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On Sombor Domination in Graphs

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Abstract

For a simple graph G, a subset $D \subseteq V(G)$ is a dominating set if $N(D) = V$, where $N(D)$ denote the open neighborhood of the set D. The Sombor index $SO(G)$ of a graph G is the sum of square root of squares of degrees of every end-vertex of an edge $E(G)$ in G. In this paper, these two classical concepts are combined and initiated the study of Sombor-domination number $\gamma^{so}(G)$ of a graph G. Further, some upper and lower bounds are obtained for $\gamma^{so}(G)$ in terms of other graph theocratical parameters. Finally, we conclude this paper by showing applications of $\gamma^{so}(G)$ in QSPR-studies of alkanes.

Keywords: *Domination number; Sombor index; Sombor domination number.*

1 Introduction

All graphs considered in this paper are finite, simple and undirected. In particular, these graphs do not possess loops. Let $G = (V, E)$ be a graph with the vertex set $V(G) = \{v_1, v_2, v_3, \cdots, v_n\}$ and the edge set $E(G) = \{e_1, e_2, e_3, \cdots, e_m\}$, that is $|V(G)| = n$ and $|E(G)| = m$. The vertex u and v are adjacent if $uv \in E(G)$. The open(closed) neighborhood of a vertex $v \in V(G)$ is $N(v) = \{u: uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$ respectively. The degree of a vertex $v \in V(G)$ is denoted by $d_G(v)$ and is defined as $d_G(v) = |N(v)|$. A vertex $v \in V(G)$ is pendant if $|N(v)| = 1$ and is called support vertex if it is adjacent to pendant vertex. Any vertex $v \in V(G)$ with $|N(v)| > 1$ is called internal vertex. If $d_G(v) = r$ for every vertex $v \in V(G)$, where $r \in \mathbb{Z}^+$ then G is called r-regular. If $r = 2$ then it is called cycle graph C_n and for $r = 3$ it is called the cubic graph. A graph G is unicyclic If $|V| = |E|$. For undefined terminologies we refer the reader to [7].

Molecular descriptors give hope that the journey throughout endless chemical space won't be a random wandering but a methodical voyage toward substances of importance to mankind. Nowadays, there is a myriad of molecular descriptors, and among them, the topological indices have a prominent place. Topological index is simply a numeric associated with the molecular graph. So far, large number of such quantities are put forward by many researchers right from 1972[6]. An useful topological index is one which has a good predicting power in QSPR studies. Therefore, topological indices can be categorized into two categories useful and not so useful TI's. One of the most useful topological index is the Sombor index $SO(G)$ which is put forward by I Gutman[4]:

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

A set $S \subseteq V$ is a *dominating set* of G if each vertex in $V - S$ is adjacent to some vertex in S. The *domination number* $\gamma(G)$ is the smallest cardinality of a dominating set. A dominating set is said to be minimal, if no proper subset of S is a dominating set of G. It is well known that, a maximal independent set of G is a minimal dominating set of G. An excellent treatment of the fundamentals of domination is given in the book by Haynes et al. [9]. A survey of several advanced topics in domination is given in the book edited by Haynes et al. [10]. Various types of domination have been defined and studied by several authors and more than 75 models of domination are listed in the appendix of Haynes et al.[8].

In this paper, we define the Sombor domination in graphs as follow:

Let $G = (V, E)$ be a graph. A subset $D \subseteq V$ of vertex set of G is said to be Sombor-dominating set if

1. for every $v \in D$ there exist $u \in V - D$ such that $uv \in E(G)$.
2. $\sum_{uv \in D \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V-D \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$.

The minimum cardinality among all Sombor dominating sets in the graph G is called the Sombor-domination number $\gamma^{so}(G)$.
For example consider the following graph G on five vertices which is depicted in Figure 1.

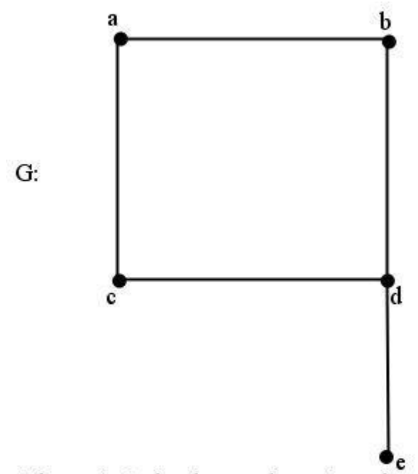

Figure 1: A simple graph on 5-vertices

In figure 1, it can be observed that $deg(a) = deg(b) = deg(c) = 2$, $deg(d) = 3$ and $deg(e) = 1$. Clearly, $D = \{b, d\}$ is a dominating set and D is also a Sombor dominating set. Because $V - D = \{a, c, e\}$ here the only existing edge is $ac \in E(G)$. Therefore,

$$\sum_{uv\in D\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} = \sqrt{deg(b)^2 + deg(d)^2}$$
$$= \sqrt{2^2 + 3^2}$$
$$= 3.3166.$$

and

$$\sum_{uv\in V-D\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} = \sqrt{deg(a)^2 + deg(c)^2}$$
$$= \sqrt{2^2 + 2^2}$$
$$= 2.828.$$

Hence, $\sum_{uv\in D\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} > \sum_{uv\in V-D\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$. Therefore, D is a minimum Sombor dominating set with $\gamma^{so}(G) = 2$.

2 Results

First, we calculate the Sombor-domination number of some standard class of graphs such as complete graph K_p, cycle graph C_p, Path Graph P_p etc.

Proposition 1

1. . For Complete graph K_p, $\gamma^{so}(K_p) = \frac{p}{2}$
2. . For cycle graph C_p, $\gamma^{so}(C_p) = \frac{p}{2}$
3. . For path graph P_p, $\gamma^{so}(P_p) = \frac{p}{2}$

Proof.

1. Let $G = K_p$ be a complete graph of order $p \geq 2$. Let $D = \{v_1, v_2, v_3, \cdots, v_{\frac{p}{2}}\}$ and clearly, $V - D = \{v_1, v_2, v_3, \cdots, v_{\frac{p}{2}}$. Since K_p is a $(p-1)-$regular graph. Therefore, it can be easily check that

$$\sum_{uv \in D \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V-D \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Hence, D is a minimal Sombor-dominating set. Therefore, $\gamma^{so}(K_p) = |D| = \frac{p}{2}$.

2. The proof follows from the same lines as in (i) due to the fact that for cycle graph C_p, $2-$regular graph.

3. Let $G = P_p$ be a path of even order. Let D be an independent dominating set of G such that D contains the every alternate vertices of P_p. Clearly, neither $\langle D \rangle$ nor $\langle V - D \rangle$ contains an edge. Now, we shall convert D into a Sombor-dominating set by by including the vertex v_{n-2} to D. Now the Sombor-dominating set $F = \{v_2, v_4, v_6, \cdots, v_{n-2}, v_{n-1}\} = |D| + 1$ contains an edge $v_{n-2}v_{n-1} \in E(P_p)$. Hence,

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} > \sum_{uv \in V-F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Proposition 2 *For any k-regular graph G with at least two vertices,* $\gamma^{so}(G) = \frac{p}{2}$.

Proof. Let G be a $k-$regular graph of order p with $V(G) = \{v_1, v_2, v_3, \cdots, v_p\}$. Let D be a dominating set with $|D| = \frac{p}{2}$. Then clearly, $|D| \geq |V - D|$. Since, $deg(v_i) = k$ for $1 \leq i \leq p$ therefore, it can be easily check that

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V-F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Hence D is a minimal Sombor-dominating set with $\gamma^{so}(G) = \frac{p}{2}$.

Theorem 1 *For any connected (p, q)-graph satisfying Sombor-dominating set,*

$$\gamma^{so}(G) \leq \frac{p}{2}$$

Further, the upper bound is attained if and only if G has a perfect matching with equal distribution of degrees of vertices.

Proof. Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, v_3, \cdots, v_p\}$ and let D be a minimum Sombor-dominating set. Then clearly $V - D$ is also a Sombor-dominating set. Hence $|D| + |V - D| = p$. Thus $\gamma^{so}(G) \leq min\{|D|, |D'|\} \leq \frac{p}{2}$.

For equality of an upper bound, let us assume that $\gamma^{so}(G) = \frac{p}{2}$ and G does not contain a perfect matching with unequal degree distribution. Then clearly,

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} < \sum_{uv \in V-F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

a contradiction to our assumption. Hence G must have perfect matching with equal degree distribution.

Theorem 2 *Let G be a connected graph satisfying Sombor-dominating set D. If D is a minimal Sombor-dominating set, then $V - D$ is also a Sombor-dominating set of G.*

Proof. Let D be a minimal Sombor-dominating set of G. Suppose $V - D$ is not an Sombor-dominating set. Then clearly,

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} < \sum_{uv \in V-F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Then there exists a vertex u such that u is not dominated by any vertex in $V - D$. Since G, a non-trivial connected graph satisfies Sombor-dominating set, u is dominated by at least one vertex in $D - \{u\}$. Thus $D - \{u\}$ is a Sombor-dominating set with

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V-F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

a contradiction. Hence $V-D$ is a Sombor-dominating set of a graph G.

Observation 3 *For a star graph* $K_{1,p-1}; p \geq 4$, $\gamma^{so}(K_{1,p-1}) = 2$.

Proof. Let G be a star graph $K_{1,p-1}$;$p \geq 4$ with central vertex v_1. Then clearly dominating sets are $D_1 = \{v_1\}$ or $D_2 = \{v_2, v_3, v_4, \cdots, v_p\}$. These dominating sets can be extended to the Sombor dominating sets as follows:

- $D_1 = \{v_1, v_2\}$
- $D_2 = \{v_1, v_3\}$
- $D_3 = \{v_1, v_4\}$

and so on $D_n = \{v_1, v_{n-1}\}$. Then clearly, $\langle V - D_i \rangle$ contains no edges. Hence, all these are minimal Sombor-dominating sets. Hence, $\gamma^{so}(K_{1,p-1}) = 2$.

Theorem 4 *For any connected graph* G *with maximum degree* $\Delta(G) \leq \frac{p}{2}$,

$$\gamma^{so}(G) \leq p - \Delta(G).$$

Proof. Let G be any connected graph of order p with maximum degree $\Delta(G) \leq \frac{p}{2}$. Let v be a vertex of maximum degree $\Delta(G)$ such that $deg(v) \leq \frac{p}{2}$. Then v is adjacent to its neighborhood vertices such that $\Delta(G) = N(v)$ and

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V - F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Hence $V - N(v)$ is Sombor-dominating set. Therefore

$$\gamma^{so}(G) \leq |V - N(V)|$$
$$= p - \Delta(G).$$

Theorem 5 *Let* $G = H \circ K_1$ *where* H *is any connected graph of even order. Then* $\gamma^{so}(G) = \frac{p}{2}$.

Proof. Consider the corona operation between the connected graph H of even order and K_1. Let $V(H) = \{v_1, v_2, v_3, \cdots, v_{\frac{p}{2}}\}$ and consider $\frac{p}{2}$ copies of K_1. Then clearly degree of each vertex $v \in V(H)$ is $deg\ _G(v) = deg\ _H(v) + 1$ and G has $\frac{p}{2}$ pendant vertices. Let D be a minimum Sombor-dominating set of G with

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V - F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

.

Such that D contains exactly half of the vertices of H together with their pendant vertices. i.e $D = \{v_1, v_2, v_3, \cdots, v_{\frac{p}{4}}\} \cup \frac{p}{4}$- copies of pendant vertices. Since the order of G is even therefore, $V - D$ also contains same number of vertices with same degree pattern. Hence clearly

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V - F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Thus D satisfies the conditions of Sombor-dominating set. Therefore, we have

$$\gamma^{so}(G) = |D|$$
$$= |\{v_1, v_2, v_3, \cdots, v_{\frac{p}{4}}\} \cup \frac{p}{4}|$$
$$= \frac{p}{4} + \frac{p}{4}$$
$$= \frac{p}{2}.$$

Theorem 3 *A dominating set* D *of a graph* G *is minimal FD-set if and only if it satisfies the following conditions,*

1. $PN(v, D) \neq \emptyset$ for every $v \in D$
2. $\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V - F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$.

Proof. Let D be a minimal Sombor-dominating set. Then every vertex $v \in D$, $D - \{v\}$ not a Sombor-dominating set, there exists a vertex $u \in V - (D - \{v\})$. Therefore $u \in PN(v, D)$. Hence for every vertex $v \in D$ has at least one neighbor. Thus $PN(v, D) \neq \emptyset$. Also,

$$\sum_{uv \in F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv \in V - F \subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Conversely, suppose $PN(v,D) \neq \emptyset$ and

$$\sum_{uv\in F\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv\in V-F\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

Now we have to prove that D is a minimal Sombor-dominating set. Assume D is not a minimal Sombor-dominating set which implies that there exists a vertex $v \in D$ such that $D - \{v\}$ a dominating set. Then v is adjacent to at least one vertex in $D - \{v\}$ and also every vertex in $V - D$ is adjacent to at least one in $D - \{v\}$. Therefore, neither (i) nor (ii) holds, which is a contradiction.

Theorem 4 *Let G be any connected graph having minimum Sombor-dominating set D. Then G is a minimal Sombor-dominating set.*

Proof. Let D be any Sombor-dominating set. If for each vertex $v \in D$, then there exist

$$\sum_{uv\in F\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2} \geq \sum_{uv\in V-F\subseteq E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

such that $uv \in E(G)$. Hence D is a minimal Sombor-dominating set.

Theorem 6 *Let G be a simple connected graph with p vertices and q edges with $\gamma^{so}(G) = k$ for some positive integer k. Then*

$$\gamma^{so}(G) \geq \frac{2kp}{\sqrt{pM_1(G)}},$$

where $M_1(G)$ is the first Zagreb index.

Proof. Let $v_1, v_2, v_3, \cdots, v_p$ be the vertices of a simple graph G. Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then by Cauchy-Schrwz inequality we have

$$(\sum_{i=1}^{p} a_i b_i)^2 \leq (\sum_{i=1}^{p} a_i^2) \cdot (\sum_{i=1}^{p} b_i^2) \qquad (2)$$

by setting $a_i = deg(v_i)$ and $b_i = \gamma^{so} = k$ we have

$$(\sum_{i=1}^{p} deg(v_i) \cdot \gamma^{so})^2 \leq (\sum_{i=1}^{p} deg(v_i)^2) \cdot (\sum_{i=1}^{p} {\gamma^{so}}^2)$$

$$k^2(\sum_{i=1}^{p} deg(v_i))^2 \leq M_1(G)(p{\gamma^{so}}^2)$$

$$p{\gamma^{so}}^2 \geq \frac{k^2(2p)^2}{M_1(G)}$$

$${\gamma^{so}}^2(G) \geq \frac{k^2(2p)^2}{pM_1(G)}$$

$$\gamma^{so}(G) \geq \frac{2kp}{\sqrt{pM_1(G)}}$$

as asserted.

We get the similar bound by applying the following inequalities:

Lemma 1 *Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then*

$$\sum_{i=1}^{n} a_i^r \geq n^{1-r}(\sum_{i=1}^{n} b_i)^r \qquad (3)$$

Lemma 2 *Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then*

$$\sum_{i=1}^{n} \frac{a_i^{r+1}}{b_i^r} \geq \frac{(\sum_{i=1}^{n} a_i)^{r+1}}{(\sum_{i=1}^{n} b_i)^r} \qquad (4)$$

Lemma 3 *Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers. Then*

$$(\sum_{i=1}^{n} b_i)^{\alpha-1}(\sum_{i=1}^{n} b_i a_i^{\alpha}) \geq (\sum_{i=1}^{n} a_i b_i)^{\alpha} \qquad (5)$$

Theorem 7 *Let G be a simple connected graph with p vertices and q edges with $\gamma^{so}(G) = k$ for some positive integer k. Then*

$$\gamma^{so} \leq \frac{\alpha(n)(\Delta-\delta)^2}{2p(p-1)}.$$

where $\alpha(n) = n\lfloor\frac{n}{2}\rfloor(1 - \frac{1}{n}\lfloor\frac{n}{2}\rfloor)$. where $\lfloor x \rfloor$ smallest integer less than or equal to x.

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Proof. Let $v_1, v_2, v_3, \cdots, v_p$ be the vertices of a simple graph G. Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be non-negative integers for which there exist real constants a, b, A and B, so that for each i, $i = 1,2, \cdots, n, a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then the following inequality is valid

$$|p \sum_{i=1}^{p} a_i b_i - \sum_{i=1}^{p} a_i \sum_{i=1}^{p} b_i| \leq \alpha(n)(A-a)(B-b) \quad (6)$$

We choose $a_i = deg_w(v_i) b_i = \gamma^{so} = k$, $A = \Delta = B$ and $a = \delta = b$, inequality (2.5), becomes

$$p \sum_{i=1}^{p} deg(v_i) \cdot \gamma^{so} - (\sum_{i=1}^{p} deg(v_i) \cdot \gamma^{so}) \leq \alpha(n)(\Delta-\delta)(\Delta-\delta)$$
$$p\gamma^{so}(2p) - \gamma^{so}(2p) \leq \alpha(n)(\Delta-\delta)^2$$
$$2p\gamma^{so}(p-1) \leq \alpha(n)(\Delta-\delta)^2$$
$$\gamma^{so} \leq \frac{\alpha(n)(\Delta-\delta)^2}{2p(p-1)}$$

Theorem 8 *Let G be a simple connected graph with p vertices and q edges with $\gamma^{so}(G) = k$ for some positive integer k. Then*

$$\gamma^{so}(G) \leq \sqrt{\frac{(\delta+\Delta)(2p) - M_1(G)}{\delta\Delta}}.$$

Proof. Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants r and R so that for each i, $i = 1,2, \cdots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid.

$$\sum_{i=1}^{p} b_i^2 + rR \sum_{i=1}^{p} a_i^2 \leq (r+R) \sum_{i=1}^{n} a_i b_i. \quad (7)$$

We choose $b_i = deg(v_i)$, $a_i = \gamma^{so} = k$, $r = \delta$ and $R = \Delta$ in inequality (2.6), then

$$\sum_{i=1}^{p} deg(v_i)^2 + \delta\Delta \sum_{i=1}^{p} \gamma_{fz}^2 \leq (\delta+\Delta) \sum_{i=1}^{p} deg(v_i)$$
$$M_1(G) + \delta\Delta p \gamma_{fz}^2 \leq (\delta+\Delta)(2p)$$
$$\delta\Delta p \gamma_{fz}^2 \leq (\delta+\Delta)(2p) - M_1(G)$$
$$\gamma_{fz}^2(G) \leq \frac{(\delta+\Delta)(2p) - M_1(G)}{\delta\Delta}$$
$$\gamma^{so}(G) \leq \sqrt{\frac{(\delta+\Delta)(2p) - M_1(G)}{\delta\Delta}}$$

as desired.

3 Applicability of the γ^{so} in QSPR-Analysis

In this section we examine the applicability of the γ^{so} with the set of 67 alkanes. For this, we consider the physical properties like [boiling points(BP), molar volumes(mv)at 20°C, molar refractions (mr) at 20°C, heats of vaporization (hv) at 25°C, surface tensions(st) 20°C, melting points(mp), acentric factor(AcentFac) and DHVAP] of octane isomers. The values are compiled in Table 1.

S.No.	Alkane	bp(°C)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct(°C)	cp(atm)	st(dyne/cm)	mp(°C)
1	Butane	-0.500				152.01	37.47		-138.35
2	2-methyl propane	-11.730				134.98	36		-159.60
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00	-129.72
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00	-159.90
5	2,2 dimethylpropane	9.503	112.074	25.7243	21.78	160.60	31.57		-16.55
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42	-95.35
7	2-methylpentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38	-153.67
8	3-methyalpentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12	-118.00
9	2,2-methylbutane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30	-99.87
10	2,3-dimethylbutane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37	-128.54
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	-90.61
12	2-methylhexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29	-118.28
13	3-methylhexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79	-119.40
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44	-118.60
15	2,2-dimethylpentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02	-123.81
16	2,3-dimethylpentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96	-119.10
17	2,4-dimethylpentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15	-119.24
18	3,3-dimethylpentane	86.064	144.530	34.3323	33.02	263.00	30	19.59	-134.46
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76	-56.79
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60	-109.04
21	3-methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17	-120.50
22	4-methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00	-120.95

S.No.	Alkane	bp(°C)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct(°C)	cp(atm)	st(dyne/cm)	mp(°C)
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51	
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60	-121.18
25	2,3-dimethylhexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99	
26	2,4-dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05	-137.50
27	2,5-dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73	-91.20
28	3,3-dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63	-126.10
29	3,4-dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64	
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52	-114.96
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99	-90.87
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67	-112.27
33	2,2,4-trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77	-107.38
34	2,3,3-trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56	-100.70
35	2,3,4-trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14	-109.21
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92	-53.52
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88	-80.40
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34	-107.64
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34	-113.20
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81	-114.90
41	4-ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81	
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80	-113.00
43	2,3-dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34	-116.00
44	2,4-dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30	
45	2,5-dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30	
46	2,6- dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83	-102.90

S.No.	Alkane	bp($°C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($°C$)	cp(atm)	st(dyne/cm)	mp($°C$)
47	3,3- dimethylheptane	137.300	176.897	43.6870	42.66	314.00	24.19	22.01	
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80	
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77	
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01	
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80	
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77	
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22	
54	2,2,4- trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51	-120.00
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04	-105.78
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41	-116.80
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80	
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27	-127.80
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27	-101.20
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75	-33.11
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38	-99.20
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87	
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80	-122.20
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38	-99.0
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98	-121.09
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37	-66.54
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31	-102.12

1. Linear Model

$$bp = 0.321 + [\gamma^{so}(G)]3.1 \quad (8)$$
$$mv = 18.7 + [\gamma^{so}(G)]2.8 \quad (9)$$
$$mr = 38.5 + [\gamma^{so}(G)]1.2 \quad (10)$$
$$hv = 48.9 + [\gamma^{so}(G)]3.8 \quad (11)$$
$$ct = 87.8 + [\gamma^{so}(G)]4.2 \quad (12)$$
$$cp = 56.3 - [\gamma^{so}(G)]2.9 \quad (13)$$
$$st = 29.6 + [\gamma^{so}(G)]3.1 \quad (14)$$
$$mp = -137.7 + [\gamma^{so}(G)]2.7 \quad (15)$$

2. Quadratic Model

$$bp = 6.7[\gamma^{so}(G)]^2 - 0.4[\gamma^{so}(G)] - 54.8 \quad (16)$$
$$mv = 6.8[\gamma^{so}(G)]^2 - 0.32[\gamma^{so}(G)] + 53.4 \quad (17)$$
$$mr = 5.3[\gamma^{so}(G)]^2 - 0.17[\gamma^{so}(G)] + 44.3 \quad (18)$$
$$hv = 6.5[\gamma^{so}(G)]^2 - 0.72[\gamma^{so}(G)] + 46.4 \quad (19)$$
$$ct = 12.3[\gamma^{so}(G)]^2 - 0.12[\gamma^{so}(G)] + 73.7 \quad (20)$$
$$cp = -4.1[\gamma^{so}(G)]^2 + 0.6[\gamma^{so}(G)] + 59.3 \quad (21)$$
$$st = 4.5[\gamma^{so}(G)]^2 - 0.57[\gamma^{so}(G)] + 42.2 \quad (22)$$
$$mp = 6.8[\gamma^{so}(G)]^2 - 0.79[\gamma^{so}(G)] - 144.8 \quad (23)$$

3. Logarithmic Model

$$bp = -121.4 + \ln[\gamma^{so}(G)]53.5 \quad (24)$$
$$mv = 33.4 + \ln[\gamma^{so}(G)]38.3 \quad (25)$$
$$mr = 0.7 + \ln[\gamma^{so}(G)]26.8 \quad (26)$$
$$hv = 36.9 + \ln[\gamma^{so}(G)]0.9 \quad (27)$$
$$ct = -49.5 + \ln[\gamma^{so}(G)]127.6 \quad (28)$$
$$cp = 42.7 - \ln[\gamma^{so}(G)]9.6 \quad (29)$$
$$st = 11.4 + \ln[\gamma^{so}(G)]8.3 \quad (30)$$
$$mp = -137.9 + \ln[\gamma^{so}(G)]36.9 \quad (31)$$

Table 2: Model summary for the boiling point of alkanes and weighted $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.91	110.5	0.000
Logarithmic	0.88	97.8	0.000
Quadratic	0.93	115.6	0.000

The above Table 2 revealed that the prediction power of the $\gamma^{so}(G)$ is good in predicting the boiling points as the correlation coefficient value $r = 0.93$ for quadratic model. i.e. our result show 93.0% of accuracy in predicting the boiling points of alkanes.

Table 3: Model summary for the critical pressure of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.84	67.8	0.000
Logarithmic	0.70	22.8	0.000
Quadratic	0.85	60.3	0.000

The above Table 3 shows that the prediction power of the $\gamma^{so}(G)$ is good in predicting the critical pressure of alkanes as the correlation coefficient value $r = 0.85$ for quadratic model. i.e. our result show 85.0% of accuracy in predicting the critical pressure of alkanes.

Table 4: Model summary for the critical temperature of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.039	0.62	0.671
Logarithmic	0.172	2.12	0.153
Quadratic	0.57	47.3	0.000

The above Table 4 revealed that the prediction power of the weighted first Zagreb index is good in predicting the critical temperature of alkanes as the correlation coefficient value $r = 0.57$ for quadratic model. i.e. our result show 57% of accuracy in predicting the critical temperature of alkanes.

Table 5: Model summary for the heats of vaporization of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.89	67.8	0.000
Logarithmic	0.88	66.9	0.000
Quadratic	0.91	76.3	0.000

The above Table 5 shows that the prediction power of the $\gamma^{so}(G)$ is good in predicting the heats of vaporization of alkanes as the correlation coefficient value $r = 0.91$ for quadratic model. i.e. our result show 91.0% of accuracy in predicting the heats of vaporization of alkanes.

Table 6: Model summary for the melting point of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.82	68.4	0.000
Logarithmic	0.613	56.7	0.000
Quadratic	0.631	58.1	0.000

The above Table 6 shows that the prediction power of the $\gamma^{so}(G)$ is not so good in predicting the melting point of alkanes as the correlation coefficient values for all models are less than 0.9.

Table 7: Model summary for the molar refraction of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.32	27.3	0.004
Logarithmic	0.38	33.7	0.001
Quadratic	0.27	25.8	0.003

The above Table 7 shows that the prediction power of the $\gamma^{so}(G)$ is not so good in predicting the molar refraction of alkanes as the correlation coefficient value for all models is less than 0.7.

Table 8: Model summary for the molar volume of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.82	54.2	0.000

Logarithmic	0.63	28.7	0.000
Quadratic	0.86	61.5	0.000

The above Table 8 revealed that the prediction power of the $\gamma^{so}(G)$ is good in predicting molar volume of alkanes as the correlation coefficient value $r = 0.86$ for quadratic model. i.e. our result show 86.0% of accuracy in predicting the molar volume of alkanes.

Table 9: Model summary for the surface tension of alkanes and $\gamma^{so}(G)$

Equation	R^2	F	Sig
Linear	0.21	0.43	0.42
Logarithmic	0.11	0.276	0.9
Quadratic	0.28	0.49	0.48

The above Table 9 shows that the prediction power of the $\gamma^{so}(G)$ is not so good in predicting the surface tension of alkanes as the correlation coefficient value for all models is less than 0.7.

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