Zagreb Domination Type Invariants in Graphs

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ABSTRACT. A set $D \subseteq V$ is a dominating set of a graph G if every vertex in $V - D$ is adjacent to one or more vertices in D. The third Zagrb index $F(G)$ is the sum of the cubes of the degree of each vertex in G. In this paper, these two classical concepts are combined and initiated the F-domination in graphs. Further, some upper and lower bounds are obtained for $F-$domination number in terms of other graph theocratical parameters. Finally, we conclude this paper by showing applications of F-domination number in QSPR-studies of alkanes.

1. INTRODUCTION

The graphs considered here are finite, undirected without loops or multiple edges. A graph with p vertices and q edges is called a (p, q) graph. Any undefined term in this paper, may be found in Harary [6]. The *neighborhood* of a vertex u in V is the set $N(u)$ consisting of all vertices v which are adjacent with u. The *closed neighborhood* is $N[u] = N(u) \cup \{u\}$. Let S be a set of vertices and let $u \in S$. A vertex v is a private neighbor of u with respect to S if $N[v] \cap S = \{u\}$. The private neighbor set of u with respect to S is the set $pn[u, S] = \{v : N[v] \cap S = \{u\}\}$. If $u \in pn[u, S]$ and u is an isolated vertex in $\langle S \rangle$, then u is called its own private neighbor. Let the vertices of degree one are called *leaves* and the vertices adjacent leaves are called *support vertices*. 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. [8]. A survey of several advanced topics in domination is given in the book edited by Haynes et al. [9]. 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. [7].

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Boris Furtula and Ivan Gutman[2] have put forward a degree based topological indices viz., a forgotten topological index which is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3 = \sum_{uv \in E(G)} \left[d_G(u)^2 + d_G(v)^2\right].$$

2. F-Dominating Set

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

(i) for every $v \in D$ there exist $u \in V - D$ such that $uv \in E(G)$.
(ii) $\sum_{v \in D} d_G(v)^3 = sum_{\{}u \in V - D\} d_G(u)^3$.

The minimum cardinality among all FD-sets of the graph G are called the F-domination number $\gamma_{fz}(G)$. Further, an FD-set D is a minimal FD-set if no proper subset of D is an FD-set. The FD-set D with minimum cardinality is called γ_{fz}-set of a graph G.

For example consider a graph $G = K_4$ depicted in Figure 1.

G:

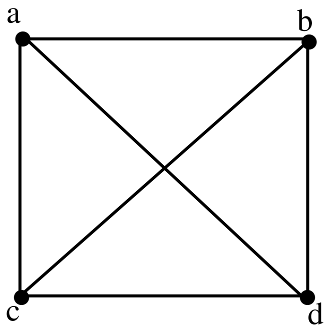

Figure 1: The complete graph on 4-vertices

In figure 1, it can be observed that $deg(a) = deg(b) = deg(c) = deg(d) = p - 1 = 4 - 1 = 3$. Further, each vertex is a dominating set in G but it is not a F- dominating set. To fulfill the conditions of $F-$dominating set, we have to consider one more vertex to dominating sets. i.e each pair of vertices of G will form a $F-$dominating sets. Hence, the domination number of G is $\gamma(G) = 1$ and the $F-$domination number of G is $\gamma_{fz}(G) = 2$. Thus it can be observed that for any connected graph G, $\gamma(G) \leq \gamma_{fz}(G)$.

2.1. F-Domination Number of Standard Class of Graphs.

In this section, we calculate the $F-$domination number of some standard class of graphs such as complete graph K_p, cycle graph C_p, Path Graph P_p etc.

Proposition 2.1. i . *For Complete graph K_p where p is even integer,* $\gamma_{fz}(K_p) = \frac{p}{2}$

ii . *For cycle graph C_p where p is even integer,* $\gamma_{fz}(C_p) = \frac{p}{2}$

iii . *For path graph P_p where p is even integer,* $\gamma_{fz}(P_p) = \frac{p}{2}$

Proof. (1) Let $G = K_p$ be a complete graph of order p with $\gamma_{fz}(K_p) = \frac{p}{2}$. Suppose the order of G is odd, then let $D = \{v_1, v_2, v_3, \cdots, v_{2k+1}\}$ will be the minimum FD-set of G. Since $G = K_p$ therefore, $\delta(G) = \Delta(G) = p - 1$. Further, $|V - D| < |D|$, which is a contradiction to the definition of $FD-$set. Hence, order of G must be even.

(2) The proof follows from the same lines as in (i) due to the fact that for cycle graph C_p, $\delta(G) = \Delta(G) = 2$.

(3) Let $G = P_p$ be a path of even order. Let $v_1, v_2, v_3, \cdots, v_p$ be the vertices of G. Then clearly, $deg(v_1) = deg(v_2) = 1$ and $deg(v_i) = 2$ where $2 \leq i \leq n - 1$. Therefore, to satisfy the condition of F- dominating set, the pendant vertices v_1 and v_p must belongs to D and $V - D$ respectively and the remaining vertices must be in alternatively D and $V - D$. Hence the cardinality of D must be $\frac{p}{2}$. Thus, $\gamma_{fz}(P_p) = |D| = \frac{p}{2}$.

□

Proposition 2.2. *For any k-regular graph G of even order, $\gamma_{fz}(G) = \frac{p}{2}$*

Proof. Let G be a $k-$regular graph of order p with $V(G) = \{v_1, v_2, v_3, \cdots, v_p\}$. Such that $\delta(G) = \Delta(G) = k$. Suppose $\gamma_{fz}(G) = \frac{p}{2}$ and p is odd. Let $D = \{v_1, v_2, v_3, \cdots, v_i\}$ be a minimum $FD-$set of G. It is assumed that $|D| = 2r + 1$ for some positive integer r. Then clearly, $|D| > |V - D|$ and

$$\left| \sum_{i=1}^{v_i} [deg(v_1^3) + deg(v_2^3) + \cdots, deg(v_i^3)] \right| > \left| \sum_{i=i+1}^{p} [deg(v_{i+1}^3) + deg(v_{i+2}^3) + \cdots, deg(v_i^p)] \right|$$

. which is a contradiction to our assumption. □

Theorem 2.1. *For any connected (p, q)-graph satisfying FD-set,*

$$\gamma_{fz}(G) \leq \frac{p}{2}$$

. 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 F-dominating set. Then clearly $V - D$ is also a $F-$dominating set. Hence $|D| + |V - D| = p$. Thus $\gamma_{fz}(G) \leq min\{|D|, |D^{'}|\} \leq \frac{p}{2}$.
For equality of an upper bound, let us assume that $\gamma_{fz}(G) = \frac{p}{2}$ and G does not contain a perfect matching with unequal degree distribution. Then there exists a vertex $v \in V(G)$ such that $v \in D$ or $v \in V - D$ which is the unique vertex of different degree. Then according to the condition of $F-$dominating set, G must contain another vertex of same degree. Which is a contradiction to our assumption. Hence G must have perfect matching with equal degree distribution. □

Theorem 2.2. *Let G be a connected graph satisfying FD-set D. If D is a minimal FD-set, then $V - D$ is also a FD-set of G.*

Proof. Let D be a minimal FD-set of G. Suppose $V - D$ is not an FD-set. 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 FD-set, u is dominated by at least one vertex in $D - \{u\}$. Thus $D - \{u\}$ is a FD-set, a contradiction. Hence $V - D$ is an FD-set of a graph G. □

There are some graphs, where the $F-$dominating sets does not exists.

Observation 2.1. *For a star graph $K_{1,p-1}; p \geq 4$ the $F-$dominating set does not exist.*

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 $D_2 = \{v_2, v_3, v_4, \cdots, v_p\}$. Further, $deg(v_1) = p - 1$ and $deg(v_i) = 1;\ 2 \leq i \leq p$. Therefore, we can see that $deg(v_1)^3 \neq deg(v_i)^3;2 \leq i \leq p$. Hence, the condition of the $F-$dominating set fails here. Further, for any combination of dominating sets results to same conclusion. Therefore, G does not contain $F-$dominating set. □

Theorem 2.1. *For any connected graph G with maximum degree $\Delta(G) \leq \frac{p}{2}$, $\gamma_{fz}(G) \leq p - \Delta(G)$.*

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 $\sum\limits_{v\in D} deg(v)^3 = \sum\limits_{v\in V-D} deg(v)^3$. Hence $V - N(v)$ is F-dominating set. Therefore

$$\begin{aligned} \gamma_{fz}(G) &\leq |V - N(V)| \\ &= p - \Delta(G). \end{aligned}$$

□

Theorem 2.2. *Let $G = H \circ K_1$ where H is any connected graph of even order. Then $\gamma_{fz}(G) = \frac{p}{2}$.*

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 $F-$dominating set of G. 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 $\sum\limits_{u\in D} deg(u)^3 = \sum\limits_{v\in V-D} deg(v)^3$. Thus D satisfies the conditions of $F-$dominating set. Therefore, we have

$$\gamma_{fz}(G) = |D|$$

$$
\begin{aligned}
&= \left|\{v_1, v_2, v_3, \cdots, v_{\frac{p}{4}}\} \cup \frac{p}{4}\right| \\
&= \frac{p}{4} + \frac{p}{4} \\
&= \frac{p}{2}.
\end{aligned}
$$

□

Theorem 2.3. *A dominating set D of a graph G is minimal FD-set if and only if it satisfies the following conditions,*

(i) $PN(v, D) \neq \emptyset$ *for every* $v \in D$

(ii) $\sum_{v\in D} d_G(v)^3 = \sum_{u\in V-D} d_G(u)^3$.

Proof. Let D be a minimal FD-set. Then every vertex $v \in D$, $D-\{v\}$ not a FD-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, $\sum_{v\in D} d_G(v)^3 = \sum_{u\in V-D} d_G(u)^3$.

Conversely, suppose $PN(v, D) \neq \emptyset$ and $\sum_{v\in D} d_G(v)^3 = \sum_{u\in V-D} d_G(u)^3$. Now we have to prove that D is a minimal FD-set. Assume D is not a minimal FD-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 2.4. *Let G be any connected graph having minimum FD-set D. Then G is a minimal FD-set.*

Proof. Let D be any FD-set. If for each vertex $v \in D$, then there exist $\sum_{v\in D} d_G(v)^3 = \sum_{u\in V-D} d_G(u)^3$ such that $uv \in E(G)$. Hence D is a minimal FD-set. □

Theorem 2.3. *Let G be a simple connected graph with p vertices and q edges with $\gamma_{fz}(G) = k$ for some positive integer k . Then*

$$\gamma_{fz}(G) \geq \frac{2kp}{\sqrt{pM_1(G)}},$$

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

$$\left(\sum_{i=1}^{p} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{p} a_i^2\right) \cdot \left(\sum_{i=1}^{p} b_i^2\right) \qquad (2.1)$$

by setting $a_i = deg(v_i)$ and $b_i = \gamma_{fz} = k$ we have

$$\left(\sum_{i=1}^{p} deg(v_i) \cdot \gamma_{fz}\right)^2 \leq \left(\sum_{i=1}^{p} deg(v_i)^2\right) \cdot \left(\sum_{i=1}^{p} \gamma_{fz}^2\right)$$

$$\begin{aligned}
k^2\left(\sum_{i=1}^{p} deg(v_i)\right)^2 &\leq M_1(G)(p\gamma_{fz}^2)\\
p\gamma_{fz}^2 &\geq \frac{k^2(2p)^2}{M_1(G)}\\
\gamma_{fz}^2(G) &\geq \frac{k^2(2p)^2}{pM_1(G)}\\
\gamma_{fz}(G) &\geq \frac{2kp}{\sqrt{pM_1(G)}}
\end{aligned}$$

as asserted. □

We get the similar bound by applying the following inequalities:

Lemma 2.1. *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*

$$\sum_{i=1}^{n} a_i^r \geq n^{1-r}\left(\sum_{i=1}^{n} b_i\right)^r \tag{2.2}$$

Lemma 2.2. *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*

$$\sum_{i=1}^{n} \frac{a_i^{r+1}}{b_i^r} \geq \frac{\left(\sum_{i=1}^{n} a_i\right)^{r+1}}{\left(\sum_{i=1}^{n} b_i\right)^r} \tag{2.3}$$

Lemma 2.3. *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*

$$\left(\sum_{i=1}^{n} b_i\right)^{\alpha-1}\left(\sum_{i=1}^{n} b_i a_i^{\alpha}\right) \geq \left(\sum_{i=1}^{n} a_i b_i\right)^{\alpha} \tag{2.4}$$

Theorem 2.4. *Let G be a simple connected graph with p vertices and q edges with $\gamma_{fz}(G) = k$ for some positive integer k . Then*

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

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.

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

$$\left| p\sum_{i=1}^{p} a_i b_i - \sum_{i=1}^{p} a_i \sum_{i=1}^{p} b_i \right| \leq \alpha(n)(A-a)(B-b) \tag{2.5}$$

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

$$\begin{aligned} p\sum_{i=1}^{p} deg(v_i)\cdot\gamma_{fz} - \left(\sum_{i=1}^{p} deg(v_i)\cdot\gamma_{fz}\right) &\leq \alpha(n)(\Delta-\delta)(\Delta-\delta) \\ p\gamma_{fz}(2p) - \gamma_{fz}(2p) &\leq \alpha(n)(\Delta-\delta)^2 \\ 2p\gamma_{fz}(p-1) &\leq \alpha(n)(\Delta-\delta)^2 \\ \gamma_{fz} &\leq \frac{\alpha(n)(\Delta-\delta)^2}{2p(p-1)} \end{aligned}$$

□

Theorem 2.5. *Let G be a simple connected graph with p vertices and q edges with $\gamma_{fz}(G) = k$ for some positive integer k. Then*

$$\gamma_{fz}(G) \leq \sqrt{\frac{(\delta+\Delta)(2p) - M_1(G)}{\delta\Delta}}.$$

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.

$$\sum_{i=1}^{p} b_i^2 + rR\sum_{i=1}^{p} a_i^2 \leq (r+R)\sum_{i=1}^{n} a_ib_i. \tag{2.6}$$

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

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

as desired. □

3. Applicability of the γ_{fz} in QSPR-Analysis

In this section we examine the applicability of the γ_{fz} 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.

Table 1.

S.No.	Alkane	bp($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
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($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
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($^\circ C$)	mv(cm^3)	mr(cm^3)	hv(kJ)	ct($^\circ C$)	cp(atm)	st(dyne/cm)	mp($^\circ C$)
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

$$bp = 1.214 + [\gamma_{fz}(G)]2.2 \quad (3.1)$$
$$mv = 112.6 + [\gamma_{fz}(G)]2.6 \quad (3.2)$$
$$mr = 32.1 + [\gamma_{fz}(G)]1.6 \quad (3.3)$$
$$hv = 26.8 + [\gamma_{fz}(G)]1.5 \quad (3.4)$$
$$ct = 139.8 + [\gamma_{fz}(G)]3.3 \quad (3.5)$$
$$cp = 36.2 - [\gamma_{fz}(G)]1.8 \quad (3.6)$$
$$st = 18.5 + [\gamma_{fz}(G)]1.8 \quad (3.7)$$
$$mp = -154.9 + [\gamma_{fz}(G)]2.2 \quad (3.8)$$

(2) Quadratic Model

$$bp = 7.5[\gamma_{fz}(G)]^2 - 0.2[\gamma_{fz}(G)] - 75.6 \quad (3.9)$$
$$mv = 4.6[\gamma_{fz}(G)]^2 - 0.2[\gamma_{fz}(G)] + 71.2 \quad (3.10)$$
$$mr = 3.1[\gamma_{fz}(G)]^2 - 0.1[\gamma_{fz}(G)] + 25.1 \quad (3.11)$$
$$hv = 4.3[\gamma_{fz}(G)]^2 - 0.5[\gamma_{fz}(G)] + 23.2 \quad (3.12)$$
$$ct = 10.1[\gamma_{fz}(G)]^2 - 0.0[\gamma_{fz}(G)] + 68.4 \quad (3.13)$$
$$cp = -2.9[\gamma_{fz}(G)]^2 + 0.4[\gamma_{fz}(G)] + 51.9 \quad (3.14)$$
$$st = 2.3[\gamma_{fz}(G)]^2 - 0.3[\gamma_{fz}(G)] + 22.4 \quad (3.15)$$
$$mp = 4.6[\gamma_{fz}(G)]^2 - 0.5[\gamma_{fz}(G)] - 134.6 \quad (3.16)$$

(3) Logarithmic Model

$$bp = -144.5 + \ln[\gamma_{fz}(G)]71.3 \quad (3.17)$$
$$mv = 44.3 + \ln[\gamma_{fz}(G)]47.1 \quad (3.18)$$
$$mr = 0.5 + \ln[\gamma_{fz}(G)]13.6 \quad (3.19)$$
$$hv = 32.8 + \ln[\gamma_{fz}(G)]0.5 \quad (3.20)$$
$$ct = -46.1 + \ln[\gamma_{fz}(G)]109.8 \quad (3.21)$$
$$cp = 54.4 - \ln[\gamma_{fz}(G)]7.9 \quad (3.22)$$
$$st = 9.2 + \ln[\gamma_{fz}(G)]4.1 \quad (3.23)$$
$$mp = -189.7 + \ln[\gamma_{fz}(G)]29.1 \quad (3.24)$$

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

Equation	R^2	F	Sig
Linear	0.8	73.3	0.000
Logarithmic	0.7	98.6	0.000
Quadratic	0.71	55.7	0.000

The above Table 2 revealed that the prediction power of the $\gamma_{fz}(G)$ is good in predicting the boiling points as the correlation coefficient value $r = 0.8$

for linear model. i.e. our result show 80.0% of accuracy in predicting the boiling points of alkanes.

Table 3: Model summary for the critical pressure of alkanes and $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.79	31.6	0.000
Logarithmic	0.51	12.4	0.001
Quadratic	0.72	27.3	0.000

The above Table 3 shows that the prediction power of the $\gamma_{fz}(G)$ is good in predicting the critical pressure of alkanes as the correlation coefficient value $r = 0.79$ for linear model. i.e. our result show 79.0% of accuracy in predicting the critical pressure of alkanes.

Table 4: Model summary for the critical temperature of alkanes and $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.059	0.83	0.456
Logarithmic	0.248	3.713	0.112
Quadratic	0.79	32.98	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 $r = 0.79$ for quadratic model. i.e. our result show 79% of accuracy in predicting the critical temperature of alkanes.

Table 5: Model summary for the heats of vaporization of alkanes and $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.81	59.7	0.000
Logarithmic	0.84	81.5	0.000
Quadratic	0.89	41.7	0.000

The above Table 5 shows that the prediction power of the $\gamma_{fz}(G)$ is good in predicting the heats of vaporization of alkanes as the correlation coefficient value $r = 0.89$ for quadratic model. i.e. our result show 89.0% of accuracy in predicting the heats of vaporization of alkanes.

Table 6: Model summary for the melting point of alkanes and $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.71	12.3	0.001
Logarithmic	0.513	11.4	0.000
Quadratic	0.564	6.8	0.003

The above Table 6 shows that the prediction power of the $\gamma_{fz}(G)$ is not so good in predicting the melting point of alkanes as the correlation coefficient values for all models are less than 0.7.

Table 7: Model summary for the molar refraction of alkanes and $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.45	10.2	0.004
Logarithmic	0.46	11.3	0.001
Quadratic	0.53	7.2	0.003

The above Table 7 shows that the prediction power of the $\gamma_{fz}(G)$ 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 $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.78	39.9	0.000
Logarithmic	0.51	11.4	0.001
Quadratic	0.82	29.3	0.000

The above Table 8 revealed that the prediction power of the $\gamma_{fz}(G)$ is good in predicting molar volume of alkanes as the correlation coefficient value $r = 0.82$ for quadratic model. i.e. our result show 82.0% of accuracy in predicting the molar volume of alkanes.

Table 9: Model summary for the surface tension of alkanes and $\gamma_{fz}(G)$

Equation	R^2	F	Sig
Linear	0.08	0.70	0.35
Logarithmic	0.16	2.4	0.1
Quadratic	0.81	29.7	0.000

The above Table 9 shows that the prediction power of the $\gamma_{fz}(G)$ is good in predicting the surface tension of alkanes as the correlation coefficient value $r = 0.81$ for quadratic model. i.e. our result show 81.0% of accuracy in predicting the quadratic model of alkanes.

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