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SOMBOR STRESS INDEX FOR GRAPHS

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ABSTRACT. We introduce a novel topological index for graphs called Sombor stress index using stresses of nodes. Some inequalities have been established, some results have been proved and Sombor stress index for some standard graphs have been computed. Further, a QSPR analysis is carried for Sombor stress index of molecular graphs and physical properties of lower alkanes and linear regression models are presented.

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KEYWORDS AND PHRASES: Graph, Geodesic, Topological index, Stress of a node.

1. INTRODUCTION

We refer to the textbook of Harary [5] 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 [26]. This centrality measure has applications in biology, sociology, psychology, etc., (See [7,24]). 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 [2]. A graph G is called k-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$.

I. Gutman [4] introduced the concept of Sombor index. The Sombor index $\mathcal{SO}(G)$ of a graph G is defined as

(1) $$\mathcal{SO}(G) = \sum_{uv \in E(G)} \sqrt{\deg(u)^2 + \deg(v)^2}$$

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K. C. Das et al. [3] have presented some novel lower and upper bounds on the Sombor index of graphs and obtained some relations on Sombor index with the first and second Zagreb indices. For new stress/degree based topological indices, we suggest the reader to refer the papers [1,6,8–10,13–23,25,27–29].

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 Sombor index discussed above, we introduce a topological index for graphs using stress on nodes. This new index is called the Sombor stress index. Further, some inequalities have been established, some results have been proved and Sombor stress index for some standard graphs have been computed. Further, a QSPR analysis is carried for Sombor stress index of molecular graphs and physical properties of lower alkanes and linear regression models are presented for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions.

2. Sombor stress index

Definition 2.1. *The Sombor stress index $\mathcal{SOS}(G)$ of a graph G is defined as*

$$\mathcal{SOS}(G) = \sum_{uv \in E(G)} \sqrt{str(u)^2 + str(v)^2} \tag{2}$$

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

$$\sqrt{2}\, m\theta_G \leq \mathcal{SOS}(G) \leq \sqrt{2}\, m\Theta_G$$

where m is the number of edges in G.

Example 2.1. *Consider the graph G given in Figure 1.*

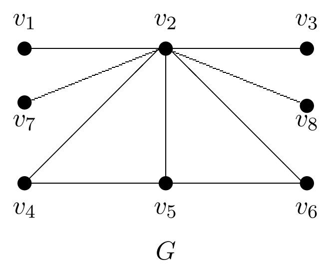

Figure 1. A graph G

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

The Sombor stress index of G is:

$$\begin{aligned}\mathcal{SOS}(G) =& \sqrt{19^2+0^2} + \sqrt{19^2+0^2} + \sqrt{19^2+0^2} + \sqrt{19^2+0^2} + \sqrt{19^2+0^2} \\ & + \sqrt{19^2+1^2} + \sqrt{19^2+0^2} + \sqrt{0^2+1^2} + \sqrt{1^2+0^2} \\ =& 135.026.\end{aligned}$$

Proposition 2.2. *For any graph G,*

$$0 \leq \mathcal{SOS}(G) \leq \sqrt{2}N|E|. \tag{3}$$

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

Corollary 2.3. *If there is no geodesic of length ≥ 2 in a graph G, then $\mathcal{SOS}(G) = 0$. Moreover, for a complete graph K_n, $\mathcal{SOS}(K_n) = 0$.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.2, we have $\mathcal{SOS}(G) = 0$.

In K_n, there is no geodesic of length ≥ 2 and so $\mathcal{SOS}(K_n) = 0$. □

Theorem 2.4. *For a graph G, $\mathcal{SOS}(G) = 0$ iff G is complete.*

Proof. Suppose that $\mathcal{SOS}(G) = 0$. Then by the Definition 2.1, $\sqrt{\mathrm{str}(u)^2 + \mathrm{str}(v)^2 = 0}$, $\forall uv \in E(G)$. 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 $\mathrm{str}(w) \geq 1$, 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 2.3, it follows that $\mathcal{SOS}(G) = 0$. □

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

$$\mathcal{SOS}(K_{m,n}) = \frac{mn}{2}\sqrt{n^2(n-1)^2 + m^2(m-1)^2}.$$

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,

$$\mathrm{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{4}$$

and

$$\mathrm{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{5}$$

Using (4) and (5) in the Definition 2.1, we have

$$\begin{aligned}
\mathcal{SOS}(K_{m,n}) &= \sum_{uv \in E(G)} \sqrt{\mathrm{str}(u)^2 + \mathrm{str}(v)^2} \\
&= \sum_{1\leq i\leq m,\ 1\leq j\leq m} \sqrt{\mathrm{str}(v_i)^2 + \mathrm{str}(u_j)^2} \\
&= \sum_{1\leq i\leq m,\ 1\leq j\leq n} \sqrt{\left(\frac{n(n-1)}{2}\right)^2 + \left(\frac{m(m-1)}{2}\right)^2} \\
&= \frac{mn}{2}\sqrt{n^2(n-1)^2 + m^2(m-1)^2}.
\end{aligned}$$

□

Proposition 2.6. *If $G=(V,E)$ is a k-stress regular graph, then*

$$\mathcal{SOS}(G)=\sqrt{2}k|E|.$$

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

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

By the Definition 2.1, we have

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

□

Corollary 2.7. *For a cycle C_n,*

$$\mathcal{SOS}(C_n)=\begin{cases}\dfrac{n(n-1)(n-3)}{4\sqrt{2}}, & \text{if } n \text{ is odd;}\\ \dfrac{n^2(n-2)}{4\sqrt{2}}, & \text{if } n \text{ is even.}\end{cases}$$

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

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

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 2.6, we have

$$\begin{aligned}\mathcal{SOS}(C_n)&=\sqrt{2}\,n\times\begin{cases}\dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd;}\\ \dfrac{n(n-2)}{8}, & \text{if } n \text{ is even.}\end{cases}\\&=\begin{cases}\dfrac{n(n-1)(n-3)}{4\sqrt{2}}, & \text{if } n \text{ is odd;}\\ \dfrac{n^2(n-2)}{4\sqrt{2}}, & \text{if } n \text{ is even.}\end{cases}\end{aligned}$$

□

Proposition 2.8. *Let T be a tree on n nodes. Then*

$$\mathcal{SOS}(T)=\sum_{uv\in J}\sqrt{\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\right)^2+\left(\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)^2}$$

$$+\sum_{w\in Q}\left(\sum_{1\le i<j\le m(w)}|C_i^w||C_j^w|\right).$$

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,

$$\text{str}(v)=\sum_{1\le i<j\le m}|C_i^v||C_j^v| \tag{6}$$

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 (6) in the Definition 2.1 ((2)), we have

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

□

Corollary 2.9. *For the path P_n on n nodes*

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

Proof. The proof of this corollary follows by above Proposition 2.8. We follow the proof of the Proposition 2.8 to compute the index. Let P_n be the path with node sequence $v_1,v_2,\ldots,v_n$ (shown in Figure 2).

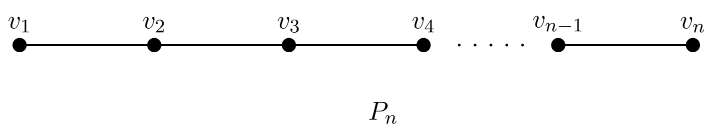

FIGURE 2. The path P_n on n nodes.

We have,

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

Then

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

□

Proposition 2.10. *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*

$$\mathcal{SOS}(Wd(n,m)) = \frac{m^2(m-1)(n-1)^3}{2}.$$

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

$$\mathcal{SOS}(F_k) = 4k^2(k-1).$$

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, $\mathrm{str}(v) = \frac{m(m-1)(n-1)^2}{2}$. 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

$$\begin{aligned}\mathcal{SOS}(Wd(n,m)) &= m(n-1)\,\mathrm{str}(v)\\ &= m(n-1)\left[\frac{m(m-1)(n-1)^2}{2}\right]\\ &= \frac{m^2(m-1)(n-1)^3}{2}.\end{aligned}$$

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

$$\mathcal{SOS}(F_k) = \frac{k^2(k-1)(3-1)^3}{2} = 4k^2(k-1).$$

□

Proposition 2.11. *Let W_n denotes the wheel graph constructed on $n \geq 4$ nodes. Then*

$$\mathcal{SOS}(W_n) = (n-1)\times\begin{cases}\sqrt{\frac{(n-1)^2(n-4)^2}{4}+\frac{(n-2)^2(n-4)^2}{64}}+\frac{(n-2)(n-4)}{4\sqrt{2}}, & \textit{if } n \textit{ is even;}\\ \sqrt{\frac{(n-1)^2(n-4)^2}{4}+\frac{(n-1)^2(n-3)^2}{64}}+\frac{(n-1)(n-3)}{4\sqrt{2}}, & \textit{if } n \textit{ is odd.}\end{cases}.$$

Proof. In W_n with $n \geq 4$, there are $(n-1)$ peripheral nodes and one central node, say v. It is easy to see that

$$\text{str}(v) = \frac{(n-1)(n-4)}{2} \tag{7}$$

Let p be a peripheral node. Since v is adjacent to all the peripheral nodes in W_n, there is no geodesic passing through p and containing v. Hence contributing nodes for str(p) are the rest peripheral nodes. So, by denoting the cycle $W_n - p$ (on $n-1$ nodes) by C_{n-1}, we have

$$\begin{aligned}
\text{str}_{W_n}(p) &= \text{str}_{W_n - v}(p) \\
&= \text{str}_{C_{n-1}}(p) \\
&= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,} \end{cases} \\
&= \begin{cases} \dfrac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases} \qquad (8)
\end{aligned}$$

Let us denote the set of all radial edges in W_n by R, and the set of all peripheral edges by Q. Note that there are $(n-1)$ radial edges and $(n-1)$ peripheral edges in W_n. Using (7) and (8) in the Definition 2.1, we have

$$\begin{aligned}
\mathcal{SOS}(W_n) &= \sum_{xy\in R}[\sqrt{\text{str}(x)^2+\text{str}(y)^2}] + \sum_{xy\in Q}[\sqrt{\text{str}(x)^2+\text{str}(y)^2}] \\
&= (n-1)[\sqrt{\text{str}(v)^2+\text{str}(p)^2}] + (n-1)\cdot\sqrt{2\cdot\text{str}(p)^2} \\
&= (n-1)\times\begin{cases} \sqrt{\left(\frac{(n-1)(n-4)}{2}\right)^2 + \left(\frac{(n-2)(n-4)}{8}\right)^2}, & \text{if } n \text{ is even;} \\ \sqrt{\left(\frac{(n-1)(n-4)}{2}\right)^2 + \left(\frac{(n-1)(n-3)}{8}\right)^2}, & \text{if } n \text{ is odd.} \end{cases} \\
&\quad + \sqrt{2}(n-1)\times\begin{cases} \frac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \frac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases} \\
&= (n-1)\times\begin{cases} \sqrt{\frac{(n-1)^2(n-4)^2}{4} + \frac{(n-2)^2(n-4)^2}{64}} + \frac{(n-2)(n-4)}{4\sqrt{2}}, & \text{if } n \text{ is even;} \\ \sqrt{\frac{(n-1)^2(n-4)^2}{4} + \frac{(n-1)^2(n-3)^2}{64}} + \frac{(n-1)(n-3)}{4\sqrt{2}}, & \text{if } n \text{ is odd.} \end{cases}
\end{aligned}$$

□

3. A QSPR Analysis

We carry a QSPR analysis for some physical properties of lower alkanes with Sombor stress index of molecular graphs. Table 1 gives the Sombor stress index $\mathcal{SOS}(G)$ of molecular graphs and the experimental values for the physical properties - Boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporization (hv) kJ, critical temperatures

(ct) $°C$, critical pressures (cp) atm, and surface tensions(st) $dyne\ cm^{-1}$ of considered alkanes. The values given in the columns 3 to 9 in the Table 1 are taken from Needham et al. [11] (the same values can be found in [30]).

TABLE 1. Sombor stress index, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

Alkane	$\mathcal{SOS}(G)$	$\frac{bp}{°C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{°C}$	$\frac{cp}{atm}$	$\frac{st}{dy\ cm^{-1}}$
Pentane	16	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	18.831	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	24	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	30.907	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	34.431	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	33.888	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	40.849	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	37.899	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	52.952	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	57.204	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	56.118	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylpentane	54	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	64.856	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	49.296	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	61.456	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	63.856	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	69	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	83.535	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	88.532	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	86.953	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	71.38	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	59.618	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	97.491	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	91.29	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	89.131	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	93.529	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	95.413	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	90.263	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	87.592	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	92.922	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	93.131	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	102.488	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	115.547	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	81.202	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	124.066	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	129.811	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	127.763	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	126.672	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	114.481	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	106.248	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	140.116	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	126.33	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	133.511	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	133.511	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	135.562	135.2	180.9	43.93	42.8	306	23.7	20.83

3,3-Dimethylheptane	137.044	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	130.244	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	131.46	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	136.984	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	124.913	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	127.229	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	131.411	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	125.014	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	142.537	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	125.813	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	127.864	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	141.506	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	135.902	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	138.078	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	142.792	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	140.54	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	128	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	125.849	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	137.287	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	130.532	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	152.795	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	138.28	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	156.166	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	147.108	141.6	169.9	43.2	41.8	334.5	26.85	23.31

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

$$P = A + B \cdot \mathcal{SOS}(G),$$

where P = Physical property and $\mathcal{SOS}(G)$ = Sombor stress index. The correlation coefficient r, its square r^2, standard error (se), t-value and p-value are computed and tabulated in Table 2 followed by linear regression models.

TABLE 2. r,r^2, se, t and p for the physical properties (P) and Sombor stress index

P	r	r^2	se	t	p
bp	0.8989	0.8080	(4.6645) (0.0433)	(8.8791) (16.7927)	$(6.30093E-13)$ $(1.04985E-25)$
mv	0.9406	0.8847	(1.9962) (0.0185)	(60.2917) (22.6704)	$(4.18484E-60)$ $(3.87304E-33)$
mr	0.9539	0.9100	(0.5366) (0.0050)	(49.2639) (26.0253)	$(2.34901E-54)$ $(9.47945E-37)$
hv	0.8676	0.7528	(0.9075) (0.0084)	(29.4028) (14.2826)	$(5.111E-40)$ $(5.2039E-22)$
ct	0.8983	0.8069	(5.6860) (0.0528)	(35.5889) (16.7315)	$(3.04537E-45)$ $(1.27991E-25)$
cp	−0.7957	0.6331	(0.5400) (0.0050)	(58.7471) (−10.7522)	$(2.30673E-59)$ $(3.12849E-16)$
st	0.7972	0.6355	(0.4340) (0.0039)	(39.8626) (9.2399)	$(6.58033E-47)$ $(2.16095E-13)$

The linear regression models for boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes are as follows:

$$bp = 41.4163 + 0.7279 \cdot \mathcal{SOS}(G) \tag{9}$$

$$mv = 120.3522 + 0.4205 \cdot \mathcal{SOS}(G) \tag{10}$$

$$mr = 26.4355 + 0.1298 \cdot \mathcal{SOS}(G) \tag{11}$$

$$hv = 26.6824 + 0.1204 \cdot \mathcal{SOS}(G) \tag{12}$$

$$ct = 202.3600 + 0.8840 \cdot \mathcal{SOS}(G) \tag{13}$$

$$cp = 31.7243 - 0.0540 \cdot \mathcal{SOS}(G) \tag{14}$$

$$st = 17.2991 + 0.0365 \cdot \mathcal{SOS}(G) \tag{15}$$

From Table 2, it follows that the linear regression models (9)-(15) can be used as predictive tools.

4. Conclusion

Table 2, reveals that the linear regression models (9)-(15) are useful tools in predicting the physical properties of low alkanes. It shows that Sombor stress index can be used as predictive means in QSPR researches.

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