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Taekyun Kim Stress Power α -Index

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ABSTRACT: In this study, we introduce the Taekyun Kim α -index, a novel topological index for graphs, where $\alpha \in \mathbb{R}$, which involves stresses and degrees of nodes. We calculate this index for a few common graphs and prove a few results. Further, a QSPR analysis is carried for Taekyun Kim 2-index and physical properties of lower alkanes and linear regression models have been provided.

Key Words: Graph, Neighborhood of a node, Stress of a node, Path, Geodesic, Topological index.

Contents

1. Introduction

For common terms and concepts in graph theory, we refer to Harary [2]'s textbook. The unconventional ideas will be provided when needed.

Let G = (V, E) be a undirected graph that is finite and connected. If v is an internal node of a shortest path (also called geodesic) P in G, then we say that P passes through v. The symbol $\deg(v)$ indicates a node v's degree in G.

In 1953, Shimbel presented the idea of a node's stress in a network (graph) as a centrality metric [27]. Numerous fields, including psychology, sociology, and biology, have used this centrality metric (see, for example, [4,25]). The number of geodesics that travel through a node v in a graph G is its stress, and it is represented as $\operatorname{str}_G(v)$ or, in short, by $\operatorname{str}(v)$ if there is no chance of misunderstanding. We designate Θ_G as the highest stress among all of the nodes in G and G as the smallest stress among all of the nodes in G.

K. Bhargava et al. have examined the ideas of total stress of a graph and stress regular graphs in [1]. A graph G is said to be k-stress regular if $\operatorname{str}(v) = k$, $\forall v \in V(G)$. The total stress of a graph G, denoted by $N_{\operatorname{str}}(G)$, is defined as

$$N_{\text{str}}(G) = \sum_{v \in V} \text{str}(v).$$

Raksha Poojary et al. [9,10] have studied the concept of total stress of G but by calling it as the stress of G.

A topological index (or connectivity index) of a chemical structure (molecular graph) is nothing but a (real) number that correlates given chemical structure with a physical property or chemical reactivity. Several topological indices have been explored for graphs with numerous applications in Chemistry [29,30], for instance, Wiener index, Harary index, Zagreb index etc.

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R. Rajendra et al. [14] introduced the first and second stress indices of graphs which are stress based topological indices. These indices of a graph G are defined as follows:

First stress index :
$$S_1(G) = \sum_{v \in V(G)} \operatorname{str}(v)^2$$
, (1.1)

Second stress index :
$$S_2(G) = \sum_{uv \in E(G)} \operatorname{str}(u) \cdot \operatorname{str}(v)$$
. (1.2)

R. Rajendra et al. [21] have carried a QSPR analysis for first stress index and demonstrated that first stress index can be used as predictive measure for physical properties of low alkanes. R. Rajendra et al. [24] have carried a QSPR analysis for total stress index and shown that the total stress index is also an useful topological index for predicting the physical properties of low alkanes. We recommend that the reader to study the publications [3,5,6,8,11-20,22-24,26,28] for novel stress/degree based topological indices.

In this work, a finite simple connected graph is referred to as a graph, G denotes a graph and \mathcal{N} denotes the number of geodesics of length ≥ 2 in G. In section 2, we introduce a novel topological index namely, Taekyun Kim stress power α -index, which involves powers of stresses of nodes, where α is a positive real number. We observe that for $\alpha = 0, 1, 2$, the Taekyun Kims stress power α -index reduces to the order of graphs, total stress index and first stress index, respectively. In section 3, some inequalities are established, some results are obtained and for some standard graphs Taekyun Kims stress power α -index is computed. In section 4, we analyze the correlation between Taekyun Kim stress power α -index of chemical structures (molecular graphs) and physical properties of lower alkanes.

2. Taekyun Kim Stress Power α -Index

Definition 2.1 The Taekyun Kim stress power α -index (or simply, TKSP α -index) $\mathcal{TKSP}_{\alpha}(G)$ of a graph (simple, connected) G is defined by

$$TKSP_{\alpha}(G) = \sum_{v \in V(G)} str(v)^{\alpha}$$
(2.1)

where α is a non-negative real number.

Observation. For any graph G = (V, E), we have

$$\mathcal{TKSP}_0(G) = \sum_{v \in V(G)} \operatorname{str}(v)^0 = |V|, \text{ the order of of } G,$$

$$\mathcal{TKSP}_1(G) = \sum_{v \in V(G)} \operatorname{str}(v) = N_{\operatorname{str}}(G), \text{ the total stress of } G \text{ (See [1])},$$

 $\mathcal{TKSP}_2(G) = \sum_{v \in V(G)} \operatorname{str}(v)^2 = \mathcal{S}_1(G)$, the first stress index of G (See [21]).

3. Some Results

Proposition 3.1 For any graph G,

$$0 \le \mathcal{TKSP}_{\alpha}(G) \le |V|\mathcal{N}^{\alpha} \tag{3.1}$$

and

$$|V|\theta_G^{\alpha} \le \mathcal{TKSP}_{\alpha}(G) \le |V|\Theta_G^{\alpha}.$$
 (3.2)

Proof: For any node v in G, we have $0 \le \operatorname{str}(v) \le \mathcal{N}$. Hence we have $0 \le \operatorname{str}(v)^{\alpha} \le \mathcal{N}^{\alpha}$ and so by Definition 2.1, the inequality (3.1) follows.

For any node v in G, $\theta_G \leq \text{str}(v) \leq \Theta_G$. Using this inequality in Definition 2.1, we establish (3.2). \square

Corollary 3.1 Let G be a graph. If $\mathcal{N} = 0$ in G, then $\mathcal{TKSP}_{\alpha}(G) = 0$. In particular, for the complete graph K_n , $\mathcal{TKSP}_{\alpha}(K_n) = 0$.

Proof: By Proposition 3.1, it follows that, if $\mathcal{N} = 0$, then $\mathcal{TKSP}_{\alpha}(G) = 0$. For K_n , N = 0 as there is no shortest path of length ≥ 2 , and consequently, $\mathcal{TKSP}_{\alpha}(K_n) = 0$.

Theorem 3.1 Let G be a graph. Then, $\mathcal{TKSP}_{\alpha}(G) = 0$ iff G is a complete graph.

Proof: Suppose that $\mathcal{TKSP}_{\alpha}(G) = 0$. Then it is evident from Definition 2.1 that $\operatorname{str}(x)^{\alpha} = 0$, $\forall x \in V(G)$ and hence $\operatorname{str}(x) = 0$, for all $x \in V(G)$. 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 G and G passing through at least one node, say G making $\operatorname{str}(w) \geq 1$, which is a contradiction. Hence, G are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then by Corollary 3.1, $\mathcal{TKSP}_{\alpha}(G) = 0$.

Proposition 3.2 For the complete bipartite graph $K_{m,n}$,

$$\mathcal{TKSP}_{\alpha}(K_{m,n}) = m \left[\frac{n(n-1)}{2} \right]^{\alpha} + n \left[\frac{m(m-1)}{2} \right]^{\alpha}.$$

Proof:

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

$$str(v_i) = \frac{1}{2}n(n-1), \quad 1 \le i \le m$$
 (3.3)

and

$$str(u_j) = \frac{1}{2}m(m-1), \quad 1 \le j \le n.$$
 (3.4)

Employing (3.3) and (3.4) in Definition 2.1, we have

$$\mathcal{TKSP}_{\alpha}(K_{m,n}) = \sum_{i=1}^{m} \operatorname{str}(v_{i})^{\alpha} + \sum_{j=1}^{n} \operatorname{str}(u_{j})^{\alpha}$$

$$= \sum_{j=1}^{m} \left[\frac{n(n-1)}{2} \right]^{\alpha} + \sum_{i=1}^{n} \left[\frac{m(m-1)}{2} \right]^{\alpha}$$

$$= m \left[\frac{n(n-1)}{2} \right]^{\alpha} + n \left[\frac{m(m-1)}{2} \right]^{\alpha}.$$

Proposition 3.3 If G is a r-stress regular graph, then

$$\mathcal{TKSP}_{\alpha}(G) = |V|r^{\alpha}.$$

Proof: Suppose that G is an r-stress regular graph. Then for any vertex x in G, str(x) = r. Using this fact in Definition 2.1, we have

$$\mathcal{TKSP}_{\alpha}(G) = \sum_{x \in V(G)} r^{\alpha} = |V|r^{\alpha}.$$

Corollary 3.2 For a cycle C_n ,

$$\mathcal{TKSP}_{\alpha}(C_n) = \begin{cases} n \left[\frac{(n-1)(n-3)}{8} \right]^{\alpha}, & \textit{when } n \textit{ is odd}; \\ n \left[\frac{n(n-2)}{8} \right]^{\alpha}, & \textit{when } n \textit{ is even}, \end{cases}$$

Proof: In the cycle C_n , for any node v, we have

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

Therefore, the cycle C_n is

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

and so by Proposition 3.3, the result follows.

Proposition 3.4 Let T be a tree on n nodes. Then

$$\mathcal{TKSP}_{\alpha}(T) = \sum_{v \in I} \left[\sum_{1 \leq i < j \leq m} |C_i^v| |C_j^v| \right]^{\alpha},$$

where I is the collection of all internal (non-pendant) nodes in T and the collections C_1^v, \ldots, C_m^v denote the node sets of the components of T-v for an internal node v of degree m=m(v).

Proof: Since a pendant node in T has 0 stress, we concentrate on internal nodes and to compute the TKSP α -index. Let v be an internal node of T of degree m = m(v). Let C_1^v, \ldots, C_m^v be the node sets of the components of T - v. As there is only one path between any two nodes in a tree, it is clear that

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

Hence by the Definition 2.1, we have

$$\mathcal{TKSP}_{\alpha}(T) = \sum_{v \in I} \left[\sum_{1 \leq i < j \leq m} |C_i^v| |C_j^v| \right]^{\alpha}.$$

where I is the collection of all internal (non-pendant) nodes in T.

Corollary 3.3 For path graph P_n on n nodes

$$\mathcal{TKSP}_{\alpha}(P_n) = \sum_{i=2}^{n-1} [(i-1)(n-i)]^{\alpha}.$$

Proof:

Let P_n be the path graph on n nodes (shown in Figure 1) with node set $\{v_1, v_2, \ldots, v_n\}$.

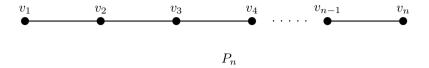


Figure 1: The path P_n on n nodes

We have, $deg(v_i) = 2$, for $2 \le i \le n-1$ and

$$\operatorname{str}(v_i) = \sum_{1 \le i < j \le 2} |C_i^{v_i}| |C_j^{v_i}| = (i-1)(n-i), \text{ for } 2 \le i \le n-1.$$

Therefore, by Proposition 3.4, the result follows.

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 common node v.

Proposition 3.5 For the windmill graph Wd(n, m),

$$\mathcal{TKSP}_{\alpha}(Wd(n,m)) = \left\lceil \frac{m(m-1)(n-1)^2}{2} \right\rceil^{\alpha}.$$

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

$$TKSP_{\alpha}(F_k) = [2k(k-1)]^{\alpha}$$
.

Proof: Any node other than the universal node has 0 stress in Wd(n,m). The only shortest paths passing through universal node v are of length 2. So, $str(v) = \frac{m(m-1)(n-1)^2}{2}$ and by Definition 2.1, we have

$$\mathcal{TKSP}_{\alpha}(Wd(n,m)) = \left\lceil \frac{m(m-1)(n-1)^2}{2} \right\rceil^{\alpha}$$

As the friendship graph F_k on 2k+1 nodes is the windmill Wd(3,k), we have

$$\mathcal{TKSP}_{\alpha}(F_k) = \left[\frac{k(k-1)(3-1)^2}{2}\right]^{\alpha} = [2k(k-1)]^{\alpha}.$$

Proposition 3.6 Let W_n denote the wheel graph on $n \geq 4$ nodes. Then

$$\mathcal{TKSP}_{\alpha}(W_n) = \left[\frac{(n-1)(n-4)}{2}\right]^{\alpha} + (n-1) \times \left\{\begin{bmatrix}\frac{(n-2)(n-4)}{8}\end{bmatrix}^{\alpha}, & \text{if n is even;} \\ \left[\frac{(n-1)(n-3)}{8}\right]^{\alpha}, & \text{if n is odd.} \end{bmatrix}$$

Proof: In W_n with $n \ge 4$, there are n-1 peripheral nodes and one central node, say v. Then

$$str(v) = \frac{(n-1)(n-4)}{2}.$$
 (3.5)

Let q be a peripheral node. Note that v is adjacent to all the peripheral nodes in W_n . So, there is no shortest path passing through q containing v. Hence contributing nodes for $\operatorname{str}(q)$ are the remaining peripheral nodes. Let us denote the cycle $W_n - v$ (on n-1 nodes) by C_{n-1} . Then

$$str_{W_n}(q) = str_{W_n - v}(q)
= str_{C_{n-1}}(q)
= \begin{cases} \frac{(n-2)(n-4)}{8}, & \text{if } n-1 \text{ is odd;} \\ \frac{(n-1)(n-3)}{8}, & \text{if } n-1 \text{ is even,} \end{cases}
= \begin{cases} \frac{(n-2)(n-4)}{8}, & \text{if } n \text{ is even;} \\ \frac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd.} \end{cases}$$
(3.6)

Let us denote the set of all the peripheral nodes in W_n by P. Then, using (3.5) and (3.6) in Definition 2.1, we have

$$\mathcal{TKSP}_{\alpha}(W_n) = \operatorname{str}(v)^{\alpha} + \sum_{q \in P} \operatorname{str}(q)^{\alpha}$$

$$= \left[\frac{(n-1)(n-4)}{2}\right]^{\alpha} + (n-1) \times \left\{\frac{\left[\frac{(n-2)(n-4)}{8}\right]^{\alpha}}{8}, \text{ if } n \text{ is even;} \right.$$

$$\left[\frac{(n-1)(n-3)}{8}\right]^{\alpha}, \text{ if } n \text{ is odd.}$$

4. Correlation between TKSP α -index and physical properties of lower alkanes

As we observed in section 2, TKSP 0-index, TKSP 1-index and TKSP 2-index are respectively, order of the (molecular) graphs, total stress index and first stress index. In [30], it is discussed that the order of the (molecular) graphs i.e. the number of carbon atoms is a valuable descriptor for the structure–property modeling of lower alkanes. R. Rajendra et al. [24] have carried a QSPR analysis for total stress index and have shown that the total stress index is an useful topological index for predicting the physical properties of low alkanes. R. Rajendra et al. [21] have carried a QSPR analysis for first stress index and have shown that the total stress index is also an useful topological index for predicting the physical properties of low alkanes. In this section, we analyze the correlation between TKSP α -index of molecular graphs and physical properties of lower alkanes.

The TKSP 3-index of chemical structures (molecular graphs) and the experimental values for the physical properties - Boiling points (bp) °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 are given in Table 1. The numerical values in columns 3 to 9 of the Table 1 are obtained from Needham et al. [7] (the same data can be found in [30]). For the values of TKSP 1-index and TKSP 2-index of molecular graphs of lower alkanes one can refer [24] and [21], respectively.

Table 1: TKSP 3-index, boiling points, molar volumes, molar refractions, heats of vaporization, critical temperatures, critical pressures and surface tensions of low alkanes

Alkane	\mathcal{TKSP}_3	$\frac{bp}{\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne \ cm^{-1}}$
Pentane	118	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	152	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	216	9.5	122.1	25.72	21.8	160.6	31.6	

Hexane									
3-Methylpentame	Hexane			130.7					18.42
22-Dimethylbstane 673 49.7 132.7 29.93 27.7 216.2 30.7 16.3 23-Dimethylbstane 686 58 130.2 22.81 22.1 22.1 22.7 20.26 2-Methylbexane 2093 98.4 146.5 34.55 36.6 267 27.2 20.26 3-Methylbexane 2093 91.9 145.8 34.8 35.7 27.6 28.6 20.41 2-Dimethylpentane 2365 79.2 148.7 34.8 32.7 27.6 28.6 20.4 2-Dimethylpentane 2187 80.5 148.9 34.3 32.2 247.1 27.4 18.15 24.2 29.8 18.70 20.2 247.1 17.4 18.15 20.2 24.1 18.1 20.2 24.7 18.1 18.0 24.2 24.2 25.6 24.2 19.6 24.2 24.2 25.6 24.1 18.1 20.2 24.2 24.2 25.6 24.1 18.2	2-Methylpentane	623	60.3	131.9	29.95	29.9	224.9	30	17.38
2.3-Dimethylbutane	3-Methylpentane				29.8		231.2		18.12
Reptane									
2.Methylhexane 2095 90.1 147.7 34.59 34.8 207.9 27.2 19.29 3.Ethylhexane 2103 93.5 143.5 34.8 35.2 207.6 28.6 20.44 2.2.Dimethylpentane 2185 89.8 144.7 34.32 34.2 204.7 28.4 18.02 2.4.Dimethylpentane 2185 89.8 144.2 34.32 34.2 204.6 29.2 19.96 2.4.Dimethylpentane 2447 86.1 144.5 34.33 33 203 30 19.99 2.3.Primethylphothane 2407 86.8 144.5 34.33 33 203 30 19.98 2.3.Primethylphothane 6003 117.6 160.6 39.91 41.5 296.2 24.64 21.76 A-Methylheptane 5904 118.5 160.1 39.1 39.8 292 25.6 21.1 2.3-Dimethylhexane 6379 106.8 161.8 39.2.5 37.3 27.2	2,3-Dimethylbutane				29.81				
3-Methylbexane 2003 91.9 145.8 34.6 35.1 202.4 28.1 19.79 2-1-Dimethylpentane 2365 79.2 148.7 34.62 32.4 24.77 28.4 18.0 2,4-Dimethylpentane 2187 80.5 148.9 34.62 32.9 24.71 22.7 18.1 3,4-Dimethylpentane 2447 86.1 144.5 34.33 33 23.3 30.3 19.59 2,3-Jirimethylpentane 6003 117.6 163.7 30.23 39.7 288 24.8 20.6 2-Methylbeptane 5904 117.7 162.1 39.12 39.7 290 25.6 21.17 4-Methylbeptane 5907 117.7 162.1 39.12 39.7 290 25.6 21.17 4-Methylbeptane 5907 117.7 162.1 39.12 39.7 290 25.6 21.17 4-Methylbeptane 5907 115.6 160.1 38.9 39.2 29.2	*	2003		146.5				27	20.26
3-Ethylpentane					34.59				
2.2 Dimethylpentane 2365 79.2 148.7 34.62 32.4 24.77 28.4 18.02 2.3-Dimethylpentane 2187 80.5 148.9 34.02 32.9 247.1 27.4 18.15 3Dimethylpentane 2447 86.1 144.5 34.3 33 263 30 19.93 2.3-Trimethylbutane 2457 80.9 145.2 34.37 32 258.3 29.8 18.66 2-Methylheptane 5904 111.6 163.7 39.23 39.7 288 24.8 20.6 2-Methylheptane 5907 111.7 162.1 39.12 39.7 290 25.6 21.1 4-Bethylhexane 5907 111.7 162.1 39.12 39.7 290 25.6 21.2 3-Ethylhexane 6379 106.8 161.3 39.23 37.3 279 25.6 21.9 2,-Dimethylhexane 6118 109.1 164.7 39.2 37.7 29.8 27.	v	2093		145.8	34.46				19.79
2,3-Dimethylpentane 2185 89,8 144,2 34,32 34,2 246,6 29,2 19,96 (2,4-Dimethylpentane 2447 86,1 144,5 34,33 33 263 30 19,59 23,3-Trimethylpentane 2447 86,1 144,5 34,33 33 263 30 19,59 23,3-Trimethylpentane 2457 86,9 145,2 34,37 32 258,3 29,8 18,76 Cctane 5888 125,7 162,6 39,19 41,5 296,2 24,64 21,76 Cctane 5888 125,7 162,6 39,19 41,5 296,2 24,64 21,76 24,76 2		2103	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,4-Dimethylpentane 2187 80.5 148.9 34.02 32.9 247.1 27.4 18.15 3.3-Dimethylpentane 2447 86.1 144.5 34.33 33 263 30 19.99 2.3-Trimethylputane 588 125.7 162.6 39.19 41.5 266.2 24.64 21.76 2-Methylheptane 5904 118.9 161.8 39.1 39.7 288 24.8 20.6 4-Methylheptane 5507 117.7 162.1 39.12 39.7 290 25.5 21.17 4-Methylheptane 5507 117.7 162.1 39.12 39.7 290 25.5 21.14 4-Hyllheptane 5607 116.8 30.1 38.9 38.7 292 25.6 21.1 2.3-Dimethylhexane 6379 106.8 16.3 38.9 38.7 29.0 25.7 25.1 19.6 2.5-Dimethylhexane 6019 109.4 16.17 39.20 37.9	2,2-Dimethylpentane	2365	79.2	148.7	34.62	32.4	247.7	28.4	18.02
3.3-Dimethylpentane									
2.3.3-frimethylbutane	2,4-Dimethylpentane	2187	80.5		34.62				
Octame 5888 125.7 162.6 39.19 41.5 296.2 24.64 20.6 2-Methylheptane 603 117.6 163.7 39.23 39.7 298 24.8 20.6 3-Methylheptane 5904 118.9 161.8 39.1 39.7 290 25.6 21.17 4-Methylhexane 5744 118.5 160.1 38.94 39.4 39.2 25.74 21.51 2,-Dimethylhexane 679 106.8 164.3 39.25 37.3 37.3 279 25.6 19.6 2,4-Dimethylhexane 6019 116.6 160.4 38.98 38.8 29.3 20.6 20.99 2,4-Dimethylhexane 6118 109.1 164.7 39.26 37.9 290 27.2 20.33 3,3-Dimethylhexane 6245 112 160.9 39.01 37.9 290 27.4 21.62 3,4-Dimethylhexane 6345 118.7 158.8 38.81 38.5 39 <td></td> <td>2447</td> <td>86.1</td> <td>144.5</td> <td>34.33</td> <td>33</td> <td>263</td> <td>30</td> <td>19.59</td>		2447	86.1	144.5	34.33	33	263	30	19.59
2-Methylheptane 6003 117.6 163.7 39.23 30.7 228 24.8 20.6 21.17 4-Methylheptane 5507 117.7 162.1 39.12 39.7 290 25.6 21 5-Ethylhexane 5544 118.5 160.1 38.94 30.4 292 25.74 21.51 2.3-Dimethylhexane 6019 106.8 164.3 39.25 37.3 279 25.6 19.6 2.3-Dimethylhexane 6019 109.4 103.1 39.13 37.8 282 28.8 20.95 2.5-Dimethylhexane 618 109.1 104.7 39.26 37.9 29.8 27.2 20.63 3.4-Dimethylhexane 655 115.7 158.8 38.85 39 298 27.4 21.62 2.5-Dimethylhexane 655 115.7 158.8 38.85 39 298 27.4 21.62 2.3-Trimethylpentane 1672 109.8 118.3 157.5 38.72 <	2,3,3-Trimethylbutane	2457	80.9	145.2	34.37	32	258.3	29.8	18.76
3-Methylheptane			125.7		39.19	41.5			21.76
4-Methylheptane 5507 117.7 162.1 39.12 39.7 290 25.6 21.1 2.2-Dimethylhexane 5744 11.85 160.1 38.94 39.4 292 25.74 21.51 2.3-Dimethylhexane 592 11.66 160.4 38.98 38.8 293 26.6 20.90 2.4-Dimethylhexane 6019 109.4 163.1 39.13 37.9 225 25.8 20.05 3.5-Dimethylhexane 618 1102 160.9 30.01 37.9 290.8 27.2 20.63 3.4-Dimethylhexane 5659 117.7 158.8 38.85 39 298 27.4 21.62 3.4-Dimethylhexane 6599 115.7 158.8 38.84 38.5 295 27.4 21.62 2.2-Trimethylpentane 1680 118.3 159.5 38.72 38 305 229.2 20.9 21.99 2.2-Trimethylpentane 1038 114.8 157.3 38.67 37.2	2-Methylheptane	6003	117.6	163.7				24.8	
2-Ethylhexane	3-Methylheptane								
2,2-Dimethylhexane 6379 106.8 164.3 39.25 37.3 279 25.6 19.6 2,3-Dimethylhexane 6019 109.4 163.1 39.13 37.8 282 25.8 20.05 2,5-Dimethylhexane 6315 112 160.9 39.01 37.9 29.8 27.2 20.63 3,4-Dimethylhexane 5920 117.7 158.8 38.85 39 298 27.4 21.62 3,4-Dimethylhexane 5920 117.7 158.8 38.85 39 298 27.4 21.62 2,23-Trimethylpentane 6480 118.3 157 38.72 38 305 28.9 21.99 2,2,3-Trimethylpentane 6434 49.2 165.1 39.26 36.1 271.2 25.5 18.77 2,3,4-Trimethylpentane 6037 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 32.2	4-Methylheptane	5807	117.7		39.12	39.7	290		
2,3-Dimethylhexane 6019 109.4 163.1 39.13 37.8 222 25.8 20.05 2,5-Dimethylhexane 6118 109.1 164.7 39.26 37.9 279 25 19.73 3,3-Dimethylhexane 5920 117.7 158.8 38.85 39 298 27.4 21.62 3.4-Dimethylhexane 5920 117.7 158.8 38.85 39 298 27.4 21.62 3.4-Dimethylhexane 6480 118.3 157 38.75 38.25 27.4 21.62 3.4-Dimethylhexane 6480 118.3 157 38.72 38 305 28.9 21.99 2,2,3-Timethylpentane 6480 118.3 157 38.72 38 305 28.9 21.99 2,2,3-Timethylpentane 6441 499.2 165.1 39.26 36.1 271.2 25.5 18.77 2,3-Timethylpentane 6444 499.2 165.1 39.26 36.1 271.2 25.5 18.77 2,3-Timethylpentane 6444 499.2 165.1 39.26 36.1 271.2 25.5 18.77 2,3-Timethylpentane 6437 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 17.87 43.84 46.4 322 2.74 22.92 2-Methyloctane 14988 151.8 178.8 43.84 46.4 322 2.74 22.92 2-Methyloctane 1478 144.2 178 43.87 44.8 318.3 23.06 22.34 4-Methyloctane 1478 144.2 178 43.87 44.8 318.3 23.06 22.34 4-Methyloctane 14376 142.5 178.2 43.77 44.8 318.3 23.06 22.34 4-Methyloctane 14376 142.5 178.2 43.77 44.8 318.3 23.9 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2.2 2	3-Ethylhexane		118.5		38.94	39.4			
2,4-Dimethylhexane 6019 109.4 163.1 39.13 37.8 282 25.8 20.05 2,5-Dimethylhexane 6118 109.1 164.7 39.26 37.9 290.8 27.2 20.63 3,4-Dimethylhexane 592 117.7 158.8 38.85 39 298 27.4 21.62 3,4-Dimethylhexane 6480 118.3 157 38.72 38 305 28.9 21.99 2,2,3-Trimethylpentane 6480 118.3 157 38.92 36.9 294 28.2 20.67 2,2,3-Trimethylpentane 16434 499.2 165.1 39.26 36.1 271.2 25.5 18.77 2,3-Trimethylpentane 1608 114.8 157.3 38.78 37.6 295 27.6 21.14 Nonane 1498 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 15114 143.3 179.8 43.73 44.8 318	2,2-Dimethylhexane								
2.5-Dimethylhexane 6118 109.1 164.7 39.26 37.9 279 25 19.73 3.3-Dimethylhexane 6345 112 160.9 39.01 37.9 290.8 27.4 21.63 3.4-Dimethylhexane 559 115.7 158.8 38.85 39 298 27.4 21.62 3.Ethyl-3-methylpentane 6480 118.3 157 38.72 38 305 28.9 21.99 2.2,4-Trimethylpentane 1672 109.8 159.5 38.92 36.9 294 28.2 20.67 2.3,4-Trimethylpentane 1684 198.2 165.1 39.26 36.1 271.2 25.5 18.77 2.3,4-Trimethylpentane 10808 114.8 157.3 38.76 37.6 292 22.5 18.77 2.3,4-Trimethylpentane 14988 150.8 178.7 43.88 44.7 315 23.6 21.88 3-Methyloctane 14988 150.8 178.7 43.88 34.7	2,3-Dimethylhexane		115.6	160.4	38.98	38.8			20.99
3.3-Dimethylhexane 5920 117.7 158.8 38.85 39 298 27.4 21.62 3-Ethyl-2-methylpentane 5859 115.7 158.8 38.85 39 298 27.4 21.62 3-Ethyl-3-methylpentane 6480 118.3 157 38.72 38 305 28.9 21.99 22,3-Trimethylpentane 1672 109.8 159.5 38.92 36.9 294 28.2 20.67 22,4-Trimethylpentane 6434 99.2 165.1 39.26 36.1 271.2 25.5 18.77 22,3-Trimethylpentane 10808 114.8 157.3 38.76 37.2 303 29 21.56 23,3-Trimethylpentane 6637 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 15114 143.3 179.8 43.88 44.7 315 23.6 21.88 3-Methyloctane 14798 144.2 178 43.73 44.8 318 23.7 22.34 3-Ethylheptane 1476 142.5 178.2 43.77 44.8 318.3 23.06 22.34 3-Ethylheptane 14476 142.5 178.2 43.77 44.8 318.3 23.98 22.81 2-Dimethylheptane 15374 132.7 180.5 43.91 44.8 318.3 23.98 22.81 2-Dimethylheptane 14502 140.5 176.7 43.49 44.8 318.3 23.98 22.81 2-Dimethylheptane 14502 140.5 176.7 43.49 44.8 318 23.79 22.34 2-Dimethylheptane 14502 135.2 180.9 43.93 42.8 306 22.7 21.3 2-Dimethylheptane 15340 135.2 180.9 43.93 42.8 306 22.7 21.3 2-Dimethylheptane 15408 135.2 176.9 43.69 42.7 31.4 24.19 22.01 3,4-Dimethylheptane 14488 140.6 175.3 43.65 43.8 32.7 24.7 22.8 3-Dimethylheptane 14488 140.6 175.3 43.65 43.8 32.7 24.7 22.8 3-Dimethylheptane 14488 140.6 175.3 43.55 43.8 32.7 24.7 22.8 3-Dimethylheptane 14488 140.6 175.3 43.55 43.8 32.7 24.7 22.8 3-Dimethylheptane 14790 135.2 176.9 43.6 42.7 31.8 24.18 22.0 3-Dimethylheptane 14790 135.2 176.9 43.6 42.8 306 22.7 21.3 3-Dimethylheptane 14788 130.8 177.4 43.66 43.8 32.7 24.77 22.8 3-Dimethylheptane 14790 135.2 176.9 43.6 42.9 30.8 32.7 24.77 22.8 3-Dimethylheptane 14790 135.2 176.9 43.6 42.8 306 22.7 21.3 3-Dimethylheptane 14788 130.8 177.4 43.66 43.8 322.7 24.77 22.8 3-Dimethylheptane 14788 133.8 177.4 43.66 43.8 322.7 24.77 22.8 3-Dimethylheptane 14790 135.2 176.9 43.6 42.9 30.8 32.7 24.77 22.8 3-Dimethylheptane 14788 133.8 177.4 43.66 43.8 322.7 24.77 22.8 3-Dimethylhexane 14762 133.6 177.9 43.66 43.8 322.7 24.77 22.8 3-Dimethylhexane 14762 133.6 177.9 43.66 43.	2,4-Dimethylhexane	6019	109.4	163.1	39.13	37.8	282	25.8	20.05
3.4-Dimethylhexane 5920 117.7 158.8 38.85 39 298 27.4 21.62 3-Ethyl-2-methylpentane 5859 115.7 158.8 38.4 38.5 295 27.4 21.52 3-Ethyl-2-methylpentane 6480 118.3 157 38.72 38 305 28.9 21.99 22.3-Trimethylpentane 6434 99.2 165.1 39.26 36.1 271.2 25.5 18.77 2.3-Trimethylpentane 6434 99.2 165.1 39.26 36.1 271.2 25.5 18.77 2.3-Trimethylpentane 6434 157.3 38.76 37.2 303 29 21.56 23.4-Trimethylpentane 6037 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 14798 144.2 178 43.73 44.8 318. 32.7 22.34 4-Methyloctane 14798 144.2 178 43.73 44.8 318. 32.30 22.84 2-Ethylheptane 14132 1413 176.4 43.64 44.8 318. 32.30 22.84 2-Ethylheptane 14132 141.2 175.7 43.9 44.8 318.3 23.96 22.34 4-Ethylheptane 15374 132.7 180.5 43.91 42.3 30.2 22.8 20.8 2.3-Dimethylheptane 14502 133.5 179.1 43.74 43.8 315. 23.79 22.34 2.5-Dimethylheptane 14502 133.5 179.1 43.74 44.8 315. 32.79 22.34 2.5-Dimethylheptane 15240 135.2 180.9 43.9 43.9 30.8 22.7 21.3 2.5-Dimethylheptane 1540 135.2 180.9 43.9 43.9 30.8 22.7 21.3 2.5-Dimethylheptane 1540 135.2 180.9 43.9 43.9 30.8 22.7 21.3 2.5-Dimethylheptane 14608 136 177.4 43.6 43.6 42.7 314 24.19 22.01 3.5-Dimethylheptane 14608 136 177.4 43.6 43.6 43.8 32.7 24.77 22.8 3.5-Dimethylheptane 14608 136 177.4 43.6 43.6 43.8 32.7 24.77 22.8 3.5-Dimethylheptane 14608 136 177.4 43.6 43.6 43.8 32.7 24.77 22.8 3.5-Dimethylheptane 1468 137.3 148.9 44.8 318.3 22.9 30.8 22.7 21.3 2.5-Dimethylheptane 1468 137.3 176.9 43.6 42.7 314 24.19 22.01 3.5-Dimethylheptane 1468 137.3 176.9 43.6 42.7 314 24.19 22.01 3.5-Dimethylheptane 1468 137.3 176.9 43.6 42.7 314 24.19 22.01 3.5-Dimethylheptane 1468 137.3 176.9 43.6 42.7 314 24.19 22.01 3.5-Dimethylheptane 1468 137.3 177.9 43.6 43.6 43.8 322.7 24.77 22.8 3.5-Dimethylheptane 1468 137.7 13.8 43.9 42.9 30.6 22.7 24.77 22.8 3.5-Dimethylheptane 1468 137.7 13.8 43.9 42.9 30.6 22.7 24.77 22.8 3.5-Dimethylhexane 1468 137.7 138.4 34.9 40.2 22.6 6.6 24.4 20.0 42.3.3-Timethylhexane	2,5-Dimethylhexane	6118	109.1	164.7	39.26	37.9	279		19.73
3-Ethyl-2-methylpentane 5859 115.7 158.8 38.84 3.5 295 27.4 21.52 2-Ethyl-3-methylpentane 6480 118.3 157 38.72 38 305 28.9 21.99 2,2,3-Trimethylpentane 6434 99.2 165.1 39.26 36.1 271.2 25.5 18.77 2,3,4-Trimethylpentane 6637 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 44.4 322 22.74 22.92 2-Methyloctane 1414 413.3 179.8 43.88 44.7 315 23.6 21.88 3-Methyloctane 14376 142.5 178.2 43.7 44.8 318 23.0 22.24 4-Ethylheptane 14132 143 176.4 43.64 44.8 318 23.9 22.81 4-Ethylheptane 14502 140.5 176.7 43.9 44.8 318									
3-Ebthyl-3-methylpentane 1680 118.3 157 38.72 38 305 28.9 21.99 2,2,3-Trimethylpentane 1672 109.8 159.5 38.92 36.9 294 28.2 20.67 2,3,4-Trimethylpentane 10808 114.8 157.3 38.76 37.2 303 29 21.56 2,3,4-Trimethylpentane 16037 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 14178 143.3 179.8 43.88 44.7 315 23.6 21.88 Methyloctane 14376 142.5 178.2 443.77 44.8 318.3 23.6 22.34 4-Ethylheptane 14376 142.5 178.2 443.77 44.8 318.3 23.98 22.81 4-Ethylheptane 15374 132.7 180.5 43.91 42.3 302 </td <td>3,4-Dimethylhexane</td> <td>5920</td> <td>117.7</td> <td>158.8</td> <td>38.85</td> <td>39</td> <td>298</td> <td>27.4</td> <td>21.62</td>	3,4-Dimethylhexane	5920	117.7	158.8	38.85	39	298	27.4	21.62
2.2.3-Trimethylpentane 1672 109.8 159.5 38.92 36.9 294 28.2 20.67 2.2.4-Trimethylpentane 10808 114.8 157.3 38.76 37.2 303 29 21.56 2.3.4-Trimethylpentane 6037 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 15114 143.3 179.8 43.88 44.7 315 23.6 21.88 3-Methyloctane 14376 142.5 178.2 43.77 44.8 318 23.7 22.3 4-Methyloctane 14376 142.5 178.2 43.77 44.8 318 23.96 22.34 4-Ethylheptane 14376 142.5 176.7 43.64 44.8 318 23.98 22.81 22.2 20.8 23.9 20.81 23.2 2.2-1 23.3 25.2 22	3-Ethyl-2-methylpentane	5859	115.7	158.8	38.84	38.5	295	27.4	21.52
2.2.4-Trimethylpentane 6434 99.2 165.1 39.26 36.1 271.2 25.5 18.77 2.3.3-Trimethylpentane 10808 114.8 157.3 38.76 37.2 303 29 21.56 2.3.4-Trimethylpentane 16988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 14798 144.2 178 43.73 44.8 318 23.7 22.34 4-Methyloctane 14376 142.5 178.2 43.77 44.8 318 23.7 22.34 4-Methyloctane 14376 142.5 178.2 43.77 44.8 318.3 23.06 22.34 4-Ethylheptane 15374 132.7 180.5 43.91 44.8 318.3 23.98 22.81 4-Ethylheptane 15574 132.7 180.5 43.91 44.8 318.3 23.98 22.81 2,2-Dimethylheptane 14502 140.5 176.7 43.63 43.8	3-Ethyl-3-methylpentane	6480	118.3	157	38.72	38	305	28.9	21.99
2,3,3-Trimethylpentane 10808 114.8 157.3 38.76 37.2 303 29 21.56 2,3,4-Trimethylpentane 6037 113.5 158.9 38.87 37.2 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 14178 144.2 178 43.88 44.7 315 23.6 21.88 3-Methyloctane 14376 142.5 178.2 43.77 44.8 318.3 23.06 22.34 4-Methyloctane 14132 143 176.4 43.64 44.8 318.3 23.96 22.34 4-Ethylheptane 14502 140.5 176.7 43.63 44.8 318.3 23.98 22.81 2,2-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.79 22.34 2,4-Dimethylheptane 14502 143.5 179.1 43.74 42.9 307.8 </td <td>2,2,3-Trimethylpentane</td> <td>1672</td> <td>109.8</td> <td>159.5</td> <td>38.92</td> <td>36.9</td> <td>294</td> <td>28.2</td> <td>20.67</td>	2,2,3-Trimethylpentane	1672	109.8	159.5	38.92	36.9	294	28.2	20.67
2,3,4-Trimethylpentane 6037 113.5 158.9 38.87 37.6 295 27.6 21.14 Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 15114 143.3 179.8 43.88 44.7 315 23.6 21.88 3-Methyloctane 14798 144.2 178 43.77 44.8 318 23.7 22.34 4-Ethylheptane 1851 141.2 175.7 43.49 44.8 318.3 23.98 22.81 2.2-Dimethylheptane 15374 132.7 180.5 43.91 42.3 302 22.8 20.8 2.3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.79 22.34 2,5-Dimethylheptane 14502 135.2 176.9 43.63 43.8 315 22.7 21.3 26Dimethylheptane 15040 135.2 180.9 43.93 42.8 306 22.7 <td>2,2,4-Trimethylpentane</td> <td>6434</td> <td>99.2</td> <td>165.1</td> <td>39.26</td> <td>36.1</td> <td>271.2</td> <td>25.5</td> <td>18.77</td>	2,2,4-Trimethylpentane	6434	99.2	165.1	39.26	36.1	271.2	25.5	18.77
Nonane 14988 150.8 178.7 43.84 46.4 322 22.74 22.92 2-Methyloctane 15114 143.3 179.8 43.88 44.7 315 23.6 21.88 3-Methyloctane 1476 142.5 178.2 43.77 44.8 318 23.06 22.34 4-Bethylheptane 14132 143 176.4 43.64 44.8 318.3 23.06 22.34 4-Ethylheptane 18581 141.2 175.7 43.49 44.8 318.3 23.98 22.81 2,3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.9 22.8 20.8 2,3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.7 22.34 2,4-Dimethylheptane 14502 135.2 180.9 43.85 42.9 306 22.7 21.3 2,6-Dimethylheptane 15050 137.3 176.9 43.69 42.7	2,3,3-Trimethylpentane	10808	114.8	157.3	38.76	37.2	303	29	21.56
2-Methyloctane	2,3,4-Trimethylpentane	6037	113.5	158.9	38.87	37.6	295	27.6	21.14
3-Methyloctane	Nonane				43.84	46.4			
4-Methyloctane 14376 142.5 178.2 43.77 44.8 318.3 23.06 22.34 3-Ethylheptane 14132 143 176.4 43.64 44.8 318.2 23.98 22.81 4-Ethylheptane 15374 132.7 180.5 43.91 42.3 302 22.8 20.8 2,3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.79 22.34 2,4-Dimethylheptane 14502 133.5 179.1 43.74 42.9 306 22.7 21.3 2,5-Dimethylheptane 19494 136 179.4 43.85 42.9 307.8 22.7 21.3 2,6-Dimethylheptane 15050 137.3 176.9 43.69 42.7 314 24.19 22.01 3,4-Dimethylheptane 14608 136 177.4 43.64 43 312.3 23.59 21.77 22.8 3,5-Dimethylheptane 14608 136 177.4 43.64 <td< td=""><td>2-Methyloctane</td><td>15114</td><td>143.3</td><td>179.8</td><td>43.88</td><td>44.7</td><td></td><td></td><td></td></td<>	2-Methyloctane	15114	143.3	179.8	43.88	44.7			
3-Ethylheptane 14132 143 176.4 43.64 44.8 318 23.98 22.81 4-Ethylheptane 8581 141.2 175.7 43.49 44.8 318.3 23.98 22.81 2,2-Dimethylheptane 15374 132.7 180.5 43.91 42.3 302 22.8 20.8 2,3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.79 22.34 2,5-Dimethylheptane 14502 133.5 179.1 43.74 42.9 306 22.7 21.3 2,6-Dimethylheptane 15240 135.2 180.9 43.93 42.8 306 23.7 20.83 3,3-Dimethylheptane 14188 140.6 175.3 43.69 42.7 314 24.19 22.01 3,4-Dimethylheptane 14608 136 177.4 43.66 43.8 322.7 24.77 22.8 3,5-Dimethylheptane 14790 135.2 176.9 43.6 42.7	3-Methyloctane	14798			43.73	44.8	318		22.34
4-Ethylheptane 8581 141.2 175.7 43.49 44.8 318.3 23.98 22.81 2,3-Dimethylheptane 14502 140.5 176.7 43.63 42.3 302 22.8 20.8 2,3-Dimethylheptane 14502 133.5 179.1 43.74 42.9 306 22.7 21.3 2,5-Dimethylheptane 19494 136 179.4 43.85 42.9 306 22.7 21.3 2,6-Dimethylheptane 15240 135.2 180.9 43.93 42.8 306 23.7 20.83 3,5-Dimethylheptane 15050 137.3 176.9 43.69 42.7 314 24.19 22.01 3,4-Dimethylheptane 14608 136 177.4 43.64 43.8 322.7 24.77 22.8 3,5-Dimethylheptane 14608 136 177.4 43.64 43 312.3 23.59 21.77 4,4-Dimethylhexane 13872 138 175.4 43.66 43.8	4-Methyloctane	14376	142.5		43.77	44.8	318.3		
2,2-Dimethylheptane 15374 132.7 180.5 43.91 42.3 302 22.8 20.8 2,3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.79 22.34 2,4-Dimethylheptane 14502 133.5 179.1 43.74 42.9 306 22.7 21.3 2,5-Dimethylheptane 15240 135.2 180.9 43.93 42.8 306 23.7 20.83 3,3-Dimethylheptane 15050 137.3 176.9 43.69 42.7 314 24.19 22.01 3,4-Dimethylheptane 14188 140.6 175.3 43.55 43.8 322.7 24.77 22.8 3,5-Dimethylheptane 14608 136 177.4 43.64 43 312.3 23.59 21.77 4,4-Dimethylheptane 14790 135.2 176.9 43.6 42.7 317.8 24.18 22.01 3,5-Dimethylhexane 13872 138 175.4 43.64 42.7 </td <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>									
2,3-Dimethylheptane 14502 140.5 176.7 43.63 43.8 315 23.79 22.34 2,4-Dimethylheptane 14502 133.5 179.1 43.74 42.9 306 22.7 21.3 2,5-Dimethylheptane 15240 135.2 180.9 43.93 42.8 306 23.7 20.83 3,3-Dimethylheptane 15050 137.3 176.9 43.69 42.7 314 24.19 22.01 3,4-Dimethylheptane 14608 136 177.4 43.65 43.8 322.7 24.77 22.8 3,5-Dimethylheptane 14608 136 177.4 43.64 43 312.3 23.59 21.77 4,4-Dimethylheptane 14790 135.2 176.9 43.6 42.7 317.8 24.18 22.01 3,5-Dimethylhexane 14879 135.2 176.9 43.6 42.7 317.8 24.18 22.01 3-Ethyl-2-methylhexane 14928 133.8 177.4 43.66									
2,4-Dimethylheptane 14502 133.5 179.1 43.74 42.9 306 22.7 21.3 2,5-Dimethylheptane 15240 135.2 180.9 43.85 42.9 307.8 22.7 21.3 2,6-Dimethylheptane 15050 137.3 176.9 43.69 42.7 314 24.19 22.01 3,4-Dimethylheptane 14188 140.6 175.3 43.55 43.8 322.7 24.77 22.8 3,5-Dimethylheptane 14608 136 177.4 43.64 43 312.3 23.59 21.77 4,4-Dimethylheptane 14790 135.2 176.9 43.6 42.7 317.8 24.18 22.01 3,5-Dimethylhexane 14879 135.2 176.9 43.6 42.7 317.8 24.18 22.01 3,5-Ethyl-2-methylhexane 14258 133.8 177.4 43.65 43 330.3 25.56 21.77 3-Ethyl-3-methylhexane 13942 140.6 173.1 43.27					43.91				
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	2,3,3,4-Tetramethylpentane	15042	141.6	169.9	43.2	41.8	334.5	26.85	23.31

Table 2: Correlation coefficient r between the physical properties (P) of lower alkanes and TKSP α -index for $\alpha = 0, 1, 2, 3$

P	\mathcal{TKSP}_0	\mathcal{TKSP}_1	\mathcal{TKSP}_2	\mathcal{TKSP}_3
\overline{bp}	0.9493	0.9087	0.9025	0.8567
mv	0.9660	0.9340	0.9507	0.9013
mr	0.9979	0.9160	0.9442	0.9074
hv	0.9107	0.9435	0.9114	0.8504
ct	0.9053	0.8377	0.8625	0.8402
cp	-0.7429	-0.9349	-0.8841	-0.7939
st	0.7464	0.7117	0.7361	0.7613

We have computed the correlation coefficient between the physical properties of lower alkanes and TKSP α -index for $\alpha=0,1,2,3$ and are presented in Table 2. The numerical values in columns 2 and 3 of the Table 2 can be found in [21] and [24], respectively. The values of the correlation coefficient r in Table 2 reveals that TKSP α -index ($\alpha=0,1,2,3$) can be used for QSPR analysis and to propose regression models to make predictions of physical properties of lower alkanes.

Conclusion

We have introduced a novel topological index for graphs namely, Taekyun Kim stress power α -index (or simply, TKSP α -index) which involves stresses of nodes, where $\alpha \geq 0$. For $\alpha = 0, 1, 2$, it is respectively, order of graphs, total stress index and first stress index. TKSP α -index ($\alpha = 0, 1, 2, 3$) can be used as a predictive measure for physical properties of low alkanes. It will be interesting to explore the properties of TKSP α -index for various real values of α .

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