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SECOND NEIGHBORHOOD STRESS INDEX FOR GRAPHS

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Abstract. We propose a new topological index for graphs, referred to as the second neighborhood stress index, which is defined based on the neighborhood stresses of individual vertices.Various inequalities involving this index are derived, and some results are proven. Additionally, the second neighborhood stress index values are calculated for certain well-known graphs. This study further explores the chemical relevance of the second neighborhood stress index by applying regression analysis to a dataset of 22 benzenoid hydrocarbons. Through power regression models, we assess the relationship between the second neighborhood stress index and multiple physicochemical properties of these hydrocarbons.

1. Introduction

We refer to the textbook of Harary [4] for standard terminology and concepts in graph theory. This article will provide non-standard information when needed.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The degree of a node v in G is denoted by $\deg(v)$. A shortest path (graph geodesic) between two nodes u and v in G is a path between u and v with the minimum number of edges. We say that a graph geodesic P is passing through a node v in G if v is an internal node of P (i.e., v is a node in P, but not an end node of P).

The concept of stress of a node (node) in a network (graph) has been introduced by Shimbel as centrality measure in 1953 [29]. This centrality measure has applications in biology, sociology, psychology, etc., (See [6, 27]). The stress of a node v in a graph G, denoted by $\mathrm{str}_G(v)$ $\mathrm{str}(v)$, is the number of geodesics passing through it. We denote the maximum stress among all the nodes of G by Θ_G and minimum stress among all the nodes of G by θ_G. Further, the concepts of stress number of a graph and stress regular graphs have been studied by Bhargava et al. in their paper [3]. A graph G is called k-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$. Many stress related concepts in graphs and topological indices have been defined and studied by several authors, see [1, 2, 5, 7–26, 28, 30–33].

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Neighborhood of a vertex v is defined as

$$N_G(v) = \{u \in V(G) \mid uv \in E(G)\}.$$

We introduce a novel index known as the neighborhood stress of a vertex v, denoted by $N_s(v)$. This index is defined as the sum of the stresses of the adjacent vertices of v, formally expressed as:

$$N_s(v) = \sum_{u \in N_G(v)} str(u)$$

The first neighborhood stress index of a graph G is defined as

$$NS_1(G) = \sum_{v \in V(G)} N_s(v)^2$$

In this work, we investigate finite simple connected graphs, collectively referred to as graphs. We denote a specific graph as G and let N represent the number of geodesics of length at least 2 in G. Motivated by the stress on vertices and their related indices, we introduce a new topological index known as the second neighborhood stress index. We establish several inequalities, prove key results, and compute this index for various standard graphs. Furthermore, we examine the chemical significance of the second neighborhood stress index through regression analysis applied to 22 benzenoid hydrocarbons, investigating its correlation with several physicochemical properties.

2. Second Neighborhood Stress Index

Definition 2.1. The second neighborhood stress index of a graph G is defined as

$$NS_2(G) = \sum_{uv \in E(G)} N_s(u)N_s(v) \tag{2.1}$$

Definition 2.2. A graph G is called k- neighborhood stress regular if $N_s(v) = k$ for all $v \in V(G)$

Example 2.3. Consider the graph G given in Figure 1.

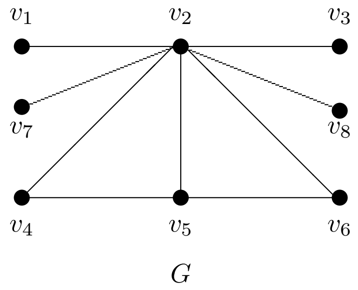


FIGURE 1. A graph G

Second neighborhood stress index of G is:

$$NS_2(G) = 895$$

Corollary 2.4. *If there is no geodesic of length* ≥ 2 *in a graph* G*, then* $NS_2(G) = 0$*. Moreover, for a complete graph* K_n*,* $NS_2(K_n) = 0$*.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N_s(v) = 0$. Hence we have $NS_2(G) = 0$.
In K_n, there is no geodesic of length ≥ 2 and so $NS_2(K_n) = 0$. □

Proposition 2.5. *For the complete bipartite* $K_{m,n}$*,*

$$NS_2(K_{m,n}) = \frac{m^3n^3(m-1)(n-1)}{4}.$$

Proof. Let $V_1 = \{v_1, \ldots, v_m\}$ and $V_2 = \{u_1, \ldots, u_n\}$ be the partite sets of $K_{m,n}$. We have,

$$N_s(v_i) = \frac{n.m(m-1)}{2} \text{ for } 1 \leq i \leq m \tag{2.2}$$

and

$$N_s(u_j) = \frac{m.n(n-1)}{2} \text{ for } 1 \leq j \leq n. \tag{2.3}$$

Using (2.2) and (2.3) in the Definition 2.1, we have

$$\begin{aligned} NS_2(K_{m,n}) &= \sum_{uv \in E(G)} N_s(u)N_s(v) \\ &= \sum_{1 \leq i \leq m,\ 1 \leq j \leq m} N_s(v_i)N_s(u_j) \\ &= \sum_{1 \leq i \leq m,\ 1 \leq j \leq m} \left[\frac{nm(m-1)}{2}\right]\left[\frac{mn(n-1)}{2}\right] \\ &= mn\left[\frac{nm(m-1)}{2}\right]\left[\frac{mn(n-1)}{2}\right] \\ &= \frac{m^3n^3(m-1)(n-1)}{4} \end{aligned}$$

□

Proposition 2.6. *For the star graph* $K_{1,n}$ *on* $n+1$ *vertices*

$$NS_2(K_{1,n}) = 0.$$

Proof. In a star graph $K_{1,n}$, internal vertex has neighborhood stress zero and remaining n have neighborhood stress $\frac{n(n-1)}{2}$ By the Definition 2.1, we have

$$\begin{aligned} NS_2(G) &= \sum_{uv \in E(G)} N_s(u)N_s(v) \\ &= 0. \end{aligned}$$

□

Proposition 2.7. *If* $G = (V, E)$ *is a* k*-neighborhood stress regular graph, then*

$$NS_2(G) = k^2|E|.$$

Proof. Suppose that G is a k-neighborhood stress regular graph. Then

$$N_s(v) = k \text{ for all } v \in V(G).$$

By the Definition 2.1, we have

$$\begin{aligned} NS_2(G) &= \sum_{uv\in E(G)} N_s(u)N_s(v) \\ &= \sum_{uv\in E(G)} k.k \\ &= k^2|E|. \end{aligned}$$

□

Corollary 2.8. *For a cycle C_n,*

$$NS_2(C_n) = \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{16}, & \textit{if } n \textit{ is odd;} \\ \dfrac{n^3(n-2)^2}{16}, & \textit{if } n \textit{ is even.} \end{cases}$$

Proof. For any node v in C_n, we have,

$$N_s(v) = \begin{cases} \dfrac{(n-1)(n-3)}{4}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{4}, & \text{if } n \text{ is even.} \end{cases}$$

Hence C_n is

$$\begin{cases} \dfrac{(n-1)(n-3)}{4}\text{-neighborhood stress regular}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{4}\text{-neighborhood stress regular}, & \text{if } n \text{ is even.} \end{cases}$$

Since C_n has n edges, by Proposition 2.7, we have

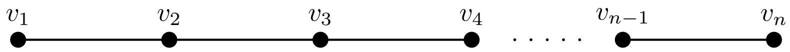
$$\begin{aligned} NS_2(C_n) &= n \times \begin{cases} \dfrac{(n-1)^2(n-3)^2}{16}, & \text{if } n \text{ is odd;} \\ \dfrac{n^2(n-2)^2}{16}, & \text{if } n \text{ is even.} \end{cases} \\ &= \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{16}, & \text{if } n \text{ is odd;} \\ \dfrac{n^3(n-2)^2}{16}, & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

□

Proposition 2.9. *For the path P_n on n nodes $NS_2(P_n)$*

$$= 4(n-2)(n-3) + \sum_{i=2}^{n-2} \left[(i-2)(n+1-i) + i(n-1-i)\right]\left[(i-1)(n-i) + (i+1)(n-i-2)\right].$$

Proof. Let P_n be the path with node sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 2).



P_n

FIGURE 2. The path P_n on n nodes.

We have ,

$$N_s(v_i) = \begin{cases} (i-2)(n+1-i)+i(n-1-i), & \text{if } 1<\text{i} < n \text{ ;} \\ (n-2), & \text{if } i\text{=1 or } i\text{=n.} \end{cases}$$

Thus by the Definition 2.1, we have

$$\begin{aligned} NS_2(P_n) &= \sum_{uv\in E(G)} N_s(u)N_s(v) \\ &= \sum_{i=1}^{n-1} N_s(v_i)N_s(v_{i+1}) \\ &= N_s(v_1)N_s(v_2) + N_s(v_{n-1})N_s(v_n) + \sum_{i=2}^{n-2} N_s(v_i)N_s(v_{i+1}) \end{aligned}$$

Thus we have $NS_2(P_n)$

$$= 4(n-2)(n-3)+\sum_{i=2}^{n-2} \left[(i-2)(n+1-i)+i(n-1-i)\right]\left[(i-1)(n-i)+(i+1)(n-i-2)\right]$$

□

Proposition 2.10. *For a fan graph* $F_{n+1} = P_n + K_1$, $n \geq 3$ *on* $n+1$ *vertices*

$$NS_2(F_{n+1}) = \frac{n^5 - 5n^4 + 17n^3 - 45n^2 + 68n - 68}{4}.$$

Proof. A fan graph $F_{n+1} = P_n + K_1$ where $V(K_1) = v_0$ and Let P_n be the path with node sequence $v_1, v_2, \ldots, v_n$.
we have

$$N_s(v_i) = \begin{cases} \frac{n^2-3n+6}{2}, & \text{if } 3 \leq i \leq n-2 \text{ ;} \\ \frac{n^2-3n+4}{2}, & \text{if } i = 1, 2, n-1, n. \end{cases}$$

and

$$N_s(v_0) = (n-2)$$

Thus by the Definition 2.1, we have

$$\begin{aligned} NS_2(F_{n+1}) &= N_s(v_1)N_s(v_2) + N_s(v_2)N_s(v_3) + N_s(v_{n-2})N_s(v_{n-1}) + N_s(v_{n-1})N_s(v_n) \\ &\quad + N_s(v_0)N_s(v_1) + N_s(v_0)N_s(v_2) + N_s(v_0)N_s(v_{n-1}) + N_s(v_0)N_s(v_n) \\ &\quad + \sum_{i=3}^{n-2} N_s(v_0)N_s(v_i) + \sum_{i=3}^{n-3} N_s(v_i)N_s(v_{i+1}) \end{aligned}$$

$$= \frac{n^5 - 5n^4 + 17n^3 - 45n^2 + 68n - 68}{4}$$

□

Proposition 2.11. *Let* $Wd(n,m)$ *denotes the windmill graph constructed for* $n \geq 2$ *and* $m \geq 2$ *by joining* m *copies of the complete graph* K_n *at a shared universal node* v*. Then*

$$NS_2(Wd(n,m)) = \frac{m^3(m-1)^2(n-1)^5}{4}.$$

Hence, for the friendship graph F_k *on* $2k+1$ *nodes,*

$$NS_2(F_k) = 8k^3(k-1)^2.$$

Proof. In the windmill graph $W_d(n,m)$, the stress of any node v_i other than the universal node v is zero. This is because the neighbors of each non-universal node induce a complete subgraph within $W_d(n,m)$. Since there are m copies of K_n (the complete graph on n vertices) in $W_d(n,m)$, and each node v_i within these copies is adjacent to the universal node v, it follows that all geodesics passing through v have length 2. Thus, the stress of v is given by $str(v) = \frac{m(m-1)(n-1)^2}{2}$. Additionally, note that v has $m(n-1)$ incident edges, and all edges not incident to v connect nodes whose stress is zero. Therefore, the neighborhood stress of the universal node v is zero, while the neighborhood stress of each remaining vertex v_i is $\frac{m(m-1)(n-1)^2}{2}$. By Definition 2.1, we obtain

$$\begin{aligned} NS_2(Wd(n,m)) &= m(n-1)N_s(v_i)^2 \\ &= m(n-1)\left[\frac{m^2(m-1)^2(n-1)^4}{4}\right] \\ &= \frac{m^3(m-1)^2(n-1)^5}{4}. \end{aligned}$$

Since the friendship graph F_k on $2k+1$ nodes is nothing but $Wd(3,k)$, it follows that

$$NS_2(F_k) = \frac{k^3(k-1)^2(3-1)^5}{4} = 8k^3(k-1)^2.$$

□

3. A QSPR Analysis

We carry a QSPR analysis for some physical properties of 22 benzenoid hydrocarbons with second neighborhood stress index of molecular graphs. Table 1 gives the second neighborhood stress index $NS_2(G)$ of molecular graphs and the experimental values for the physical properties - boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO),molar volume (MV), and molar refractivity (MR) of benzenoid hydrocarbons

Table 1. Second neighborhood stress index ($NS_2(G)$), boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR) of benzenoid hydrocarbons

Derivatives of benzene	$NS_2(G)$	**BP**	**π-ele**	**MW**	**PO**	**MV**	**MR**
Benzene	216	78.8	8	78.11	10.4	89.4	26.3
Naphthalene	8370	221.5	13.683	128.17	17.5	123.5	44.1
Phenanthrene	73034	337.4	19.448	178.23	24.6	157.7	61.9
Anthracene	78464	337.4	19.314	178.23	24.6	157.7	61.9
Chrysene	420747	448	25.192	228.3	31.6	191.8	79.8
Benzo[a]anthracene	391280	436.7	25.101	228.3	31.6	191.8	79.8
Triphenylene	294705	425	25.275	228.3	31.6	191.8	79.8
Tetracene	405482	436.7	25.188	228.3	31.6	191.8	79.8
Benzo[a]pyrene	703714	495	28.222	252.3	35.8	196.1	90.3
Benzo[e]pyrene	524357	467.5	28.336	252.3	35.8	196.1	90.3
Perylene	513128	467.5	28.245	252.3	35.8	196.1	90.3
Anthanthrene	1154490	497.1	31.253	276.3	40	200.4	100.8
Benzo[ghi]perylene	907940	501	31.425	276.3	40	200.4	100.8
Dibenz[a,c]anthracene	1105605	518	30.942	278.3	38.7	225.9	97.6
Dibenz[a,h]anthracene	1808618	524.7	30.881	278.3	38.7	225.9	97.6
Dibenz[a,j]anthracene	1142712	524.7	30.88	278.3	38.7	225.9	97.6
Picene	2027142	519	30.943	278.3	38.7	225.9	97.6
Coronene	1545868	525.6	34.572	300.4	44.1	204.7	111.4
Dibenzo[a,h]pyrene	2686828	552.3	33.928	302.4	42.9	230.2	108.1
Dibenzo[a,i]pyrene	2872065	552.3	33.954	302.4	42.9	230.2	108.1
Dibenzo[a,l]pyrene	1578179	552.3	34.031	302.4	42.9	230.2	108.1
Pyrene	150700	404	22.506	202.25	28.7	162	72.5

Regression Models. Using Table 1, a study was carried out with a power regression model

$$P = A \cdot (NS_2(G))^B,$$

where P = Physical property and $NS_2(G)$ = Second neighborhood stress index.

Table 2. The correlation coefficient r from power regression model between second neighborhood stress index and physicochemical properties (BP, π-ele,MW, PO, MV, MR) of benzenoid hydrocarbons.

BP	$\pi - ele$	MW	PO	MV	MR
0.971	0.982	0.987	0.979	0.979	0.979

The power regression models for boiling point , π-electron energy , molecular weight, polarizability, molar volume, and molar refractivity of benzenoid hydrocarbons are as follows:

$$BP = 34.585 \cdot (NS_2(G))^{0.1944} \tag{3.1}$$

$$\pi - ele = 3.3701 \cdot (NS_2(G))^{0.1581} \tag{3.2}$$

$$MW = 34.572 \cdot (NS_2(G))^{0.1481} \tag{3.3}$$

$$PO = 4.4307 \cdot (NS_2(G))^{0.1551} \tag{3.4}$$

$$MV = 49.711 \cdot (NS_2(G))^{0.1039} \tag{3.5}$$

$$MR = 11.198 \cdot (NS_2(G))^{0.1549} \tag{3.6}$$

Table 3. Comparison of boiling point(BP) between experimental and predicted values

Derivatives of benzene	BP from experiments	BP computed using the regression model
Benzene	78.80	98.33
Naphthalene	221.50	200.20
Phenanthrene	337.40	305.04
Anthracene	337.40	309.32
Chrysene	448.00	428.74
Benzo[a]anthracene	436.70	422.73
Triphenylene	425.00	400.07
Tetracene	436.70	425.67
Benzo[a]pyrene	495.00	473.83
Benzo[e]pyrene	467.50	447.49
Perylene	467.50	445.61
Anthanthrene	497.10	521.69
Benzo[ghi]perylene	501.00	497.89
Dibenz[a,c]anthracene	518.00	517.33
Dibenz[a,h]anthracene	524.70	569.27
Dibenz[a,j]anthracene	524.70	520.66
Picene	519.00	582.03
Coronene	525.60	552.16
Dibenzo[a,h]pyrene	552.30	614.80
Dibenzo[a,i]pyrene	552.30	622.82
Dibenzo[a,l]pyrene	552.30	554.38
Pyrene	404.00	351.17

Table 4. Comparison of π-ele between experimental and predicted values.

Derivatives of benzene	π-ele from experiments	π-ele computed using the regression model
Benzene	8.00	7.88
Naphthalene	13.68	14.05
Phenanthrene	19.45	19.80
Anthracene	19.31	20.02

Derivatives of benzene	π-ele from experiments	π-ele computed using the regression model
Benzene	8.00	7.88
Naphthalene	13.68	14.05
Phenanthrene	19.45	19.80
Anthracene	19.31	20.02
Chrysene	25.19	26.11
Benzo[a]anthracene	25.10	25.81
Triphenylene	25.28	24.68
Tetracene	25.19	25.96
Benzo[a]pyrene	28.22	28.32
Benzo[e]pyrene	28.34	27.03
Perylene	28.25	26.94
Anthanthrene	31.25	30.63
Benzo[ghi]perylene	31.43	29.49
Dibenz[a,c]anthracene	30.94	30.42
Dibenz[a,h]anthracene	30.88	32.88
Dibenz[a,j]anthracene	30.88	30.58
Picene	30.94	33.48
Coronene	34.57	32.07
Dibenzo[a,h]pyrene	33.93	35.00
Dibenzo[a,i]pyrene	33.95	35.37
Dibenzo[a,l]pyrene	34.03	32.18
Pyrene	22.51	22.20

Table 5. Comparison of molecular weight(MW) between experimental and predicted values

Derivatives of benzene	MW from experiments	MW computed using the regression model
Benzene	78.11	76.64
Naphthalene	128.17	131.73
Phenanthrene	178.23	181.56
Anthracene	178.23	183.50
Chrysene	228.30	235.31
Benzo[a]anthracene	228.30	232.79
Triphenylene	228.30	223.22
Tetracene	228.30	234.03
Benzo[a]pyrene	252.30	253.94
Benzo[e]pyrene	252.30	243.11
Perylene	252.30	242.33
Anthanthrene	276.30	273.25
Benzo[ghi]perylene	276.30	263.70
Dibenz[a,c]anthracene	278.30	271.51

Derivatives of benzene	MW from experiments	MW computed using the regression model
Dibenz[a,h]anthracene	278.30	292.04
Dibenz[a,j]anthracene	278.30	272.84
Picene	278.30	297.01
Coronene	300.40	285.33
Dibenzo[a,h]pyrene	302.40	309.67
Dibenzo[a,i]pyrene	302.40	312.74
Dibenzo[a,l]pyrene	302.40	286.20
Pyrene	202.25	202.12

Table 6. Comparison of polarizabiity (PO) between experimental and predicted values.

Derivatives of benzene	PO from experiments	PO computed using the regression model
Benzene	10.40	10.20
Naphthalene	17.50	17.98
Phenanthrene	24.60	25.17
Anthracene	24.60	25.45
Chrysene	31.60	33.02
Benzo[a]anthracene	31.60	32.65
Triphenylene	31.60	31.24
Tetracene	31.60	32.83
Benzo[a]pyrene	35.80	35.76
Benzo[e]pyrene	35.80	34.17
Perylene	35.80	34.05
Anthanthrene	40.00	38.61
Benzo[ghi]perylene	40.00	37.20
Dibenz[a,c]anthracene	38.70	38.36
Dibenz[a,h]anthracene	38.70	41.40
Dibenz[a,j]anthracene	38.70	38.55
Picene	38.70	42.14
Coronene	44.10	40.40
Dibenzo[a,h]pyrene	42.90	44.02
Dibenzo[a,i]pyrene	42.90	44.48
Dibenzo[a,l]pyrene	42.90	40.53
Pyrene	28.70	28.16

Table 7. Comparison of molar volume(MV) between experimental and predicted values.

Derivatives of benzene	MV from experiments	MV computed using the regression model
Benzene	89.4	86.90
Naphthalene	123.5	127.06

Derivatives of benzene	MV from experiments	MV computed using the regression model
Phenanthrene	157.7	159.14
Anthracene	157.7	160.33
Chrysene	191.8	190.89
Benzo[a]anthracene	191.8	189.46
Triphenylene	191.8	183.96
Tetracene	191.8	190.16
Benzo[a]pyrene	196.1	201.37
Benzo[e]pyrene	196.1	195.31
Perylene	196.1	194.87
Anthanthrene	200.4	212.00
Benzo[ghi]perylene	200.4	206.77
Dibenz[a,c]anthracene	225.9	211.05
Dibenz[a,h]anthracene	225.9	222.12
Dibenz[a,j]anthracene	225.9	211.77
Picene	225.9	224.77
Coronene	204.7	218.53
Dibenzo[a,h]pyrene	230.2	231.45
Dibenzo[a,i]pyrene	230.2	233.06
Dibenzo[a,l]pyrene	230.2	219.00
Pyrene	162	171.58

Table 8. Comparison of molar refractivity(MR) between experimental and predicted values

Derivatives of benzene	MR from experiments	MR computed using the regression model
Benzene	26.3	25.75
Naphthalene	44.1	45.37
Phenanthrene	61.9	63.46
Anthracene	61.9	64.17
Chrysene	79.8	83.23
Benzo[a]anthracene	79.8	82.30
Triphenylene	79.8	78.77
Tetracene	79.8	82.76
Benzo[a]pyrene	90.3	90.14
Benzo[e]pyrene	90.3	86.12
Perylene	90.3	85.83
Anthanthrene	100.8	97.32
Benzo[ghi]perylene	100.8	93.77
Dibenz[a,c]anthracene	97.6	96.67
Dibenz[a,h]anthracene	97.6	104.33
Dibenz[a,j]anthracene	97.6	97.17
Picene	97.6	106.19

Derivatives of benzene	MR from experiments	MR computed using the regression model
Coronene	111.4	101.82
Dibenzo[a,h]pyrene	108.1	110.93
Dibenzo[a,i]pyrene	108.1	112.08
Dibenzo[a,l]pyrene	108.1	102.15
Pyrene	72.5	71.00

4. Conclusion

Table 2, reveals that the power regression models (3.1)-(3.2)-(3.3)-(3.4)-(3.5)-(3.6) are useful tools in predicting the physical properties of benzenoid hydrocarbons. It shows that second neighborhood stress index can be used as predictive means in QSPR researches.

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