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ELLIPTIC SOMBOR STRESS INDEX FOR GRAPHS

HAKEEM A. OTHMAN, M. KIRANKUMAR, HUSNIYAH ALZUBAIDI,
P. SIVA KOTA REDDY*, AND SAMI H. ALTOUM

Abstract. We introduce a novel topological index for graphs called elliptic Sombor stress index using stresses of nodes. Some inequalities have been established, some results have been proved and elliptic Sombor stress index of some standard graphs have been computed. This study examines the chemical significance of the elliptic Sombor stress index through regression analysis applied to 22 benzenoid hydrocarbons. Using power regression models, we investigate how the elliptic Sombor stress index correlates with several physicochemical properties of these hydrocarbons.

1. Introduction

We refer to the textbook of Harary [6] 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 [40]. This centrality measure has applications in biology, sociology, psychology, etc., (See [9, 38]). The stress of a node v in a graph G, denoted by $\mathrm{str}_G(v)$ or $\mathrm{str}(v)$, 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 [1–4, 7, 8, 10–20, 22–37, 39, 41–45].

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*Corresponding author.

Gutman et al. [5] introduced the concept of elliptic Sombor index. The elliptic Sombor index EI of a graph G is defined as

$$EI(G) = \sum_{uv \in E(G)} (deg(u) + deg(v))\sqrt{\deg(u)^2 + \deg(v)^2}. \tag{1.1}$$

In this work, a finite simple connected graph is referred to as a graph, G denotes a graph and N denotes the number of geodesics of length ≥ 2 in G. Motivated by the elliptic Sombor index discussed above, we introduce a topological index for graphs using stress on nodes, in section 2. This new index is called the elliptic Sombor stress index. Further, some inequalities have been established, some results have been proved and elliptic Sombor stress index of some standard graphs have been computed. In section 3, we examine the chemical significance of the elliptic Sombor stress index through regression analysis applied to 22 benzenoid hydrocarbons. Using power regression models, we investigate how the elliptic Sombor stress index correlates with several physicochemical properties of these hydrocarbons.

2. Elliptic Sombor Stress Index

Definition 2.1. The elliptic Sombor stress index $ESI(G)$ of a graph G is defined as

$$ESI(G) = \sum_{uv \in E(G)} (str(u) + str(v))\sqrt{\mathrm{str}(u)^2 + \mathrm{str}(v)^2}. \tag{2.1}$$

Observation: From the Definition 2.1, it follows that, for any graph G,

$$2\sqrt{2}\, m^2\theta_G \leq ESI(G) \leq 2\sqrt{2}\, m^2\Theta_G$$

where m is the number of edges in G.

Example 2.2. Consider the graph G given in Figure 1.

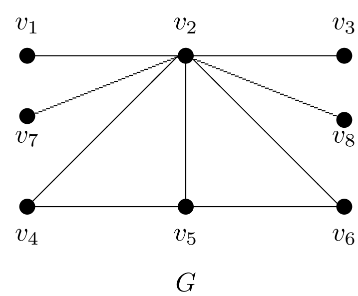


Figure 1. A graph G

The stresses of the nodes of G are as follows:
$\mathrm{str}(v_1) = \mathrm{str}(v_3) = \mathrm{str}(v_7) = \mathrm{str}(v_8) = \mathrm{str}(v_4) = \mathrm{str}(v_6) = 0$,
$\mathrm{str}(v_2) = 19$, $\mathrm{str}(v_5) = 1$.

The elliptic Sombor stress index of G is:

$$ESI(G) = 19\sqrt{19^2 + 0^2} + 19\sqrt{19^2 + 0^2} + 19\sqrt{19^2 + 0^2} + 19\sqrt{19^2 + 0^2}$$

$$+ 19\sqrt{19^2+0^2} + 20\sqrt{19^2+1^2} + 19\sqrt{19^2+0^2} + \sqrt{0^2+1^2}$$
$$+ \sqrt{1^2+0^2}$$
$$=2548.526.$$

Proposition 2.3. *For any graph G,*

$$0 \le ESI(G) \le 2\sqrt{2}N^2|E|. \tag{2.2}$$

Proof. For any node v in G, we have $0 \le \mathrm{str}(v) \le N$. Hence by Definition 2.1, it follows that $0 \le ESI \le 2\sqrt{2}N^2|E|$. □

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

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.3, we have $ESI(G) = 0$.

In K_n, there is no geodesic of length ≥ 2 and so $ESI(K_n) = 0$. □

Theorem 2.5. *For a graph G, $ESI(G) = 0$ iff G is complete.*

Proof. Suppose that $ESI(G) = 0$. Then by the Definition 2.1, $(str(u) + str(v))\sqrt{\mathrm{str}(u)^2 + \mathrm{str}(v)^2} = 0$, $\forall uv \in E(G)$. Hence $\mathrm{str}(v) = 0$, $\forall v \in V(G)$. If $|V(G)| = 1$ or 2, then G is a complete graph as $G \cong K_1$ or K_2. Assume that $|V(G)| > 2$. Let u, v be any two distinct nodes in G. We claim that u, v are adjacent in G. For, if u, v are not adjacent in G, then there is a geodesic in G between u and v passing through at least one node, say w making $\mathrm{str}(w) \ge 1$, which a contradiction. Hence, u, v are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then by Corollary 2.4, it follows that $ESI(G) = 0$. □

Proposition 2.6. *For the complete bipartite $K_{m,n}$,*

$$ESI(K_{m,n}) = \frac{mn}{4}\left(n(n-1) + m(m-1)\right)\sqrt{n^2(n-1)^2 + m^2(m-1)^2}.$$

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

$$\mathrm{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \le i \le m \tag{2.3}$$

and

$$\mathrm{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \le j \le n. \tag{2.4}$$

Using (2.3) and (2.4) in the Definition 2.1, we have

$$ESI(K_{m,n}) = \sum_{uv \in E(G)} (str(u) + str(v))\sqrt{\mathrm{str}(u)^2 + \mathrm{str}(v)^2}$$
$$= \sum_{1 \le i \le m,\ 1 \le j \le m} (str(v_i) + str(u_j))\sqrt{\mathrm{str}(v_i)^2 + \mathrm{str}(u_j)^2}$$

$$= \sum_{1\leq i\leq m,\ 1\leq j\leq n} \frac{n(n-1)+m(m-1)}{2}\sqrt{\left(\frac{n(n-1)}{2}\right)^2+\left(\frac{m(m-1)}{2}\right)^2}$$
$$= \frac{mn}{4}\left(n(n-1)+m(m-1)\right)\sqrt{n^2(n-1)^2+m^2(m-1)^2}.$$

□

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

$$ESI(G)=2\sqrt{2}k^2|E|.$$

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

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

By the Definition 2.1, we have

$$\begin{aligned} ESI(G) &= \sum_{uv\in E(G)} (str(u)+str(v))\sqrt{\mathrm{str}(u)^2+\mathrm{str}(v)^2} \\ &= \sum_{uv\in E(G)} 2k\sqrt{k^2+k^2} \\ &= 2\sqrt{2}k^2|E|. \end{aligned}$$

□

Corollary 2.8. *For a cycle C_n,*

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

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

$$\mathrm{str}(v)=\begin{cases} \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

Hence C_n is

$$\begin{cases} \dfrac{(n-1)(n-3)}{8}\text{-stress regular}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{8}\text{-stress regular}, & \text{if } n \text{ is even.} \end{cases}$$

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

$$\begin{aligned} ESI(C_n) &= 2\sqrt{2}\,n\times\begin{cases} \dfrac{(n-1)^2(n-3)^2}{64}, & \text{if } n \text{ is odd;} \\ \dfrac{n^2(n-2)^2}{64}, & \text{if } n \text{ is even.} \end{cases} \\ &= \begin{cases} \dfrac{n(n-1)^2(n-3)^2}{16\sqrt{2}}, & \text{if } n \text{ is odd;} \\ \dfrac{n^3(n-2)^2}{16\sqrt{2}}, & \text{if } n \text{ is even.} \end{cases} \end{aligned}$$

□

Proposition 2.9. *Let T be a tree on n nodes. Then*

$$\begin{aligned}ESI(T) = \sum_{uv\in J}\Bigg[&\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u| + \sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)\\ &\qquad\sqrt{\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\right)^2 + \left(\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)^2}\ \Bigg]\\ &+\sum_{w\in Q}\left(\sum_{1\le i<j\le m(w)}|C_i^w||C_j^w|\right)^2.\end{aligned}$$

where J is the set of internal(non-pendant) edges in T, Q denotes the set of all nodes adjacent to pendent nodes in T, and the sets $C_1^v,\ldots,C_m^v$ denotes the node sets of the components of $T-v$ for an internal node v of degree $m=m(v)$.

Proof. We know that a pendant node in T has zero stress. Let v be an internal node of T of degree $m=m(v)$. Let $C_1^v,\ldots,C_m^v$ be the components of $T-v$. Since there is only one path between any two nodes in a tree, it follows that,

$$\operatorname{str}(v) = \sum_{1\le i<j\le m}|C_i^v||C_j^v| \tag{2.5}$$

Let J denotes the set of internal(non-pendant) edges, and P denotes pendant edges and Q denotes the set of all nodes adjacent to pendent nodes in T. Then using (2.5) in the Definition 2.1 ((2.1)), we have

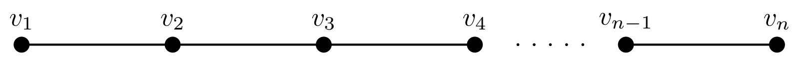
$$\begin{aligned}ESI(T) &= \sum_{uv\in J}(str(u)+str(v))\sqrt{\operatorname{str}(u)^2+\operatorname{str}(v)^2}\\ &\qquad+\sum_{uv\in P}(str(u)+str(v))\sqrt{\operatorname{str}(u)^2+\operatorname{str}(v)^2}\\ &= \sum_{uv\in J}(str(u)+str(v))\sqrt{\operatorname{str}(u)^2+\operatorname{str}(v)^2}+\sum_{w\in Q}\operatorname{str}(w)^2\\ &= \sum_{uv\in J}\Bigg[\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u| + \sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)\\ &\qquad\sqrt{\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\right)^2 + \left(\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)^2}\ \Bigg]\\ &\qquad+\sum_{w\in Q}\left(\sum_{1\le i<j\le m(w)}|C_i^w||C_j^w|\right)^2.\end{aligned}$$

□

Corollary 2.10. *For the path P_n on n nodes*

$$ESI(P_n) = \sum_{i=1}^{n-1} ((i-1)(n-i) + i(n-i-1)) \sqrt{(i-1)^2(n-i)^2 + i^2(n-i-1)^2}.$$

Proof. The proof of this corollary follows by above Proposition 2.9. We follow the proof of the Proposition 2.9 to compute the index. Let P_n be the path with node sequence $v_1, v_2, \dots, v_n$ (shown in Figure 2).



P_n

Figure 2. The path P_n on n nodes.

We have,

$$\text{str}(v_i) = (i-1)(n-i),\ 1 \le i \le n.$$

Then

$$\begin{aligned} ESI(P_n) &= \sum_{uv \in E(P_n)} (str(u) + str(v)) \sqrt{\text{str}(u)^2 + \text{str}(v)^2} \\ &= \sum_{i=1}^{n-1} (str(v_i) + str(v_{i+1})) \sqrt{\text{str}(v_i)^2 + \text{str}(v_{i+1})^2} \\ &= \sum_{i=1}^{n-1} ((i-1)(n-i) + i(n-i-1)) \sqrt{(i-1)^2(n-i)^2 + i^2(n-i-1)^2}. \end{aligned}$$

□

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

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

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

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

Proof. Clearly the stress of any node other than universal node is zero in $Wd(n,m)$, because neighbors of that node induces a complete subgraph of $Wd(n,m)$. Also, since there are m copies of K_n in $Wd(n,m)$ and their nodes are adjacent to v, it follows that, the only geodesics passing through v are of length 2 only. So, $\text{str}(v) = \dfrac{m(m-1)(n-1)^2}{2}$. Note that there are $m(n-1)$ edges incident on v and the edges that are not incident on v have end nodes of stress zero. Hence by the Definition 2.1, we have

$$ESI(Wd(n,m)) = m(n-1)\,\text{str}(v)^2$$

$$= m(n-1)\left[\frac{m^2(m-1)^2(n-1)^4}{4}\right]$$
$$= \frac{m^3(m-1)^2(n-1)^5}{4}.$$

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

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

□

3. A QSPR Analysis

We carry a QSPR analysis for some physical properties of 22 benzenoid hydrocarbons with elliptic Sombor stress index of molecular graphs. Table 1 gives the elliptic Sombor stress index $ESI(G)$ 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. Elliptic Sombor stress index, 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	**ESI**	**BP**	**π-ele**	**MW**	**PO**	**MV**	**MR**
Benzene	152.73	78.8	8	78.11	10.4	89.4	26.3
Naphthalene	5274.46	221.5	13.683	128.17	17.5	123.5	44.1
Phenanthrene	41132.79	337.4	19.448	178.23	24.6	157.7	61.9
Anthracene	42352.30	337.4	19.314	178.23	24.6	157.7	61.9
Chrysene	220644.78	448	25.192	228.3	31.6	191.8	79.8
Benzo[a]anthracene	203083.27	436.7	25.101	228.3	31.6	191.8	79.8
Triphenylene	147906.95	425	25.275	228.3	31.6	191.8	79.8
Tetracene	202256.62	436.7	25.188	228.3	31.6	191.8	79.8
Benzo[a]pyrene	339777.16	495	28.222	252.3	35.8	196.1	90.3
Benzo[e]pyrene	251772.52	467.5	28.336	252.3	35.8	196.1	90.3
Perylene	251145.97	467.5	28.245	252.3	35.8	196.1	90.3
Anthanthrene	527254.88	497.1	31.253	276.3	40	200.4	100.8
Benzo[ghi]perylene	418822.73	501	31.425	276.3	40	200.4	100.8
Dibenz[a,c]anthracene	527032.29	518	30.942	278.3	38.7	225.9	97.6
Dibenz[a,h]anthracene	913843.88	524.7	30.881	278.3	38.7	225.9	97.6
Dibenz[a,j]anthracene	583385.30	524.7	30.88	278.3	38.7	225.9	97.6
Picene	1020139.13	519	30.943	278.3	38.7	225.9	97.6
Coronene	682838.95	525.6	34.572	300.4	44.1	204.7	111.4
Dibenzo[a,h]pyrene	1251375.98	552.3	33.928	302.4	42.9	230.2	108.1
Dibenzo[a,i]pyrene	1345921.18	552.3	33.954	302.4	42.9	230.2	108.1
Dibenzo[a,l]pyrene	728731.37	552.3	34.031	302.4	42.9	230.2	108.1
Pyrene	77194.74	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

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

where P = Physical property and $ESI(G)$ = Sombor stress index.

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

BP	$\pi - ele$	MW	PO	MV	MR
0.968	0.977	0.983	0.973	0.981	0.973

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

$$BP = 35.26 \cdot (ESI(G))^{0.2037} \tag{3.1}$$

$$\pi - ele = 3.4338 \cdot (ESI(G))^{0.1654} \tag{3.2}$$

$$MW = 35.159 \cdot (ESI(G))^{0.155} \tag{3.3}$$

$$PO = 4.5155 \cdot (ESI(G))^{0.1622} \tag{3.4}$$

$$MV = 50.116 \cdot (ESI(G))^{0.1091} \tag{3.5}$$

$$MR = 11.412 \cdot (ESI(G))^{0.1621} \tag{3.6}$$

From Table 2, it follows that the power regression models: (3.1)-(3.2)-(3.3)-(3.4)-(3.5)-(3.6) can be used as predictive tools.

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 elliptic Sombor stress index can be used as predictive means in QSPR researches.

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Department of Mathematics, Albaydha University, Al Bayda, Yemen.
Email address: hakim_albdoie@yahoo.com

Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru-570 006, India
Email address: kiran.maths@vvce.ac.in

Department of Mathematics, AL-Qunfudhah University college, Umm Al-Qura University, Kingdom of Saudi Arabia
Email address: hazbaidi@uqu.edu.sa

P. Siva Kota Reddy: Department of Mathematics, JSS Science and Technology University, Mysuru-570 006, India.
and
Universidad Bernardo O'Higgins, Facultad de Ingeniería, Ciencia y Tecnología, Departamento de Formación y Desarrollo Científico en Ingeniería, Av. Viel 1497, Santiago, Chile
Email address: pskreddy@jssstuniv.in; pskreddy@sjce.ac.in

Sami H. Altoum: Manar Al Janoub College of Science and Technology, Jazan, Kingdom of Saudi Arabia
Email address: s.altom@mjc.edu.sa