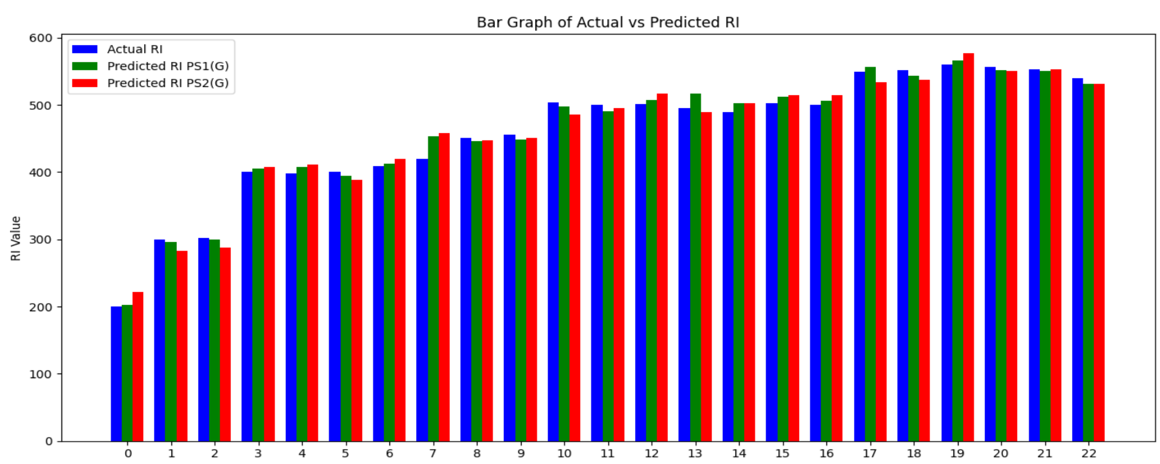

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Figure 4 : *Bar graph of Actual vs Predicted RI*

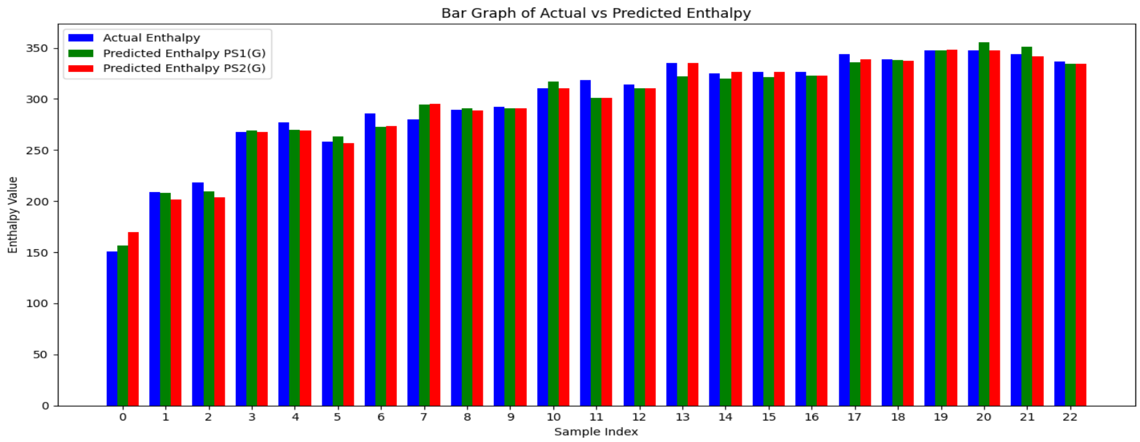

Figure 5: *Bar graph of Actual vs Predicted Enthalpy*

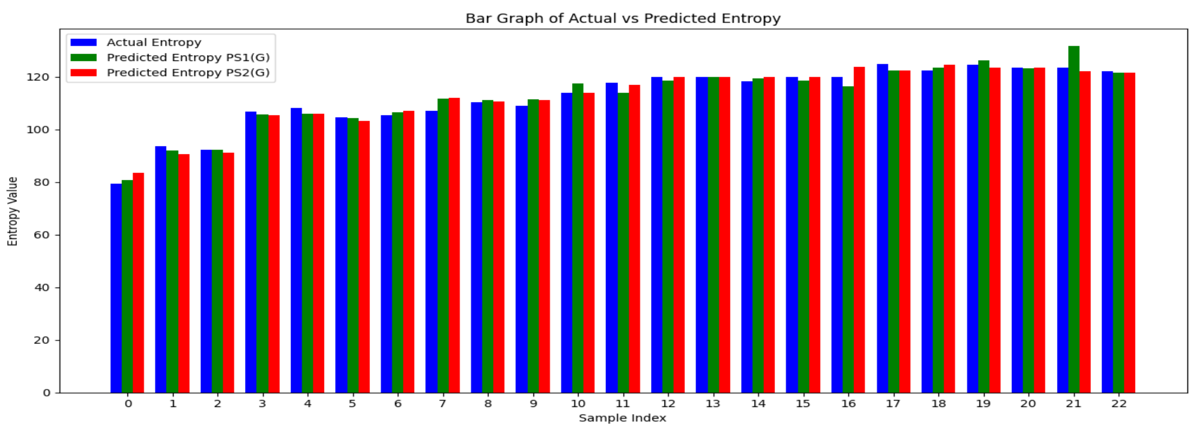

Figure 6: *Bar graph of Actual vs Predicted Entropy*

5 Conclusion

In this study, we introduced two new graph indices, $PS_1(G)$ and $PS_2(G)$, and studied their properties for different classes of graphs, and investigated some bounds. We also tested their ability to predict physicochemical properties of benzenoid hydrocarbons using cubic regression models. The results show that $PS_1(G)$ works better than $PS_2(G)$ and gives more accurate predictions. Comparing actual and predicted values confirms that these indices, especially $PS_1(G)$, are effective tools for linking graph structure to molecular properties. This work shows the usefulness of these indices in chemical graph theory and suggests that they could be applied to larger molecules or combined with other descriptors in future studies.

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